Advanced Quantum Mechanics

— Incomplete Notes —

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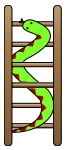

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Warm-up

To warm up, let's recall the most basic notations from undergraduate quantum mechanics. For more details, consult Sec. A of the Appendix.

- With every quantum system, one associates a Hilbert space $\mathcal{H}$.
- Each state corresponds to a normalized vector $|\psi\rangle \in \mathcal{H}$.
- Observable quantities are associated with Hermitian operators on $\mathcal{H}$. If $A = A^\dagger$ is Hermitian, it has an eigendecomposition

  $$A = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|,$$

  where the $\{|\phi_i\rangle\}_i$ are an ortho-normal basis for $\mathcal{H}$ and the $\lambda_i \in \mathbb{R}$ the eigenvalues of A. The possible numerical outcomes of a measurement process are then the λ_i, the i-th one occurring with probability

  $$\mathrm{Pr}_\psi[i] = |\langle\phi_i|\psi\rangle|^2 = \mathrm{tr}(|\psi\rangle\langle\psi|\phi_i\rangle\langle\phi_i|)$$

  if the system is in a state described by $|\psi\rangle$. If one repeats the measurement many times, the average of the observed outcomes will then tend to the expectation value

  $$\langle A\rangle_\psi = \sum_i \lambda_i \mathrm{Pr}_\psi[i] = \sum_i \lambda_i |\langle\phi_i|\psi\rangle|^2 = \langle\psi|A|\psi\rangle = \mathrm{tr}(|\psi\rangle\langle\psi|A).$$

- Also, every system is associated with a distinguished Hermitian operator, the Hamiltonian H. It serves two roles:
  - It is the observable describing energy measurements.
  - It determines the time evolution of the system via Schrödinger's equation

    $$i\hbar\partial_t|\psi(t)\rangle = H|\psi(t)\rangle.$$

- We usually choose a preferred basis for every Hilbert space $\mathcal{H}$, ideally with a clear physical interpretation. If the Hamiltonian is non-degenerate, the eigenbasis of H is a natural choice. In this case, saying that the system is in an eigenstate with given energy completely specifies the state vector.
  - Example: The harmonic oscillator, with $|n\rangle$ defined by

    $$H|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle.$$

  If the Hamiltonian *is* degenerate, it is natural to add additional observables commuting with H until their common eigenbasis is unique.
  - Example: The bound states of the hydrogen atom, for which $|n, l, m\rangle$ is defined by

    $$\begin{aligned} H|n,l,m\rangle &= E_n|n,l,m\rangle, \\ L^2|n,l,m\rangle &= \hbar^2 l(l+1)|n,l,m\rangle, \\ L_z|n,l,m\rangle &= \hbar m|n,l,m\rangle. \end{aligned}$$

Chapter 1

Multi-partite quantum systems

1.1 Mixed states

Goals

In undergraduate QM, "state" means "Hilbert space vector". To describe noisy systems (not terribly deep, but practically important) or entangled systems (much deeper and increasingly important!) one needs to widen the concept of "state" to include *mixed states* represented by *density operators*.

Imagine a process that prepares the state $|\psi_j\rangle$ with probability q_j. The probabilities could e.g. reflect fluctuations of control fields, see below. The collection of states $|\psi_j\rangle$ and probabilities q_j is called an *ensemble*. We do not require that the states $|\psi_j\rangle$ be orthogonal to each other.

If we measure an observable A on this ensemble, the expected value will be

$$\sum_j q_j \Big(\operatorname{tr} |\psi_j\rangle\langle\psi_j| A \Big) = \operatorname{tr} \Big(\Big(\sum_j q_j |\psi_j\rangle\langle\psi_j| \Big) A \Big).$$

Thus, the statistics of the experiment are described by replacing the projection $|\psi\rangle\langle\psi|$ with the more general *density operator*

$$\rho := \sum_j q_j |\psi_j\rangle\langle\psi_j| \tag{1.1}$$

so that $\langle A\rangle = \operatorname{tr}(\rho A)$. The density operator ρ has the following properties:

1. It is Hermitian $\rho^\dagger = \rho$,
2. Its eigenvalues form a probability distribution (which is equal to the q_j if and only if the states $|\psi_j\rangle$ are orthogonal).

Conversely, every operator with these two properties can be realized by an ensemble as in (1.1).

Here's the proof. Equation (1.1) implies the normalization property

$$\operatorname{tr} \rho = \sum_j q_j \operatorname{tr} |\psi_j\rangle\langle\psi_j| = \sum_j q_j = 1. \tag{1.2}$$

and the positivity property

$$\langle\phi|\rho|\phi\rangle = \sum_j q_j \langle\phi|\psi_j\rangle\langle\psi_j|\phi\rangle = \sum_j q_j |\langle\phi|\psi_j\rangle|^2 \geq 0. \tag{1.3}$$

The density operator ρ is Hermitian because every summand in (1.1) is. It thus has an eigendecomposition $\rho = \sum_j \lambda_j |\phi_j\rangle\langle\phi_j|$, and the above implies

$$\sum_j \lambda_j = \operatorname{tr}\rho = 1, \qquad \lambda_j = \langle\phi_j|\rho|\phi_j\rangle \geq 0,$$

which shows the first claim. Conversely, if $\rho = \sum_j p_j |\phi\rangle\langle\phi|$ with p_j a distribution, then the eigendecomposition already forms an ensemble realization.

If ρ is a density operator with only one non-zero eigenvalue, then $\rho = |\psi\rangle\langle\psi|$. In this case, we say that ρ describes a *pure state*. Otherwise, the state is *mixed*.

Example: Canonical ensemble. Consider a classical system where the i-th microstate has energy E_i. In the *Gibbs ensemble*, we expect to find the i-th state with probability

$$p_i = \frac{1}{Z} e^{-E_i/(kT)}, \qquad Z = \sum_i e^{-E_i/(kT)}.$$

Here, k is the Boltzmann constant, T the temperature, and Z the partition function. Now let $H = \sum_i E_i |E_i\rangle\langle E_i|$ be a quantum-mechanical Hamiltonian. The *quantum Gibbs ensemble* is, by definition, the one described by the density operator

$$\rho = \frac{1}{Z} \sum_i p_i |E_i\rangle\langle E_i| = \frac{1}{Z} e^{-H/(kT)}, \qquad Z = \operatorname{tr} e^{-H/(kT)}.$$

Thus, ρ is the operator that is diagonal in the eigenbasis of the Hamiltonian and has the classical canonical probabilities as eigenvalues. Convince yourself: ρ is pure if and only if $T = 0$ and there is a unique ground state.

von Neumann entropy. Density matrices allow us to define a quantum-mechanical notion of *entropy*. Indeed, recall that with a classical probability distribution p, one associates the *Shannon entropy*

$$S(p) = -\sum_i p_i \log p_i, \qquad \text{with convention: } 0 \log 0 = 0.$$

If ρ is a density operator, then the *von Neumann entropy* $H(\rho)$ is defined as the Shannon entropy of its eigenvalues. In addition to its central role in statistical physics, von Neumann entropy can also be used to quantify entanglement, as we will see later.

1.1.1 Visualizing mixed states: The Bloch ball

For spin-$1/2$ degrees of freedom, one can easily visualize the set of density operators. Indeed, any 2×2 matrix is of the form

$$A = \frac{1}{2} \begin{pmatrix} a_0 + a_3 & a_1 - i a_2 \\ a_1 + i a_2 & a_0 - a_3 \end{pmatrix} = \frac{1}{2} \sum_{i=0}^{3} a_i \sigma_i, \qquad a_i = \operatorname{tr} \sigma_i A \tag{1.4}$$

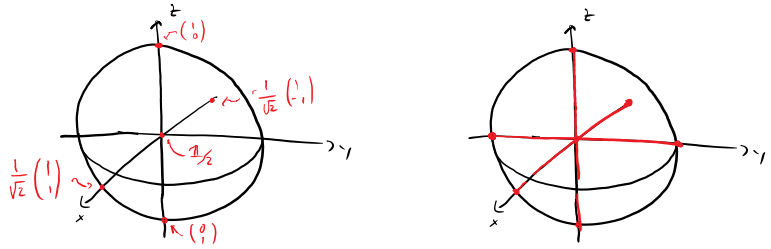


Figure 1.1: Up to a factor of $\frac{\hbar}{2}$, the i-th component $a_i = \operatorname{tr}\rho\sigma_i$ of the Bloch vector is the expectation values of the angular momentum along the $\boldsymbol{e}_i$-axis. The length of the Bloch vector encodes the "purity" of the state. Take an ensemble decomposition $\rho = \sum_j q_j|\psi_j\rangle\langle\psi_j|$ of a density operator ρ. If $\boldsymbol{a}^{(j)}$ is the Bloch vector of the j-th state, then the Bloch representation of ρ is the convex combination $\boldsymbol{a} = \sum_j q_j\boldsymbol{a}^{(j)}$.

(this is just saying that the Pauli matrices form a basis of the linear space of matrices). One directly sees that the matrix is Hermitian iff the a_i are real and has trace equal to one iff $a_0 = 1$. Thus density operators are of the form

$$\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{a}\cdot\boldsymbol{\sigma}), \tag{1.5}$$

where $\boldsymbol{a} \in \mathbb{R}^3$ is the *Bloch vector*. The eigenvalues of ρ are non-negative iff the Bloch vector lies in the unit ball of $\mathbb{R}^3$; it lies on the unit sphere exactly if ρ is pure.

> To see this, use (1.4) to compute $\det\rho = \frac{1}{4}(1-\|\boldsymbol{a}\|^2)$. Because $\operatorname{tr}\rho = 1$, the eigenvalues are of the form $\lambda, (1-\lambda)$. The determinant is the product of the eigenvalues, so that
>
> $$\lambda(1-\lambda) = \frac{1}{4}(1-\|\boldsymbol{a}\|^2) \quad\Leftrightarrow\quad \lambda = \frac{1}{2}(1\pm\|\boldsymbol{a}\|).$$

The maximally mixed state. The center point of the Bloch ball seems special. From (1.5), it corresponds to $\rho = \frac{1}{2}\mathbb{1}$. For a d-dimensional Hilbert space, $\rho = \frac{1}{d}\mathbb{1}$ is called the *maximally mixed state*. It has eigenvalues $(1/d,\ldots,1/d)$ and thus entropy $\log d$, which is the highest one can get in d dimensions. In statistical physics language, the maximally mixed state is thus the Gibbs state for $T\to\infty$.

Non-uniqueness of ensemble decompositions. From Fig. 1.1, it is geometrically obvious that there are many different ensembles that realize any given mixed state. In particular, the maximally mixed state in d dimensions can be expressed as

$$\frac{1}{d}\mathbb{1} = \sum_{i=1}^{d}|\psi_j\rangle\langle\psi_j|$$

for *any* ONB $\{|\psi_j\rangle\}_j$. (This is just the completeness relation for the basis). What seems like a geometric curiosity at this point is in fact fundamental for a number of uniquely quantum phenomena, in particular to *quantum steering*. We'll come back to this point later.

1.1.2 Time evolution of density operators

The noise-free dynamics of pure states is described by the Schrödinger equation. What is the analogue for density matrices?

Applying the formal solution $|\psi(t)\rangle = e^{\frac{t}{i\hbar}H}|\psi(0)\rangle$ of the Schrödinger equation to an ensemble, we get

$$\rho(t) = \sum_i q_i |\psi_i(t)\rangle\langle\psi_i(t)| = \sum_i q_i e^{\frac{t}{i\hbar}H}|\psi_i(0)\rangle\langle\psi_i(0)|e^{-\frac{t}{i\hbar}H} = e^{\frac{t}{i\hbar}H}\rho(0)e^{-\frac{t}{i\hbar}H}.$$

Differentiating with respect to t:

$$\partial_t\rho = \partial_t\left(e^{\frac{t}{i\hbar}H}\rho(0)e^{-\frac{t}{i\hbar}H}\right) = \frac{1}{i\hbar}(H\rho - \rho H)$$

which gives the *quantum Liouville equation*:

$$i\hbar\partial_t\rho = [H,\rho]. \tag{1.6}$$

It is called that, because it is the quantum analogue of the classical Liouville equation $\partial_t\rho = \{H,\rho\}$, which governs the time evolution of a probability density ρ on phase space. Up to a sign, the quantum Liouville equation is the same as the Heisenberg picture time evolution for observables (why?):

$$A(t) = e^{-\frac{t}{i\hbar}H}Ae^{\frac{t}{i\hbar}H}, \qquad i\hbar\partial_t A = [A,H].$$

1.1.3 Dynamics of a noisy spin

Lamor precession

Recall the noise-free time evolution of a spin in a magnetic field. Plugging the Hamiltonian

$$H = -\frac{\gamma\hbar}{2}\boldsymbol{B}\cdot\boldsymbol{\sigma}$$

and the Bloch ball description of the state $\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{a}\cdot\boldsymbol{\sigma})$ into the Liouville equation gives

$$i\hbar\frac{1}{2}\partial_t\big(\boldsymbol{a}(t)\cdot\boldsymbol{\sigma}\big) = [H,\rho] = -\frac{\gamma\hbar}{4}\sum_{ij=1}^{3}[B_i\sigma_i, a_j\sigma_j] = -i\frac{\gamma\hbar}{2}\sum_{ijk}\epsilon_{ijk}B_i a_j\sigma_k,$$

or $\partial_t\boldsymbol{a} = \gamma\boldsymbol{a}\times\boldsymbol{B}$. In particular, for $\boldsymbol{B} = B\boldsymbol{e}_z$, with $\omega := \gamma B$ the *Lamor frequency*,

$$\boldsymbol{a}(t) = \begin{pmatrix} a_x\cos(\omega t) + a_y\sin(\omega t) \\ -a_x\sin(\omega t) + a_y\cos(\omega t) \\ a_z \end{pmatrix} \;\Rightarrow\; \rho(t) = \frac{1}{2}\begin{pmatrix} 1+a_z & (a_x - ia_y)e^{i\omega t} \\ (a_x+ia_y)e^{-i\omega t} & 1-a_z \end{pmatrix}.$$

Thus, the main diagonal of the density matrix (corresponding to the spin component parallel to the field) remains constant, while the off-diagonal (corresponding to the spin components orthogonal to the field) picks up a complex phase factor oscillating with the Lamor frequency.

Dephasing of a spin

So far, we have just re-packaged undergrad calculations in new language. Let's go further, by treating a *noisy* time evolution of a spin-$1/2$ system in a magnetic field.

Assume that during the time period $t \in [0, T]$, the field strength is not B, but $B + \Delta B$. Then the Lamor frequency adapts accordingly, so that the phase factor picked up by the upper-right term of the density matrix during the time interval changes as

$$e^{iT\omega} \mapsto e^{iT\omega} e^{i\phi}, \qquad \phi = \gamma T \Delta B.$$

We say the system experiences of *phase kick* by $e^{i\phi}$.

Now imagine the changes ΔB and thus the phases ϕ fluctuate probabilistically. For concreteness assume that the ϕ follow a Gaussian distribution

$$p(\phi) = \frac{1}{\sqrt{4\pi\Lambda}} e^{-\phi^2/(4\Lambda)}$$

with mean 0 and variance 2Λ for some $\Lambda \in \mathbb{R}$. Then the expected value of the phase factor is

$$\mathbb{E}[e^{i\phi}] = \frac{1}{\sqrt{4\pi\Lambda}} \int_{-\infty}^{\infty} e^{i\phi} e^{-\phi^2/(4\Lambda)} \, \mathrm{d}\phi = e^{-\Lambda}$$

(c.f. Eq. (B.1)). We see that random phase kicks cause the off-diagonal terms of the density operator to attenuate:

$$\rho(T) = \begin{pmatrix} 1 + a_z & (a_x - i a_y) e^{i\omega T} e^{-\Lambda} \\ (a_x + i a_y) e^{-i\omega T} e^{-\Lambda} & 1 - a_z \end{pmatrix}.$$

Now assume that during the following time periods $t \in [(n-1)T, nT]$, the system experiences independent phase kicks. Taking expectations again gives rise to additional factors of $e^{-\Lambda}$ so that the upper-right matrix element at time nT reads $(a_x - i a_y) e^{i\omega nT} e^{-n\Lambda}$. Under reasonable independence assumptions on the distribution of the fluctuations, it is then justified to interpolate to arbitrary times, so that, with $\lambda = T/\Lambda$, the system evolves according to

$$\rho(t) = \begin{pmatrix} 1 + a_z & (a_x - i a_y) e^{i\omega t} e^{-\lambda t} \\ (a_x + i a_y) e^{-i\omega t} e^{-\lambda t} & 1 - a_z \end{pmatrix}$$

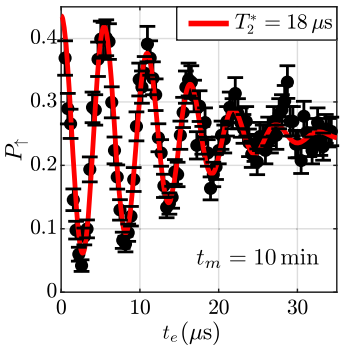
(see Fig. 1.2).

We have seen that unavoidable fluctuations in the control fields lead to the off-diagonal elements of the density matrix to tend to zero exponentially fast. The characteristic time scale $1/\lambda$ is called the T_2 *relaxation time*. (As the name suggests, there's also a T_1 *time*, which is the time scale during which the *diagonal* elements of ρ tend to their thermal equilibrium values.) The limiting density matrix

$$\rho(t \to \infty) = \begin{pmatrix} 1 + a_z & 0 \\ 0 & 1 - a_z \end{pmatrix} \tag{1.7}$$

is a probabilistic mixture of energy eigenstates. The lack of superposition terms means that (1.7) can be interpreted as a "classical state".

> Quantum computers rely on interference effects. Therefore, a system can serve as a qubit only if its T_2-time is long enough that the computation can conclude before phase coherence is lost (else, costly *quantum error correction* procedures become necessary).



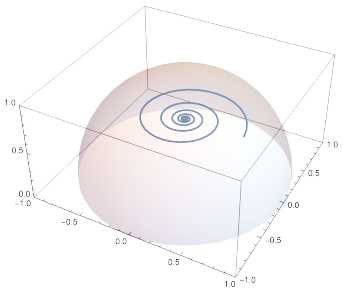


Figure 1.2: Left panel: Decoherence time measurement on a spin qubit operated at the Research Center Jülich and RWTH Aachen with support of the project Matter and Light for Quantum Computing. From [Struck et al., *Low-frequency spin qubit energy splitting noise in highly purified* ^{28}*Si/SiGe*, npj Quantum Information (2020). Right panel: The trajectory of a dephasing spin in the Bloch ball.

It is instructive to work out how the Liouville equation has to be modified to take dephasing into account. Noting that one can write the projection of the density matrix onto its off-diagonal as

$$\frac{1}{2}(\rho - \sigma_z \rho \sigma_z^\dagger),$$

it is easy to verify that $\rho(t)$ satisfies the differential equation

$$\partial_t \rho(t) = -\frac{i}{\hbar}[H, \rho] + \frac{\lambda}{2}\big(\sigma_z \rho \sigma_z^\dagger - \rho\big).$$

Such differential equations that describe the time evolution of noisy quantum systems are called *quantum master equations*.

Summary

- General states are described by *density operators*, Hermitian operators whose eigenvalues form a probability distribution.
- Reversible time evolution of density operators is determined by the *quantum Liouville equation* $i\hbar\partial_t\rho = [H, \rho]$.
- In $d = 2$, density operators can be described using their *Bloch vector* $\boldsymbol{a}$ as $\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{a} \cdot \boldsymbol{\sigma})$.
- Phase noise attenuates off-diagonal coefficients of density operators.

1.2 Multi-partite Hilbert space

Goals

We will introduce tensor product Hilbert spaces, and argue why this is the right space for multiple distinguishable particles. We'll have to spend a lot of time on notation (boring, but necessary) and have a first look at entanglement.

1.2.1 Tensor product Hilbert spaces

Two particles are *distinguishable* if one can construct measurement devices that are sensitive to one of the particles, but are not influenced by the other. (In contrast, try to build a detector that will be triggered only by one specific electron!)

More precisely, let $\mathcal{H}_1, \mathcal{H}_2$ be the Hilbert spaces of two particles. We say they are *distinguishable* if:

$$\text{For any state } |\alpha\rangle \in \mathcal{H}_1 \text{ and observable } A = \sum_i a_i |e_i\rangle\langle e_i| \text{ on } \mathcal{H}_1,$$
$$\text{and any state } |\beta\rangle \in \mathcal{H}_2 \text{ and observable } B = \sum_j b_j |f_j\rangle\langle f_j| \text{ on } \mathcal{H}_2,$$

it makes physical sense to prepare the first particle in the state $|\alpha\rangle$, the second one in the state $|\beta\rangle$, and perform the measurements A and B. We also demand that in this case, the outcome probabilities are independent:

$$\Pr[a_i \text{ and } b_j] = |\langle\alpha|e_i\rangle|^2 \, |\langle\beta|f_i\rangle|^2. \tag{1.8}$$

We now construct the Hilbert space $\mathcal{H}_{12}$ associated with the combined system. The above implies that $\mathcal{H}_{12}$ contains vectors associated with the outcomes a_i, b_j. Let's call them $|e_i, f_j\rangle$. Because they correspond to different outcomes of an observable, they have to be orthogonal. The Hilbert space must also contain a vector associated with the preparation procedure, let's call it $|\alpha, \beta\rangle$. The independence condition (1.8) is fulfilled if, for

$$|\alpha\rangle = \sum_i \alpha_i |e_i\rangle, \quad |\beta\rangle = \sum_j \alpha_j |f_j\rangle,$$

we define

$$|\alpha, \beta\rangle = \sum_{ij} \alpha_i \beta_j |e_i, f_j\rangle \tag{1.9}$$

(One can show that this is essentially the only way to satisfy independence.) The resulting Hilbert space

$$\mathcal{H}_{12} = \Big\{ \sum_{ij} \psi_{ij} |e_i, f_j\rangle \,|\, \psi_{ij} \in \mathbb{C} \Big\},$$

together with the rule (1.9), is called the *tensor product space* $\mathcal{H}_1 \otimes \mathcal{H}_2$.

States that describe independent preparations of the particles, i.e. those of the form given in (1.9), are called *product states*. Alternative notations:

$$|\alpha, \beta\rangle = |\alpha\beta\rangle = |\alpha\rangle|\beta\rangle = |\alpha\rangle \otimes |\beta\rangle,$$

and, if the bases referenced are (hopefully) clear from context:

$$|e_i, f_j\rangle = |i, j\rangle.$$

For general elements $|\psi\rangle = \sum_{ij} \psi_{ij}|ij\rangle \in \mathcal{H}_{12}$, the coefficients ψ_{ij} need not factorize as in (1.9). Such states are called *entangled*, and we'll have more to say about them.

The observables A, B associated with the individual particles act on product vectors in the obvious way:

$$A|\alpha, \beta\rangle = (A|\alpha\rangle)|\beta\rangle, \qquad B|\alpha, \beta\rangle = |\alpha\rangle(B|\beta\rangle).$$

This defines A, B on all of $\mathcal{H}_{12}$, because the product vectors $|e_i, f_j\rangle$ form a basis.

Notation and conventions If not clear from context, the system on which an operator acts is explicitly specified

$$C^{(1)}|\alpha, \beta\rangle = (C|\alpha\rangle)|\beta\rangle, \qquad C^{(2)}|\alpha, \beta\rangle = |\alpha\rangle(C|\beta\rangle).$$

There's also the "tensor product of operators" notation (sometimes called the *Kronecker product*, in particular in computer algebra systems):

$$C^{(1)}D^{(2)} = C \otimes D, \qquad C^{(1)} = C \otimes \mathbb{1}, \qquad C^{(2)} = \mathbb{1} \otimes C.$$

This implies that "tensor products of outer products" equal "outer products of tensor products" (yeah, I know... you'll get used to it):

$$|\alpha\rangle\langle\gamma| \otimes |\beta\rangle\langle\delta| = |\alpha\beta\rangle\,\langle\gamma\delta|. \tag{1.10}$$

Example: The singlet state. In the theory of the addition of angular momentum (every student's favorite topic!), one comes across the *singlet* state

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

in $\mathcal{H}_1 \otimes \mathcal{H}_2$, where the $\mathcal{H}_i$ are two-dimensional with basis $\{|\uparrow\rangle, |\downarrow\rangle\}$.

1.2.2 The partial trace

Let's recall the classical notion of a *marginal distribution*. The statistics of a pair X_1, X_2 of random variables is described by their *joint distribution* $p^{(2)}$:

$$p^{(2)}(x_1, x_2) = \Pr[X_1 = x_1 \text{ and } X_2 = x_2].$$

If one has access only to the first variable, one can obtain its distribution from the joint one by summing over the irrelevant outcomes

$$p^{(1)}(x_1) = \Pr[X_1 = x_1] = \sum_y p^{(2)}(x_1, x_2). \tag{1.11}$$

The result $p^{(1)}$ is called the *marginal distribution* associated with X_1.

Let's work out the quantum analogue of the "partial sum" in Eq. (1.11). Assume we are given a joint state of two particles, described by a density operator $\rho^{(12)}$ on the tensor product Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$. We would like to compute an effective state $\rho^{(1)}$ that

describes measurements performed on the first particle alone. More precisely, for every observable A on $\mathcal{H}_1$, we demand

$$\operatorname{tr} \rho^{(1)} A = \operatorname{tr}(\rho^{(12)}(A \otimes \mathbb{1})). \tag{1.12}$$

To solve this problem, define the *partial trace* tr_2 of a product operator by computing the usual trace of the second factor only:

$$\operatorname{tr}_2(C \otimes D) = C \operatorname{tr}(D).$$

Note that the partial trace maps an operator on the tensor product Hilbert space to an operator on the first system alone. Next, because any operator M on $\mathcal{H}_1 \otimes \mathcal{H}_2$ can be expanded in terms of product operators

$$M = \sum_{ijkl} M_{ijkl} |ij\rangle\langle kl| = \sum_{ijkl} M_{ijkl} |i\rangle\langle k| \otimes |j\rangle\langle l|,$$

one can extend tr_2 linearly to all operators:

$$\operatorname{tr}_2 M = \sum_{ijkl} M_{ijkl} |i\rangle\langle k| \otimes \operatorname{tr}(|j\rangle\langle l|) = \sum_{ik} \Big(\sum_j M_{ijkj} \Big) |i\rangle\langle k|.$$

Using this expression:

$$\begin{aligned} \operatorname{tr}\big(\rho^{(12)}(A \otimes \mathbb{1})\big) &= \sum_{ijkl} \underbrace{\langle ij|\rho^{(12)}|kl\rangle}_{\rho^{(12)}_{ijkl}} \underbrace{\langle kl|A \otimes \mathbb{1}|ij\rangle}_{\langle k|A|i\rangle \delta_{lj}} \\ &= \sum_{ik} \langle k|A|i\rangle \Big(\sum_j \rho^{(12)}_{ijkj} \Big) \langle k|k\rangle = \operatorname{tr} A\big(\operatorname{tr}_2 \rho^{(12)} \big). \end{aligned}$$

We have found that

$$\rho^{(1)} = \operatorname{tr}_2 \rho^{(12)}$$

solves Eq. (1.12). In this sense, the partial trace is the quantum analogue of the "partial sum" of Eq. (1.11). The density matrix $\rho^{(1)}$ is called the *marginal state* or the *reduced density matrix*.

Pure product states. For pure product states, we find

$$\rho^{(12)} = |\alpha\beta\rangle\langle\alpha\beta| = |\alpha\rangle\langle\alpha| \otimes |\beta\rangle\langle\beta| \quad \Rightarrow \quad \rho^{(1)} = |\alpha\rangle\langle\alpha| \operatorname{tr}(|\beta\rangle\langle\beta|) = |\alpha\rangle\langle\alpha|.$$

Physically, this says that measurements on the first particle are sensitive only to the preparation of the first particle, which reflects the independence property (1.8) we have required in the distinguishable case.

The singlet state. The partial trace of the singlet state is much more interesting:

$$\begin{aligned} \operatorname{tr}_2 |\Psi^-\rangle\langle\Psi^-| =& \frac{1}{2} \operatorname{tr}_2 \big(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\uparrow\downarrow\rangle\langle\downarrow\uparrow| - |\downarrow\uparrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow| \big) \\ =& \frac{1}{2} |\downarrow\rangle\langle\downarrow| + \frac{1}{2} |\uparrow\rangle\langle\uparrow| = \frac{1}{2} \mathbb{1}. \end{aligned}$$

While the global state $\rho = |\Psi^-\rangle\langle\Psi^-|$ was pure, the partial trace $\operatorname{tr}_2 \rho = \frac{1}{2}\mathbb{1}$ is maximally mixed! If ρ describes a thermodynamic equilibrium state, the total system is at temperature 0, while Alice's subsystem has temperature ∞. In classical physics, this is impossible. This example shows that mixed states can occur in QM even in the absence of any form of classical randomness. We'll explore the conceptual implication in the next section.

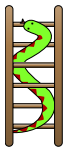
Entropy of entanglement Let $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$. If $|\Psi\rangle = |\alpha\beta\rangle$ is a product state, then the reduced density matrix $\rho^{(1)} = \mathrm{tr}_2 |\Psi\rangle\langle\Psi| = |\beta\rangle\langle\beta|$ is pure and thus has vanishing von Neumann entropy $S(\rho^{(1)}) = 0$. Since we have defined "entanglement" to be the property of not-being-a-product-state, it is natural to define $S(\mathrm{tr}_2 |\Psi\rangle\langle\Psi|)$ as a quantitative measure of entanglement. For the singlet state, this *entropy of entanglement* is 1 bit, the highest value realizable in two dimensions. For this reason, the singlet is called a *maximally entangled state*.

Summary

- The global Hilbert space of particles with individual Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$ with bases $\{|e_i\rangle\}, \{|f_j\rangle\}$ is the tensor product space

$$\mathcal{H}_{12} = \Big\{ \sum_{ij} \psi_{ij} |e_i f_j\rangle \,|\, \psi_{ij} \in \mathbb{C} \Big\}.$$

- The restriction of a global density operator $\rho^{(12)}$ to one subsystem is given by the *partial trace* $\rho^{(2)} = \mathrm{tr}_2 \rho^{(12)}$.
- Globally pure states can look locally mixed. This is a sign of entanglement.



The rest of this chapter present some topics in multi-partite quantum systems, which are, I think, conceptually highly interesting. But we won't build on them in the remainder. So it's fine to skip ahead to Chapter 2.

1.3 Dynamics of coupled systems

Goals

Things will get much more interesting! Our direct objective in this section is to work out a model in which entangled states arise naturally. Even though the model is extremely simple, we will, as a by-product, be able to make progress on issues that seem to pose conceptual problems to QM: The *measurement problem* and the question of why the world looks classical, even though it seems to be fundamentally governed by QM.

1.3.1 The measurement problem and the classicality problem

The measurement problem

Elementary QM provides two *very* different rules for time evolution:

- Hamiltonian time evolution: $|\psi\rangle \mapsto e^{\frac{1}{i\hbar}\Delta t H}|\psi\rangle$. Change is continuous in time, reversible, deterministic, and linear in the state vector.
- Projective measurements: $|\psi\rangle \mapsto P_j|\psi\rangle/\sqrt{p_j}$ with probability $p_j = \langle\psi|P_j|\psi\rangle$. Change is discontinuous in time, irreversible, non-deterministic, non-linear in the wave function.

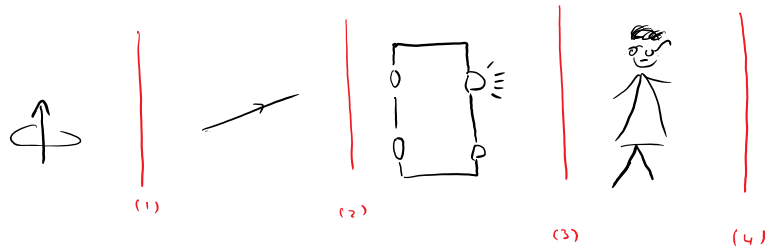


Figure 1.3: The formalism of QM divides the universe into degrees of freedom that are modeled quantum-mechanically and those that are classical. The boundary between these two regimes is the *Heisenberg cut*. For a Stern-Gerlach experiment, the quantum side could include just the spin (1), but also the motional degrees of freedom (2) of the silver atom, or the measurement device (3) that records its final position, or even the experimentalist (4) observing the outcome.

Given that these are completely different, quantum physicists take great care to very carefully explain when to use the one and when to use the other. ... Huh huh, just kidding. Check out your introductory textbook and try to find a definition of which properties exactly a physical process has to fulfill in order to qualify as a "measurement". I wish you good luck!

The standard presentation of quantum mechanics divides the world into a "quantum part" and a "classical part". The measurement rules connect the two. But it is not clear which degrees of freedom belong to which side of this *cut*.

Example: In the standard treatment of the Stern-Gerlach experiment, the spin is modeled quantum mechanically, but the spatial position of the atom classically. The spin-dependent movement of the atom is treated as a measurement. But it also seems reasonable to put the atom's position to the quantum side of the cut (Fig. 1.3). The interaction between spin and spatial coordinates is then described by a coherent Hamiltonian time evolution. A measurement only takes place once an observer records the atom's position.

We can now state to aspects of quantum mechanic's *measurement problem*:

- *The pragmatic problem*: Why can physicists get away with being so vague about the notion of "measurement"? Why don't different modeling decisions produce different predictions? (We'll be able to answer this).

- *The philosophical problem*: Given that quantum mechanics is supposedly more fundamental than classical theories, how do we deal with the fact that its predictions are stated with respect to a classical world? Who's measuring the wave function of the universe? (We won't make progress here. In fact, there's no agreement what's the best solution to this issue. Or whether there is a solution. Or whether there was a problem in the first place. It's a mess.)

Why is the macroscopic world classical?

The gravitational potential describing planetary motion and the Coulomb potential binding an electron to a nucleus are mathematically equivalent. Why then is it the case that we describe states of bound electrons in terms of delocalized orbitals, whereas Venus seems to occupy a pretty definite spot in the night sky (however, see Fig. 1.4)?

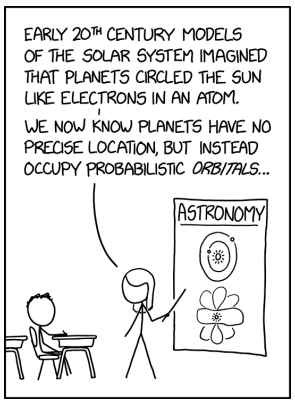


Figure 1.4: Why do planets and electrons behave differently? An unconventional take. Source: xkcd.com.

Likewise, why do marbles seem to be in one place at any one time, while from the perspective of elementary QM, it would be much more natural to assign a momentum eigenstate to them (which diagonalizes the free Hamiltonian)? Due to the their macroscopic mass, it is *compatible* with Heisenberg's uncertainty relation that a marble can be in a state in which both position and momentum are very precisely determined – but it is by no means *necessary* that such a state be adopted. So why then does this seem to happen?

More generally: *Which process breaks the unitary invariance of quantum state space and selects the basis in which we encounter physical objects?*

1.3.2 A quantum model for measurements

With these fundamental questions at the back of our heads, let's start with the Hamiltonian for a particle with spin interacting with an external magnetic field:

$$H = \frac{P^2}{2m} - \frac{\gamma\hbar}{2}\boldsymbol{B}\cdot\boldsymbol{\sigma}$$

Assume that $\boldsymbol{B} = Bz\boldsymbol{e}_z$. Then only the z-coordinate participates in the interaction, so nothing is lost by only treating the spin and the spatial z-coordinate explicitly.

Let's further assume that B is zero except for a brief period $t \in [0, T]$, where it is large. In this case, we can approximately time-evolve the system under

$$H_0 = \frac{P_z^2}{2m} \quad \text{for } t \notin [0,T], \qquad H_I = -\frac{\gamma\hbar}{2}\boldsymbol{B}\cdot\boldsymbol{\sigma} \quad \text{for } t \in [0,T].$$

First treat the case where the particle is initially in a momentum-0 eigenstate:

$$|\psi(t=0)\rangle = (\alpha|\uparrow\rangle + \beta|\downarrow\rangle)|(k=0)\rangle.$$

Using that the position operator induces a shift on momenta, $e^{i\delta tz}|k\rangle = |k+\delta t\rangle$ (why?),

$$\begin{aligned}|\psi(T)\rangle &= e^{\frac{i\gamma}{2}TBz\sigma_z}|\psi(0)\rangle \\ &= \alpha\, e^{\frac{i\gamma}{2}TBz}|\uparrow\rangle|0\rangle + \beta\, e^{-\frac{i\gamma}{2}TBz}|\downarrow\rangle|0\rangle \\ &= \alpha|\uparrow\rangle|\delta T\rangle + \beta|\downarrow\rangle|-\delta T\rangle, \qquad \delta := \frac{\hbar\gamma B}{2}. \end{aligned} \tag{1.13}$$

This is an entangled state! A measurement of spin and momentum gives correlated outcomes:

$$\Pr[s, k + \mathrm{d}k] = \begin{cases} |\alpha|^2 & (s,k) = (\uparrow, +\delta t) \\ |\beta|^2 & (s,k) = (\downarrow, -\delta t) \end{cases} .$$

The marginal distribution for the spin variable alone is

$$\Pr[s] = \begin{cases} |\alpha|^2 & s = \uparrow \\ |\beta|^2 & s = \downarrow \end{cases} .$$

This is *exactly* what we would have obtained by treating just the spin quantum mechanically! Thus: Using a quantum model for the spatial z-component does *not* change the prediction about the measured spin state. All it does is to entangle the measured and the measuring degree of freedom so that the global state becomes a superposition of consistent configurations. Indeed, we could have included further degrees of freedom – e.g. the experimentalist observing the particle momentum. If we model them – simplifying slightly – as a two-dimensional system with (mental) states $|\text{☺}\rangle$ when seeing an upwards moving atom, and $|\text{☹}\rangle$ when encountering one moving downwards, an analogous calculation would have resulted in

$$|\psi(t)\rangle = \alpha|\uparrow\rangle|\delta t\rangle|\text{☺}\rangle + \beta|\downarrow\rangle|-\delta t\rangle|\text{☹}\rangle, \tag{1.14}$$

with a similar interpretation if now the experimentalist's state gets measured.

Instead of a momentum eigenstate, let's use a more realistic Gaussian initial state. Write $|\psi_{k_0}\rangle$ for a Gaussian wave packet centered around k_0 in momentum space:

$$\langle k|\psi_{k_0}\rangle = (\pi)^{-1/4} e^{-\frac{(k-k_0)^2}{2}}.$$

Then

$$e^{\frac{i\gamma}{2}Btz}|\psi_{k_0}\rangle = |\psi_{k_0+\delta t}\rangle, \qquad t \in [0, T],$$

so that, if we take $|\psi(0)\rangle = |\psi_0\rangle$,

$$|\psi(t)\rangle = \alpha|\uparrow\rangle|\psi_{\delta t}\rangle + \beta|\downarrow\rangle|\psi_{-\delta t}\rangle.$$

The correlations between spin and position now build up over time. Indeed:

$$\Pr[s, k + \mathrm{d}k] = \frac{1}{\sqrt{\pi}} \begin{cases} |\alpha|^2 e^{-(k-\delta t)^2}\mathrm{d}k & s = \uparrow \\ |\beta|^2 e^{-(k+\delta t)^2}\mathrm{d}k & s = \downarrow \end{cases} .$$

At $t = 0$, the momentum distribution is independent of the spin state. For times $t \simeq 1/\delta$, the two spin-dependent Gaussian distributions become distinct, but overlap significantly. Only for $t \gg 1/\delta$ does the sign of a measured momentum value identify the spin state with certainty.

Let's summarize: The coupling term ($z\sigma_z$) caused the spin and the positional degree of freedom to become entangled over time. A measurement on the entangled state in the eigenbases of the two factors z, σ_z leads to correlated outcomes. Asymptotically, the correlations are perfect, and a direct measurement of one observable on the initial state is equivalent to a measurement of the other observable on the final state. One can then *define* a measurement to be any process to which the above analysis applies. In this case,

the measuring degree of freedom (called a *pointer* in this context) can be treated either classically or quantum-mechanically.

The same framework can be used to identify the basis in which objects present. To see how, compute the reduced density matrix for the spin. From

$$|\psi(t)\rangle\langle\psi(t)| = |\alpha|^2 |\uparrow\rangle\langle\uparrow| \otimes |\psi_{\delta t}\rangle\langle\psi_{\delta t}| + \alpha\beta^* |\uparrow\rangle\langle\downarrow| \otimes |\psi_{\delta t}\rangle\langle\psi_{-\delta t}| + \dots$$

and

$$\begin{aligned}\operatorname{tr} |\psi_{\delta t}\rangle\langle\psi_{-\delta t}| = \langle\psi_{-\delta t}|\psi_{\delta t}\rangle &= \frac{1}{\sqrt{\pi}} \int e^{-\frac{(k+\delta t)^2+(k-\delta t)^2}{2}} \mathrm{d}k \\ &= \frac{1}{\sqrt{\pi}} \int e^{-(k^2+(\delta t)^2)} \mathrm{d}k = e^{-(\delta t)^2},\end{aligned}$$

we can read off the reduced density matrix in the $\{|\uparrow\rangle, |\downarrow\rangle\}$-basis:

$$\rho_{\text{spin}}(t) = \operatorname{tr}_{\text{space}} |\psi_I(t)\rangle\langle\psi_I(t)| = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* e^{-(\delta t)^2} \\ \alpha^*\beta e^{-(\delta t)^2} & |\beta|^2 \end{pmatrix}.$$

Thus, the state of the spin part alone dephases from a pure state at $t = 0$ to a probabilistic mixture of $|\uparrow\rangle$ and $|\downarrow\rangle$ for times $t \gg 1/\delta$. The entropy (of entanglement) gradually builds up from $S(t = 0) = 0$ to

$$S(t \to \infty) = -|\alpha|^2 \log |\alpha|^2 - |\beta|^2 \log |\beta|^2.$$

Let's again interpret this calculation from a broader perspective. After the dephasing time, an unrelated observer will find the spin in a σ_z-eigenstate and will not encounter superpositions. Recall what distinguishes the z-axis: It is the one in which the interaction takes place! The bases which we perceive as "classical" are the ones in which the interaction terms are diagonal, and the emergence of probabilistic mixtures is a result of entanglement building up. Interactions are *local*, which is why quantum systems usually appear to be well-localized in space. However, some interactions select for different bases: e.g. electrons bound in an atom couple to the environment via the electromagnetic field. This interaction is sensitive to atomic energy scales and angular momentum – but the wave lengths of the involved photons is too large for the position of the electron within the atom to make a meaningful difference. Therefore, the semi-classical description of electrons in terms of atomic quantum numbers ("n, l, m") makes sense in this case. In contrast, whether or not a photon is scattered off the surface of venus depends on the planet's *position* within its orbit, not on its internal energy or angular momentum.

Further conceptual points:

- Q.: *Are measurements discontinuous in time?*
  A.: Nope! Correlations between the measured system and the environment are built up at a time scale proportional to the inverse coupling strength. The instantaneous process postulated in introductory QM can be understood as an effective description valid for times much larger than that.

- Q: *Are these these processes irreversible?*
  A.: The dynamics on the quantum side of the cut is reversible in theory – the final measurement still isn't. This doesn't lead to practical contradictions, though. Assume we put the whole universe, except for ourselves, on the quantum side. What would it take to reverse the measurement after a blob of silver (in the Stern-Gerlach

case) has been deposited on a screen, but before we have looked at it? The deposit will have interacted with an enormous number of degrees of freedom: phonons in the screen, the cosmic background radiation, thermal photons that have since zoomed off into the sky at the speed of light. Clearly, for all practical purposes ("FAP"), it is impossible to reverse those interactions. Thus, once a macroscopic record of an event exists, the irreversibility introduced by QM's measurement postulate does not change anything FAP. Philosophically, it might still be a thorny issue though! This is all good news if you like to compute things (no immediate contradiction). It's bad news if you like to understand foundational questions, because there seems little empirical guidance on offer for how to handle this conceptual inconsistency.

- Q.: *In thermodynamics, there's tension between the fact that entropy increases, while microscopic dynamics is reversible. The buildup of entanglement seems like an elegant solution: Local randomness is created from globally reversible dynamics. Maybe "*all *entropy is entanglement entropy"! Is that a good way to think about the apparent increase of entropy?*
  A.: You betcha!

Concrete estimates for decoherence rates can be found in Table 2 of Tegmark, *Apparent wave function collapse caused by scattering*.

1.4 Quantum many-body systems as computers

Goals

Quantum computing is all the rage! We'll introduce the basic concepts here and discuss one very cool and comparatively simple application: Grover's algorithm, which can search through N times in $\sqrt{N}$ time. You heard me right.

One can iterate the construction of the two-particle Hilbert space to find the space for $n > 2$ systems. Assume, for simplicity, that every single-system Hilbert space $\mathcal{H}_i$ has dimension d and basis $\{|1\rangle, \ldots, |d\rangle\}$. Then a general state vector in the joint Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ is of the form

$$|\psi\rangle = \sum_{i_1, i_2, \ldots, i_n = 1}^{d} \psi_{i_1, \ldots, i_n} |i_1, \ldots, i_n\rangle.$$

You should immediately notice that the sum is over d^n terms, i.e. the dimension of the joint space is exponentially large in the number of constituents! For a collection of spin-$1/2$s arranged on a cube with side length only 10, this gives an *way*-bigger-than-merely-astronomical 2^{1000}. This is:

- **Bad news** if you work in computational physics. It is absolutely out of the question even to just store the coefficients $\psi_{i_1, \ldots, i_n}$ in memory. Fortunately, one can sometimes use clever tricks to make statements about large-n systems without having to work with explicit representations. More on this: See rest of these notes.
- **Potentially good news** if you can carefully control large quantum systems. Because Nature seems to be able to track quantum states that our classical computers can't, it stands to reason that quantum systems could be used to solve otherwise intractable computational problems. More on this: See Sec. 1.4.

Many-body Hamiltonians *can* usually be efficiently represented, though. The reason is that physical interaction involve only few particles at a time. A Hamiltonian with only single- and two-body terms is of the form

$$H = \sum_k h^{(k)} + \frac{1}{2}\sum_{k\neq l} h^{(k,l)}$$

where $h^{(ij)}$ acts non-trivially only on the i-th and j-th Hilbert spaces and can therefore be specified as a $d^2 \times d^2$-matrix (or, if $d = \infty$, will typically be a simple function of position and momentum operators).

Given the Hamiltonian, typical questions of interest are:

1. Obtain information about the eigenvalues of H, e.g. the energies of the ground states and of low-lying excitations.

2. Compute thermodynamical potentials, e.g. the free energy

$$\log Z = \log \operatorname{tr} e^{-\beta H}.$$

3. Compute the expectation value $\langle\psi(t)|A^{(i)}|\psi(t)\rangle$ of a local observable. Here, $|\psi(t)\rangle = e^{\frac{t}{i\hbar}H}|\psi(0)\rangle$ is the time evolution of a state that started out in a simple form, say $|\psi(0)\rangle = |i_1, \ldots, i_n\rangle$.

In general, finding answers to these questions is intractable. The task of *quantum many-body theory* is to find special cases or approximations where progress can be made.

Quantum algorithms

It is not *obvious* that simulating the time evolution of quantum many-body systems actually is classically intractable. Sure, we have argued above that storing a many-body wave function in memory is impossible. But we have also seen that any physical time evolution can be described using only a small number of parameters (the local terms of the Hamiltonian, a simple initial state). So it is conceivable that there exists a smart universal way of keeping track of $|\psi(t)\rangle$ that does not involve working with the full state vector.

Today, there is strong evidence that such a universal strategy does *not* exist[1].

One piece of evidence is given by the existence of *quantum algorithms*. These are methods that allow one to solve a difficult classical computational problem efficiently by outsourcing parts of the calculation to a quantum device.

1.4.1 Grover's algorithm

Here, we will look at one example: *Grover's algorithm*. As we'll see, it is simultaneously: (i) comparatively easy to understand, (ii) highly surprising in what it achieves, and (iii) probably of limited practical value even if big quantum computers can be constructed.

[1] There is no rigorous proof of this, though! The issue is that is has so far been beyond the wit of humankind to prove *any* reasonable problem to be computationally hard. For example, the infamous "P vs NP" problem asks for a proof that *finding* solutions to problems is generally harder than *verifying* that a proposed solution indeed works. An imprecise analogue would be: Appreciating classical music is easier than becoming the next Mozart. *Of course* this is true – so the fact that there is no mathematical proof that "P $\neq$ NP" is not generally be taken to be indicative of there being serious doubts about the statement, but rather as testament to the limitations of the human mind. Sadly, a detailed account is beyond the scope of this lecture.

```
davidg@repos:~$ sudo grep davidg /etc/shadow
davidg:$6$2kjoNwafEvibRYry$BzfBTGfk0wY2nk3c05OAucPXQPIP8
dWMFGbCNoAs7B1dacUNNUn5fDMyOorDu4QSaxOWZskpObEz3dlBbfI3f
/:19425:0:99999:7:::
davidg@repos:~$
```

Figure 1.5: Stored SHA-512 hash of *my actual university login*. If you find a pre-image, you can read my emails and adjust your grades. Knock yourself out! [If you do succeed, you could also *answer* my emails. Come to think of it, maybe I should just post my password...].

Overview

There are some computational puzzles for which the best-known approach is to just try every possible input to see whether it is a solution.

The most clear-cut cases are used in cryptography. For example, your computer does not actually know your password! Instead, it stores an n-bit image $y^\star = h(x^\star)$ of the password $x^\star$ under a *cryptographic hash function* h. It is designed such that computing $y = h(x)$ for an input x is easy, but the best-known way of finding a pre-image $x \in h^{-1}(\{y\})$ given y is to try $\simeq 2^n$ random inputs (Fig. 1.5). To authenticate a user who claims their password is x, the computer compares $y = h(x)$ to the hash $y^\star$ on file. The advantage of such an indirect procedure is that not much harm is done if the stored hashes fall into the wrong hands: A typical value of n is 512 and $2^{512} \gg$ (hadrons in universe), so recovering the passwords $x^\star$ is impractical. (Unless, of course, the user chooses a password that can be guessed with reasonable effort. No hash magic makes "date-of-birth-of-romantic-partner123lol" a secure choice.)

Finding an inverse by trying random inputs does not require that we understand anything about the inner workings of h. All we need is the ability to compute $h(x)$ given x. Methods that interact with h only in this way are called *black box* (or *oracle*) algorithms.

Are black box algorithms really the best way to invert a hash function? Don't take my word for it! The vast wealth stored in "crypto currencies" is secure only to the degree that this assumption is true. BitCoin is effectively a multi-billion dollar bounty on an improved algorithm. It hasn't been claimed as of 2023 (Fig. 1.6).

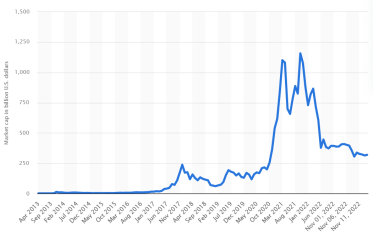


Figure 1.6: Left: Cryptocurrency mines consists of racks of computers that try random inputs hoping to find a solution to a mathematical puzzle. Right: If you can do better, there's 300b dollars on the table (as of early 2023). Credit: Wikipedia, Statista.

In light of this, it is truly remarkable that in 1996, Lov Grover showed that a quantum computer can find x from y in roughly $\sqrt{2^n} = 2^{n/2}$ time steps. In fact, this *square root*

speedup is possible for *any* puzzle for which a solution can be efficiently recognized!

Here's a high-level overview: We model "puzzle for which a solution can be recognized" by a function f that maps n-bit strings x ("candidates") to 0 ("no solution") or 1 ("solution!"). In the above example: $f(x) = 1$ if $h(x) = y^\star$ and 0 else. Assume you have a piece of code that evaluates f on a classical computer in T_n time steps. Then Grover's recipe turns that code into a time-dependent two-body Hamiltonian $H(t)$ such that if $|\psi(0)\rangle = |0, \ldots, 0\rangle$, then

$$\big|\psi\big(t = cT_n\sqrt{2^n}\big)\big\rangle \simeq |x_1^\star, \ldots, x_n^\star\rangle,$$

where $x^\star$ is such that $f(x^\star) = 1$ and c a (reasonably small) constant. A measurement will then reveal the bits of $x^\star$ with high probability.

Grover's algorithm is also "black box" in the sense that no understanding of "the inner workings" of f beyond the ability to compute it is required. So how is it possible to find a solution in drastically less time than it would take to consider a fixed fraction of all inputs? The answer is that Grover constructs a *quantum* black box $U_f : |x, 0\rangle \mapsto |x, f(x)\rangle$ that *can be run on a superposition of inputs*

$$U_f\Big(\sum_x c_x|x, 0\rangle\Big) = \sum_x c_x|x, f(x)\rangle.$$

Thus, just a *single* invocation of the quantum black box results in a wave function that carries information about *all possible inputs*. The tricky part is then to read this information out. Grover's contribution was to find a clever trick for getting the amplitudes for all $|x, f(x)\rangle$ with $f(x) = 0$ to interfere destructively, so that only the solutions survive.

We'll work our way through the details next.

The gate model

The connection between classical computer code and quantum Hamiltonians goes via the *gate model* of computation.

A classical computer operators on *bits*, physical systems that can be in one of two states. Traditionally, these are labeled 0 and 1. A *logic gate* (or just *gate*) is a process that changes the state of a small number of bits in a defined way, see Fig. 1.7. It is known in classical computer science that any function that can be computed at all can also be computed by a circuit formed by concatenating reversible logic gates.

We now consider a quantum generalization. To this end, replace each bit by a two-level quantum system and fix some basis with states labeled $|0\rangle, |1\rangle$. Voilà, a *quantum bit* (or *qubit*). We assume that we have detailed control over the dynamics: By adjusting classical control parameters (external fields, position of the qubits, etc.), we are able to switch off the time evolution $H = 0$, or to realize single qubit $H = h^{(i)}$ or two-qubit $H = h^{(ij)}$ Hamiltonians.

Let's look at the single-qubit case first. If we set, e.g., $H = h^{(i)} = \frac{\hbar}{2}\sigma_x^{(i)}$ for a duration $\delta t = \pi$, then the time evolution $U(\delta t) = e^{-i\frac{\pi}{2}\sigma_x^{(i)}} = -i\sigma_x^{(i)}$ acts on the i-th qubit like the classical NOT gate (ignoring a global phase factor of $-i$):

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} : |0\rangle \mapsto |1\rangle, |1\rangle \mapsto |0\rangle \quad \text{or} \quad |x_i\rangle \mapsto |\text{NOT}(x_i)\rangle.$$

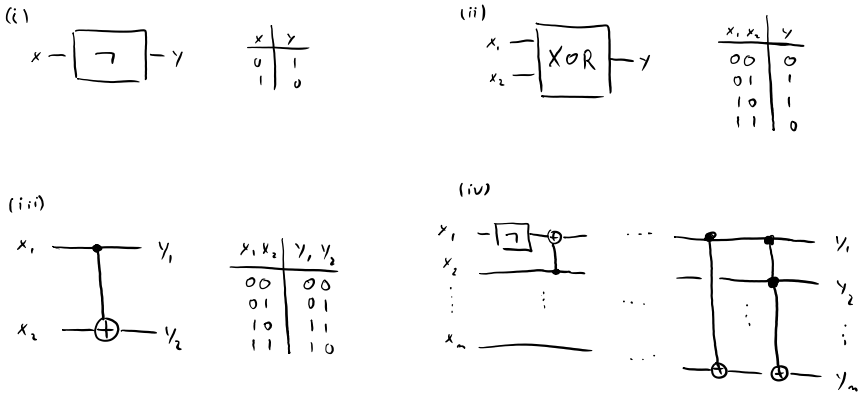


Figure 1.7: Classical gates and circuits. *(i)* The NOT gate inverts the state of a single bit. *(ii)* The XOR gate computes the *exclusive or* $x \oplus y$ of its inputs. *(iii)* The CNOT (or *controlled not*) gate toggles the state of the second bit if and only if the first bit is in the 1-state. Note that the CNOT and the NOT gate are reversible: I.e. the input can be reconstructed given the output. *(iv)* A reversible circuit. It turns out that anything a classical computer can do can be represented in this way.

Likewise, the matrix that is represented in the $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$-basis by

$$\textsc{Cnot} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix} : \qquad \begin{array}{c|c} |x_i x_j\rangle & \textsc{Cnot}|x_i x_j\rangle \\ \hline |00\rangle & |00\rangle \\ |01\rangle & |01\rangle \\ |10\rangle & |11\rangle \\ |11\rangle & |10\rangle \end{array}$$

acts like the CNOT gate, but on qubits. Because U is unitary, it can be implemented by a suitable two-qubit Hamiltonian (homework). This construction generalizes to all reversible logic gates and, as per our previous comment, any classical computation can thus be realized by a time-dependent Hamiltonian on qubits.

But of course, most unitaries are not permutations! A *quantum gate* is any unitary that acts on a small number of qubits. Prominent examples with no classical counterpart are

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \textit{Z-gate}, \tag{1.15}$$

$$P = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \qquad \textit{phase gate}, \tag{1.16}$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad \textit{Hadamard gate}. \tag{1.17}$$

The Hadamard gate, e.g., turns basis states into uniform superpositions:

$$\begin{aligned} H|0\rangle &= 2^{-1/2}(|0\rangle + |1\rangle), \\ (H \otimes H)|0\rangle|0\rangle &= (H|0\rangle)(H|0\rangle) = 2^{-1}(|00\rangle + |01\rangle + |10\rangle + |11\rangle), \\ &\vdots \\ H^{\otimes n}|0, \ldots, 0\rangle &= 2^{-n/2} \sum_{x_1,\ldots,x_n=0}^{n} |x_1, \ldots, x_n\rangle. \end{aligned}$$

Grover iterations

Let $f : \{0,1\}^{\times n} \to \{0,1\}$ be a classical function as introduced in Sec. 1.4.1. To represent f in a quantum computer, we have to consider a reversible version. The common choice is this:

$$(x, y) \mapsto (x, y \oplus f(x)) \qquad x \in \{0,1\}^{\times n}, y \in \{0,1\}.$$

As is the case for any reversible function, it can be expressed as a circuit consisting of reversible classical gates. Re-interpreting these as quantum gates, we arrive at the $(n+1)$-qubit unitary

$$U_f : |x, y\rangle \mapsto |x, y \oplus f(x)\rangle$$

which can indeed be realized by a time-dependent Hamiltonian running in time proportional to T_n.

At this point, we have constructed the quantum black box, and have seen how to create superposition states using Hadamard gates. Let's combine these two steps. For simplicity, assume that there is a unique $x^\star$ such $f(x^\star) = 1$. Then:

$$U_f \left(H^{\otimes n} \otimes \mathbb{1}\right) |0, ..., 0\rangle = 2^{-n/2} \sum_x |x, f(x)\rangle = 2^{-n/2} \sum_{x \neq x^\star} |x, 0\rangle + 2^{-n/2} |x^\star, 1\rangle.$$

That's promising, because a single invocation of the quantum black box did indeed leave information about $x^\star$ in the output. But it's not yet useful, because the coefficient in front of $|x^\star, 1\rangle$ is exponentially small. Performing a measurement will reveal it only with probability 2^{-n}, exactly the same as a classical random guess would give.

Grover found a way to *amplify* the coefficient in front of the solution. His construction involves the following elements, whose relevance will become clear soon:

1. Instead of U_f, which indicates whether a solution has been first by flipping an auxiliary qubit, use

   $$V_f : |x\rangle \mapsto (-1)^{f(x)} |x\rangle$$

   which changes the sign of the coefficient for the solution. One can construct V_f from U_f by throwing in an extra Hadamard gate. Verifying this is homework.

2. Introduce a second unitary

   $$V_\delta : |x\rangle \mapsto (-1)^{\delta(x)} |x\rangle,$$

   where f is replaced by the "Kronecker delta for bit-strings", i.e. V_δ flips the sign of the coefficient for $x = 0$.

3. Define the *Grover operator* to be

$$G = (-H^{\otimes n} V_\delta H^{\otimes n}) V_f.$$

The big claim now is that starting from $H^{\otimes n}|0\rangle$, every application of the Grover operator G will rotate the state vector closer to $|x^\star\rangle$, hitting the target after $\simeq \frac{\pi}{4}\sqrt{2^n}$ iterations.

Proof: Define

$$|\skull\rangle = \frac{1}{\sqrt{2^n - 1}} \sum_{x \neq x^\star} |x\rangle$$

to be the uniform superposition of all non-solutions. Then $\{|\skull\rangle, |\smiley\rangle := |x^\star\rangle\}$ form on ONB for a two-dimension subspace. Remarkably, the state vector will regularly end up in this 2-dimensional space, so we can track the progress of the algorithm solely by considering the dynamics in this small space. (This makes Grover comparatively easy to analyze. Don't get your hopes up, though. This never happens again). Indeed, the state $|+\rangle = H^{\otimes n}|0\rangle$ can be expanded as

$$|+\rangle = \sqrt{\frac{2^n - 1}{2^n}}|\skull\rangle + \frac{1}{\sqrt{2^n}}|\smiley\rangle.$$

As you can see, the initial superposition is almost parallel to the non-solutions $|\skull\rangle$. Call the angle they enclose $\vartheta/2$ (the factor $1/2$ will be motivated momentarily). Then

$$\vartheta := 2\,\angle(|\psi_1\rangle, |\skull\rangle) = 2\arcsin\left(\frac{1}{\sqrt{2^n}}\right) \simeq \frac{2}{\sqrt{2^n}}$$

(an *excellent* approximation for reasonably large n). Now the application of V_f changes the sign of the coefficient in front of $|\smiley\rangle$. Geometrically, this corresponds to a reflection about the plane orthogonal to $|\smiley\rangle$. Likewise,

$$-H^{\otimes n} V_\delta H^{\otimes n} = H^{\otimes n}(-\mathbb{1} + 2|0\rangle\langle 0|)H^{\otimes n} = -\mathbb{1} + 2|+\rangle\langle +|$$

is a reflection about $|+\rangle$. The combinations of two reflections is a rotation, and a simple geometric analysis in the $|\skull\rangle$–$|\smiley\rangle$–plane (Fig. 1.8) shows it is by an angle of ϑ toward the solution vector $|\smiley\rangle$. It is reached after k iterations of G, for

$$\vartheta/2 + k\vartheta = \frac{\pi}{2} \quad \Leftrightarrow \quad k = \frac{\pi}{2\vartheta} - \frac{1}{2} \simeq \frac{\pi}{4}\sqrt{2^n} \tag{1.18}$$

as claimed. □

Remarks:

- Don't run Grover for too long! Otherwise, you'll rotate past the solution $|\smiley\rangle$.
- Don't worry if (1.18) has no integer solution. If $\langle\psi|x^\star\rangle = 1 - \epsilon$, you'll get a wrong solution $x \neq x^\star$ with probability $\simeq 2\epsilon$. But by assumption, we can *check the solution efficiently* by computing $f(x)$. If $f(x) = 0$, just rerun the algorithm.
- While impressive in its generality, the practical utility of Grover's algorithm is limited. The "square root speedup" isn't as large as the *exponential* speedup some quantum algorithms promise. What is more, quantum computers are much harder to build than classical ones and might require a substantial overhead to compensate for errors. On top of all that, Grover, unlike an exhaustive classical search, cannot be parallelized. Thus the square root advantage might only materialize for n's such that not only 2^n, but already $\sqrt{2^n}$ is astronomical.

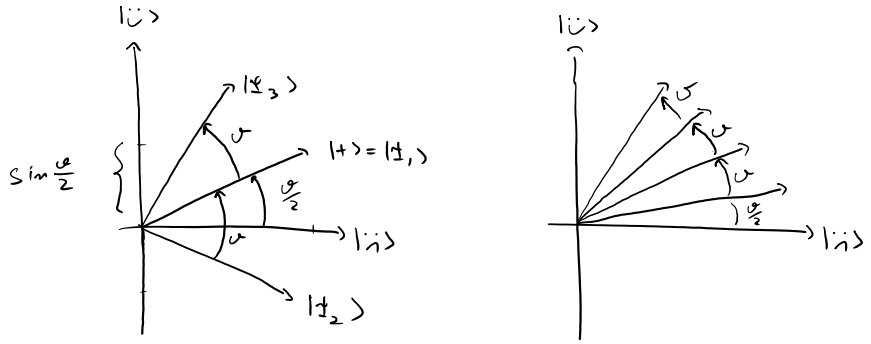


Figure 1.8: Time evolution of the Grover algorithm. Left panel: A Grover iteration performs two reflections that combine to a rotation by θ toward the target state $|\☺\rangle = |x^\star\rangle$. Angles not to typical scale! Right panel: The effect of consecutive Grover rotations.

Summary

- The exponential size of the many-body Hilbert space can potentially be put to use to solve classically hard computational problems.
- Time evolutions of few qubits are described by small unitaries, which are called *quantum gates* and generalize classical logic gates.
- Classical computations can be made reversible and reversible gates reinterpreted as unitaries. This way, classical subroutines can be can be evaluated on superpositions of inputs. The resulting state carries information about their global behavior. Putting this information into a form that can be read out may require non-trivial efforts (e.g. Grover iterations).

1.5 Bell inequalities and their implications

Classical mechanics tells you what is happening. Quantum mechanics only tells you what you will observe when you measure. It does not assign values to unmeasured physical properties.

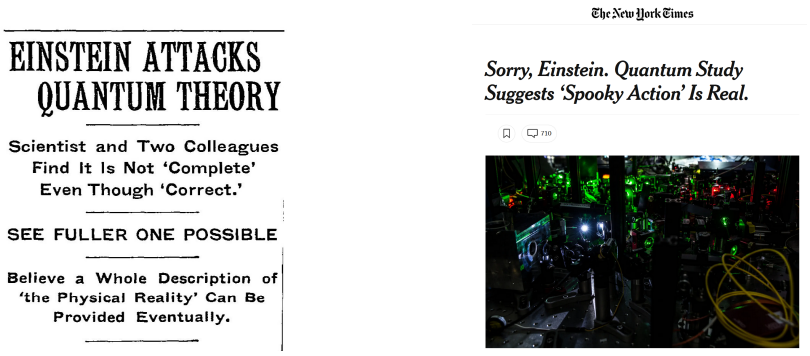
From the early days of the theory, some scientists – famously Albert Einstein (Fig. 1.9 – saw this as a sign that quantum mechanics was *incomplete*, and should be supplanted by a more detailed description of Nature that does track the time evolution of all physical properties, measured or not.

In what I feel is one of the most profound findings of modern physics, this program has since been proven to be impossible: The hypothesis

"Physical properties exist independently of measurements" (1.19)

has been *experimentally falsified* as a general property of Nature! On top of the surprising conclusion, this is remarkable because (1.19) feels like a philosophical statement that is too vague to have testable implications. Yet here we are.

In the following derivation, we have to keep in mind that we want to reason about theories different from quantum mechanics. This means that we cannot use any concept



EINSTEIN ATTACKS QUANTUM THEORY

Scientist and Two Colleagues Find It Is Not 'Complete' Even Though 'Correct.'

SEE FULLER ONE POSSIBLE

Believe a Whole Description of 'the Physical Reality' Can Be Provided Eventually.

The New York Times

Sorry, Einstein. Quantum Study Suggests 'Spooky Action' Is Real.

Figure 1.9: Left panel: 1935 New York Times headline reporting on Einstein-Podolsky-Rosen paper arguing that quantum mechanics was incomplete. I wonder how Podolsky and Rosen felt about the framing. Right panel: 2015 New York Times headline reporting on Einstein being wrong.

that has a meaning only in the context of QM. "Hilbert space", "entanglement", "commutators", even "photon"... ...all these terms are verboten until further notice.[2]

Goals

The goals of this section? You got to be kidding me! Understand that, of course. This has got to be one of the coolest things physics has to offer.

1.5.1 The CHSH scenario

Our challenge now is to come up with a setting in which the vague statement (1.19) leads to quantitative predictions that can be compared to experiments. The most important case is the so-called *CHSH scenario* (Fig. 1.10). While not difficult to understand, it does contain quite a number of elements that seem ill-motivated at this point. Please bear with me for a moment.

The scenario contains two observers, Alice and Bob, located at different ends of a laboratory. There's a box in the middle. In regular intervals, it emits two systems, one flying to Alice and one to Bob. Each observer has two measurement devices, labeled 1 and 2. The devices work like this: They have an entry port and when one of the systems coming from the central box enters a device, one of two lights will flash. The lights are labeled $+1$ and -1 respectively. Every time a pair of systems leaves the central box, Alice and Bob choose one of their measurement devices at random, put it in the path, and record the observed outcomes.

OK, some Q&A's:

- Q.: *So what's up with the talk of "systems"? What are these? Photons? Spins?*
  A.: Unspecified. For now, these could be puffs of hot air and the measurement

[2] Physicists talking about Bell inequalities have a tendency of emphasizing entanglement, or the singlet state and how the fact that it's spin-0 means that angular momentum measurements are anti-correlated, and some such things. These are not wrong and even mildly helpful for the design of experiments that lead to the falsification we are after. All this is also completely secondary to the main point; a case of people sticking to their comfort zone.

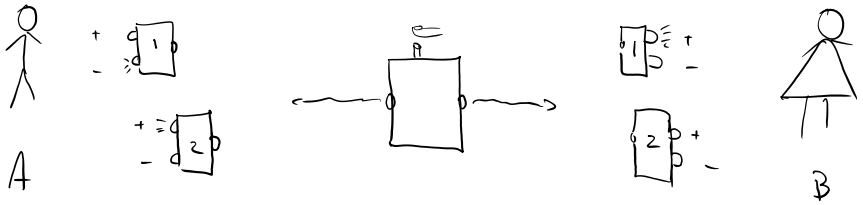


Figure 1.10: The ingredients of the CHSH scenario (for Clauser, Horne, Shimony and Holt). Two experimentalists are located at different ends of a laboratory. Each can perform one of two measurements on systems emanating from a box in the middle. Surprisingly, the analysis of the set of correlations that are compatible with this extremely vaguely defined scenario offers profound insights!

devices random number generators. Our analysis does not depend on assumptions about their nature. (Also, what's a photon?)

- Q.: *Are Alice's devices* 1 *and* 2 *different? Is Alice's device 1 different from Bob's device 1?*
  A.: We do not need to make any assumptions about this.

- Q.: *Why are the outcomes labeled* ± 1*?*
  A.: That's not really essential. This particular choice will work well with our analysis, though.

- Q.: *Can Alice rig her boxes together such that she can perform both measurement on the same incoming system?*
  A.: For all we know at this point... maybe?

- Q.: *Look man. You are clearly just avoiding my questions. Why don't you study your system first, and come back once you can give specific answers?!*
  A.: You got it backwards! The fewer assumptions I need to make, the more generally applicable my conclusions will be.[3]

- Q.: *How in the world does one come up with this?*
  A.: Well, it took physics a few decades. Also, literal Einstein missed it.

With the setup established, let's look at the lab book produced by A&B. Here's a possible snapshot:

	Alice		**Bob**	
i	A_1	A_2	B_1	B_2
1	$+$		$-$	
2	$+$			$+$
3	$-$			$-$
4		$+$	$+$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

[3] I once had a long discussion with colleague who refused to conceit this point, despite me applying all the logic, persuasion, and appeals to authority I could muster. Very frustrating.

Obviously, in each round i, both Alice and Bob can fill out only the column corresponding to the measurement they chose to make.

We will now argue that Assumption (1.19) puts quantitative constraints on the type of data that can appear in this setting. Later, we will see that there are experiments that violate these constraints—thereby disproving the general validity of (1.19). (Also, QM predicts the violations correctly. That's also interesting, but less relevant).

Concretely, if physical properties exist independently of observations, then there exits a complete table, say

	Alice		**Bob**	
i	A_1	A_2	B_1	B_2
1	$+$	$-$	$-$	$-$
2	$+$	$-$	$+$	$+$
3	$-$	$-$	$+$	$-$
4	$+$	$+$	$+$	$-$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

and in each round, A&B just decide which of the pre-existing values to uncover.

In what may feel like an unmotivated move even by the standards of the present discussion, associate the expression

$$C = A_1B_1 + A_1B_2 + A_2B_1 - A_2B_2$$

which each complete row. There's an elegant geometric construction that leads to this particular formula (the keyword is *Bell polytope*) – but it takes some time to develop, so let's just work with C regardless of where it comes from. In our example:

	Alice		**Bob**		
i	A_1	A_2	B_1	B_2	C
1	$+$	$-$	$-$	$-$	-2
2	$+$	$-$	$+$	$+$	2
3	$-$	$-$	$+$	$-$	2
4	$+$	$+$	$+$	$-$	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Despite being the sum of four terms each valued ± 1, the expression (in fact: its absolute value) is upper-bounded by 2: Factoring out Alice's variables and applying the triangle inequality,

$$|C| = |A_1(B_1 + B_2) + A_2(B_1 - B_2)| \leq |B_1 + B_2| + |B_1 - B_2| = 2.$$

It may seem that we can't extract observable predictions out of this discussion, because the expression C involves all four variables, and by assumption, we only have access to two of them in each round. But there's a nice trick to get around this! Indeed, if $C \leq 2$ in every run, then so is the *average*

$$\langle C \rangle = \frac{1}{N} \sum_{i=1}^{N} C^{(i)}$$

over N runs. But averages are linear, and therefore $\langle C \rangle$ equals

$$\langle A_1B_1 + A_1B_2 + A_2B_1 - A_2B_2 \rangle = \langle A_1B_1 \rangle + \langle A_1B_2 \rangle + \langle A_2B_1 \rangle - \langle A_2B_2 \rangle.$$

Each of the four terms $\langle A_iB_j \rangle$ *can* be estimated by A&B! If they choose their settings at random, then by the law of large numbers (or, quantitatively, by the *Chernoff bound*), their observed mean will converge to the true expected value in the limit of large N. Thus, Assumption (1.19) implies that the linear combination of these four experimentally accessible numbers is no larger than 2, up to statistical fluctuations that vanish in the large-N limit. Such a test of (1.19) is called a *Bell inequality*.

Following up on pioneering works that led to the 2022 Nobel Prize, it is today fairly routine to perform experiments that are compatible with the CHSH setup and yield a value of $\langle C \rangle \simeq 2.7$.

Thus, Assumption (1.19) must be rejected as a general feature of Nature.

1.5.2 Operational consequences of Bell inequality violations

The existence of Bell inequality violations imply some interesting "no-go theorems", i.e. statements showing that certain processes are impossible (similar to how the second law of thermodynamics rules out the existence of perpetual motion machines). In the literature, these results are usually derived relying on the quantum mechanical formalism. But it's both easier and more fundamental to conclude them purely from empirically observed violations of (1.19).

Further reading: The exposition in this section is, unfortunately, not commonly found in textbooks. It is based on this paper, which should be better known!

Joint measurements

Recall the Heisenberg uncertainty principle $\mathrm{Var}_\psi[X]\,\mathrm{Var}_\psi[P] \geq \frac{\hbar^2}{4}$. It is often verbally summarized as stating that "position and momentum can't be measured simultaneously." But the relation says no such thing. (Rather, it says that there's no state $|\psi\rangle$ that would cause both position and momentum measurements to produce arbitrarily sharply concentrated outcomes.)

It is still *true*, however, that position and momentum cannot be measured simultaneously. What is more, this is true for any pair of observables that Alice can use in an experiment that violates the CHSH inequality. Even better: This no-go statement does not assume the validity of QM, but is an empirical fact about the universe we live in.

To state the result, we first have to say what we mean by "joint measurement", again without using quantum-mechanical concepts. Let's say two measurement devices are *equivalent* if give the same probability distribution over outcomes for every possible input (Fig 1.11). Now consider two measurements $1, 2$, say with two outcomes each. A *joint measurement machine* for $1, 2$ is a device J with *two* pairs of outcomes (Fig. 1.12). It must be such that if one only considers the first pair, one obtains a measurement procedure equivalent to 1; and if one only considers the second pair, one obtains a measurement procedure equivalent to 2. The two original machines are said to be *jointly measurable* if there exists a joint measurement machine for them.

Now assume that the two properties probed by Alice in the CHSH scenario are jointly measurable and that the same is true for the two properties measured by Bob. They could then use joint measurement machines to produce a complete table, with all properties A_1, A_2, B_1, B_2 provided in every round. The definition of a joint measurement machine and of equivalent measurement implies that each pair i, j, the marginal distributions for

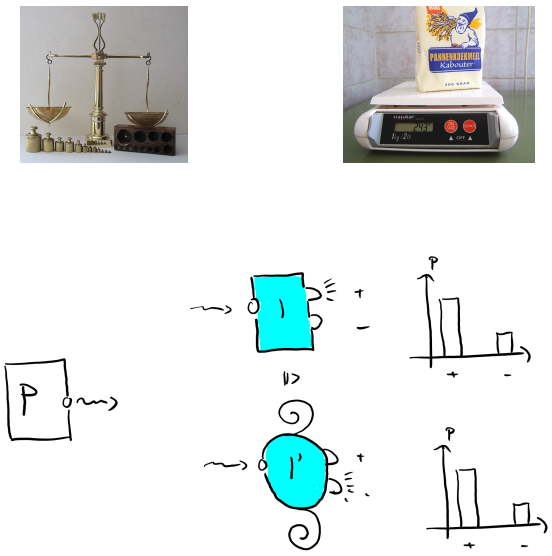


Figure 1.11: Top panel: Each physical property can be measured in many equivalent ways. Bottom panel: Formalization this observation for probabilistic theories. Two measurement devices 1, $1'$ are *equivalent* if for every preparation procedure P, measuring 1 or $1'$ leads to identical probability distribution over outcomes.

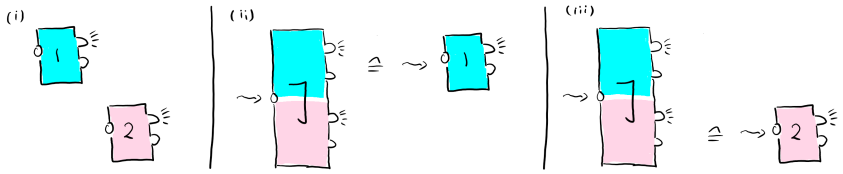


Figure 1.12: (i) Two two-outcome measurement devices, 1 and 2, like the ones held by Alice in the CHSH scenario. They are *jointly measurable* if there exists a measurement device J that produces two pairs of outcomes such that: (ii) The first pair (cyan) alone defines a measurement that is equivalent to 1, and (iii) The second pair (pink) alone defines a measurement that is equivalent to 2.

A_iB_j the arise this way are identical to the ones that the original measurement devices realize. In particular, the correlation function C must be the same in both cases. But, as proven above, in this case $|C| \leq 2$.

The contrapositive: In a universe where the CHSH inequality can be violated (such as ours), there must be pairs of physical properties that cannot, as a matter of principle, be jointly measured. This is a remarkably far-reaching statement to follow from empirical observations alone!

- Q.: *Wait. In our earlier Q&A, you said that as far as you knew, Alice* could *measure her two properties jointly.*
  A.: And that was the right answer at that point in the analysis! We didn't have to *assume* incompatibility. We *derived* it. Like the cool kids.

No cloning

Define a *universal cloning machine* to be a process that takes one physical system as input and outputs two systems such that: Applying any measurement device to the first or to the second output is equivalent to applying it to the input. It is clear that the existence of a universal cloner implies the existence of a joint measurement machine for any pair of properties (Fig. 1.13). Again, we conclude that in a universe where CHSH violations are observed, cloning is impossible.

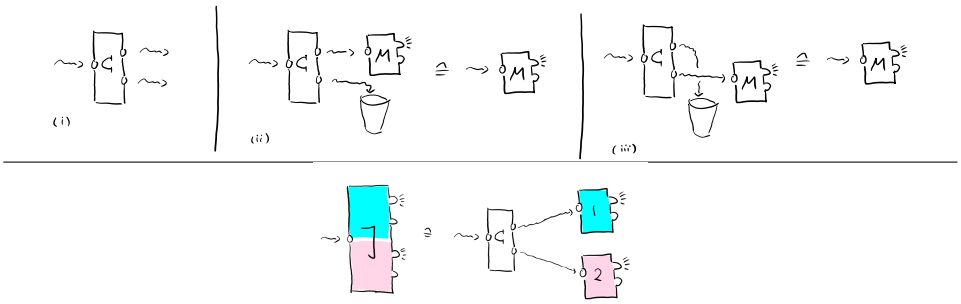


Figure 1.13: Top: A *universal cloning machine* (i) is a device that takes one physical system as input and outputs two physical systems, where each of the outputs is indistinguishable from the input under any measurement (ii), (iii). Bottom: A cloner can be used to construct a joint measurement machine.

There's a famous paper (cited in an academic publication about once every day!) that derives the no-cloning theorem from quantum mechanics. Here's their proof: If U is an operator that "clones two orthogonal states" in that

$$U|0\rangle = |00\rangle, \qquad U|1\rangle = |11\rangle,$$

then by linearity,

$$U\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \neq \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle),$$

so it necessarily fails to clone superpositions of the two states. That's cool and all, but note that it assumes the validity of quantum mechanics, whereas our argument doesn't!

True randomness

Assume I put a dice in a cup, shake it vigorously, and put the cup upside down on a table. Nobody will have any idea how many eyes the dice shows, so one might well model the situation by ascribing a probability of $1/6$ to any of the possible outcomes. But note that this description only reflects my ignorance about the true state of the dice. There is no doubt that *some* side is facing up even before I lift the cup. In fact, it is conceivable in principle that a computer coupled to a camera that captured my motions might solve Newton's equations and predict the state of the dice accurately. Let's refer to a variable as *pseudo-random* if such a prediction is possible in principle, and as *truly random* otherwise.

A priori, it is unclear whether true randomness exists at all.

But CHSH violations are only possible if the outcomes of Alice and Bob are truly random. For if some process could predict the outcomes, it could do so independently of

which property they choose to measure. It could therefore predict the full table, and we are back at the proof by contradiction outlined above.

The fact that no outside observer can predict the outcomes of Alice and Bob means that they are, in this sense, "private" to them. This observation is the basis of provably secure *quantum key distribution* protocols.

1.5.3 Interpretations

We have presented a *negative* argument that rules out the classical model of a world that evolves independently from observations. It is widely argument accepted today. However, there is no *positive* agreement what, if anything, should replace it. Below are some common reactions as I see them.

The orthodox position is to say that the purpose of science is to make empirically testable predictions. QM excels at this task. Counterfactual questions about "what would have happened had you measured something else" just amount to storytelling and lie outside the remit of science. So Bell is interesting for its operational consequences (Sec. 1.5.2), but philosophically, there's not much to be done other than to shrug and move on.

Problems with this position: (1) It is rather unambitious. Theoretical physics has historically offered more than just the ability to predict detector click patterns. To just disallow hypotheticals feels like giving up too early. (2) The *elements of reality* critique explained next.

The Bohmians point out that sometimes, one *can* predict the outcome of a measurement with 100% certainty. (E.g., for a system in the singlet state, when Alice measured spin along one axis and obtained $\uparrow$, Bob will definitely obtain $\downarrow$ w.r.t. the same axis). They argue that in such situations, reality doesn't change if the now somewhat redundant measurement is performed – so that if we consider outcomes to be real, there must already have been some *element or reality* representing them before the measurement. Speaking in terms of the lab books we analyzed above, they therefore posit that there always is a full table representing the true state of all elements of reality at any time, measured or not.

By Bell's argument, the table can't be *independent* of the measurements made. A more detailed analysis shows that one can accommodate CHSH violations only if Bob's variables change as a result of Alice interacting with her side of the joint system (and / or vice versa). There is a simple model developed by David Bohm showing that QM can in principle be interpreted in such a *realistic* (i.e. properties have values whether measured or not) but *non-local* (i.e. the unmeasured parameters change due to actions far away) way. In Bohm's model, the change of unmeasured parameters happens in a subtle way that is strong enough to enable CHSH violations, but too weak to allow for the exchange faster-than-light signals between far away parties.

Therefore, the Bohmians argue, such a description is both necessary (by the elements--of-reality argument) and possible (by Bohm's model). There is thus no paradox, and we should concentrate on working out the details.

The problem with this position is that you get into tension with special relativity even in the absence of superluminal signals. Recall that if A&B's actions are space-like separated, their order in time is observer-dependent. So how can I think about Alice's actions *causing* change at Bob's end, when in some reference frames, Bob acted first?

Some proponents of Bohm's program bite this bullet and acknowledge that realist interpretations of QM imply that there must be a distinguished frame of reference in the universe. They may not *like* having to break Lorentz invariance, but they like attempts to discuss away the elements-of-reality critique even less. Needless to say, having seen what

the Michelson–Morley experiment did to the concept of the *luminiferous ether*, mainstream physicists are highly reluctant to re-introduce distinguished reference frames.

The loopholers maintain that there are further implicit assumptions in the analysis, some of which have to be rejected. After improvements of experimental techniques in the past few years, the (unfortunately-named) *free will loophole* is the last major one standing.

Recall that we have assumed that A&B choose their settings randomly. More precisely, the empirical means for A_iB_j only converge to the expected values $\langle A_iB_j\rangle$ if the probability of choosing a setting is independent of its value. (Think of an election pollster calling random citizens on their landlines during work hours, to ask about their voting intentions. Retired people are more likely to answer the phone—potentially skewing the result, as their voting preferences are different from the population as a whole). But A&B are physical systems, too! They share a common history with the central box. It is therefore unjustified, it is argued, to assume that they can make independent choices.

Problems: (i) The position "proves too much". It seems like it can be used as a general argument against all of empirical science ("apples mostly fall upwards, but we only look when they happen to fall down"). (ii) One can design the choice function of A&B in such a way that it would take one sophisticated cosmic conspiracy to still produce a CHSH value of 2.7. People have performed Bell experiments where the settings were driven by fluctuations in the cosmic background radiation measured at different sections of the night sky, XOR'ed against the input of internet users participating in an online action game.

The many-worlders will remind you that QM anyway has a philosophical problem (the one we didn't address in Sec. 1.3.1), and propose to fix all issues in one fell swoop. They then throw out the measurement postulate and posit that there exists a "wave function of the universe" that evolves under a global Hamiltonian. The reality we experience is an emergent feature of this wave function – not a pre-existing concept like in standard QM.

Without a measurement postulate that will probabilistically pick one "branch of a superposition", all of them have an equal right to being considered as "real". Let's apply this way of thinking to the superposition $\alpha|\uparrow\rangle|\delta t\rangle|\text{☺}\rangle + \beta|\downarrow\rangle|(-\delta t)\rangle|\text{☹}\rangle$ which showed up in Eq. (1.14) as the result of a spin degree of freedom interacting with the particle's position and an observer. Proponents of this interpretation would say that there are now two co-existing realities (the *worlds*), one associated with each summand (or *branch*). In the first, the spin points up, the particle is deflected by δt and the observer is happy. Things are reversed in the second world.

In particular, in a CHSH experiment, all possible outcomes are simultaneously realized in different *branches of the wave function*. Any philosophical problem tied to the assumption that only one branch actually occurs is thus spurious.

The problem here is that the measurement postulate, clunky as it may be, is what connects the formalism to reality! If you claim it's unnecessary, it's on you to re-derive the empirical content of the theory in this reduced framework. One important touchstone is the *Born rule* which says in this language that "if my wave function splits into two branches with amplitudes α and β, I experience these with probability $|\alpha|^2, |\beta|^2$ respectively". Researchers working on many-world formulations therefore spend a lot of time thinking about probabilities and their interpretation (but, to my personal taste, haven't cracked this nut yet).

1.6 Further reading

To repeat the basics:

- *Quantum Mechanics* by Leslie Ballentine is a nice presentation that's somewhat more careful than many textbooks without being too mathematical.
- *Quantum Mechanics 1 & 2* by Cohen-Tannoudji and friends contains an enormous amount of optional material for each chapter. It can thus both be used as an introductory textbook and as a reference.
- *Modern Quantum Mechanics* and *Advanced Quantum Mechanics* by Sakurai will also be used for later parts of this course.

The quantum model of the measurement process is described in Chapter 12 of *Quantum Theory* by Asher Peres. A classic volume on decoherence theory is *Decoherence and the Appearance of a Classical World in Quantum Theory* by Jost, Zeh, (Cologne's very own) Kiefer, Giulini, Kupsch, and Stamtescu. A standard introduction to quantum computing is *Quantum Information and Computation* by Nielsen and Chuang. The operational consequences of Bell violations follow *Quantum Information Theory: An Invitation* by Werner.

Chapter 2

Indistinguishable particles

2.1 Bosonic and Fermionic Hilbert spaces

The tensor product construction (Sec. 1.2.1) of the Hilbert space of two distinguishable particles was guided by the need to represent observables for properties of the first or second particle alone. (For example, "What is the expected position of the first particle?", or "Does the second particle's spin point up?"). However, electrons, say, seem to be *indistinguishable* in the sense that any experiment that is sensitive to one electron will be equally sensitive to any other. It thus makes sense to search for a joint Hilbert space that only supports observables like "What is the expected center of mass of the particle configuration?" or "How many particles have their spins pointing up?" that do not involve unphysical references to specific particles.

> The same issue already arises in *classical mechanics*, where e.g. the two configurations $\begin{pmatrix} \boldsymbol{q}_1 \\ \boldsymbol{q}_2 \end{pmatrix}, \begin{pmatrix} \boldsymbol{q}_2 \\ \boldsymbol{q}_1 \end{pmatrix} \in \mathbb{R}^6$ of two point particles describe the same physics. In mechanics, this redundancy does not usually seem to lead to wrong predictions (unlike the QM case, as we will see shortly). There's *some* indication that things are amiss, though. The *Gibbs paradox* says that the classical thermodynamical treatment of a gas of identical particles does give wrong results unless indistinguishable configurations are counted only once. However, this doesn't quite show that the redundant formulation of classical mechanics is inconsistent, as the connection between this microscopic theory and thermodynamics depends on unproven assumptions (e.g. the *maximum entropy principle*), and so the problem could lie somewhere else.

There's a simple construction that seems to account for all fundamental particles. Let $\mathcal{H}^{(1)}$ be a single-particle Hilbert space with basis $\{|i\rangle\}$. If the particles were distinguishable, a general element of the n-body joint Hilbert space would be

$$|\psi\rangle = \sum_{i_1,\dots,i_n} \psi_{i_1,\dots,i_n} |i_1,\dots,i_n\rangle \in (\mathcal{H}^{(1)})^{\otimes n}.$$

Let's look for subspaces of $(\mathcal{H}^{(1)})^{\otimes n}$ that make sense for indistinguishable particles. Let τ_{kl} be the operator that exchanges the k-th and the l-th factor:

$$\tau_{kl}\left(|\dots,i_k,\dots,i_l,\dots\rangle\right) = |\dots,i_l,\dots,i_k,\dots\rangle.$$

If the particles are indistinguishable, then $|\psi\rangle$ and $\tau_{kl}|\psi\rangle$ should describe the same physics. This is certainly true if they differ at most by a phase factor. Because $\tau_{kl}^2 = \mathbb{1}$, such a

phase must be ± 1. The *totally symmetric* or *Bosonic* subspace $\mathrm{Sym}^n(\mathcal{H}^{(1)})$ consists of all vectors such that

$$\tau_{kl}|\psi\rangle = |\psi\rangle \qquad \forall k, l.$$

The *totally anti-symmetric* or *Fermionic* subspace $\wedge^n(\mathcal{H}^{(1)})$ ("*wedge-n*") consists of all vectors such that

$$\tau_{kl}|\psi\rangle = -|\psi\rangle \qquad \forall k, l.$$

> At this point, many texts "prove" that the construction leading to Fermions and Bosons are the only conceivable ways for building a quantum theory of indistinguishable particles. I find these textbook arguments inconsistent and unhelpful to the degree that I'm prepared to claim the world would be better if they all just be forgotten. Ask me about it, or maybe don't.

2.1.1 Permutations and occupation numbers

The operators τ_{kl} (called *transpositions*) generate the group S_n of all *permutations* of the n factors. Recall that a permutation is a way of re-arranging the symbols $1, 2, \ldots, n$ (Fig. 2.1). The *sign* of a permutation π is

$$\mathrm{sgn}(\sigma) = \begin{cases} +1 & \sigma \text{ is product of an even number of transpostions} \\ -1 & \sigma \text{ is product of an odd number of transpositions} \end{cases}.$$

The Bosonic and Fermionic Hilbert spaces can therefore also be defined as the sets of vectors such that

$$\begin{aligned} \pi|\psi\rangle &= |\psi\rangle, && \text{Bosons} \\ \pi|\psi\rangle &= \mathrm{sgn}(\pi)|\psi\rangle && \text{Fermions} \end{aligned}$$

for all permutations $\pi \in S_n$.

> You have encountered this concept before, in the definition of the *determinant* of an $(n \times n)$-matrix:
>
> $$\det M = \sum_{\pi \in S_n} \mathrm{sgn}(\pi) \prod_{i=1}^{n} M_{i,\pi(i)}. \tag{2.1}$$

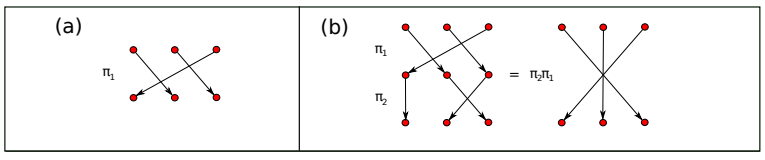


Figure 2.1: (a) A permutation can be represented as a graph, where each position indicates a letter, and where the arrows points to where each letter is mapped. (b) One can multiply permutations σ_1 and σ_2 by performing one after the other.

How many permutations of n letters are there? There are n ways of choosing a new place for the first symbol, then $n-1$ remaining possibilities for the second symbol, etc, for a total of

$$|S_n| = n(n-1)\cdots 2\cdot 1 = n!\,.$$

This explains the various "factorials" that will appear in formulas below.

We can now find bases for the Bosonic / Fermionic subspaces. Indeed, if

$$|\psi\rangle = \sum_{i_1,\dots,i_n} \psi_{i_1,\dots,i_n} |i_1,\dots,i_n\rangle$$

is Bosonic, then $|\psi\rangle = \pi|\psi\rangle$ for all π and thus

$$|\psi\rangle = \frac{1}{n!}\sum_\pi \pi|\psi\rangle = \sum_{i_1,\dots,i_n} \psi_{i_1,\dots,i_n}\Big(\frac{1}{n!}\sum_\pi \pi|i_1,\dots,i_n\rangle\Big). \tag{2.2}$$

The vector in parentheses only depends on the number of times n_k each single-particle basis element $|k\rangle$ appears in the product $|i_1\rangle\dots|i_n\rangle$. This motivates the definition of the *occupation number basis*. For $n_i \in \{0,1,2,\dots\}$ such that $\sum_i n_i = n$, set

$$\begin{aligned}|n_1,n_2,\dots\rangle &:= \frac{1}{\sqrt{n!\prod_k n_k!}}\sum_{\pi\in S_n}\pi|\underbrace{1,\dots,1}_{n_1\times},\underbrace{2,\dots,2}_{n_2\times},\dots\rangle \\ &= \frac{1}{\sqrt{n!\prod_k n_k!}}\sum_{\pi\in S_n}\pi(|1\rangle^{\otimes n_1}|2\rangle^{\otimes 2}\dots).\end{aligned} \tag{2.3}$$

The funky factorial factor makes the vector normalized (check it!). By (2.2), any Bosonic state vector can be expanded in the occupation number basis.

> Recall the *triplet states* of two spin-$1/2$ particles
>
> $$|\uparrow\uparrow\rangle,\quad \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\big),\quad |\downarrow\downarrow\rangle.$$
>
> They are clearly invariant under permutations of the particles. In occupation number notation with respect to the $|\uparrow\rangle, |\downarrow\rangle$-basis, the triplet states are
>
> $$|2,0\rangle,\quad |1,1\rangle,\quad |0,2\rangle.$$

If $|\psi\rangle$ is Fermionic, then arguing as above gives

$$|\psi\rangle = \sum_{i_1,\dots,i_n} \psi_{i_1,\dots,i_n}\Big(\frac{1}{n!}\sum_\pi \operatorname{sgn}(\pi)\,\pi|i_1,\dots,i_n\rangle\Big). \tag{2.4}$$

Anti-symmetry makes things a bit more exciting, though: Again look at the vector in parentheses for some choice $i_1,\dots,i_n$ of single-particle states. If one state occurs twice (say $i_k = i_l$), then

$$|\dots,i_k,\dots,i_l,\dots\rangle + \operatorname{sgn}(\tau_{kl})\,\tau_{kl}|\dots,i_k,\dots,i_l,\dots\rangle = 0$$

which implies that the sum is 0. Therefore, in the Fermionic occupation number basis

$$|n_1,n_2,\dots\rangle := \frac{1}{\sqrt{n!}}\sum_{\pi\in S_n}\operatorname{sgn}(\pi)\pi\big(|1\rangle^{\otimes n_1}|2\rangle^{\otimes n_2}\dots\big), \tag{2.5}$$

n_k must be either 0 or 1. This explains the *Pauli principle*! Beware that in the Fermi case, the sign of the occupation number basis elements (2.5) depend on an ordering of single-particle basis vectors.

For the anti-symmetrization of general single-particle vectors $|\alpha_1\rangle, \dots, |\alpha_n\rangle$, one also uses the *wedge product notation*

$$|\alpha_1\rangle \wedge \cdots \wedge |\alpha_n\rangle := \frac{1}{\sqrt{n!}} \sum_{\pi \in S_n} \operatorname{sgn}(\pi) \pi\big(|\alpha_1\rangle \otimes \cdots \otimes |\alpha_n\rangle\big)$$

pronounced "*alpha one, wedge alpha two, ...*". Wedge products are also called *Slater determinants*. That's because one can express the wedge product as a "formal determinant":

$$|\alpha_1\rangle \wedge \cdots \wedge |\alpha_n\rangle = \frac{1}{\sqrt{n!}} \det \begin{pmatrix} |\alpha_1\rangle^{(1)} & |\alpha_2\rangle^{(1)} & \dots & |\alpha_n\rangle^{(1)} \\ |\alpha_1\rangle^{(2)} & |\alpha_2\rangle^{(2)} & \dots & |\alpha_n\rangle^{(2)} \\ \vdots & \vdots & & \vdots \\ |\alpha_1\rangle^{(n)} & |\alpha_2\rangle^{(n)} & \dots & |\alpha_n\rangle^{(n)} \end{pmatrix}.$$

Here, the super-scripts indicate which tensor factor the vector belongs to.

The singlet state $\frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\big) = |\uparrow\rangle \wedge |\downarrow\rangle$ is clearly anti-symmetric. In occupation number notation with respect to the $|\uparrow\rangle, |\downarrow\rangle$-basis, it is given by $|1, 1\rangle$.

Assume $\dim \mathcal{H}^{(1)} = d < \infty$. In both the Bose and the Fermi case, the occupation number bases give us a combinatorial way to compute the dimension of the Hilbert spaces.

Fermions: Basis elements are labeled by subsets $S \subset \{1, \dots, 1\}$ of size $|S| = n$. Thus

$$\dim \wedge^n\big(\mathbb{C}^d\big) = \binom{d}{n}.$$

Bosons: Basis elements are labeled by a *partition* $n = \sum_{i=1}^d n_i$ of n into d non-negative parts. There's a cute combinatorial argument for computing the number of such partitions. The answer is

$$\dim \operatorname{Sym}^n\big(\mathbb{C}^d\big) = \binom{n+d-1}{n}. \tag{2.6}$$

Can you find it? (Spoiler: Search for "stars and bars").

The occupation number basis adds another possible meaning to the heavily overloaded notation of "a list of numbers in a ket". In particular, in $|n_1, n_2, \dots\rangle = \frac{1}{\sqrt{n! \prod_k n_k!}} \sum_\pi \pi |1, \dots, 1, 2, \dots, 2, \dots\rangle$ the numbers in the ket on the l.h.s. count occupations, while the numbers in the ket on the r.h.s. are indices of some single-particle basis. Which of these definitions is meant, and which single-particle basis it is relative to, and whether the occupation numbers are for Fermions or for Bosons, or whether the numbers have nothing to do with these many-body concepts and are more general "quantum numbers" (like the labels $|n, l, m\rangle$ of the atomic basis) has to be inferred from context. There's no general, reliable rule.

Look. If I were the emperor of physics, I'd outlaw this mess. But I'm not and everybody is using it. After you got used to it, you'll find that this convention causes surprisingly few catastrophic misunderstandings.

Summary

Let $\mathcal{H}^{(1)}$ be a single-body Hilbert space with basis $\{|i\rangle\}$. Then a general state of n indistinguishable particles can be expressed in the occupation number basis as

$$|\psi\rangle = \sum_{n_1,n_2,\dots} c_{n_1,n_2,\dots}|n_1, n_2, \dots\rangle,$$

where the sum is over $n_i \in \{0, 1, 2, \dots\}$ for Bosons and $n_i \in \{0, 1\}$ for Fermions, and where $\sum_i n_i = n$. The occupation number basis is defined as

$$|n_1, n_2, \dots\rangle = \frac{1}{\sqrt{n! \prod_k n_k!}} \sum_{\pi \in S_n} (\operatorname{sgn} \pi)^\zeta \pi(|1\rangle^{\otimes n_1}|2\rangle^{\otimes 2} \dots), \tag{2.7}$$

where $\zeta = 0$ for Bosons and $\zeta = 1$ for Fermions.

2.1.2 Single-particle operators

We started this section remarking that a full tensor product Hilbert space supports more observables than are physically meaningful for indistinguishable particles. Let $A^{(i)}$ be an operator acting on the i-th particle. Then (why?)

$$\pi A^{(i)} \pi^{-1} = A^{(\pi_i)}.$$

Thus, if $|\psi\rangle$ is Bosonic or Fermionic,

$$\begin{aligned}\operatorname{tr}\left(A^{(i)}|\psi\rangle\langle\psi|\right) &= \frac{1}{n!}\sum_{\pi\in S_n} \operatorname{tr}\left(A^{(i)}\pi|\psi\rangle\langle\psi|\pi^{-1}\right) = \frac{1}{n!}\sum_{\pi\in S_n} \operatorname{tr}\left(\pi^{-1}A^{(i)}\pi|\psi\rangle\langle\psi|\right) \\ &= \frac{1}{n}\sum_{j=1}^{n} \operatorname{tr}\left(A^{(j)}|\psi\rangle\langle\psi|\right).\end{aligned} \tag{2.8}$$

A measurement on any one particle is thus equal to the average over all of them – the formalism no longer allows us to pick out the properties of individual particles.

Now assume A has an eigendecomposition

$$A = \sum_i \lambda_i |i\rangle\langle i|.$$

Then for an element of the occupation number basis with respect to the eigenbasis $\{|i\rangle\}$ of A, one computes from (2.7)

$$\sum_{j=1}^{n} A^{(j)}|n_1, n_2, \dots\rangle = \Big(\sum_i \lambda_i n_i\Big)|n_1, n_2, \dots\rangle. \tag{2.9}$$

In particular, single-body operators are diagonal in the occupation number basis. If the single-body eigenvalues are sorted $\lambda_0 \le \lambda_1 \le \dots$, then the lowest n-body eigenvalue in the Bosonic case is $n\lambda_0$ and in the Fermionic case $\lambda_0 + \dots + \lambda_{n-1}$. For Fermions, if the λ_i's describe energies, then λ_{n-1}, the largest energy still occupied in the ground state, is called the *Fermi energy*.

2.1.3 The exchange interaction

Goals

The Coulomb repulsion term between two electrons, $h^{(1,2)} \propto \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^{-1}$, does not depend on spin. However, when combined with the anti-symmetrization postulate for Fermions, an effective coupling between electron spins arises. It is important, e.g. in magnetism and atomic physics. We'll look at a simple case: the electrons of the helium atom in first-order perturbation theory.

Treating the nucleus as fixed, the Hamiltonian for the helium atom is

$$H = H_0 + h^{(1,2)}, \qquad H_0 = h^{(1)} + h^{(2)},$$
$$h^{(i)} = \frac{P_i^2}{2m} - \frac{2e^2}{4\pi\epsilon_0}\frac{1}{\|\boldsymbol{x}_i\|}, \qquad h^{(1,2)} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|}.$$

The eigenfunctions of the single-body Hamiltonian are the same as those for hydrogen (with Bohr radius halved on account of the higher charge), and with arbitrary spin:

$$|\phi_{n,l,m}\rangle|s\rangle, \qquad n \geq 0, l \leq n-1, -m \leq l \leq m, -\frac{1}{2} \leq s \leq \frac{1}{2}.$$

By Sec. 2.1.2, their Slater determinants diagonalize the non-interacting part H_0.

Warm up: The ground state

Write $|1\rangle := |\phi_{1,0,0}\rangle$ for short. The ground state of H_0 is given by

$$|1\uparrow\rangle \wedge |1\downarrow\rangle = \frac{1}{\sqrt{2}}\big(|1\uparrow\rangle|1\downarrow\rangle - |1\downarrow\rangle|1\uparrow\rangle\big).$$

That is: both electrons are in the single-body ground state (spectroscopic notation: $1s^2$), with anti-parallel spins. The ground state vector becomes a lot clearer when we group the spatial and the spin degrees of freedom together:

$$|1\rangle|\uparrow\rangle \wedge |1\rangle|\downarrow\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle|1\rangle|\uparrow\rangle|\downarrow\rangle - |1\rangle|1\rangle|\downarrow\rangle|\uparrow\rangle\right) = |1\rangle|1\rangle\frac{1}{\sqrt{2}}\big(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\big) \quad (2.10)$$

Let's analyze this. The permutation τ exchanges *all* degrees of freedom of the electrons:

$$\tau\Big((|\phi_1\rangle|s_1\rangle)(|\phi_2\rangle|s_2\rangle)\Big) = (|\phi_2\rangle|s_2\rangle)(|\phi_1\rangle|s_1\rangle)$$

We could also define operators $\tau^{(\text{space})}$ and $\tau^{(\text{spin})}$ that only act on one of them:

$$\tau^{(\text{space})}\Big((|\phi_1\rangle|s_1\rangle)(|\phi_2\rangle|s_2\rangle)\Big) = (|\phi_2\rangle|s_1\rangle)(|\phi_1\rangle|s_2\rangle),$$
$$\tau^{(\text{spin})}\Big((|\phi_1\rangle|s_1\rangle)(|\phi_2\rangle|s_2\rangle)\Big) = (|\phi_1\rangle|s_2\rangle)(|\phi_2\rangle|s_1\rangle)$$

so that $\tau = \tau^{(\text{space})}\tau^{(\text{spin})}$. The Hamiltonian H commutes not only with τ, but (in this case) with $\tau^{(\text{space})}$ and $\tau^{(\text{spin})}$ individually. We can therefore find a common eigenbasis, i.e. energy eigenvectors that also have well-defined parity with respect to the exchange of each of the spatial and the spin parts. To get anti-symmetry under τ, exactly one of these two parts has to be anti-symmetric. That's what happened in (2.10).

The energy correction induced by the interaction in first-order perturbation theory is

$$\begin{aligned}&\langle 1|\langle 1|\langle \Psi^-|h^{(1,2)}|1\rangle|1\rangle|\Psi^-\rangle = \langle 1|\langle 1|h^{(1,2)}|1\rangle|1\rangle \\ =&\frac{2e^2}{4\pi\epsilon_0}\int |\langle \boldsymbol{x}_1|1\rangle|^2\,|\langle \boldsymbol{x}_2|1\rangle|^2 \frac{1}{\|\boldsymbol{x}_1-\boldsymbol{x}_2\|}\,\mathrm{d}^3\boldsymbol{x}_1\,\mathrm{d}^3\boldsymbol{x}_2. \end{aligned} \tag{2.11}$$

This expression – called the *Coulomb* or *direct integral* – equals the expected value of the repulsion term experienced by two classical electrons that are found at $\boldsymbol{x}$ with probability density $|\langle \boldsymbol{x}|1\rangle|^2$.

Excited states

The first excited states of H_0 are the ones where one electron remains in the ground state and one is in the state $|\phi_{2,0,0}\rangle =: |2\rangle$ (spectroscopic: "$1s, 2s$"). Taking spin into account, the first excited energy of the non-interacting Hamiltonian is thus four-fold degenerate:

$$|1\rangle|s_1\rangle \wedge |2\rangle|s_2\rangle \qquad s_i \in \{\uparrow,\downarrow\}.$$

As discussed above, we can choose a basis of states that are symmetric / anti-symmetric in the spatial and spin degrees individually:

$$\left.\begin{array}{l} \frac{1}{\sqrt{2}}\big(|1\rangle|2\rangle + |1\rangle|2\rangle\big)\frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\big) \end{array}\right\} \qquad (S=0, \text{“singlet”})$$

$$\left.\begin{array}{l} \frac{1}{\sqrt{2}}\big(|1\rangle|2\rangle - |1\rangle|2\rangle\big)\frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\big) \\ \frac{1}{\sqrt{2}}\big(|1\rangle|2\rangle - |1\rangle|2\rangle\big)|\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\big(|1\rangle|2\rangle - |1\rangle|2\rangle\big)|\downarrow\downarrow\rangle \end{array}\right\} \qquad (S=1, \text{“triplet”})$$

Again, the energy correction only depends on the spatial part. In particular it is the same for the last three vectors. For the first two, we get

$$\frac{1}{2}\big(\langle 1|\langle 2| \pm \langle 1|\langle 2|\big)h^{(1,2)}\big(|1\rangle|2\rangle \pm |1\rangle|2\rangle\big) = \langle 1|\langle 2|h^{(1,2)}|1\rangle|2\rangle \pm \mathrm{Re}\langle 1|\langle 2|h^{(1,2)}|2\rangle|1\rangle.$$

The first matrix element is again a "Coulomb integral"

$$I := \langle 1|\langle 2|h^{(1,2)}|1\rangle|2\rangle = \frac{2e^2}{4\pi\epsilon_0}\int |\langle \boldsymbol{x}_1|1\rangle|^2\,|\langle \boldsymbol{x}_2|2\rangle|^2 \frac{1}{\|\boldsymbol{x}_1-\boldsymbol{x}_2\|}\,\mathrm{d}^3\boldsymbol{x}_1\,\mathrm{d}^3\boldsymbol{x}_2 > 0,$$

which allows for the same probabilistic interpretation as given for Eq. (2.11). The second one is called the *exchange integral*

$$J := \langle 1|\langle 2|h^{(1,2)}|2\rangle|1\rangle = \frac{2e^2}{4\pi\epsilon_0}\int \overline{\langle 1|\boldsymbol{x}_1\rangle}\,\overline{\langle 2|\boldsymbol{x}_2\rangle}\frac{1}{\|\boldsymbol{x}_1-\boldsymbol{x}_2\|}\langle 2|\boldsymbol{x}_1\rangle\,\langle 1|\boldsymbol{x}_2\rangle\,\mathrm{d}^3\boldsymbol{x}_1\,\mathrm{d}^3\boldsymbol{x}_2.$$

The exchange integral is also positive, although that's less obvious.

To see this, rewrite the exchange integral as

$$J = \frac{2e^2}{\epsilon_0}\int \overline{\langle 1|\boldsymbol{x}_1\rangle}\,\langle 2|\boldsymbol{x}_1\rangle \frac{1}{4\pi\|\boldsymbol{x}_1-\boldsymbol{x}_2\|}\,\langle 1|\boldsymbol{x}_2\rangle\overline{\langle 2|\boldsymbol{x}_2\rangle}\,\mathrm{d}^3\boldsymbol{x}_1\,\mathrm{d}^3\boldsymbol{x}_2.$$

Defining

$$\phi(\boldsymbol{x}) := \overline{\langle 1|\boldsymbol{x}\rangle}\langle 2|\boldsymbol{x}\rangle, \qquad A := \int |\boldsymbol{x}_1\rangle\frac{1}{4\pi\|\boldsymbol{x}_1-\boldsymbol{x}_2\|}\langle \boldsymbol{x}_2|\,\mathrm{d}^3\boldsymbol{x}_1\,\mathrm{d}^3\boldsymbol{x}_2,$$

the integral is of the form $\langle\phi|A|\phi\rangle$ with A a translation-invariant. By Eq. (A.25), A is diagonal in the Fourier basis, with eigenvalues given by $(2\pi)^{3/2}$ times the Fourier transform of $f(\boldsymbol{x}) = 1/(4\pi\|\boldsymbol{x}\|)$. From Eq. (C.20), $(2\pi)^{3/2}\tilde{f}(\boldsymbol{k}) = \frac{1}{\|\boldsymbol{k}\|^2}$, so that

$$J = \frac{2e^2}{\epsilon_0}\int \frac{|\langle\phi|\boldsymbol{k}\rangle|^2}{\|\boldsymbol{k}\|^2}\,\mathrm{d}^3\boldsymbol{k} > 0.$$

The effect of the interaction is thus twofold: (i) It uniformly increase the energies by the Coulomb term I describing the expected repulsion felt by the two electrons (as one would expect). (ii) It introduces a splitting by $2J$ of the energies between the symmetric $S = 1$ and anti-symmetric $S = 0$ spin states. The physical way to think about the second effect is that anti-symmetry in the spatial part "allows the electrons to avoid each other", thus decreasing the energy penalty due to electron-electron repulsion.

The Heisenberg model

We have seen that within the $1s, 2s$-space, the energy depends only on the spin configuration. Let's map it to an effective 2-spin model by setting:

$$|s_1, s_2\rangle := |1\rangle|s_1\rangle \wedge |2\rangle|s_2\rangle.$$

In this two-spin Hilbert space, the effective Hamiltonian is, up to an irrelevant global shift of energies,

$$H_{\text{eff}} = -J\tau.$$

We can write the transposition τ as (excercise!)

$$\tau = \sum_{j\in 0,x,y,z} \sigma_j^{(1)}\sigma_j^{(2)} = \mathbb{1} + \boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(2)}$$

and thus, up to another shift,

$$H_{\text{eff}} = -J\,\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(2)}. \tag{2.12}$$

The exchange principle can thus be described as an effective interaction between the two spins. Equation (2.12) is an embryonic version of the *Heisenberg model* of magnetism.

2.2 Second quantization

Goals

This section is mostly formal (definitions, generic constructions). Not too exciting? Maybe. But familiarizing you with the formalism of "second quantization" is one of the most important goals of this lecture. Much builds on it. Be alert!

So far, we have considered systems with a fixed number n of particles. We will now treat the particle number as variable. Mathematically, this actually simplifies some calculations (we won't have to worry about combinatorial expressions like (2.6) any more). Physically, this step is necessary e.g. for relativistic theories, where different species of particles can be converted into each other.

2.2.1 Fock space

Start with a single-particle Hilbert space $\mathcal{H}^{(1)}$. To describe systems with an indefinite particle number, we'll use superpositions

$$|\psi\rangle = \sum_{n=0}^{\infty} |\psi_n\rangle$$

with $|\psi_n\rangle \in \mathrm{Sym}^n(\mathcal{H}^{(1)})$ (Bosons) or $|\psi_n\rangle \in \wedge^n(\mathcal{H}^{(1)})$ (Fermions). Terms corresponding to different particle numbers are taken to be orthogonal, so that inner products are

$$\langle\psi|\psi'\rangle = \sum_{n=0}^{\infty} \langle\psi_n|\psi'_n\rangle.$$

The resulting Hilbert space is called the symmetric/anti-symmetric *Fock space*

$$\mathcal{F}_S\big(\mathcal{H}^{(1)}\big) = \bigoplus_{n=0}^{\infty} \mathrm{Sym}^n(\mathcal{H}^{(1)}) \qquad \text{(Bosons)},$$

$$\mathcal{F}_A\big(\mathcal{H}^{(1)}\big) = \bigoplus_{n=0}^{\infty} \wedge^n(\mathcal{H}^{(1)}) \qquad \text{(Fermions)}.$$

Wait, $n = 0$ is included? That's right, we allow for systems with zero particles. To make sense of that, define

$$(\mathcal{H}^{(1)})^{\otimes 0}, \wedge^{(0)}(\mathcal{H}^{(1)}), \mathrm{Sym}^{(0)}(\mathcal{H}^{(1)}) := \mathbb{C}^1,$$

the Hilbert space of one-component vectors. Up to a phase, it only contains a single normalized vector, which is called the *vacuum* and denoted as $|\mathrm{vac}\rangle$ or $|0\rangle$.

This construction is very transparent in the occupation number basis, where it basically amounts to removing the constraint $\sum_i n_i = n$ (and all the combinatorial nastiness that comes with it). With respect to a basis $\{|i\rangle\}$ of $\mathcal{H}^{(1)}$, Fock space is the Hilbert space with basis $|n_1, n_2, \dots\rangle$, where $n_i \in \{0, 1, 2, \dots\}$ for Bosons and $n_i \in \{0, 1\}$ for Fermions. The vacuum is $|0, 0, \dots\rangle = |\mathrm{vac}\rangle = |0\rangle$.

2.2.2 Creation and annihilation operators

Recall the treatment of the quantum harmonic oscillator (Appendix A.3.1). There, one introduces the *ladder operators* that create/destroy excitations in the sense that

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad \Leftrightarrow \quad a|n\rangle = \sqrt{n}|n-1\rangle. \tag{2.13}$$

The definition might feel a bit unmotivated at first, but it turns out to radically simplify the analysis. Ladder operators can likewise be introduced on Fock space, and once more, they turn out to simplify calculations with indistinguishable particles much more than one could expect.

For any single-particle state $|\alpha\rangle$, the *creation operator* $a^\dagger_\alpha$ is defined via its action on n-particle states $|\psi_n\rangle$ as

$$a^\dagger_\alpha|\psi_n\rangle = \underbrace{\sqrt{n+1}}_{\text{scale to match (2.13)}} \underbrace{\frac{1}{(n+1)!}\sum_{\pi\in S_{n+1}} (\mathrm{sgn}\,\pi)^\zeta\, \pi}_{\text{(anti-)symmetrize}} \underbrace{\big(|\alpha\rangle \otimes |\psi_n\rangle\big)}_{\text{add particle in state } |\alpha\rangle} \tag{2.14}$$

with $\zeta = 0$ (Bosons) and $\zeta = 1$ (Fermions). The associated *annihilation operator* is the adjoint: $a_\alpha = (a_\alpha^\dagger)^\dagger$.

> Equation (2.14) is commonly summarized as "$a_\alpha^\dagger$ creates a particle in state $|\alpha\rangle$". This phrase should be thought of as a mnemonic, not as a precise statement. For one, it omits the crucial scale factor $\sqrt{n+1}$. What is more, a creation operator by itself doesn't usually have a direct physical interpretation (Sec. 2.3.2). Rather, these operators appear as mathematical building blocks that allow for a convenient representation of local operators (Sec. 2.2.3).
>
> It is slightly unfortunate that $a^\dagger$ is a more natural starting point than a, requiring the round-about definition of a as $(a^\dagger)^\dagger$. On the upside, the "dagger" symbol used by physicists to denote the adjoint looks a bit like a "+", so one can easily remember that $a^\dagger$ is the one that "adds" a particle.

We'll usually fix a basis $\{|i\rangle\}$ of the single-body Hilbert space and work in the associated occupation number basis, where the ladder operators act in a transparent way. Eq. (2.14) implies

$$a_i^\dagger|\dots n_{i-1}, n_i, n_{i+1}\dots\rangle = \sqrt{n_i+1}(-1)^{\zeta\sum_{j<i}n_j}|\dots n_{i-1}, n_i+1, n_{i+1}\dots\rangle.$$

Here, we use the convention that $|n_1\dots\rangle$ equals 0 if one of the occupation numbers is negative, or, in the Fermionic case, additionally if one occupation number exceeds 1. Explicitly, for Bosons:

$$\begin{aligned} a_i^\dagger|\dots n_{i-1}, n_i, n_{i+1}\dots\rangle &= \sqrt{n_i+1}|\dots n_{i-1}, n_i+1, n_{i+1}\dots\rangle, \\ a_i|\dots n_{i-1}, n_i, n_{i+1}\dots\rangle &= \sqrt{n_i}|\dots n_{i-1}, n_i-1, n_{i+1}\dots\rangle, \end{aligned} \tag{2.15}$$

and for Fermions

$$\begin{aligned} a_i^\dagger|\dots n_{i-1}, n_i, n_{i+1}\dots\rangle &= (-1)^{\sum_{j<i}n_j}|\dots n_{i-1}, n_i+1, n_{i+1}\dots\rangle, \\ a_i|\dots n_{i-1}, n_i, n_{i+1}\dots\rangle &= (-1)^{\sum_{j<i}n_j}|\dots n_{i-1}, n_i-1, n_{i+1}\dots\rangle. \end{aligned} \tag{2.16}$$

Iterating, any basis element can be written using creation operators acting on the vacuum:

$$|n_1, \dots\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}}\frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}}\dots|0\rangle. \tag{2.17}$$

Basis expansions and field operators

Choose a single-body basis $\{|i\rangle\}$ and a state $|\alpha\rangle \in H^{(1)}$. Plugging the expansion

$$|\alpha\rangle = \sum_i |i\rangle\langle i|\alpha\rangle$$

into (2.14) shows that "creation operators can be expanded like kets and annihilation operators like bras":

$$a_\alpha^\dagger = \sum_i \langle i|\alpha\rangle a_i^\dagger \quad \Rightarrow \quad a_\alpha = \sum_i \langle\alpha|i\rangle a_i. \tag{2.18}$$

We don't need to restrict ourselves to normalizable states. For example, if $|\alpha\rangle = |\boldsymbol{x}\rangle$ is a delta function centered at $\boldsymbol{x} \in \mathbb{R}^3$ and $|i\rangle = |\phi_i\rangle$ for some smooth function $\phi_i(\boldsymbol{x})$ in $L^2(\mathbb{R}^3)$, then the above reads

$$|\boldsymbol{x}\rangle = \sum_i |\phi_i\rangle\langle\phi_i|\boldsymbol{x}\rangle = \sum_i \bar{\phi}_i(\boldsymbol{x})|\phi_i\rangle,$$

and thus the operators "creating / destroying a particle at position $\boldsymbol{x}$" are

$$a^\dagger_{\boldsymbol{x}} = \sum_i \bar{\phi}_i(\boldsymbol{x}) a_i^\dagger \quad \Rightarrow \quad a_{\boldsymbol{x}} = \sum_i \phi_i(\boldsymbol{x}) a_i.$$

Recall that a classical field is any physical quantity that depends on points in space. The $a_{\boldsymbol{x}}$ are quantum operators depending on points in space, and thus a first example of a *quantum field*. These annihilation field operators and their Heisenberg-picture time evolution are commonly written as

$$\hat{\Psi}(\boldsymbol{x}) := a_{\boldsymbol{x}}, \qquad \hat{\Psi}(t, \boldsymbol{x}) := a_{\boldsymbol{x}}(t) = e^{-\frac{t}{i\hbar}H} a_{\boldsymbol{x}} e^{\frac{t}{i\hbar}H}.$$

Despite the similarity in notation, the field operators $\hat{\Psi}(\boldsymbol{x})$ should not be confused with wave functions $\psi(\boldsymbol{x}) \in L^2(\mathbb{R}^3)$!

> All the caveats that apply to delta functions (App. A.1.8) likewise apply to the $\hat{\Psi}(\boldsymbol{x})$. In particular, formulas involving field operators have physical content only when integrated against smooth functions. (In the mathematical literature, the $\hat{\Psi}(\boldsymbol{x})$ are therefore referred to as *operator-valued distributions*, to indicate that they give proper operators only after an integration). See the discussion around (2.23) for an example of how this pans out.

The converse of the above construction also works. From the completeness relation for delta functions (A.14):

$$|\alpha\rangle = \int \alpha(\boldsymbol{x}) \, |\boldsymbol{x}\rangle \, \mathrm{d}^3\boldsymbol{x} \quad \Rightarrow \quad a^\dagger_\alpha = \int \alpha(\boldsymbol{x}) \, \hat{\Psi}^\dagger(\boldsymbol{x}) \, \mathrm{d}^3\boldsymbol{x}. \tag{2.19}$$

Commutation relations

As is the case for the treatment of the harmonic oscillators with ladder operators, their commutation relations are important in calculations.

To treat the Bosonic and Fermionic cases in parallel, introduce the notation

$$[A, B]_\zeta := AB - (-1)^\zeta BA$$

so that

$$\begin{aligned} [A, B]_\zeta &= AB - BA = [A, B] && \text{(Bosons, } \zeta = 0\text{)}, \\ [A, B]_\zeta &= AB + BA = \{A, B\} && \text{(Fermions, } \zeta = 1\text{)}. \end{aligned}$$

From (2.15, 2.16), one finds

$$[a_i, a_j^\dagger]_\zeta = \delta_{ij} \mathbb{1}, \qquad [a_i, a_j]_\zeta = [a_i^\dagger, a_j^\dagger]_\zeta = 0. \tag{2.20}$$

More generally, combining these basis-dependent relations with (2.18) gives

$$[a_\alpha, a_\beta^\dagger]_\zeta = \langle \alpha | \beta \rangle \, \mathbb{1} \tag{2.21}$$

which for field operators formally reads

$$[\hat{\Psi}(\boldsymbol{x}), \hat{\Psi}^\dagger(\boldsymbol{y})]_\zeta = \delta(\boldsymbol{x} - \boldsymbol{y}) \, \mathbb{1}. \tag{2.22}$$

How should one interpret Eq. (2.22)? Recall the general rule that expressions involving delta functions carry meaning only when integrated against smooth functions. Viewed this way, (2.22) turns out to be an equivalent restatement of the unproblematic version (2.21). Indeed, for smooth functions $\alpha(\boldsymbol{x}), \beta(\boldsymbol{x})$, combining Eq. (2.19) and Eq. (2.22) gives

$$\begin{aligned}[a_\alpha, a_\beta^\dagger]_\zeta &= \int\int \bar{\alpha}(\boldsymbol{x})\beta(\boldsymbol{y})[\hat{\Psi}(\boldsymbol{x}), \hat{\Psi}(\boldsymbol{y})^\dagger]\,\mathrm{d}^3\boldsymbol{x}\,\mathrm{d}^3\boldsymbol{y} \\ &= \int\int \bar{\alpha}(\boldsymbol{x})\beta(\boldsymbol{y})\delta(\boldsymbol{x}-\boldsymbol{y})\,\mathbb{1}\,\mathrm{d}^3\boldsymbol{x}\,\mathrm{d}^3\boldsymbol{y} \\ &= \int \bar{\alpha}(\boldsymbol{x})\beta(\boldsymbol{y})\mathbb{1}\,\mathrm{d}^3\boldsymbol{y} = \langle\alpha|\beta\rangle\mathbb{1}.\end{aligned} \tag{2.23}$$

2.2.3 Single- and two-particle operators

An n-particle Hamiltonian is typically of the form

$$H = \sum_{k=1}^{n} h^{(k)} + \frac{1}{2}\sum_{k\neq l=1}^{n} h^{(k,l)}$$

for a single-particle term $h^{(k)}$ (e.g. $h^{(k)} = P_k^2/(2m)$) and an interaction term $h^{(k,l)}$ (e.g. $h^{(k,l)} = V(\boldsymbol{x}_k - \boldsymbol{x}_l)$). On Fock space, we have to sum over all possible particle numbers n, so that, e.g., the single-particle term becomes

$$\bigoplus_{n=1}^{\infty}\sum_{k=1}^{n} h^{(k)}.$$

These formulas become much cleaner when expressed in terms of creation and annihilation operators.

Indeed, choose a single-particle basis $\{|i\rangle\}$ and consider the expansion

$$h = \sum_{ij}\big(\langle i|h|j\rangle\big)\,|i\rangle\langle j| = \sum_{ij} h_{ij}|i\rangle\langle j|. \tag{2.24}$$

We claim that for both Bosons and Fermions, the following holds:

$$\bigoplus_{n=1}^{\infty}\sum_{k=1}^{n} h^{(k)} = \sum_{ij} h_{ij}\, a_i^\dagger a_j. \tag{2.25}$$

In other words: We can formally move from single-body operators to many-body operators replacing "ket's by creation operators and bra's by annihilation operators".

This is not so surprising if we look at (2.24) in the right way. The bra $\langle j|$ is a linear map from $\mathcal{H}^{(1)}$ to the complex numbers, a space that we have since identified as the "vacuum sector". In this sense, $\langle j|$ maps the single-particle state $|j\rangle$ to $|\mathrm{vac}\rangle$. Dually, we can re-interpret the ket $|i\rangle$ as a linear map $\mathbb{C}^{(1)} \to \mathcal{H}^{(1)}$, $(z) \mapsto z|i\rangle$, or $|\mathrm{vac}\rangle \mapsto |i\rangle$. Thus, the familiar matrix element expansion (2.24) can be interpreted as a superposition of processes that "destroy a particle in state $|j\rangle$ and create one in state $|i\rangle$, weighted by the amplitude h_{ij}". From this point of view, (2.25) amounts to the claim that the same description remains valid in higher particle number sectors.

To verify (2.25) start with the case where $\{|i\rangle\}$ is an eigenbasis of h. We have already found in (2.9) that in this case, the occupation number basis diagonalizes the single-body operator, so that

$$\Big(\bigoplus_{n=1}^{\infty}\sum_{k=1}^{n} h^{(k)}\Big)|n_1\dots\rangle = \Big(\sum_i \lambda_i n_i\Big)|n_1, n_2, \dots\rangle = \Big(\sum_i \lambda_i a_i^\dagger a_i\Big)|n_1, n_2, \dots\rangle$$

as claimed. The general case follows from the fact that, as remarked around (2.18), "creation operators transform like kets and annihilation operators like bras": If $\{|\alpha_i\rangle\}$ is another single-particle basis, then inserting completeness relations and using (2.18) gives

$$\begin{aligned}
\sum_i \langle i|h|i\rangle a_i^\dagger a_i &= \sum_{ij} \langle i|h|j\rangle a_i^\dagger a_j \qquad (h \text{ is diagonal in } \{|i\rangle\}\text{-basis}) \\
&= \sum_{ijkl} \langle i|\alpha_k\rangle\langle\alpha_k|h|\alpha_l\rangle\langle\alpha_l|j\rangle a_i^\dagger a_j \\
&= \sum_{kl} \langle\alpha_k|h|\alpha_l\rangle \Big(\sum_i \langle i|\alpha_k\rangle a_i^\dagger\Big)\Big(\sum_j a_j\langle\alpha_l|j\rangle\Big) \\
&= \sum_{kl} \langle\alpha_k|h|\alpha_l\rangle a_{\alpha_k}^\dagger a_{\alpha_l}.
\end{aligned}$$

Likewise, if h is a two-particle operator on $\mathcal{H}^{(1)} \otimes \mathcal{H}^{(1)}$, then the symmetrized n-body version is

$$\frac{1}{2}\sum_{k\neq l=1}^{n} h^{(k,l)},$$

where the super-script denotes the two particles on which the operator acts non-trivially. The factor $1/2$ is there to avoid double-counting of (k,l) and (l,k). As above, one can show that

$$\frac{1}{2}\bigoplus_{n=1}^{\infty}\sum_{k\neq l=1}^{n} h^{(k,l)} = \frac{1}{2}\sum_{ijrs} h_{ijrs}\, a_i^\dagger a_j^\dagger a_s a_r, \qquad h_{ijrs} = \langle ij|h|rs\rangle.$$

Note that the indices s, r of the annihilation operators are *reversed* as compared to the indices in the matrix element! This makes the sign come out right in the Fermionic case. We omit the proof.

Some concrete operators

Let's apply the framework developed above to some important examples, both in position and in momentum representation.

Single-particle potential. The single-particle potential operator is

$$U = \int U(\boldsymbol{x})|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\,\mathrm{d}^3\boldsymbol{x}.$$

We can directly read off the corresponding expressions in second quantization

$$\int \Psi^\dagger(\boldsymbol{x})U(\boldsymbol{x})\Psi(\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{x}$$

("destroy a particle at $\boldsymbol{x}$, multiply with potential at this point, re-create it").

Its matrix elements in the Fourier basis are

$$\langle \boldsymbol{k}'|U|\boldsymbol{k}\rangle = (2\pi)^{-3}\int U(\boldsymbol{x})e^{i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{x}}\,\mathrm{d}^3\boldsymbol{x} = (2\pi)^{-3/2}\,\tilde{U}(\boldsymbol{k}'-\boldsymbol{k}).$$

leading to

$$(2\pi)^{-3/2}\int \tilde{U}(\boldsymbol{k}'-\boldsymbol{k})a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}}\,\mathrm{d}^3\boldsymbol{k}'\,\mathrm{d}^3\boldsymbol{k}. \tag{2.26}$$

Read that as: A potential term can change the momentum of particles. The amplitude associated with a change of $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$ is proportional to the Fourier transform $\tilde{U}(\boldsymbol{q})$ of the potential.

If one works in a box of finite volume $V = L^3$, then (in the sense of App. A.2), the expression becomes

$$\frac{1}{\sqrt{V}}\sum_{\boldsymbol{k},\boldsymbol{k}''\in\mathbb{Z}^3/(2\pi L)} \tilde{U}(\boldsymbol{k}'-\boldsymbol{k})a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}}\,\mathrm{d}^3\boldsymbol{k}'\,\mathrm{d}^3\boldsymbol{k}.$$

Momentum and kinetic energy. In the Fourier basis, we directly get

$$\begin{aligned}\boldsymbol{P} = \hbar\int \boldsymbol{k}\,|\boldsymbol{k}\rangle\langle\boldsymbol{k}|\,\mathrm{d}^3\boldsymbol{k} \quad &\mapsto \quad \hbar\int \boldsymbol{k}\,a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}\,\mathrm{d}^3\boldsymbol{k},\\ \frac{P^2}{2m} = \frac{\hbar^2}{2m}\int \|\boldsymbol{k}\|^2\,|\boldsymbol{k}\rangle\langle\boldsymbol{k}|\,\mathrm{d}^3\boldsymbol{k} \quad &\mapsto \quad \frac{\hbar^2}{2m}\int \|\boldsymbol{k}\|^2 a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}\,\mathrm{d}^3\boldsymbol{k}.\end{aligned}$$

In the sense of App. A.1.8, one can also express these in position basis:

$$\begin{aligned}\boldsymbol{P} &\mapsto -i\hbar\int \hat{\Psi}^\dagger(\boldsymbol{x})\,\boldsymbol{\nabla}\,\hat{\Psi}(\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{x},\\ \frac{P^2}{2m} &\mapsto \frac{-\hbar^2}{2m}\int \hat{\Psi}^\dagger(\boldsymbol{x})\,\boldsymbol{\nabla}^2\,\hat{\Psi}(\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{x} = \frac{\hbar^2}{2m}\int (\boldsymbol{\nabla}\hat{\Psi}(\boldsymbol{x})^\dagger)(\boldsymbol{\nabla}\hat{\Psi}(\boldsymbol{x}))\,\mathrm{d}^3\boldsymbol{x}.\end{aligned}$$

> These expressions are very suggestive, but also easy to misinterpret. Keep in mind that $\hat{\Psi}(\boldsymbol{x}) = a_{\delta_{\boldsymbol{x}}}$ is not a complex function on $\mathbb{R}^3$, but rather a field of annihilation operators for delta functions indexed by $\boldsymbol{x}$. If you are confused, read the explanation in App. A.1.8. If you are not confused, then you're probably missing something (confusion is the natural state at this point!), so you should *really* read App. A.1.8!

Chemical potential. The point of Fock space is that the particle number is variable. The problem with Fock space is that the particle number is variable. Let's say you want to find the ground state of a gas (as we'll do later). There will be some mechanism (walls of a container, pressure exerted by other gases, ...) that controls at least the average number of particles in the gas. We could explicitly describe this mechanism (sounds complicated), or just follow the lead of the grand canonical ensemble of stat mech and add an effective term $-\mu\hat{N}$ that formally adjusts the energy carried by a particle, and then vary μ until the ground state shows the right average particle number. The operator implementing this is just

$$\int \hat{\Psi}(\boldsymbol{x})^\dagger(-\mu)\hat{\Psi}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int a^\dagger_{\boldsymbol{k}}\,(-\mu)\,a_{\boldsymbol{k}}\,\mathrm{d}\boldsymbol{k}.$$

Interaction potential. Now consider an interaction potential $V(\boldsymbol{x}_1, \boldsymbol{x}_2) = V(\boldsymbol{x}_1 - \boldsymbol{x}_2)$ that only depends on the relative position of two particles. The most prominent example is, of course, the Coulomb potential. In position basis, the second quantized version is:

$$\frac{1}{2}\int V(\boldsymbol{x}_1 - \boldsymbol{x}_2)\Psi^\dagger(\boldsymbol{x}_1)\Psi^\dagger(\boldsymbol{x}_2)\Psi(\boldsymbol{x}_2)\Psi(\boldsymbol{x}_1)\,\mathrm{d}^3\boldsymbol{x}_1\mathrm{d}^3\boldsymbol{x}_2. \tag{2.27}$$

The Fourier transform that turns (2.27) into its momentum representation is already slightly annoying to perform. To guide us, let's first guess the structure of the momentum representation. Recall that potentials that are invariant under a simultaneous translation of all particles conserve total momentum. The most general two-particle process compatible with that conservation law is one that shifts the two momenta in a symmetric way, say by $\pm\boldsymbol{q}$. We thus expect an integral over terms

$$f(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{q})\, a^\dagger_{\boldsymbol{k}_1+\boldsymbol{q}} a^\dagger_{\boldsymbol{k}_2-q} a_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1}$$

where the amplitude $f(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{q})$ remains to be found. Comparison with (2.26) suggests that f might be related to the Fourier transform of the potential. That turns out to be true:

$$\begin{aligned}
\langle \boldsymbol{k}_1', \boldsymbol{k}_2'|V|\boldsymbol{k}_1, \boldsymbol{k}_2\rangle &= \int \frac{\mathrm{d}^3\boldsymbol{x}_1}{(2\pi)^3}\frac{\mathrm{d}^3\boldsymbol{x}_2}{(2\pi)^3} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_1')\boldsymbol{x}_1 + i(\boldsymbol{k}_2-\boldsymbol{k}_2')\boldsymbol{x}_2} V(\boldsymbol{x}_1-\boldsymbol{x}_2) \\
&= \int \frac{\mathrm{d}^3\boldsymbol{x}_1}{(2\pi)^3}\frac{\mathrm{d}^3\boldsymbol{x}_2}{(2\pi)^3} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_1')\boldsymbol{x}_1 + i(\boldsymbol{k}_2-\boldsymbol{k}_2')\boldsymbol{x}_2} \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^{3/2}} e^{i\boldsymbol{q}(\boldsymbol{x}_1-\boldsymbol{x}_2)}\tilde{V}(\boldsymbol{q}) \\
&= \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^{3/2}}\tilde{V}(\boldsymbol{q}) \int \frac{\mathrm{d}^3\boldsymbol{x}_1}{(2\pi)^3} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_1'+\boldsymbol{q})\boldsymbol{x}_1} \int \frac{\mathrm{d}^3\boldsymbol{x}_2}{(2\pi)^3} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_2'-\boldsymbol{q})\boldsymbol{x}_2} \\
&= \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^{3/2}}(2\pi)^{-3/2}\,\tilde{V}(\boldsymbol{q})\,\delta(\boldsymbol{k}_1+\boldsymbol{q}-\boldsymbol{k}_1')\delta(\boldsymbol{k}_2-\boldsymbol{q}-\boldsymbol{k}_2').
\end{aligned}$$

Therefore, the momentum representation of an interaction term is

$$\frac{1}{2}\frac{1}{(2\pi)^{3/2}}\int \tilde{V}(\boldsymbol{q})\, a^\dagger_{\boldsymbol{k}_1+\boldsymbol{q}} a^\dagger_{\boldsymbol{k}_2-\boldsymbol{q}} a_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1}\,\mathrm{d}^3\boldsymbol{k}_1\,\mathrm{d}^3\boldsymbol{k}_2\,\mathrm{d}^3\boldsymbol{q}.$$

Summary

- Action of ladder operators on occupation number basis:

$$a_i^\dagger|\dots,n_i,\dots\rangle = \sqrt{n_i+1}(-1)^{\zeta\sum_{j<i}n_i}|\dots,n_i+1,\dots\rangle.$$

- Commutation relations

$$[a_i,a_j^\dagger]_\zeta = \delta_{ij}\mathbb{1}, \qquad [a_i,a_j]_\zeta = [a_i^\dagger,a_j^\dagger]_\zeta = 0.$$

- "Creation operators can be expanded like kets":

$$a_\alpha^\dagger = \sum_i \langle i|\alpha\rangle a_i^\dagger$$

- Annihilation field operators in position basis (not wave functions!):

$$\hat{\Psi}(t,\boldsymbol{x}) := e^{-\frac{t}{i\hbar}H}\, a_{\boldsymbol{x}}\, e^{\frac{t}{i\hbar}H}.$$

- In second quantization, kets $\mapsto$ creation ops and bras $\mapsto$ annihilation ops.

2.3 Quasiparticles and collective excitations

The Bosonic Fock space ladder operators act on the occupation number basis in exactly the same way as the ladder operators associated with quantum harmonic oscillators act on their energy eigenbasis (compare e.g. Eq. (2.17) to Eq. (A.28)) In fact, other than the way they have been constructed, there is no systematic way of distinguishing between an n-dimensional harmonic oscillator and non-interacting Bosons with an n-dimensional single-particle Hilbert space. Because any Hamiltonian that is quadratic in position and momentum operators is equivalent to a collection of uncoupled Harmonic oscillators when expressed in normal modes (Sec. A.3.2), such models are widely applicable. Excitations arising this way are called *quasiparticles* or *collective excitations*.

> Formally, one says that the two systems are *unitarily equivalent*. Define a linear map U from $L^2(\mathbb{R}^n)$ to $\mathcal{F}_S(\mathbb{C}^n)$ by requiring that it sends an element $|n_1,\dots\rangle^{L^2(\mathbb{R}^n)}$ of the eigenbasis of n harmonic oscillators as constructed in (A.28) to the element $|n_1,\dots\rangle^{\mathcal{F}_S(\mathbb{C}^n)}$ of the occupation number basis as constructed in (2.17). Then U, mapping an ONB to an ONB, is unitary and one immediately verifies that $Ua_i^{L^2(\mathbb{R}^n)}U^\dagger = a_i^{\mathcal{F}_S(\mathbb{C}^n)}$.

The most elementary case are lattice vibrations, or *phonons*. Let's have a look.

2.3.1 Phonons

Goals

The phonon Hamiltonian is conceptually easy to solve (by undergrad mechanics tools), but has much to teach us! Here, phonons will serve as an example of how Fock space describes collective excitations, rather than arising from a single-particle space. We'll also have the opportunity to recall normal mode expansions. A continuum limit will later motivate rules for field quantization.

We consider N particles in one dimension whose interaction potential has a minimum at distance a and goes to 0 for large distances. There is therefore an equilibrium configuration where the particles are arranged in a linear chain, with the k-th particle at position ka. Let X_k be the position of the k-th particle, measured relative to its equilibrium value. Expanding the potential around the minimum to second order,

$$H = \sum_{r=1}^{N} \left(\frac{P_r^2}{2m} + \frac{\kappa}{2}(X_r - X_{r+1})^2 \right). \tag{2.28}$$

We have to specify boundary conditions. If the chain is longer than the length scale of any phenomenon we'll be studying, boundary effects shouldn't matter much (c.f. App. A.2). We therefore opt for the mathematically simplest case: cyclic boundary conditions, i.e. we assume that the indices of the operators in (2.28) only depend on r modulo N.

The chain Hamiltonian is quadratic in positions and momenta and can therefore be diagonalized using canonical transformations (App. A.3.2). Working out the details is an excellent exercise, so we only present the final result here.

For $n = 1 \dots N$ and $k = n\frac{2\pi}{L}$ with $L = Na$ the total length, define

$$\phi_k = \sqrt{\frac{1}{N}} \sum_{r=1}^{N} e^{-ikra} X_r, \quad \pi_k = \sqrt{\frac{1}{N}} \sum_{r=1}^{N} e^{ikra} P_r.$$

In the sense of App. A.3.2, the ϕ_k, π_k correspond to complex normal coordinates associated with standing waves with quasi-momentum k. Then

$$a_k = \frac{1}{\sqrt{2}} \Big(\sqrt{\frac{m\omega_k}{\hbar}} \phi_k + i \sqrt{\frac{1}{m\hbar\omega_k}} \pi_{-k} \Big), \quad \omega_k = \sqrt{\frac{\kappa}{m}} 2|\sin(ka/2)|$$

define annihilation operators ($[a_k, a_{k'}^\dagger] = \delta_{k,k'}$) that diagonalize the Hamiltonian

$$H = \sum_k \frac{1}{2m} \pi_k \pi_{-k} + 2\kappa \sum_k \sin^2(ka/2) \phi_k \phi_{-k} = \sum_k \hbar\omega_k \Big(a_k^\dagger a_k + \frac{1}{2} \Big).$$

The (Heisenberg picture) equations of motion $i\hbar\partial_t a_k(t) = [a_k, H]$ are then solved by $a_k(t) = e^{-i\omega_k t} a_k(0)$. For the original observables this means

$$\begin{aligned} X_r(t) &= \sqrt{\frac{\hbar}{Nm}} \sum_k \frac{1}{\sqrt{2\omega_k}} (a_k e^{-i\omega_k t + ikar} + a_k^\dagger e^{i\omega_k t - ikar}), \\ P_r(t) &= -i \sqrt{\frac{m\hbar}{N}} \sum_k \sqrt{\frac{\omega_k}{2}} (a_k e^{-i\omega_k t + ikar} - a_k^\dagger e^{i\omega_k t - ikar}). \end{aligned} \tag{2.29}$$

In these expressions, we've grouped adjoint terms together, to emphasize that X_r is Hermitian. Sometimes it's more advantageous to group terms by complex normal modes instead:

$$\begin{aligned} X_r(t) &= \sqrt{\frac{\hbar}{Nm}} \sum_k \frac{1}{\sqrt{2\omega_k}} \big(a_k(t) + a^\dagger_{-k}(t)\big) e^{ikar}, \\ P_r(t) &= -i\sqrt{\frac{m\hbar}{N}} \sum_k \sqrt{\frac{\omega_k}{2}} \big(a_k(t) - a^\dagger_{-k}(t)\big) e^{ikar}. \end{aligned} \tag{2.30}$$

Finally, note that every formula in this section equally applies to the classical case, with the only exception that the Hamilton function reads (c.f. App. A.3.2):

$$H = \sum_k \hbar\omega_k |a_k|^2.$$

2.3.2 Global phase gauge symmetry and particle number conservation

A *gauge symmetry* is a mathematical redundancy in the description of physical objects. In quantum mechanics, a global phase change $|\psi\rangle \mapsto e^{i\phi}|\psi\rangle$ is such a redundancy. It is implemented by the 1×1 unitary "matrix" $(e^{i\phi}) \in U(1)$, and therefore called *global* $U(1)$ *gauge symmetry*.

When we constructed Fock space, we inadvertently got in tension with that symmetry! That's because multiplying all single-particle vectors by $e^{i\phi}$ means that a tensor product of n such vectors changes by $e^{in\phi}$. In other words, if

$$\hat{N} = \sum_i \hat{n}_i = \sum_i a_i^\dagger a_i$$

is the total particle number operator, then $U(1)$ acts on Fock space as $e^{i\phi\hat{N}}$. Thus, $U(1)$-transformations induce *relative* phases between subspaces of different particle numbers. These will change the expectation values of observables that do not commute with $\hat{N}$.

So can we observe global phase changes of single-particle states when working with many-body systems?

For non-relativistic massive particles (i.e. the kind of systems treated in undergraduate QM courses), the answer is "no". Loosely speaking, we expect that in a "non-relativistic theory" deserving of that name, massive particle cannot be created or destroyed. We should then require that all physical observables commute with total particle number. The requirement that all physical observables obey an extra symmetry (i.e. $[A, \hat{N}] = 0$) is called a *superselection rule*. In particular, because

$$a^\dagger_{e^{i\phi}\psi} = e^{i\phi} a^\dagger_\psi, \qquad a_{e^{i\phi}\psi} = e^{-i\phi} a_\psi \tag{2.31}$$

linear expressions in ladder operators are not directly observable in the presence of this superselection rule.

The Fock space for phonons was *not* constructed starting from a single-particle Hilbert space of a non-relativistic massive particle, so the argument does not apply in this case. And indeed, the observable (2.29) corresponding to the displacement of the r-th particle (clearly a measurable quantity, at least in principle) is a linear combination of ladder operators. Also, as we'll see next, when the particle number tends to infinity, the physical and mathematical definition of $\hat{N}$ becomes iffy, which may lead to non-relativistic systems to behave as if particle number conservation is violated.

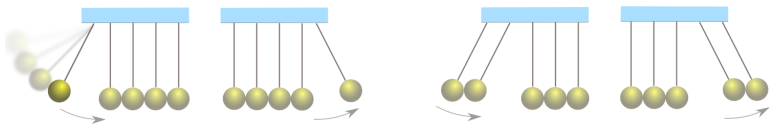


Figure 2.2: The motion in a Newton cradle is determined by energy and momentum conservation alone. (Figure adapted from Wikipedia.)

2.4 Spin chains

TBD.

Move Ising part here. Discuss SSB.

Solve transverse field by Jordan-Wigner.

Maybe organize this like this:

Chapter: Examples of many-body systems.

Sections: * Phonons * Spin chains (and Jordan-Wigner) * SSB (example of spin chains) * Bose gas

2.5 Bose gas: Take 1

Indistinguishable particles with interaction potential V are described by the Hamiltonian

$$H = \int \hat{\Psi}^\dagger(\boldsymbol{x})\Big(\frac{-\hbar^2\boldsymbol{\nabla}^2}{2m} - \mu\Big)\hat{\Psi}(\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{x} + \int \hat{\Psi}^\dagger(\boldsymbol{x})\hat{\Psi}^\dagger(\boldsymbol{y})V(\boldsymbol{x}-\boldsymbol{y})\hat{\Psi}(\boldsymbol{x})\hat{\Psi}(\boldsymbol{y})\,\mathrm{d}^3\boldsymbol{x}\,\mathrm{d}^3\boldsymbol{y}.$$

Simplify: Restrict the gas to a box of finite volume V (App. A.2); choose a "hard core interaction potential" $V(\boldsymbol{x}-\boldsymbol{y}) = U\delta(\boldsymbol{x}-\boldsymbol{y})$, with Fourier transform $\tilde{V}(\boldsymbol{q}) = V^{-1}U$; switch to momentum representation; suppress vector notation; set $\epsilon_k = \frac{\hbar^2k^2}{2m}$. Then

$$H = \sum_k(\epsilon_k - \mu)a_k^\dagger a_k + \frac{U}{2V}\sum_{k,k',q} a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'}a_k. \tag{2.32}$$

This still is difficult to treat, so let's get some intuition first, to guide our analysis.

Superfluidity

At very low temperature, helium becomes superfluid: A particle slowly passing through it does not experience friction. Here's a way to think about that: Recall the Newton cradle (Fig. 2.2), where one can uniquely determine the number of balls being excited merely from energy and momentum conservation. Likewise, one may model the interaction between the particle and the gas as a scattering process, where the particle transfers energy and momentum to the gas. Now imagine that the energy-momentum relations of the particle and the excitations of the gas are "out of tune" in the sense that there is *no* process that would respect both conservation laws. In this case, no scattering is possible and one would expect the particle to pass through the gas uninhibited.

With this model in mind, we set it as our goal to work out the energy-momentum relation of the low-lying excitations of H.

Bose-Einstein condensation

Recall that for non-interacting Bosons (i.e. when $V = 0$), the ground state is achieved when all particles are in the lowest-energy state of the single-particle term. It is plausible (though a very difficult question to treat rigorously) that remnants of this behavior persist for non-zero interaction V and for low-lying states. We will thus treat H under the assumption that there is a finite density

$$\rho = \frac{n_0}{V} = \frac{1}{V}\langle a_0^\dagger a_0 \rangle \tag{2.33}$$

of particles occupying the $k = 0$ mode. To achieve this, we add a "chemical potential term" $-\mu\hat{N}$ to the Hamiltonian and will later adjust μ to achieve (2.33).

2.5.1 Approximate solution part 1

Because for low-lying many-body states $|\psi\rangle$, we expect the occupation number $\langle\psi|a_0^\dagger a_0|\psi\rangle$ of the single-particle ground state to be much larger than the ones for other modes, we neglect all terms that are of third order or higher in creation/annihilation operators for $k \neq 0$.

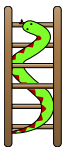
A lengthy but uneventful calculation leads to

$$\begin{aligned} H = &\sum_k (\epsilon_k - \mu) a_k^\dagger a_k + \frac{U}{2V} a_0^\dagger a_0 a_0^\dagger a_0 + \frac{2U}{V}\sum_{k\neq 0} a_0^\dagger a_0 a_k^\dagger a_k \\ &+ \frac{U}{2V}\sum_{k\neq 0}(a_0^\dagger a_0^\dagger a_k a_{-k} + a_0 a_0 a_k^\dagger a_{-k}^\dagger) + O(a_k^3). \end{aligned} \tag{2.34}$$

To make further progress, we employ *Bogoliubov's c-number substitution*: Replace the operator $\frac{1}{\sqrt{V}}a_0$ with a complex number $\sqrt{\rho}e^{i\theta}$.

Wait, we do what? Why would that be justified? The minimal story goes like this: In the limit $V \to \infty$, the number of Bosons n_0 in the $k = 0$-mode is expected to be macroscopic $n_0 = \rho V \to \infty$. Because we cannot physically resolve the number of Bosons in the mode, $a_0|n_0\rangle = \sqrt{n_0}|n_0 - 1\rangle$ "behaves just like" $\sqrt{n_0}|n_0\rangle$ with respect to any measurement we can actually implement. So switching to a mathematical model where a_0 is not a ladder operator at all, but rather equal to $\sqrt{\rho V}\,\mathbb{1}$ should give similar results.

Well, OK. That always seemed at most mildly convincing to me. To get a better feeling for why this is a justified way of arguing, let's take a detour and introduce a broader framework for such phenomena, which are connected to *spontaneous symmetry breaking*.



If you are already fully convinced, or if "mildly convincing" is anyway all you aim for at this moment, you can skip ahead to Sec. 2.7.

2.6 Detour: Spontaneous symmetry breaking

Broadly interpreted, the concept of *spontaneous symmetry breaking* (SSB) refers to any situation where the solutions of a problem are less symmetric than the problem itself. There are banal ways in which this can manifest (Fig. 2.3), but there's also deep ones. In the examples we'll look at, the technical origin of the effect may be traced back to the (vague, for now) principle

"One cannot implement operators that act on macroscopically many particles." (2.35)

Figure 2.3: SSB. TBD.

2.6.1 Ferromagnetism

The guiding phenomenlogical example is *ferrogmagnetism*. If cooled below its Curie temperature, a ferromagnet develops a magnetic moment $\boldsymbol{M} \neq 0$. In the absence of external fields, the moment $\boldsymbol{M}$ is equally likely to point into any direction. Thus, *statistically*, the behavior is rotationally invariant. But every time the magnet is cooled down, it "spontaneously" singles out one direction in space, thereby "breaking the symmetry".

The simplest case of a model exhibiting ferromagnetic behavior is the Ising model. It involves N spin-$1/2$ particles – and in fact, we can learn a lot by looking at their Hilbert space in the limit $N \to \infty$, even before introducing the Hamiltonian.

Indeed, consider the two states (depending on the relative phase)

$$|\psi_\pm^N\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle^{\otimes N} \pm |\downarrow\rangle^{\otimes N}).$$

The $|\psi_\pm^N\rangle$ are eigenvectors of $\sigma_x^{\otimes N}$ with eigenvalue $+1$ and -1 respectively. Despite them being orthogonal, I claim that as N gets macroscopic, the two states become effectively indistinguishable.

To justify this outrageous claim, assume that just one of the macroscopically many particles is lost (as will always, realistically, be the case). Then any measurement effectively takes place on the reduced density matrix

$$\mathrm{tr}_1\, |\psi_\pm^N\rangle\langle\psi_\pm^N| = \frac{1}{2}(|\uparrow\rangle\langle\uparrow|)^{\otimes(N-1)} + \frac{1}{2}(|\downarrow\rangle\langle\downarrow|)^{\otimes(N-1)},$$

which is a uniform mixture of $|\uparrow\ldots\rangle, |\downarrow\ldots\rangle$, and independent of the relative phase. In this sense: The operator $\sigma_x^{\otimes N}$ does not actually describe a physically realizable measurement in the limit $N \to \infty$.

Sometimes, it is beneficial to keep idealized mathematical objects around (like δ functions) even if they are not directly physical. In this case, however, it turns out that we'll attain a cleaner understanding of ferromagnetism, superfluidity, and many other important quantum many-body phenomena, if we commit to the principle (2.35) and declare operators like $\sigma_x^{\otimes N}$ to be unphysical in the limit $N \to \infty$.

Let's explore this further. Define $\mathcal{H}_\uparrow$ to be the space of states that can be reached by physical operations starting from $|\uparrow\rangle^{\otimes N}$ and define $\mathcal{H}_\downarrow$ analogously. For microscopic N, the two spaces are identical, but as $N \to \infty$, they become orthogonal. A good way to see this is to consider the *average magnetization*. For a state $|\psi\rangle$, it is defined as

$$m := \frac{1}{N}\sum_{k=1}^{N}\langle\psi|\sigma_z^{(k)}|\psi\rangle. \tag{2.36}$$

The average magentization is $+1$ on $|\uparrow\rangle^{\otimes N}$ and -1 on $|\downarrow\rangle^{\otimes N}$. If A is any physical operator, then by (2.35), $A|\psi\rangle$ differs from $|\psi\rangle$ only on a microscopic number of spins. For $N \to \infty$, this doesn't affect the average in (2.36), and we conclude that no quantum-mechanical process can change m in that limit.

One consequence is that within each of these two physically separated Hilbert spaces, the average magnetization operator $\frac{1}{N}\sum_{k=1}^{N}\sigma_z^{(k)}$ can be replace by a number, namely by

± 1 respectively. (Spoiler alert: That's the mechanism that will allow us to replace $\frac{a_0}{\sqrt{V}}$ by a complex number for Bose-Einstein condensates.)

We can still mathematically write down superpositions $|\psi\rangle = \sqrt{p}|\psi_\uparrow\rangle + e^{i\phi}\sqrt{1-p}|\psi_\downarrow\rangle$ between vectors $|\psi_\uparrow\rangle \in \mathcal{H}_\uparrow, |\psi_\downarrow\rangle \in \mathcal{H}_\downarrow$, of the two disjoint spaces. But because for every physical operation A, the matrix elements between them vahish $\langle\psi_\uparrow|A|\psi_\downarrow\rangle = 0$, these coherent superpositions cannot be experimentally distinguished from the incoherent mixture

$$\rho = p|\psi_\uparrow\rangle\langle\psi_\uparrow| + (1-p)|\psi_\downarrow\rangle\langle\psi_\downarrow|.$$

That's a generalization of the example we started with.

It's time to have a look at the Hamiltonian of the Ising model:

$$H = -J\sum_{i,j}\sigma_z^{(i)}\sigma_z^{(j)}, \qquad J > 0,$$

where the sum is over nearest neighbors. The summands give

$$-J\sigma_z^{(i)}\sigma_z^{(j)}|s_i s_j\rangle = \begin{cases} -J & |s_i s_j\rangle = |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, \\ +J & |s_i s_j\rangle = |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle. \end{cases}$$

We immediately see that the Hamiltonian is invariant under a simultaneous flip of all spins, realized by the operator $\sigma_x^{\otimes N}$. Also, the ground state energy is $-J$ times the number of neighboring pairs. It is attained on the subspace with basis $|\uparrow\rangle^{\otimes N}, |\downarrow\rangle^{\otimes N}$, or, equivalently, with basis the $|\psi_\pm^N\rangle$.

Given the discussion above, it is now easy to see what happens. The spin flip symmetry of the Hamiltonian is implemented by $\sigma_x^{\otimes N}$, which "breaks" in the sense that it becomes unphysical for $N \to \infty$. For microscopic N, the $|\psi_\pm^N\rangle$ are pure ground states that are invariant under the spin flip symmetry (up to phase). As $N \to \infty$, they remain invariant, but they become effectively mixed. In fact, any ground state $\alpha|\uparrow\rangle^{\otimes N} + \beta|\downarrow\rangle^{\otimes N}$ becomes a mixture of the two non-symmetric ones $|\uparrow\rangle^{\otimes N}, |\downarrow\rangle^{\otimes N}$. We can now connect back to the loose definition of "symmetry breaking" in the very beginning: The restriction on physical observables in macroscopic systems means that there is no longer a pure ground state that shares the symmetry of the Hamiltonian.

Further comments (not needed in the sequel)

- Because $\sigma_x\sigma_z\sigma_x^\dagger = -\sigma_z$, the average magnetization vanishes for every state (possibly mixed) that is spin flip invariant. An observable that "witnesses the lack of symmetry" in this way is called an *order parameter*.

- In reality, there's at least some tiny external fields around, so we should modify the Hamiltonian to read $H_\lambda = H + \lambda\sum_k \sigma_z^{(k)}$, where λ corresponds to the net external field. The sign of λ lifts the degeneracy of the ground space. SSB is then witnessed by the fact that when taking limits $\lim_{\lambda\to 0}\lim_{N\to\infty} H_\lambda$ (in that order!), the resulting ground state depends on whether λ approaches 0 from above or from below.

- In elementary QM, one often associates different Hilbert spaces with the same quantum system, as a matter of convenience. For example, a single harmonic oscillator can be described by the Hilbert space $L^2(\mathbb{R})$ of square-integrable functions, or by the Fock space $\mathcal{F}(\mathbb{C})$. These choices are equivalent: Every basis vector $|n\rangle \in \mathcal{F}(\mathbb{C})$ can be mapped to a wave function (in terms of Gaussians and Hermite polynomials) and this way, every set of expectation values realizable on one of the Hilbert spaces

can be reproduced on the other. In contrast, the fact that the average magnetization takes on different values in the two Hilbert spaces constructed above, shows that the representation of the observables of the Ising model on them are *inequivalent*.

2.6.2 SSB and Bose-Einstein condensation

We are now ready to argue that Bose-Einstein condensation of a macroscopic number of particles leads to spontaneous symmetry breaking, this time of a continuous symmetry.

Consider a Bose gas contained in a box of volume V. Recall from (2.33) that we are interested in states $|\psi\rangle$ that have a fixed density $\rho = n_0/V$ of particles in the $k = 0$-mode:

$$\frac{1}{V}\langle\psi|a_0^\dagger a_0|\psi\rangle = \langle\psi|\big(\frac{1}{\sqrt{V}}a_0^\dagger\big)\big(\frac{1}{\sqrt{V}}a_0\big)|\psi\rangle = \rho. \tag{2.37}$$

In the limit $V \to \infty$, measuring the precise occupation number

$$\langle\psi|a_0^\dagger a_0|\psi\rangle = V\rho \to \infty$$

would require us to count a macroscopic number of particles. Consistent with the principle (2.35), we reject his as unphysical. The density, however, should be measurable. Hence we posit that an observable is physical only if it can be expressed in terms of the re-scaled ladder operators

$$\frac{1}{\sqrt{V}}a_0, \quad \frac{1}{\sqrt{V}}a_0^\dagger \tag{2.38}$$

as well as the $a_k, a_k^\dagger$ for $k \neq 0$ (with coefficients that do not depend on V, of course).

This seemingly minor restriction has dramatic effects in the limit $V \to \infty$. Indeed,

$$\Big[\frac{1}{\sqrt{V}}a_0, \frac{1}{\sqrt{V}}a_0^\dagger\Big] = \frac{1}{V} \to 0, \tag{2.39}$$

so that in the thermodynamic limit, the operators (2.38) commute! But then *all* physical observables commute with $\frac{1}{\sqrt{V}}a_0$ (why?). This operator therefore plays the same role as the average magnetization in the Ising model: Its eigenspaces are physically separated in the sense that relative phases between them are not observable and no vector can be mapped from one eigenspace to another. If $\frac{a_0}{\sqrt{V}}|\psi\rangle = \lambda|\psi\rangle$ then (2.37) implies that $\lambda = \sqrt{\rho}e^{i\theta}$ for some $\theta \in [0, 2\pi)$

Thus, we may always assume that the dynamics takes place in one of the eigenspaces

$$\mathcal{H}_\theta = \Big\{|\psi\rangle \;\Big|\; \frac{a_0}{\sqrt{V}}|\psi\rangle = \sqrt{\rho}e^{i\theta}|\psi\rangle\Big\},$$

where $\frac{a_0}{\sqrt{V}}$ acts like $\sqrt{\rho}e^{i\theta}$. This is what we set out to justify.

$U(1)$ symmetry breaking

Just like spin flip symmetry before, there are unphysical operations that do connect different eigenspaces. This role is played by the $U(1)$ symmetry $e^{i\phi\hat{N}}$ (Sec. 2.3.2). It "breaks" in the $V \to \infty$ limit, because it involves the diverging total particle number operator $\hat{N}$. Mathematically, however, it holds that

$$e^{i\phi\hat{N}}\,\mathcal{H}_\theta = \mathcal{H}_{\theta+\phi}.$$

That's because annihilation operators transform as

$$e^{-i\phi\hat{N}} a_\alpha e^{i\phi\hat{N}} = e^{i\phi} a_\alpha \tag{2.40}$$

(the positive phase gets applied to one more particle than the negative one). Some consequences:

By (2.40), the expectation value $\langle \frac{a_0}{\sqrt{V}} \rangle$ vanishes in any state that is $U(1)$ invariant. The operator $\frac{a_0}{V}$ therefore constitutes an order parameter. Now comes a big difference to the Ising example. On Fock space for massive non-relativistic particles, we have a second condition for an observable to be physical: In addition to fulfilling (2.35), observables also have to be gauge invariant (Sec. 2.3.2). Hence in this case, the order parameter is not measurable (unlike the average magnetization, which is the central physical quantity associated with the Ising magnet). It also means that the physical behavior of the Bose gas can only depend on ρ, not on θ, so we are free to restrict to the case $\theta = 0$ below.

We found that a state $|\psi\rangle$ is pure with respect to the physical observables only if it is contained in one of the $\mathcal{H}_\theta$ spaces. But then, it isn't $U(1)$-invariant. Only the mixed state

$$\rho = \int e^{i\phi\hat{N}} |\psi\rangle\langle\psi| e^{-i\phi\hat{N}} \frac{\mathrm{d}\theta}{2\pi}$$

is. We're again encountering the dichotomy that states are symmetric or pure, but not both.

2.7 Bose gas: Take 2

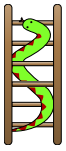
Back to the Bose gas. We (reasonably) assume that each low-lying state has a non-zero density $\rho = n_0/V$ of particles occupying the single-body ground state. The value of ρ will be determined momentarily. For now, following the discussion on SSB, we just make the substitution $\frac{a_0}{\sqrt{V}} \mapsto \sqrt{\rho}$. Then (2.34) becomes

$$H \simeq V\Big(-\mu\rho + \frac{U}{2}\rho^2 \Big) + \sum_{k\neq 0} \big(\epsilon_k - \mu + 2U\rho\big) a_k^\dagger a_k + \frac{U\rho}{2} \sum_{k\neq 0} (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger).$$

The effect of ρ on the energy will, in the limit $V \to \infty$, be dominated by the first term, which is the only one proportional to V. Thus, low-lying states will have a density ρ minimizing that term. Setting its derivative to zero gives the relation $\rho = \mu/U$. We keep ρ and eliminate μ, to get

$$H = \text{const.} + \sum_{k\neq 0} \big(\epsilon_k + U\rho\big) a_k^\dagger a_k + \frac{U\rho}{2} \sum_{k\neq 0} (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger). \tag{2.41}$$

This is a quadratic expression in ladder operators, so we know from general principles (Sec. A.3.2) that it can be diagonalized using a canonical transformation. Let's find it in two (and a half) easy steps!



The result of the following "2½ easy steps" is summarized in (2.46). In principle, one can just check directly that the form of H given there is indeed equal to (2.41). Below, we only describe a somewhat natural thought process that leads to (2.46). If you're in a hurry, skip ahead.

Step 1: Decouple. Start with the rightmost term. It creates / destroys pairs of particles of opposite momentum. This suggests switching the basis of the single-particle space to

one that consists of superpositions of states moving in opposite directions. Remembering that $|\pm k\rangle$ are represented in position space by complex exponentials that are each other's conjugates, the cosine / sine basis

$$\frac{1}{\sqrt{2}}(|k\rangle + |-k\rangle), \qquad \frac{-i}{\sqrt{2}}(|k\rangle - |-k\rangle). \tag{2.42}$$

seems like a natural candidate. Let's agree that a vector k is *positive* if its first non-zero component is. Then there is exactly one positive wave vector in every pair $+k, -k$. For $k > 0$, define the annihilation operators

$$b_k = \frac{1}{\sqrt{2}}(a_k + a_{-k}) \qquad (\text{"positive } k \text{ label the cosines"})$$
$$b_{-k} = \frac{i}{\sqrt{2}}(a_k - a_{-k}) \qquad (\text{"negative } k \text{ label the sines"})$$

associated with the new basis. Inverting,

$$a_k = \frac{1}{\sqrt{2}}(b_k - ib_{-k}), \quad a_{-k} = \frac{1}{\sqrt{2}}(b_k + ib_{-k}) \qquad k > 0. \tag{2.43}$$

Plugging in, the pair term decouples, as hoped:

$$H = \text{const.} + \sum_{k\neq 0}\Big(\big(\epsilon_k + U\rho\big)b_k^\dagger b_k + \frac{U\rho}{2}(b_k b_k + b_k^\dagger b_k^\dagger)\Big).$$

Step 2: Solve harmonic oscillator. It turns out that each summand represents a harmonic oscillator and that a simple re-scaling of position and momentum coordinates will put it into standard form. To see how this works, we switch to Hermitian operators for the moment:

$$X = \frac{1}{\sqrt{2}}(b_k + b_k^\dagger), \qquad P = \frac{-i}{\sqrt{2}}(b_k - b_k^\dagger).$$

Abbreviating $A = \epsilon_k + U\rho, B = U\rho$ one directly finds

$$A\, b_k^\dagger b_k + \frac{B}{2}\,(b_k b_k + b_k^\dagger b_k^\dagger) = \frac{A-B}{2}P^2 + \frac{A+B}{2}X^2. \tag{2.44}$$

Well, we know how to solve these using undergrad methods (App. A.3.1)! The transformation

$$\tilde{X} = \sqrt[4]{\frac{A+B}{A-B}}X, \qquad \tilde{P} = \sqrt[4]{\frac{A-B}{A+B}}P, \qquad E_k = \sqrt{A^2 - B^2}$$

is obviously canonical, $[\tilde{X}, \tilde{P}] = [X, P]$, and puts the oscillator into standard form:

$$\frac{1}{2}E_k(\tilde{X}^2 + \tilde{P}^2) = \frac{1}{2}\sqrt{(A+B)(A-B)}\Big(\sqrt{\frac{A-B}{A+B}}P^2 + \sqrt{\frac{A+B}{A-B}}X^2\Big) = (2.44).$$

Therefore, setting $\tilde{b}_k = \frac{1}{\sqrt{2}}(\tilde{X} + i\tilde{P})$, we have diagonalized H (that wasn't too hard ☺):

$$H = \text{const.} + \sum_{k\neq 0} E_k \tilde{b}_k^\dagger \tilde{b}_k, \qquad E_k = \sqrt{\epsilon_k^2 + \epsilon_k 2U\rho}. \tag{2.45}$$

Step 2.5: Cleanup. Because $E_{-k} = E_k$, the Hamiltonian is degenerate and any unitary transformation within the $\pm k$-subspaces will leave its form invariant. Choosing

$$c_k := \frac{1}{\sqrt{2}}(\tilde{b}_k + \tilde{b}_{-k}) \quad \text{for } k > 0, \qquad c_k := \frac{1}{\sqrt{2}}(\tilde{b}_k - \tilde{b}_{-k}) \quad \text{for } k < 0$$

turns out to lead to the cleanest theory. Plugging in all the nested definitions gives

$$\begin{aligned} &c_k = u_k a_k - v_k a_{-k}^\dagger, \quad u_k = \frac{1}{2}\Big(\sqrt{\frac{\epsilon_k}{E_k}} + \sqrt{\frac{E_k}{\epsilon_k}}\Big), \quad v_k = \frac{1}{2}\Big(\sqrt{\frac{\epsilon_k}{E_k}} - \sqrt{\frac{E_k}{\epsilon_k}}\Big), \\ &E_k = \sqrt{\epsilon_k^2 + \epsilon_k 2U\rho}, \qquad H = \text{const.} + \sum_{k\neq 0} E_k c_k^\dagger c_k. \end{aligned} \tag{2.46}$$

The coefficients lie on the unit hyperbola:

$$u_k^2 - v_k^2 = \frac{1}{4}\left(\frac{\epsilon_k}{E_k} + 2 + \frac{E_k}{\epsilon_k}\right) - \frac{1}{4}\left(\frac{\epsilon_k}{E_k} - 2 + \frac{E_k}{\epsilon_k}\right) = 1$$

which implies (exercise) that the inverse transformation is

$$a_k = u_k c_k + v_k c_{-k}^\dagger. \tag{2.47}$$

Discussion

We have found that the elementary excitations of the Bose gas are given by quasi-particles created by the $c_k^\dagger$. The ground state is the *quasi-particle* vacuum characterized by

$$c_k|0\rangle^{(\mathrm{q})} = 0 \qquad \forall k.$$

It is not to be confused with the *particle* vacuum $|0\rangle^{(\mathrm{p})}$ characterized by $a_k|0\rangle^{(\mathrm{p})} = 0$! For example, using (2.47), the expected number of particles with momentum k in the quasi-particle vacuum is

$$\langle 0|^{(\mathrm{q})} a_k^\dagger a_k |0\rangle^{(\mathrm{q})} = \langle 0|^{(\mathrm{q})}(u_k c_k^\dagger + v_k c_{-k})(u_k c_k + v_k c_{-k}^\dagger)|0\rangle^{(\mathrm{q})} = v_k^2.$$

While the above shows that quasi-particle occupation number states $|\dots n_k \dots\rangle^{(\mathrm{q})}$ do not have definite particle numbers, it turns out that they do have definite momentum! In the exercise, you will show that $c_k^\dagger$ creates quasi-particles with momentum $\hbar k$. Thus, $E(k)$ found in (2.45) describes their energy-momentum (or dispersion) relation. Compared to a free particle, $E(k)$ involves the additional term $\epsilon_k 2U\rho$. It dominates if

$$\epsilon_k = \frac{\hbar^2\|\boldsymbol{k}\|^2}{2m} \ll 2U\rho \quad \Leftrightarrow \quad \frac{\|\hbar\boldsymbol{k}\|}{m} \ll \sqrt{\frac{U\rho}{m}} =: c,$$

i.e. for velocities much smaller than c. In this regime, we have $E_k \simeq c\|\hbar\boldsymbol{k}\|$, that is, energy scales *linearly* with momentum. Beyond that, E_k is convex ("bends upwards", Fig. 2.4), so that $E_k \geq c\|\hbar k\|$ holds in general.

As alluded to in the very beginning, this means that a particle moving through the Bose gas at low velocity cannot slow down by transferring energy and momentum to a quasi-particle. Quantitatively: Let M be the mass of the test particle and $\boldsymbol{p}$ its initial momentum. Assume it excites a quasi-particle of momentum $\boldsymbol{q}$. Then energy conservation demands

$$0 = \frac{\|\boldsymbol{p}\|^2}{2M} - \frac{\|\boldsymbol{p}-\boldsymbol{q}\|^2}{2M} - E_q = -\frac{\boldsymbol{p}\boldsymbol{q}}{M} - \frac{\|\boldsymbol{q}\|^2}{2M} - E_q \leq \frac{\|\boldsymbol{p}\|\,\|\boldsymbol{q}\|}{M} - c\|\boldsymbol{q}\| = \left(\frac{\|\boldsymbol{p}\|}{M} - c\right)\|\boldsymbol{q}\|$$

which has a solution only if the test particle has initial velocity $\|\boldsymbol{p}\|/M$ at least c.

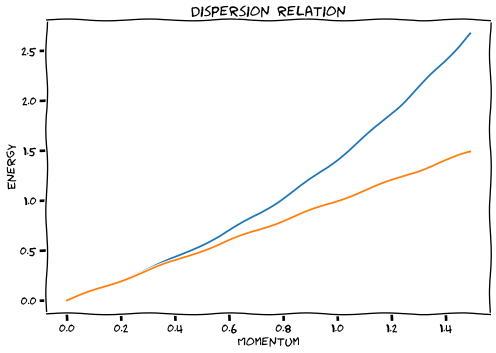


Figure 2.4: Blue line: Dispersion relation $E(\|\boldsymbol{k}\|)$ for the Bose gas. Orange line: $E = c\hbar\|\boldsymbol{k}\|$ is a good approximation for small $\|\boldsymbol{k}\|$, and a lower bound for all $\boldsymbol{k}$. The x-axis is in units of $mc/\hbar$, y-axis in units of mc^2.

2.8 Further reading

A good presentation of many-body theory is *Advanced Quantum Mechanics* by Schwabl, which also covers the Bose gas. Spontaneous symmetry breaking is a complex phenomenon that can be approached from many points of view that might feel quite different. I enjoy the presentations by Strocchi (*Elements of Quantum Mechanics in Infinite Systems* and *Symmetry Breaking*), but they might be a little too mathematical for the average taste. A more phenomenological approach in the language of path integrals is in Chapter 6 of *Condensed Matter Field Theory* by Alexander Altland (of Cologne) and Ben Simons.

Chapter 3

Field quantization and quantum theory of light

Our goal is to construct a quantum theory for the EM field. Since quantum mechanics is more fundamental than classical physics, one cannot hope to *derive* a quantum theory from its classical limit. "Quantization" thus always involves educated guesses.

To educate ourselves, we'll first have another look at lattice vibrations (Sec. 2.3.1). For both their classical and their quantum model, one can easily construct a continuum limit. The result is a classical and a quantum field theory. Their relation will serve as a template for quantizing other fields.

3.1 Phonon continuum limit

Recall our treatment of N coupled particles arranged in a line of length L (Sec. 2.3.1). For phenomena that have length scales much larger than the equilibrium spacing $a = L/N$, the behavior of the model should not depend on the precise value of a. (Try to infer the lattice spacing from listening to the sound of a string instrument...). More precisely, the family of models with parameters

$$N^{(\lambda)} = \lambda N, \qquad m^{(\lambda)} = \frac{1}{\lambda} m, \qquad a^{(\lambda)} = \frac{1}{\lambda} a, \qquad \kappa^{(\lambda)} = \lambda \kappa,$$

for $\lambda \in \mathbb{N}$ should all behave similarly (Fig. **??**). It thus make sense to investigate the limit $\lambda \to \infty$.

Quantities that do not depend on λ include the total length $L = Na$, the mass density $\rho = m/a$, and the velocity $c := \sqrt{\frac{\kappa a}{\rho}}$. Asymptotically, also the dispersion relation becomes independent:

$$\omega_k^{(\lambda)} = 2\sqrt{\frac{\kappa}{m}\lambda^2} |\sin(ka\lambda^{-1}/2)| \to 2\sqrt{\frac{\kappa}{m}} \lambda \lambda^{-1} |ka/2| = c|k|.$$

Recall the formula (2.29) for the displacement of the r-th particle in terms of the normal coordinates

$$X_r(t) = \sqrt{\frac{\hbar}{Nm}} \sum_k \frac{1}{\sqrt{2\omega_k}} (a_k e^{-i\omega_k t + ikar} + a_k^\dagger e^{i\omega_k t - ikar}).$$

Let's rewrite it in a form suitable for our limit. The product Nm is just the total mass, invariantly expressed as $L\rho$. Also, it makes sense to label the particles not by their index $r = 1, \dots N$, but by their equilibrium position $x = ra \in [0, L]$. With these substitutions, we obtain the "displacement field"

$$\phi(t,x) = \sqrt{\frac{\hbar}{L\rho}} \sum_k \frac{1}{\sqrt{2\omega_k}} (a_k e^{-i\omega_k t + ikx} + a_k^\dagger e^{i\omega_k t - ikx}). \tag{3.1}$$

The continuum model is now defined as an infinite collection of harmonic oscillators indexed by $k \in \frac{2\pi}{L}\mathbb{Z}$ with Hamiltonian

$$H = \sum_k \hbar c|k|\, a_k^\dagger a_k + \text{const.} \tag{3.2}$$

and associated displacement field $\phi(t,x)$ given by (3.1).

> There's some trouble brewing in (3.2): The "constant" is $\sum_k \frac{1}{2}\hbar c|k|$, which diverges. This is the first of the many infinities of quantum field theory. This one is easy to deal with: For finite N, the sum over the ground state energies of the harmonic oscillators is finite. Subtracting this constant from the total energy does not alter physical predictions, so as long as we do not dynamically change the ground state energy (e.g. by putting stress on the material in a way that affects the equilibrium separation a) or get into the realm of general relativity. Thus, the *renormalization* $\sum_k \hbar c|k| \left(a_k^\dagger a_k + \frac{1}{2}\right) \mapsto \sum_k \hbar c|k|\, a_k^\dagger a_k$, while maybe not very principled, does not affect predictions and makes the continuum limit converge. So let's adopt this convention. (We'll encounter more troubling infinities later).

As in Sec. 2.3.1 and App. A.3.1, the definitions so far make sense equally in classical and in quantum mechanics. In QM, the a_k's are annihilation operators that are taken to act on Fock space with occupation number basis $|\dots n_k \dots\rangle$. Classically, the a_k's are complex numbers and (3.1) is the most general real-valued solution of the wave equation

$$\left(\frac{1}{c^2}\partial_t^2 - \partial_x^2\right)\phi(t,x) = 0 \tag{3.3}$$

under cyclic boundary conditions.

We went through this exercise in order to find a strategy for quantizing Maxwell's equations. The relation between the classical and the quantum continuum model found here suggests the following recipe for quantizing classical wave equations:

Summary

- Consider a classical wave equation whose solutions are of the form

  $$\phi(t,x) = \mathcal{N} \sum_k \frac{1}{\sqrt{2\omega_k}} \left(a_k e^{-i\omega_k t} f_k(x) + a_k^\dagger e^{i\omega_k t} f_k(x)^\dagger\right)$$

  for some set of modes $\{f_k(x)\}_k$, a constant $\mathcal{N}$ and $a_k \in \mathbb{C}$.
- Choose normalization such that $H = \sum_k \hbar\omega_k a_k^\dagger a_k$ is the energy of the field.
- The quantized field is obtained by associating an oscillator with every mode and replacing the complex coefficients a_k by annihilation operators acting on a Bosonic or Fermionic Fock space.

Fields for which this program can be implemented are called *free*. We'll only work with free field in this course. General, *interacting* fields, are treated in the QFT courses. How to decide whether to use Fermionic or Bosonic Fock spaces will be a major topic in Chap. 6.

Further comments

It is also of interest to write down a momentum field $\pi(x)$ which describes the continuum limit of the P_r. Because the mass of the individual particles goes to 0 for $\lambda \to \infty$, only the momentum *density* defines an interesting quantity in the limit. Thus, starting from

$$\frac{1}{a}P_r = -i\frac{1}{a}\sqrt{\frac{\hbar m}{N}}\sum_k \sqrt{\frac{\omega_k}{2}}(a_k e^{ikar} - a_k^\dagger e^{-ikar}),$$

and arguing as above, we get for the momentum density field

$$\pi(x) = -i\sqrt{\frac{\hbar\rho}{L}}\sum_k \sqrt{\frac{\omega_k}{2}}(a_k e^{ikx} - a_k^\dagger e^{-ikx}).$$

In the continuum limit, the commutation relation (or $i\hbar$ times the Poisson bracket) between the displacement and the momentum density fields is

$$\begin{aligned}[\phi(x), \pi(y)] &= \frac{-i\hbar}{2L}\sum_{k,k'}[(a_k e^{ikx} + a_k^\dagger e^{-ikx}), (a_{k'} e^{ik'y} - a_{k'}^\dagger e^{-ik'y})] \\ &= \frac{i\hbar}{L}\sum_{k,k'} e^{ikx-k'y}[a_k, a_{k'}^\dagger] = \frac{i\hbar}{L}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}} e^{ik(x-y)} = i\hbar\delta(x-y).\end{aligned}$$

3.2 Quantization of the EM field

Classical electrodynamics can be described either in terms of $\boldsymbol{E}$- and $\boldsymbol{B}$-fields, or in terms of scalar and vector potential Φ, $\boldsymbol{A}$ such that

$$\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}, \qquad \boldsymbol{E} = -\boldsymbol{\nabla}\Phi - \partial_t\boldsymbol{A}. \tag{3.4}$$

The classical Hamilton function

$$H = \frac{1}{2m}(\boldsymbol{P} - q\boldsymbol{A})^2 + q\Phi$$

for a charged particle is expressed in terms of the potential. This suggests that Φ, $\boldsymbol{A}$, rather than $\boldsymbol{E}$, $\boldsymbol{B}$, are the right fields to base a quantum theory on.

However, this immediately leads to a problem: Φ, $\boldsymbol{A}$ are determined by the physical state of the EM field only up to gauge transformations

$$\boldsymbol{A} \mapsto \boldsymbol{A} + \nabla\chi, \qquad \Phi \mapsto \Phi - \partial_t\chi$$

with an arbitrary function χ. Here, we get rid of the ambiguity by adopting the *Coulomb gauge*, fixed by the gauge condition

$$\boldsymbol{\nabla}\cdot\boldsymbol{A}(t,\boldsymbol{x}) = 0. \tag{3.5}$$

Further, we restrict to the free-space version of Maxwell's equation, i.e. we assume that there are no charges or currents $\rho = j = 0$. In this case, the Maxwell equations become

$$\Phi(t, \boldsymbol{x}) = 0, \qquad \Big(\frac{1}{c^2}\partial_t^2 - \partial_x^2 - \partial_y^2 - \partial_z^2\Big)\boldsymbol{A}(t, \boldsymbol{x}) = 0. \tag{3.6}$$

In a box with side length L and cyclic boundary conditions, the space of complex solutions to Eq. (3.6) is spanned by plane waves of the form

$$\boldsymbol{A_k}\, e^{\pm i\omega_k t + i\boldsymbol{k}\boldsymbol{x}}, \qquad \boldsymbol{A}_k \in \mathbb{C}^3, \quad \boldsymbol{k} \in \frac{2\pi}{L}\mathbb{Z}^3, \quad \omega_k := c\|\boldsymbol{k}\|.$$

The gauge condition (3.5) requires the coefficients $\boldsymbol{A_k}$ to be "transversal" to the wave vector $\boldsymbol{k}$:

$$0 = \boldsymbol{\nabla} \cdot \big(\boldsymbol{A_k}\, e^{\pm i\omega_k t + i\boldsymbol{k}\boldsymbol{x}}\big) = i\boldsymbol{k} \cdot \boldsymbol{A_k}\, e^{\pm i\omega_k t + i\boldsymbol{k}\boldsymbol{x}} \quad \Leftrightarrow \quad \boldsymbol{k} \cdot \boldsymbol{A_k} = 0.$$

We can take this into account by choosing, for each $\boldsymbol{k}$, an ortho-normal basis (the *polarization vectors*)

$$\big\{\boldsymbol{e}_1(\boldsymbol{k}), \boldsymbol{e}_2(\boldsymbol{k})\big\} \subset \{\boldsymbol{k}\}^\perp \subset \mathbb{R}^3 \qquad \text{with} \qquad \boldsymbol{e}_\lambda(-\boldsymbol{k}) = \boldsymbol{e}_\lambda(\boldsymbol{k})$$

for the space orthogonal to $\boldsymbol{k}$ (Fig. **??**). Then a general real-valued solution to the Maxwell equations in Coulomb gauge is

$$\boldsymbol{A}(t, \boldsymbol{x}) = \sqrt{\frac{\hbar}{\epsilon_0 L^3}} \sum_{\boldsymbol{k},\lambda} \frac{1}{\sqrt{2\omega_k}} \boldsymbol{e}_\lambda(\boldsymbol{k}) \big(a_{\boldsymbol{k}\lambda} e^{-i\omega_k t + i\boldsymbol{k}\boldsymbol{x}} + a^\dagger_{\boldsymbol{k}\lambda} e^{+i\omega_k t - i\boldsymbol{k}\boldsymbol{x}}\big), \tag{3.7}$$

where the sum is over wave vectors $\boldsymbol{k} \in \frac{2\pi}{L}\mathbb{Z}^3$ and polarization directions $\lambda \in \{1, 2\}$. As discussed before for phonons (Eq. (2.30), it is often convenient to re-arrange the sum in (3.7) so that terms corresponding to the same complex mode are grouped together:

$$\boldsymbol{A}(t, \boldsymbol{x}) = \sqrt{\frac{\hbar}{\epsilon_0 L^3}} \sum_{\boldsymbol{k},\lambda} \frac{1}{\sqrt{2\omega_k}} \boldsymbol{e}_\lambda(\boldsymbol{k}) \big(a_{\boldsymbol{k}\lambda}(t) + a^\dagger_{-\boldsymbol{k}\lambda}(t)\big) e^{i\boldsymbol{k}\boldsymbol{x}}, \tag{3.8}$$

The time evolution of the $\boldsymbol{E}$ and $\boldsymbol{B}$-fields follows by applying (3.4). Setting $\boldsymbol{\kappa} = \frac{\boldsymbol{k}}{\|k\|}$,

$$\boldsymbol{E}(t, \boldsymbol{x}) = i\sqrt{\frac{\hbar}{\epsilon_0 L^3}} \sum_{\boldsymbol{k},\lambda} \sqrt{\frac{\omega_k}{2}}\, \boldsymbol{e}_\lambda(\boldsymbol{k}) \big(a_{\boldsymbol{k}\lambda} e^{-i\omega_k t + i\boldsymbol{k}\boldsymbol{x}} - a^\dagger_{\boldsymbol{k}\lambda} e^{+i\omega_k t - i\boldsymbol{k}\boldsymbol{x}}\big) \tag{3.9}$$

$$= i\sqrt{\frac{\hbar}{\epsilon_0 L^3}} \sum_{\boldsymbol{k},\lambda} \sqrt{\frac{\omega_k}{2}}\, \boldsymbol{e}_\lambda(\boldsymbol{k}) \big(a_{\boldsymbol{k}\lambda}(t) - a^\dagger_{-\boldsymbol{k}\lambda}(t)\big) e^{i\boldsymbol{k}\boldsymbol{x}}, \tag{3.10}$$

$$\boldsymbol{B}(t, \boldsymbol{x}) = i\sqrt{\frac{\hbar}{\epsilon_0 L^3 c^2}} \sum_{\boldsymbol{k},\lambda} \sqrt{\frac{\omega_k}{2}}\, \boldsymbol{\kappa} \times \boldsymbol{e}_\lambda(\boldsymbol{k}) \big(a_{\boldsymbol{k}\lambda} e^{-i\omega_k t + i\boldsymbol{k}\boldsymbol{x}} - a^\dagger_{\boldsymbol{k}\lambda} e^{+i\omega_k t - i\boldsymbol{k}\boldsymbol{x}}\big), \tag{3.11}$$

$$= i\sqrt{\frac{\hbar}{\epsilon_0 L^3 c^2}} \sum_{\boldsymbol{k},\lambda} \sqrt{\frac{\omega_k}{2}}\, \boldsymbol{\kappa} \times \boldsymbol{e}_\lambda(\boldsymbol{k}) \big(a_{\boldsymbol{k}\lambda}(t) + a^\dagger_{-\boldsymbol{k}\lambda}(t)\big) e^{i\boldsymbol{k}\boldsymbol{x}}. \tag{3.12}$$

Plugging these expressions into the formula

$$H_{\mathrm{em}} = \frac{\epsilon_0}{2} \int \boldsymbol{E}^2(t, \boldsymbol{x}) + c^2 \boldsymbol{B}^2(t, \boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}$$

for the energy of the EM field, one finds after some calculations

$$H_{\mathrm{em}} = \sum_{\boldsymbol{k},\lambda} \hbar\omega_{\boldsymbol{k}} |a_{\boldsymbol{k}\lambda}|^2.$$

The $\boldsymbol{A}$-field is thus of the form discussed in Sec. 3.1 so that one can perform a free-field quantization. From now on, we will thus treat the $a_{\boldsymbol{k}\lambda}$'s as annihilation operators for a collection of harmonic oscillators acting on the Fock space $\mathcal{H}_{\mathrm{em}}$.

Notation

For increased legibility, we'll now write k for $(\boldsymbol{k}, \lambda)$, with the convention that $-k$ corresponds to $(-\boldsymbol{k}, \lambda)$. Also, for an element $|\dots n_k \dots\rangle$ of the occupation number basis of the harmonic oscillators, write $|\{n\}\rangle$.

3.3 States of the EM field

3.3.1 Number states

Elements $|\{n\}\rangle$ of the occupation number basis – i.e. states with a definite number of photons in each mode – are called *number states* or *Fock states*. The expected electric field strength in any number state is

$$\langle\{n\}|\boldsymbol{E}(\boldsymbol{x})|\{n\}\rangle \propto \sum_k \langle\{n\}|(a_k e^{i\boldsymbol{k}\boldsymbol{x}} - a_k^\dagger e^{-i\boldsymbol{k}\boldsymbol{x}})|\{n\}\rangle = 0.$$

Zero on average does not imply zero with probability one. Indeed, compute the variance:

$$\begin{aligned}
&\langle\{n\}|\boldsymbol{E}(\boldsymbol{x})\cdot\boldsymbol{E}(\boldsymbol{x})|\{n\}\rangle \\
=&\frac{-\hbar}{\epsilon_0 L^3}\sum_{k,k'}\frac{\sqrt{\omega_k\omega_{k'}}}{2}\big(\boldsymbol{e}_k\cdot\boldsymbol{e}_{k'}\big)\langle\{n\}|\big(a_k e^{i\boldsymbol{k}\boldsymbol{x}} - a_k^\dagger e^{-i\boldsymbol{k}\boldsymbol{x}}\big)\big(a_{k'} e^{i\boldsymbol{k}'\boldsymbol{x}} - a_{k'}^\dagger e^{-i\boldsymbol{k}'\boldsymbol{x}}\big)|\{n\}\rangle \\
=&\frac{\hbar}{2\epsilon_0 L^3}\sum_k \omega_k \langle\{n\}|a_k e^{i\boldsymbol{k}\boldsymbol{x}} a_k^\dagger e^{-i\boldsymbol{k}\boldsymbol{x}} + a_k^\dagger e^{-i\boldsymbol{k}\boldsymbol{x}} a_k e^{i\boldsymbol{k}\boldsymbol{x}}|\{n\}\rangle = \sum_k \frac{\hbar\omega_k}{\epsilon_0 L^3}(n_k + 1/2),
\end{aligned}$$

which diverges. Another infinity!

The infinity encountered in (3.2) was easy to dismiss, as it related to an unobservable choice of energy zero point. This one is a somewhat tougher nut to crack, because electric field strength (proportional to the force exerted on a charged body) has direct physical consequences. One can argue as follows: Any test particle used to measure the field strength will have finite extent, so it cannot be concentrated on just one point $\boldsymbol{x}$ in space. If we replace the point-sized probe by one with a charge density $\rho(\boldsymbol{x})$, then one can show (excercise!) that the spatially averaged force

$$\boldsymbol{F} = \int \rho(\boldsymbol{x})\boldsymbol{E}(\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{x}$$

has finite fluctuations, if ρ is sufficiently spread out. This is physically plausible. The sum diverges because there are infinitely many summands with increasingly large wave vector $\boldsymbol{k}$. But these correspond to fields that oscillate rapidly, so that cancellations over any finite region cause the net force to be small. Mathematically speaking, we found again

Figure 3.1: Net force is zero, so QFT would presumably be OK with it. (Scene from the Caucasian Chalk Circle, as depicted on in this poster).

(c.f. Sec. 2.2.2) that field operators should be thought of as distributions that have to be integrated against smooth functions to be meaningful.

Is this a satisfactory solution?

Yes, in that it gives a good reason for why extended bodies don't regularly get accelerated into orbit due to vacuum fluctuations. *No*, because it paints quite the violent picture of the microscopic world, where, supposedly, unbounded forces constantly tear at objects and only cancellations prevent mayhem (Fig. 3.1). It sure feels like an indication that our current theories of light and matter become invalid at very short length scales.

3.3.2 Coherent states

Number states have zero expected field strength. Since we expect classical electrodyndamics to emerge as a limiting case, there should be states for which the expectation values $\langle \boldsymbol{E}(\boldsymbol{x},t)\rangle$ resemble the classical behavior.

To construct these, recall the *coherent states* of a single harmonnic oscillator. For $\alpha \in \mathbb{C}$, define

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle.$$

Coherent states are eigenvectors of the annihilation operator

$$a|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n}|n-1\rangle = e^{-|\alpha|^2/2} \sum_{n'=0}^{\infty} \frac{\alpha^{n'+1}}{\sqrt{(n'+1)!}} \sqrt{n'+1}|n'\rangle = \alpha\,|\alpha\rangle.$$

A coherent state $|\{\alpha\}\rangle$ of the entire EM field is one where each mode $k \equiv (\boldsymbol{k},\lambda)$ is in a coherent state $|\alpha_k\rangle$. Let's compute the expectation value of the E-field:

$$\begin{aligned}\langle\{\alpha\}|\hat{\boldsymbol{E}}(\boldsymbol{x},t)|\{\alpha\}\rangle &= -i\sqrt{\frac{2\hbar\pi}{L^3}} \sum_k \sqrt{\omega_k}\boldsymbol{e}_k \langle\{\alpha\}|(a_k^\dagger e^{-i\boldsymbol{k}\boldsymbol{x}+\omega_k t} - a_k e^{i\boldsymbol{k}\boldsymbol{x}-\omega_k t})|\{\alpha\}\rangle \\ &= -i\sqrt{\frac{2\hbar\pi}{L^3}} \sum_k \sqrt{\omega_k}\boldsymbol{e}_k \big(\alpha_k^\dagger e^{-i\boldsymbol{k}\boldsymbol{x}+\omega_k t} - \alpha_k e^{i\boldsymbol{k}\boldsymbol{x}-\omega_k t}\big)\end{aligned}$$

which is indeed the classical value (3.9).

3.4 Light-matter interaction

The Hamiltonian of a single spinless particle with charge q, position and momentum operators $\boldsymbol{X}, \boldsymbol{P}$, subject to a field in Coulomb gauge is

$$H = \frac{\big(\boldsymbol{P} - q\boldsymbol{A}(\boldsymbol{X})\big)^2}{2m} + U(\boldsymbol{X}) + \sum_k \hbar\omega_k a_k^\dagger a_k. \tag{3.13}$$

It acts on a total Hilbert space $\mathcal{H} = \mathcal{H}_{\mathrm{par}} \otimes \mathcal{H}_{\mathrm{em}}$ that is the tensor product between the spaces of the particle $\mathcal{H}_{\mathrm{par}} = L^2(\mathbb{R}^3)$ and of the field $\mathcal{H}_{\mathrm{em}}$. Here, $\boldsymbol{A}(\boldsymbol{X})$ is defined by (3.7), where the ladder operators $a_k, a_k^\dagger$ act on $\mathcal{H}_{\mathrm{em}}$, but the parameter $\boldsymbol{x}$ is evaluated on the position of the particle. In other words

$$\boldsymbol{A}(\boldsymbol{X})\,|\boldsymbol{x}\rangle|\psi\rangle = |\boldsymbol{x}\rangle\big(\boldsymbol{A}(\boldsymbol{x})|\psi\rangle\big) \qquad \boldsymbol{x} \in \mathbb{R}^3, |\psi\rangle \in \mathcal{H}_{\mathrm{em}}. \tag{3.14}$$

We will now go through a sequence of simplifications and transformations. Start with

$$\frac{1}{2m}\big(\boldsymbol{P} - q\boldsymbol{A}(\boldsymbol{X})\big)^2 = \frac{\boldsymbol{P}^2}{2m} - \frac{q}{2m}(\boldsymbol{P}\boldsymbol{A}(\boldsymbol{X}) + \boldsymbol{A}(\boldsymbol{X})\boldsymbol{P}) + \frac{q^2}{2m}\boldsymbol{A}(\boldsymbol{X})^2.$$

As a first step, we will neglect the square $\boldsymbol{A}(\boldsymbol{X})^2$, which describes two-photon processes. Next, verify that in Coulomb gauge, momentum and the vector potential commute:

$$\boldsymbol{P}\big(\boldsymbol{A}(\boldsymbol{X})|\phi\rangle\big) = -i\hbar\boldsymbol{\nabla}\big(\boldsymbol{A}(\boldsymbol{X})|\phi\rangle\big) = -i\hbar(\boldsymbol{\nabla}\cdot\boldsymbol{A}(\boldsymbol{X}))|\phi\rangle + \boldsymbol{A}(\boldsymbol{X})\cdot\boldsymbol{P}|\phi\rangle = \boldsymbol{A}(\boldsymbol{X})\cdot\boldsymbol{P}|\phi\rangle,$$

so that we can write $H \simeq H_{\mathrm{par}} + H_{\mathrm{em}} + H_I$, with

$$H_{\mathrm{par}} = \frac{\boldsymbol{P}^2}{2m} + U(\boldsymbol{X}), \quad H_{\mathrm{em}} = \sum_k \hbar\omega_k a_k^\dagger a_k, \quad H_I = -\frac{q}{m}\boldsymbol{P}\cdot\boldsymbol{A}(\boldsymbol{X}).$$

So far, we have worked in a "mixed picture", where the EM field was expressed in second quantization, but only a single particle in first quantization was present. We now also pass to the second-quantized picture for the particle. To this end, let $\{|\phi_i\rangle\}_i$ be an eigenbasis of H_{part} and denote the corresponding creation operators as $b_i^\dagger$, so that

$$H_{\mathrm{part}} = \sum_i E_i\, b_i^\dagger b_i.$$

It remains to treat the interaction Hamiltonian. Even without doing any calculations, we can see from (3.8) that H_I will be of the form

$$\sum_{ijk} g_{ijk}(a_k + a_{-k}^\dagger)b_i^\dagger b_j.$$

It thus describes a superposition of processes where a photon is removed from or added to the field, while the state of the particle gets switched. Let's calculate the amplitudes:

$$\begin{aligned}\sum_{ij}\big\langle\phi_i\big|H_I\big|\phi_j\big\rangle b_i^\dagger b_j &= -\frac{q}{m}\sum_{ij}\big\langle\phi_i\big|\boldsymbol{P}\cdot\boldsymbol{A}\big|\phi_j\big\rangle b_i^\dagger b_j \\ = -\frac{q}{m}\sqrt{\frac{\hbar}{\epsilon_0 L^3}}\sum_{ijk}\int \phi_i^\dagger(\boldsymbol{x})\frac{1}{\sqrt{2\omega_k}}\big((a_k + a_{-k}^\dagger)e^{-i\boldsymbol{k}\boldsymbol{x}}\big)\boldsymbol{e}_k\cdot\boldsymbol{P}\phi_j(\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{x}\; b_i^\dagger b_j &\end{aligned} \tag{3.15}$$

so that

$$g_{ijk} = -\frac{q}{m}\sqrt{\frac{\hbar}{\epsilon_0 L^3 2\omega_k}}\int \phi_i^\dagger(\boldsymbol{x}) e^{-i\boldsymbol{k}\boldsymbol{x}} \boldsymbol{e}_k \cdot \boldsymbol{P}\phi_j(\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{x}.$$

The wave lengths associated with atomic transitions are much longer than the length scales of the atoms themselves. This justifies the *dipole approximation*, in which the dependencies of the EM field on position is neglected by substituting $e^{i\boldsymbol{x}\boldsymbol{k}} \simeq 1$. Then

$$g_{ijk} \simeq -\frac{q}{m}\sqrt{\frac{\hbar}{\epsilon_0 L^3 2\omega_k}}\int \phi_i^\dagger(\boldsymbol{x}) \boldsymbol{e}_k \cdot \boldsymbol{P}\phi_j(\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{x}.$$

In the expression, the momentum operator acts on energy eigenfunctions in position representation. One can eliminate momentum using

$$[\boldsymbol{X}, H_{\mathrm{part}}] = \frac{i\hbar}{m}\boldsymbol{P} \qquad \Rightarrow \qquad \boldsymbol{P} = \frac{m}{i\hbar}[\boldsymbol{X}, H_{\mathrm{part}}],$$

so that the coupling constants become

$$g_{ijk} = \frac{-q}{m}\sqrt{\frac{\hbar}{\epsilon_0 L^3 2\omega_k}}\big\langle\phi_i\big|(\boldsymbol{e}_k \cdot \boldsymbol{P})\big|\phi_j\big\rangle = iq\sqrt{\frac{1}{\epsilon_0 L^3 2\hbar\omega_k}}(E_j - E_i)\big\langle\phi_i\big|(\boldsymbol{e}_k \cdot \boldsymbol{X})\big|\phi_j\big\rangle. \tag{3.16}$$

Because this expression is symmetric under inversion of $\boldsymbol{k}$, the minus sign of $a_{-k}^\dagger$ in (3.15) can be dropped, so that

$$\sum_{ij}\big\langle\phi_i\big|H_I\big|\phi_j\big\rangle b_i^\dagger b_j = \sum_{ijk} g_{ijk}(a_k + a_k^\dagger) b_i^\dagger b_j. \tag{3.17}$$

3.4.1 Spontaneous emission

The goal is to compute the life time of the first excited state $n = 2$ of a hydrogen atom. We will employ first-order time-dependent perturbation theory in the form of *Fermi's Golden Rule* (Sec. A.4.1), which says that H_I will cause an initial state $|i\rangle$ to decay at a rate

$$\Gamma \simeq \frac{2\pi}{\hbar}\int |\langle f|H_I|i\rangle|^2\,\delta(E_i - E_f)\rho(f)\,\mathrm{d}f. \tag{3.18}$$

Here, $|i\rangle = |\phi_{2,l,m}\rangle|0\rangle$ (we'll choose l and m later). The delta function ensures that total energy is conserved. Because the EM field is already in its lowest-energy state, only final states where the atom has transitioned into its ground state and has emitted photons are permitted. Because, by Eq. (3.17), H_I is linear in ladder operators, the coupling matrix element is non-zero only for final states that contain a single photon: $|f\rangle = |\phi_{1,0,0}\rangle|k\rangle$, where $k = (\boldsymbol{k}, \lambda)$ labels the state of the emitted photon. (This is an artifact of the approximations we have made – multiple-photon processes are, in principle, possible).

The energy difference between the two lowest levels (the *Lyman-α line*) is (Sec. A.3.3)

$$E_{1,2} := \Big(1 - \frac{1}{4}\Big)E_I = \frac{3}{4}E_I = \frac{3\alpha^2}{8}mc^2.$$

The photon energy is $\hbar\omega_k = \hbar c\|\boldsymbol{k}\|$ and energy conservation is thus equivalent to $\|\boldsymbol{k}\| = \frac{E_{1,2}}{\hbar c}$.

It follows that the integral in (3.18) is over states labeled by $f = (\boldsymbol{k}, \lambda)$, where $\boldsymbol{k}$ lies on a sphere of radius $\frac{E_{1,2}}{\hbar c}$. For fixed λ, the density of states in $\boldsymbol{k}$-space is $\rho(\boldsymbol{k})\mathrm{d}^3\boldsymbol{k} = \left(\frac{L}{2\pi}\right)^3 \mathrm{d}^3\boldsymbol{k}$. Switching to spherical coordinates,

$$\rho(\boldsymbol{k})\,\mathrm{d}^3\boldsymbol{k} = \left(\frac{L}{2\pi}\right)^3 \mathrm{d}^3\boldsymbol{k} = \left(\frac{L}{2\pi}\right)^3 r^2\,\mathrm{d}r\sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta = \left(\frac{L}{2\pi}\right)^3 \frac{E^2}{\hbar^3 c^3}\,\mathrm{d}E\sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta.$$

Using (3.16, 3.17), the coupling constant for $\hbar\omega_k = E_{1,2}$ is

$$|\langle\phi_{2,l,m}|\langle 0|H_I|\phi_{1,0,0}\rangle|k\rangle|^2 = \frac{e^2\,E_{1,2}}{2\epsilon_0 L^3}\left|\left\langle\phi_{2,l,m}\right|(\boldsymbol{e}_k\cdot\boldsymbol{X})\left|\phi_{1,0,0}\right\rangle\right|^2.$$

To evaluate the matrix element, we need to borrow some results on atomic eigenstates.

> Four facts: (F1) The *dipole matrix elements* $\langle\phi_{2,l,m}|\boldsymbol{e}\cdot\boldsymbol{X}|\phi_{1,0,0}\rangle$ are non-zero only if $l = 1$. (F2) $\langle\phi_{2,l,0}|x|\phi_{1,0,0}\rangle = \langle\phi_{2,l,0}|y|\phi_{1,0,0}\rangle = 0$. (F3) States that differ only in the magnetic quantum number m can be mapped onto each other by a rotation. (F4) Using the explicit form of the functions $\phi_{n,l,m}(\boldsymbol{x})$, a tedious integral gives
>
> $$|\langle\phi_{2,1,0}|z|\phi_{1,0,0}\rangle|^2 = \frac{2^{15}}{3^{10}}a_0^2 = \frac{\hbar^2}{m^2c^2}\frac{2^{15}}{3^{10}\alpha^2}.$$

Fact (F1) implies that in first-order perturbation theory, the states $|\phi_{2,l,0}\rangle$ have infinite life time unless $l = 1$, i.e. only the $2p \to 1s$ transition can be computed in this approximation. By (F3), m can be changed by rotating the atom. But the life time of a level is independent of the atom's orientation and hence of m. We trust that our approximations reproduce this rotational invariance (they do), and compute Γ only for $m = 0$:

$$\Gamma = \frac{2\pi}{\hbar}\int \frac{e^2}{2\epsilon_0 L^3}\sum_\lambda \left|\left\langle\phi_{2,1,0}\right|(\boldsymbol{e}_k\cdot\boldsymbol{X})\left|\phi_{1,0,0}\right\rangle\right|^2 \left(\frac{L}{2\pi}\frac{E_{1,2}}{\hbar c}\right)^3 \sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta.$$

Then by (F2, F4), only the z-component of $\boldsymbol{e}_k\cdot\boldsymbol{X} = \boldsymbol{e}_\lambda(\boldsymbol{k})\cdot\boldsymbol{X}$ gives a non-zero contribution, namely

$$\sum_\lambda \left|\left\langle\phi_{2,1,0}\right|(\boldsymbol{e}_\lambda(\boldsymbol{k})\cdot\boldsymbol{X})\left|\phi_{1,0,0}\right\rangle\right|^2 = \frac{2^{15}}{3^{10}}a_0^2\sum_\lambda(\boldsymbol{e}_\lambda(\boldsymbol{k}))_z^2.$$

To evaluate the sum, note that with $\boldsymbol{e}_0(\boldsymbol{k}) := \frac{\boldsymbol{k}}{\|\boldsymbol{k}\|}$, the set $\{\boldsymbol{e}_\lambda(\boldsymbol{k})\}_{\lambda=0}^2$ forms on orthonormal basis. Expressing the length-squared of $\boldsymbol{e}_z$ in that basis gets us

$$1 = \sum_{\lambda=0}^2 |\boldsymbol{e}_\lambda(\boldsymbol{k})\cdot\boldsymbol{e}_z|^2 = \cos^2\theta + \sum_{\lambda=1}^2(\boldsymbol{e}_\lambda(\boldsymbol{k}))_z^2 \quad\Rightarrow\quad \sum_{\lambda=1}^2(\boldsymbol{e}_\lambda(\boldsymbol{k}))_z^2 = \sin^2\theta.$$

Using the identity $\sin^3\theta\,\mathrm{d}\theta = -\sin^2\theta\,\mathrm{d}(\cos\theta) = (z^2-1)\,\mathrm{d}z$, the integration results in

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\sin^3\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = 2\pi\int_{-1}^{1}(z^2-1)\,\mathrm{d}z = 2\pi\frac{4}{3}.$$

To express all quantities in relativistic units, eliminate e^2 in favor of the fine structure constant $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$. Now brew some coffee, close the door, and plug in:

$$\begin{aligned}
\Gamma &= \frac{2\pi}{\hbar}\,\frac{\alpha 4\pi\epsilon_0\hbar c}{2\epsilon_0 L^3}\,\frac{\hbar^2}{m^2c^2}\,\frac{2^{15}}{3^{10}\alpha^2}\left(\frac{L}{2\pi}\,\frac{3\alpha^2\,mc^2}{8\hbar c}\right)^3 2\pi\frac{4}{3} && \text{(don't think, just copy)}\\
&= 2^{17}8^{-3}3^{-8}\pi^0 L^0\epsilon_0^0\alpha^5\hbar^{-1}m^1c^2 && \text{(sort by units)}\\
&= \left(\frac{2}{3}\right)^8\alpha^5\frac{mc^2}{\hbar} = 6.27\times10^8\,\mathrm{Hz} = 1/(1.6\,\mathrm{ns}) && \text{(yeah, go ahead and click).}
\end{aligned}$$

Amazingly, given the number of approximations made, this is the accepted value [Radzig, Smirnov, *Reference Data on Atoms, Molecules, and Ions*, Table 7.4].

3.5 Further reading

For field quantization, see *Photons and Atoms* by Cohen-Tannoudji, Dupont-Roc, and Grynberg. Matter-light interaction follows *Quantum Optics* by Walls and Milburn and *Advanced Quantum Mechanics* by Sakurai (who uses Heaviside-Lorentz units instead of SI units employed by the other authors – consult Wikipedia to convert).

Chapter 4

Scattering theory

Chapter 5

Symmetries in quantum mechanics

Chapter 6

Relativistic QM

Appendix A

Quantum mechanics recap

In this chapter, we recall some facts that should be familiar from linear algebra and introductory quantum mechanics courses. The textbook *Quantum Mechanics* by L. Ballentine is a good source for this material.

A.1 Linear algebra of Hilbert spaces

A.1.1 Hilbert spaces

A *Hilbert space* $\mathcal{H}$ is a complex vector space with a *sesquilinear* inner product $\langle\cdot|\cdot\rangle$. Sesquilinearity means that for all vectors

$$\alpha, \beta, \gamma \in \mathcal{H}$$

and complex numbers $z \in \mathbb{C}$, we have

$$\langle\alpha|\beta+\gamma\rangle = \langle\alpha|\beta\rangle + \langle\alpha|\gamma\rangle, \tag{A.1}$$
$$\langle\alpha|z\beta\rangle = z\langle\alpha|\beta\rangle, \tag{A.2}$$

as well as

$$\langle\alpha|\beta\rangle = \overline{\langle\beta|\alpha\rangle}. \tag{A.3}$$

From this, it follows that

$$\langle\alpha+\beta|\gamma\rangle = \langle\alpha|\gamma\rangle + \langle\beta|\gamma\rangle,$$
$$\langle z\alpha|\beta\rangle = \bar{z}\langle\alpha|\beta\rangle,$$

i.e. the inner product is anti-linear w.r.t. the first entry and linear w.r.t. the second one.

> Beware that mathematicians usually employ the opposite convention, where the sesquilinear inner product is linear in the first entry!

The *norm* of a vector $\alpha \in \mathcal{H}$ is given by

$$\|\alpha\| := \sqrt{\langle\alpha|\alpha\rangle}.$$

Recall that inner products are required to be *definite*, i.e. to fulfill

$$\|\alpha\| > 0 \quad \forall\alpha \neq 0.$$

There are two examples of Hilbert spaces you should be acquainted with: *column vectors* and *square-integrable functions*. Let's look at both in turn.

The vector space $\mathbb{C}^d$ is formed by d-dimensional complex column vectors

$$\alpha = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_d \end{pmatrix}$$

with sesquilinear inner product

$$\langle \alpha | \beta \rangle = \sum_{i=1}^{d} \bar{\alpha_i} \beta_i. \tag{A.4}$$

Hilbert spaces appears e.g. in the description of spin degrees of freedom.

More involved is the Hilbert space $L^2(\mathbb{R}^n)$ of square-integrable complex functions on $\mathbb{R}^n$. Given two functions $\alpha, \beta : \mathbb{R}^n \to \mathbb{C}$, we can define a "continuous analogue" of Eq. (A.4):

$$\langle \alpha | \beta \rangle = \int \bar{\alpha}(x) \beta(x) \, \mathrm{d}^n x. \tag{A.5}$$

For the non-pedantic physicist, the space of all wave functions, together with (A.5) defines a Hilbert space. It is associated with a point particle with n degrees of freedom.

> There are three technical problems that one has to address to define the Hilbert space of functions with mathematical rigor.
>
> The first problem is the integral is not actually defined for all functions. Set, for example
>
> $$\psi(x) = \begin{cases} \sin(1/x) & x \neq 0, \\ 0 & x = 0. \end{cases}$$
>
> Then
>
> $$\int |\alpha(x)|^2 \, \mathrm{d}^n x$$
>
> does not exist (in either the Riemann or the Lebesque sense). The second problem is that the integral may be defined, but infinite – take e.g. $\alpha(x) = 1$ and compute $\langle \alpha | \alpha \rangle$. To get rid of both problems, we define a function α to be *square-integrable* if
>
> $$\|\alpha\|^2 = \langle \alpha | \alpha \rangle = \int |\alpha(x)|^2 \, \mathrm{d}^n x$$
>
> exists and is finite. If α, β are square-integrable, then the product $\bar{\alpha}\beta$ is integrable, and the *Cauchy-Schwarz inequality* says that
>
> $$|\langle \alpha | \beta \rangle|^2 \leq \|\alpha\|^2 \, \|\beta\|^2 < \infty,$$
>
> so that, by restricting to square-integrable functions, we have rid outselves of undefined and infinite integrals!
>
> The third problem is that the norm is no longer definite. Indeed, define a function
>
> $$\alpha(x) = \begin{cases} 1 & x = 0 \\ 0 & x \neq 0 \end{cases} .$$

Then $\alpha \neq 0$, but $\|\alpha\|^2 = 0$. Circumventing this problem requires some mathematical gymnastics: We say that two functions are *equivalent* if they differ only on a set of measure zero. This means e.g. that the function α is equivalent to the 0-function, as the two differ only at one point. If we define the Hilbert space $L^2(\mathbb{R}^n)$ to be the *complex vector space of equivalence classes* of square-integrable functions, then one can show that (A.5) becomes a *definite* inner product. Problem solved.

Another technical issue with function spaces concerns physical units. Let me say upfront that one can represent all physical quantities just by real numbers relative to some fixed set of units, and that in this case, none of the issues below arise. (This is what we will mainly do in this document). However, attaching a dimension to every physical quantity has some value in that it can highlight certain inconsistencies and guide heuristic arguments. So let's briefly discuss how this would be done in QM. For example, we may want $\psi(x)$ to be defined not on the set of real numbers, but on a set representing physical positions ($[x] = \mathrm{L}$) measured in some concrete unit of length, say meters m. Then $[\mathrm{d}x] = \mathrm{L}$ as well, and for the normalization property to work out, we can either stick with the scalar product

$$\langle\phi|\psi\rangle = \int_{\mathbb{R}} \bar{\phi}(x)\psi(x)\,\mathrm{d}x,$$

in which case the wave function needs to have the dimension $[\psi(x)] = \mathrm{L}^{1/2}$, or we retain dimensionless wave functions, in which case we have to redefine the scalar product

$$\langle\phi|\psi\rangle = \int_{\mathbb{R}\cdot\mathrm{m}} \bar{\phi}(x)\psi(x)\,\mathrm{d}\mu(x),$$

with respect to a dimension-carrying measure

$$\mathrm{d}\mu(x) := \frac{1}{\mathrm{m}}\mathrm{d}x.$$

When working in another continuous representation (e.g. momentum, see below), the units will have to be adapted accordingly. Unlike functions that depend on continuous parameters, discrete coefficients remain dimensionless (so that $[\sum_i |\alpha_i|^2] = 1$) and thus do not carry information about their physical interpretation.

We will sometimes consider slight modifications, e.g. by choosing some region $R \subset \mathbb{R}^d$ and working with the space $L^2(R)$ of square-integrable functions on R, subject to appropriate boundary conditions.

A.1.2 Linear operators

A map A between two vector spaces is *linear* if

$$A(\phi + \psi) = A(\phi) + A(\psi), \qquad A(\lambda\phi) = \lambda A(\phi).$$

In QM, linear maps between Hilbert spaces are traditionally called *operators*.

Examples:

- $\mathcal{H} = \mathbb{C}^d$: In this case, operators can conveniently be specified as matrices, which act on column vectors in the usual way. For example, we will have ample opportunity to work with the *Pauli matrices*:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- $\mathcal{H} = L^2(\mathbb{R})$: The *position operator* acts on a function $\psi : \mathbb{R} \to \mathbb{C}$ by multiplying it with its argument

$$(X\psi)(x) = x\psi(x).$$

The *momentum operator* maps a function to $-i\hbar$ times its derivative

$$P = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x} : \psi \mapsto P\psi = -i\hbar\psi'.$$

A.1.3 Dirac notation

Physicists often use notational aids to delinate vector-valued quantities from scalars. In quantum mechanics, the suggestive *Dirac* notation (or "bra-ket" notation) is usually employed. Here, a vector $\alpha \in \mathcal{H}$ is written as $|\alpha\rangle$. This is called a *ket*, for reasons that will be obvious momentarily.

Every vector $\psi \in \mathcal{H}$ defines a linear function

$$\mathcal{H} \to \mathbb{C}, \qquad \phi \mapsto \langle\psi|\phi\rangle,$$

the "projection onto ψ". In quantum, we denote this function as $\langle\psi|$ and call it a *bra*. Then we can write

$$\langle\psi|(|\phi\rangle) = \langle\psi|\phi\rangle, \tag{A.6}$$

so a "bra-ket" is a "braket". This passes for humor around here.

> Linear functions from a vector spaces to $\mathbb{C}$ are also called *dual vectors* or *(linear) functionals*. In the calculus of variation – i.e. the branch of calculus that turns the action principle into the Euler-Langrange equation – the word "functional" is used instead to refer to a function that takes other functions as arguments. Don't be confused by this ambiguity!
> In math and engineering, is is common to use a star or sometimes a dagger superscript to denote the functional associated with a vector in a Hilbert space:
>
> $$|\psi\rangle \leftrightarrow \psi, \qquad \langle\psi| \leftrightarrow \psi^* \text{ or } \psi^\dagger.$$

The genius of this notation is that one doesn't need to expend any thoughts on concepts like "dual vectors" or "linear functionals" – the formalism almost forces one to use these object correctly.

Let's play around with this. Equation (A.6) is the *inner product* between $|\psi\rangle$ and $|\phi\rangle$. One can combine two vectors also to form an *outer product*, namely the linear operator $\mathcal{H} \to \mathcal{H}$ defined as

$$|\beta\rangle \mapsto |\phi\rangle\langle\psi|\left(|\beta\rangle\right) := |\phi\rangle\left(\langle\psi|\beta\rangle\right). \tag{A.7}$$

Definition (A.7) implies that composing bra's and ket's is associative: One can read the expression

$$|\phi\rangle\langle\psi|\beta\rangle$$

as either

$$\left(|\phi\rangle\langle\psi|\right)\left(|\beta\rangle\right) \qquad \text{"operator acting on vector"}$$

or as

$$|\phi\rangle\left(\langle\psi|\beta\rangle\right) \qquad \text{"vector times inner product"},$$

getting the same result.

A.1.4 Bases

Let $\mathcal{H}$ be a Hilbert space. A set $\{|e_i\rangle\}_i \subset \mathcal{H}$ is called *ortho-normal* if

$$\langle e_i|e_j\rangle = \delta_{i,j}.$$

If in addition, every element $|\psi\rangle \in \mathcal{H}$ can be expressed as a liner combination

$$|\psi\rangle = \sum_i \psi_i |e_i\rangle \tag{A.8}$$

with suitable *expansion coefficients* $\psi_i \in \mathbb{C}$, then we have an *ortho-normal basis* (ONB).

> In physics, unless stated otherwise, "basis" always means "ortho-normal basis". Also, one usually assumes that every Hilbert space comes with some distinguished basis, ideally with a clear physical interpretation.
>
> Hilbert spaces are often infinite-dimensional. In this case, the "sum" in (A.8) is actually an infinite series, and the equality sign is to be interpreted as the statement
>
> $$\lim_{n\to\infty} \left\| \left(\sum_{i=1}^{n} \psi_i |e_i\rangle \right) - |\psi\rangle \right\| = 0.$$
>
> Experience has it that ignoring all these mathematical subtleties tends to not create major problems in physics. If you are bothered by this, it pays to pick up a book on functional analysis.

Every ONB fulfills the *completness relation*

$$\sum_i |e_i\rangle\langle e_i| = \mathbb{1}, \tag{A.9}$$

where $\mathbb{1} : |\psi\rangle \mapsto |\psi\rangle$ is the identity map.

> To prove it, calculate for an arbitrary $|\psi\rangle = \sum_i \psi_i |i\rangle$,
>
> $$\left(\sum_i |e_i\rangle\langle e_i| \right) \left(\sum_j \psi_j |e_j\rangle \right) = \sum_{i,j} \psi_j |e_i\rangle \underbrace{\langle e_i|e_j\rangle}_{\delta_{i,j}} = |\psi\rangle.$$
>
> The converse is *not* true: There are complete sets that are not ortho-normal bases.

Using just the completeness relation, the following important properties of ONBs can be easily verified:

1. Expansion coefficients are given by inner products

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \Big(\sum_i |e_i\rangle\langle e_i| \Big) |\psi\rangle = \sum_i \underbrace{\langle e_i|\psi\rangle}_{\psi_i} |e_i\rangle.$$

2. Expansion coefficients of bras are the complex conjugate:

$$\langle\psi| = \langle\psi|\mathbb{1} = \sum_i \underbrace{\langle\psi|e_i\rangle}_{\bar{\psi}_i} \langle e_i|.$$

3. Inner products with respect to an arbitrary ONB:

$$\langle\psi|\phi\rangle = \langle\psi|\mathbb{1}|\phi\rangle = \sum_i \langle\psi|e_i\rangle\langle e_i|\phi\rangle = \sum_i \bar{\psi}_i\phi_i.$$

The special case where $\phi = \psi$ is sometimes called the *Parseval relation*:

$$\|\psi\|^2 = \langle\psi|\psi\rangle = \sum_i |\psi_i|^2.$$

4. Description of operators via *matrix elements*

$$A = \mathbb{1}A\mathbb{1} = \sum_{i,j} |e_i\rangle\langle e_i|A|e_j\rangle\langle e_j| = \sum_{i,j} A_{i,j}|e_i\rangle\langle e_j|, \quad A_{i,j} := \langle e_i|A|e_j\rangle. \tag{A.10}$$

so that

$$\langle\phi|A|\psi\rangle = \langle\phi|\mathbb{1}A\mathbb{1}|\psi\rangle = \sum_{ij} \bar{\phi}_j A_{ij}\psi_i.$$

The expression (A.10) also shows that for every basis $\{|e_i\rangle\}_i$ of the Hilbert space, the set $\{|e_i\rangle\langle e_j|\}_{ij}$ is a basis for the vector space of linear operators.

The Dirac notation allows one to save a bit of ink when working with one fixed ONB. Say we have agreed to work with $\{|e_i\rangle\}_i$. Then quantum physicists (and no-one else…) commonly drop the symbol e and just put the index into the ket:

$$|i\rangle := |e_i\rangle.$$

Vector and matrix representations

Assume that $\mathcal{H}$ is finite-dimensional and that some ONB $\{|i\rangle\}_{i=1}^d$ has been fixed. Then the calculations above define a one-one relation between $\mathcal{H}$ and the Hilbert space $\mathbb{C}^d$ of row vectors. Concretely, take the dictionary

$$\text{kets} \leftrightarrow \text{column vectors} \qquad |\psi\rangle \leftrightarrow \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_d \end{pmatrix}$$

$$\text{bras} \leftrightarrow \text{row vectors} \qquad \langle\psi| \leftrightarrow (\bar{\psi}_1, \ldots, \bar{\psi}_d)$$

$$\text{operators} \leftrightarrow \text{matrices} \qquad A \leftrightarrow \begin{pmatrix} A_{1,1} & \ldots & A_{1,d} \\ \vdots & & \vdots \\ A_{d,1} & \ldots & A_{d,d} \end{pmatrix}$$

with

$$\psi_i = \langle i|\psi\rangle, \qquad A_{i,j} = \langle i|A|j\rangle.$$

Under this identification, the composition rules of bra's, ket's, and operators correspond to the usual rules of matrix-vector multiplication. This representation is particularly useful for computer implementations!

For example, a spin-$1/2$-degree of freedom is associated with the Hilbert space

$$\mathcal{H} = \{\alpha|\uparrow\rangle + \beta|\downarrow\rangle \,|\, \alpha, \beta \in \mathbb{C}\}$$

with basis $\{|\uparrow\rangle, |\downarrow\rangle\}$. Then one can introduce operators either abstractly or as matrices, e.g.:

$$\begin{aligned} \sigma_x &= |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| \quad \text{“}=\text{”} \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \sigma_z &= |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow| \quad \text{“}=\text{”} \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned}$$

A.1.5 The adjoint

Recall that in $\mathbb{R}^d$ with Euclidean scalar product

$$(u, v) = \sum_i u_i v_i$$

one can “move a matrix from one entry of the scalar product to the other by taking its transpose”

$$(u, Av) = (A^t u, v), \qquad (A^t)_{i,j} = A_{j,i}.$$

Likewise, if $\mathcal{H}$ is a Hilbert space and A an operator on $\mathcal{H}$, then there is a unique *adjoint operator* $A^\dagger$ such that

$$\langle\phi|A\psi\rangle = \langle A^\dagger\phi|\psi\rangle \qquad \forall\, \psi, \phi \in \mathcal{H}.$$

With respect to a basis, one finds the formula

$$\langle\phi|A\psi\rangle = \sum_{ij} \bar{\phi}_i A_{ij} \psi_j = \sum_j \overline{\left(\sum_i \phi_i \bar{A}_{ij}\right)} \psi_j = \langle A^\dagger\phi|\psi\rangle \quad \Rightarrow \quad (A^\dagger)_{ij} = \bar{A}_{ji}.$$

The matrix representation of $A^\dagger$ is therefore the “conjugate transpose” of the one of A. The expression $A^\dagger$ for the adjoint is pronounced “A dagger”. An operator A is *self-adjoint* or *Hermitian* if $A = A^\dagger$.

If one chooses a basis of $\mathcal{H}$ and expands

$$A = \sum_{ij} A_{ij} |i\rangle\langle j|,$$

then, just as in

$$\langle i|A^\dagger|j\rangle = \overline{\langle j|A|i\rangle} = \bar{A}_{ji} \qquad \Rightarrow \qquad A^\dagger = \sum_{ij} \bar{A}_{ji} |i\rangle\langle j|.$$

The matrix representation of $A^\dagger$ is therefore the “conjugate transpose” of the one of A. An operator A is *self-adjoint* or *Hermitian* if $A = A^\dagger$.

Properties. It is easy to see that taking the adjoint

- ...is anti-linear $(A + zB)^\dagger = A^\dagger + \bar{z}A^\dagger$,
- ...reverses products $(AB)^\dagger = B^\dagger A^\dagger$,
- ...exchanges "bras" and "kets" $\big(|\alpha\rangle\langle\beta|\big)^\dagger = |\beta\rangle\langle\alpha|$.

One can unify the last two properties by slightly generalizing the definition of the adjoint. If $\mathcal{H}$ and $\mathcal{K}$ are two Hilbert spaces, then it is still true that for every operator $A : \mathcal{H} \to \mathcal{K}$, there is a unique adjoint $A^\dagger : \mathcal{K} \to \mathcal{H}$, such that

$$\langle\phi|A\psi\rangle_\mathcal{K} = \langle A^\dagger\phi|\psi\rangle_\mathcal{H} \qquad \phi \in \mathcal{K}, \psi \in \mathcal{H}.$$

Now $\mathbb{C} = \mathbb{C}^1$ is itself is a Hilbert space, and we can identify a ket $|\beta\rangle \in \mathcal{H}$ with the map $\mathbb{C} \to \mathcal{H}$ sending $z \in \mathbb{C}$ to $z|\beta\rangle$. Then one directly verifies that $|\beta\rangle^\dagger = \langle\beta|$ and that the first two properties listed above still hold in the generalized setting. The third property is then a special case of the second one.

We'll also use the following consequence

$$(A|\beta\rangle)^\dagger = \langle\beta|A^\dagger. \tag{A.11}$$

Examples.

- The Pauli matrices are self-adjoint, as is evident by taking the conjugate-transpose.
- The momentum operator is self-adjoint:

$$\begin{aligned}\langle\phi|P|\psi\rangle &= \int_{-\infty}^{\infty} \bar{\phi}(x)(-i\hbar)\psi'(x)\,\mathrm{d}x \\ &= -\int_{-\infty}^{\infty} (\bar{\phi})'(x)(-i\hbar)\psi(x)\,\mathrm{d}x \qquad \text{(integration by parts)} \\ &= \overline{\int_{-\infty}^{\infty} \bar{\psi}(x)(-i\hbar)\phi'(x)\,\mathrm{d}x} = \overline{\langle\psi|P|\phi\rangle},\end{aligned}$$

where we have used that for square-integrable functions $\lim_{x\to\pm\infty}\psi(x) = 0$ so that no boundary terms appear when integrating by parts.

A.1.6 Spectral decomposition (discrete case)

Recall our old friend, the *eigenvalue problem*: Given an operator $A : \mathcal{H} \to \mathcal{H}$, find all $\lambda_i, |\psi_i\rangle$ such that

$$A|\psi_i\rangle = \lambda_i|\psi_i\rangle$$

Of course, the λ_i's are the *eigenvalues* and the $|\psi_i\rangle$'s the *eigenvectors* of A.

A *spectral decomposition* (or *eigendecomposition*) of A is a representation of the form

$$A = \sum_i \lambda_i|\psi_i\rangle\langle\psi_i|, \qquad \mathbb{1} = \sum_i |\psi_i\rangle\langle\psi_i|. \tag{A.12}$$

Given a spectral decomposition, compute

$$A|\psi_j\rangle = \sum_i \lambda_i|\psi_i\rangle \underbrace{\langle\psi_i|\psi_j\rangle}_{\delta_{ij}} = \lambda_j|\psi_j\rangle.$$

It follows that A has an eigendecomposition if and only if one can find an ONB comprised of eigenvectors. In this case, one refers to it as A's *eigenbasis*, and the λ_i's appearing in the decomposition are exactly the eigenvalues of A.

Not every operator has an eigenbasis, e.g. the spin-$1/2$ *raising operator*

$$\sigma_+ = \frac{1}{2}(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

does not (why?). There's a theorem in functional analysis that essentially says that A has an eigendecomposition if and only if A commutes with its adjoint, i.e. $AA^\dagger = A^\dagger A$. (Though the case when there is a continuum of eigenvalues needs more attention, see section below).

The most important class of operators for which this holds are, of course, the self-adjoint ones $A = A^\dagger$. What is more, in this case, all eigenvalues are real. Indeed, $A|\psi\rangle = \lambda|\psi\rangle$ implies (taking $|\psi\rangle$ to be normalized without loss of generality)

$$\lambda = \langle\psi|A|\psi\rangle = \overline{\langle\psi|A^\dagger|\psi\rangle} = \overline{\langle\psi|A|\psi\rangle} = \bar{\lambda}.$$

Thus the self-adjoint operators are exactly those of the form

$$A = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|, \qquad \lambda_i \in \mathbb{R}, \{|\phi_i\rangle\}_i \text{ an ONB}.$$

A.1.7 Spectral decomposition (continuous case)

When working out eigendecompositions in infinite dimensions, we can run into trouble. Let's see what can go wrong.

First, consider the momentum operator $P = -i\frac{\mathrm{d}}{\mathrm{d}x}$. The eigenvalue equation is trivial to solve:

$$-i\psi' = \lambda\psi \quad \Leftrightarrow \quad \psi(x) = c\, e^{i\lambda x}.$$

Trouble is that these solutions are not square integrable:

$$\|\psi\|^2 = \int_{-\infty}^{\infty} |c|^2 \,\mathrm{d}x = \infty. \qquad \text{☹}$$

There are additional problems! For the position operator $(X\psi)(x) = x\psi(x)$, the eigenvalue equation

$$x\psi(x) = \lambda\psi(x) \qquad \forall x$$

is solved by

$$\psi(x) = \begin{cases} c & x = \lambda \\ 0 & \text{else} \end{cases},$$

which has norm $\|\psi\| = 0$. So it seems like there are no eigendecompositions for the two most important operators of QM. ☹☹

To get around the problem, we widen our domain of discourse by allowing for more general objects than just square-integrable functions. Let's first see how this formally solves our problem. Whether we are "allowed to do this", i.e. whether the formal construction will lead to inconsistencies, is something we'll worry about later.

Delta distributions

The *distribution* δ_y is a formal object whose inner product with a smooth function ψ is *defined* to be

$$\langle \delta_y | \psi \rangle = \int \bar{\delta}_y(x)\psi(x)\,\mathrm{d}x := \psi(y).$$

Then the expression

$$\int_x x|\delta_x\rangle\langle\delta_x|\,\mathrm{d}x$$

provides an eigendecomposition of the position operator X *in the sense* that for any pair of smooth functions ϕ, ψ we get the correct result

$$\langle\phi|\left(\int_x x|\delta_x\rangle\langle\delta_x|\,\mathrm{d}x\right)|\psi\rangle = \int x\langle\phi|\delta_x\rangle\langle\delta_x|\psi\rangle = \int x\bar{\phi}(x)\psi(x) = \langle\phi|X|\psi\rangle. \quad \text{(A.13)}$$

Likewise, we have the completeness relation

$$\int_x |\delta_x\rangle\langle\delta_x|\,\mathrm{d}x = \mathbb{1} \quad \text{(A.14)}$$

in the same sense, i.e.

$$\langle\phi|\left(\int_x |\delta_x\rangle\langle\delta_x|\,\mathrm{d}x\right)|\psi\rangle = \int\langle\phi|\delta_x\rangle\langle\delta_x|\psi\rangle = \int \bar{\phi}(x)\psi(x) = \langle\phi|\psi\rangle.$$

So *when integrated against smooth functions*, the expressions above behave just like an eigendecomposition should. We can work this that! ☺

Plane waves

We now turn to eigendecomposition of the momentum operator. For $k \in \mathbb{R}$, define the non-normalizable eigenfunction

$$\phi_k(x) = (2\pi)^{-1/2}e^{ikx}.$$

We claim that

$$\int_k |\phi_k\rangle\langle\phi_k|\,\mathrm{d}k = \mathbb{1}, \qquad \int_k \hbar k\,|\phi_k\rangle\langle\phi_k|\,\mathrm{d}k = P,$$

in the sense that for ψ, ϕ vanishing at infinity

$$\langle\phi|\left(\int_k |\phi_k\rangle\langle\phi_k|\,\mathrm{d}k\right)|\psi\rangle = \langle\phi|\psi\rangle, \quad \text{(A.15)}$$

$$\langle\phi|\left(\int_k \hbar k\,|\phi_k\rangle\langle\phi_k|\,\mathrm{d}k\right)|\psi\rangle = \langle\phi|P|\psi\rangle. \quad \text{(A.16)}$$

To see that this is true, note that the inner product with a function ψ

$$\langle\phi_k|\psi\rangle = (2\pi)^{-1/2}\int e^{-ikx}\psi(x)\,\mathrm{d}x = \tilde{\psi}(k)$$

gives the *Fourier transform* $\tilde{\psi}$ of ψ evaluated at k. Recall that the inverse transform is

$$(2\pi)^{-1/2}\int e^{ikx}\tilde{\psi}(k)\,\mathrm{d}k = \psi(x).$$

The completeness relation Eq. A.15 thus follows from

$$\langle\delta_x|\left(\int_k |\phi_k\rangle\langle\phi_k|\,\mathrm{d}k\right)|\psi\rangle = (2\pi)^{-1/2}\int_k e^{ikx}\tilde{\psi}(k)\,\mathrm{d}k = \psi(x).$$

Next, for ψ vanishing at infinity, integration by parts give

$$\begin{aligned}\hbar k\langle\phi_k|\psi\rangle &= (2\pi)^{-1/2}\int \hbar k e^{-ikx}\psi(x)\,\mathrm{d}x\\ &= (2\pi)^{-1/2}\int\left(i\hbar\frac{\mathrm{d}}{\mathrm{d}x}e^{-ikx}\right)\psi(x)\,\mathrm{d}x\\ &= (2\pi)^{-1/2}\int\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)\right)e^{-ikx}\,\mathrm{d}x = \langle\phi_k|P|\psi\rangle\end{aligned}$$

which implies Eq. (A.16):

$$\langle\phi|\left(\int_k \hbar k|\phi_k\rangle\langle\phi_k|\,\mathrm{d}k\right)|\psi\rangle = \langle\phi|\left(\int_k |\phi_k\rangle\langle\phi_k|\,\mathrm{d}k\right)P|\psi\rangle = \langle\phi|P|\psi\rangle. \quad ☺☺$$

General eigendecompositions

We can now sketch the way in which a general Hermitian operator A has an eigendecomposition. Consider all solutions to the eigenvalue equation

$$A|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle,$$

regardless of whether $|\psi_\lambda\rangle$ is square-integrable or not. Assume for simplicity that A is non-degenerate, i.e. that for every $\lambda\in\mathbb{R}$, there is at most one eigenfunction $|\psi_\lambda\rangle$. An eigenvalue $\lambda\in\mathbb{C}$ is called *discrete* if it is separated from all other eigenvalues by a finite distance. Let D be the set of discrete eigenvalues. Eigenvalues that are not discrete are called *continuous*. Collect them in another set C. Choose normalization such that

$$\begin{aligned}\langle\psi_{\lambda'}|\psi_\lambda\rangle &= \delta_{\lambda',\lambda} && \lambda\in D,\\ \langle\psi_{\lambda'}|\psi_\lambda\rangle &= \delta(\lambda'-\lambda) && \lambda\in C.\end{aligned}$$

Then we have the completeness relation and *spectral decomposition*

$$\begin{aligned}\mathbb{1} &= \int_C |\psi_\lambda\rangle\langle\psi_\lambda|\,\mathrm{d}\lambda + \sum_{\lambda\in D}|\psi_\lambda\rangle\langle\psi_\lambda|,\\ A &= \int_C \lambda|\psi_\lambda\rangle\langle\psi_\lambda|\,\mathrm{d}\lambda + \sum_{\lambda\in D}\lambda|\psi_\lambda\rangle\langle\psi_\lambda|.\end{aligned} \tag{A.17}$$

We can unify the treatment of the discrete and the continuous part. Define

$$\rho = \sum_{\lambda\in D}\delta_\lambda + I_C \quad \text{in terms of the } \textit{indicator function } I_C(\lambda') = \begin{cases}1 & \lambda'\in C\\ 0 & \text{else}\end{cases}.$$

The delta functions allow us to incorporate the sums in (A.17) into the integral:

$$A = \int \lambda |\psi_\lambda\rangle\langle\psi_\lambda| \rho(\lambda)\, \mathrm{d}\lambda. \tag{A.18}$$

The completeness relation generalizes like this: For any subset $S \subset \mathbb{R}$,

$$\int_S |\psi_\lambda\rangle\langle\psi_\lambda| \rho(\lambda)\, \mathrm{d}\lambda = P_S, \tag{A.19}$$

where P_S projects onto the space spanned by $\{|\psi_\lambda\rangle \,|\, \lambda \in S\}$. This looks somewhat like the formula

$$\int_S \rho(\lambda)\, \mathrm{d}\lambda = \mu(S)$$

for computing the measure of a set S given a density ρ. Therefore, the map $S \mapsto P_S$ is called a *projection-valued measure* and ρ the *density of states* (with respect to $\mathrm{d}\lambda$). The interpretation of ρ is particularly clear when applied to sets S that do not intersect the continuous part $S \cap C = \emptyset$. Then

$$\int_S \rho(\lambda)\, \mathrm{d}\lambda = |S \cap D|$$

equals the number of eigenvalues of A in S.

See Chapter 1 of *Quantum Mechanics* by Ballentine for a more careful, but not too technical exposition. A rigorous version is the *spectral theorem* of functional analysis.

A.1.8 More on delta distributions

How to think about distributions

Our account of general eigendecompositions and distributions is not mathematically rigorous. It *can* be made precise, but doing so takes a lecture in functional analysis (c.f. the *spectral theorem* and the theory of *distributions*). Given that we won't take the time here to go into more details, how should one deal with distributions that pop up in equations? Some strategies:

1. *Integrate against smooth functions that quickly vanish at infinity*. As in (A.13), even if the intermediate mathematical expression contains δ's, they should have all vanished after one has integrated the expression over smooth functions in order to extract physical quantities. The mathematically rigorous approach is based on this strategy, and it is the one we will have at the back of our heads in this document.

2. *Think of δ is an idealization of "highly concentrated"*. One can in principle replace $\delta_{\boldsymbol{x}}$ by functions $\delta_{\boldsymbol{x}}^{(\epsilon)}$ that are supported on an ϵ-ball around $\boldsymbol{x}$, where ϵ is much smaller than any relevant length scale. The final physical results should then only weakly depend on the actual choice of ϵ, and one should, in fact, be able to take a limit $\epsilon \to 0$. In this sense, the actual distribution is an idealization that allows one to directly obtain the limit, without first introducing an ϵ and eliminating it again in the end.

3. *Shut-up-and-calculate*. The reason δ's are so ubiquitous is that they work well as a computational tool. So in *reality*, people just use them whenever they would have used a Kronecker delta in a discrete analogue, and pretend that all algebraic manipulations that are valid for Kronecker deltas also extend to distributions. This *mostly* works.

Derivatives of delta functions

While the mathematicians look the other way, let's get adventurous and represent the momentum operator in *position* basis.

The *derivative of the delta function* $\delta'_y(x)$ is a formal object whose inner product with smooth functions vanishing at infinity is defined so that formally the rule of *integration by parts* holds:

$$\langle \delta'_y | \psi \rangle = \int \delta'_x(x)\psi(x)\,\mathrm{d}x := -\int \delta_x(x)\psi'(x)\,\mathrm{d}x = -\phi'(y)$$

and therefore

$$P = i\hbar \int |\delta_x\rangle\langle\delta'_x|\,\mathrm{d}x$$

is valid in the sense that for all smooth ψ, ϕ vanishing at infinity,

$$i\hbar \int \langle\psi|\delta_x\rangle\langle\delta'_x|\phi\rangle\,\mathrm{d}x = -i\hbar \int \bar{\psi}(x)\phi(x')\,\mathrm{d}x = \langle\psi|P|\phi\rangle. \tag{A.20}$$

Other expressions are

$$P = -i\hbar \int |\delta'_x\rangle\langle\delta_x|\,\mathrm{d}x = -i\hbar \int |\delta_x\rangle\partial_x\langle\delta_x|\,\mathrm{d}x = i\hbar \int\int |\delta_y\rangle\, \delta'_y(z)\, \langle\delta_z|\,\mathrm{d}y\,\mathrm{d}z.$$

The first holds because shifting the derivative to the bra means that in (A.20), ψ instead of ϕ gets differentiated, and to remedy that, we need to use integration by parts once more, which causes the change in sign. The second one holds because $\partial_x\delta_x(y) = \partial_x\delta(y-x) = -\delta'_x(y)$, so differentiating the index rather than the argument of the delta function also incurs a sign change. A similar argument verifies the third expression. This last one is interesting, because it is a formal generalization of (A.10) to continuous bases. It expresses P in terms of its "matrix elements"

$$\langle\delta_y|P|\delta_z\rangle = -i\hbar \int \delta_y(x)\delta'_z(x)\,\mathrm{d}x = i\hbar \int \delta'_y(x)\delta_z(x)\,\mathrm{d}x = i\hbar\delta'_y(z).$$

Using these formulas, the kinetic energy operator reads

$$\frac{P^2}{2m} = -\frac{\hbar^2}{2m}\int |\delta_x\rangle\partial_x^2\langle\delta_x|\,\mathrm{d}x = \frac{\hbar^2}{2m}\int |\delta'_x\rangle\langle\delta'_x|\,\mathrm{d}x.$$

A.1.9 Functions of operators

Let

$$A = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$$

be the eigendecomposition of an operator. Then

$$A^2 = \sum_{ij} \lambda_i\lambda_j |\phi_i\rangle \underbrace{\langle\phi_i|\phi_j\rangle}_{\delta_{ij}}\langle\phi_j| = \sum_i \lambda_i^2 |\phi_i\rangle\langle\phi_i|$$

and likewise

$$A^k = \cdots = \sum_i \lambda_i^k |\phi_i\rangle\langle\phi_i|.$$

Thus, if $p(x) = \sum_k c_k x^k$ is a polynomial, then

$$p(A) = \sum_k c_k A^k = \sum_i p(\lambda_i)|\phi_i\rangle\langle\phi_i|.$$

For an arbitrary function $f : \mathbb{C} \to \mathbb{C}$, one can thus consistently *define* its action on operators with an eigendecomposition as

$$f(A) := \sum_i f(\lambda_i)|\phi_i\rangle\langle\phi_i|.$$

(This convention is sometimes called the *spectral calculus*).

A.1.10 Unitary operators

Unitary operators are the Hilbert space analogue of orthogonal rotations in Euclidean vector spaces: Invertible linear operators that preserve inner products. Let's work out what that means.

The inner product between $U|\phi\rangle, U|\psi\rangle$ is $\langle\phi|U^\dagger U|\psi\rangle$ (recall Eq. (A.11)). Thus U preserves the inner product between any pair of operators if and only if

$$\langle\phi|U^\dagger U|\psi\rangle = \langle\phi|\psi\rangle \quad \forall\, \phi, \psi \in \mathcal{H}.$$

We thus define: An operator is *unitary* if it is invertible and fulfills $U^\dagger U = \mathbb{1}$.

One can work out that these characterizations are equivalent:

1. U is unitary.
2. U has a spectral decomposition of the form

$$U = \sum_i e^{i\phi_i}|\psi_i\rangle\langle\psi_i|, \qquad \phi_i \in \mathbb{R},$$

   i.e. all eigenvalues $\lambda_i = e^{i\phi_i}$ have absolute value equal to 1.
3. There is a Hermitian operator A such that $U = e^{iA}$ (in the sense of Sec. A.1.9).
4. U is such that $U^\dagger U = \mathbb{1}$ *and* $UU^\dagger = \mathbb{1}$ (in which case U is automatically invertible, so we do not have to list this as an extra requirement).
5. If $\{|e_i\rangle\}_i$ is an ONB, then so is $\{U|e_i\rangle\}_i$.

In quantum mechanics, unitary operators describe symmetries. The most important symmetry is of course time evolution! The Hermitian operator that generates time evolution $U(t)$ in the sense that $U(t) = e^{-it/\hbar H}$ (as in Point 3.) is nothing but $-1/\hbar$ times the Hamiltonian.

A.1.11 Projections

Recall (see Fig. A.1) that in $\mathbb{R}^d$ with Euclidean scalar product $(u, v) = \sum_i u_i v_i$, there is a one-one relation between

- Subspaces $V \subset \mathbb{R}^d$, and
- *orthogonal projections* P, i.e. linear maps fulfilling $P = P^t$, $P^2 = P$.

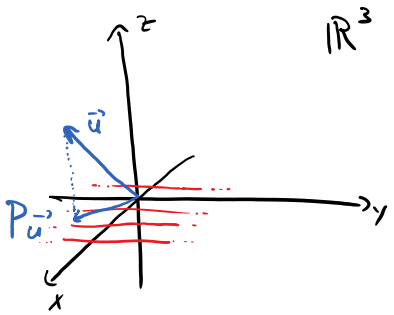


Figure A.1: Orthogonal projection of $\boldsymbol{u}$ onto the x-y-plane.

The Hilbert space analogue works like this: An operator P is a *projector* (or *projection*) if

1. $P = P^\dagger$, and
2. $P^2 = P$.

The first property means that P has a spectral decomposition. The second property then implies that the eigenvalues are elements of $\{0, 1\}$. Thus,

$$P = \sum_i |\psi_i\rangle\langle\psi_i|,$$

where the $\{|\psi_i\rangle\}$ form an ONB for the subspace $V \subset \mathcal{H}$ onto which P projects.

Examples:

- For every normalized vector $|\psi\rangle \in \mathcal{H}$, the outer product $P = |\psi\rangle\langle\psi|$ is the projection onto the one-dimensional subspace $V = \{z|\psi\rangle \,|\, z \in \mathbb{C}\}$.
- Define the *parity operator* Π on $\mathcal{H} = L^2(\mathbb{R})$ by

  $$\Pi|\delta_x\rangle = |\delta_{-x}\rangle, \quad \text{that is} \quad (\Pi\phi)(x) = \phi(-x).$$

  Then it's easy to see that $P_\pm = \frac{1}{2}(\mathbb{1} + \Pi)$ are projection operators onto the space of even and odd functions respectively (why?).

A.1.12 The trace

The *trace* of an operator is the sum over its eigenvalues. It can be expressed as

$$\operatorname{tr} A = \sum_i \langle i|A|i\rangle,$$

where the sum is over *any* ONB $\{|i\rangle\}_i$.

Some properties:

- Cyclic invariance:

$$\operatorname{tr} AB = \sum_{ij} \langle i|A|j\rangle\langle j|B|i\rangle = \sum_{ij} \langle j|B|i\rangle\langle i|A|j\rangle = \operatorname{tr} BA.$$

- Trace of outer products are inner products:

$$\operatorname{tr} |\alpha\rangle\langle\beta| = \sum_i \langle i|\alpha\rangle\langle\beta|i\rangle = \sum_i \langle\beta|i\rangle\langle i|\alpha\rangle = \langle\alpha|\beta\rangle.$$

A.1.13 Commuting operators

Assume that two operators A, B have a *joint eigenbasis* $\{|\psi_i\rangle\}$:

$$A|\psi_i\rangle = a_i|\psi_i\rangle, \qquad B|\psi_i\rangle = b_i|\psi_i\rangle.$$

Then

$$[A, B]|\psi_i\rangle = (AB - BA)|\psi_i\rangle = (a_i b_i - b_i a_i)|\psi_i\rangle = 0 \qquad \forall\, i.$$

so the operators commute.

Less obvious, but still true is that the converse also holds: If two operators commute, one can construct a joint eigenbasis. In fact, the conclusion also holds for any set of mutually commuting operators.

Warning: If two operators commute then it does *not* follow that *every* eigenbasis of one is also an eigenbasis of the other (why?).

A.2 More on Fourier transforms

Let's have a closer look at the n-dimensional Fourier basis $\phi_{\boldsymbol{k}}(\boldsymbol{x}) = (2\pi)^{-n/2} e^{i\boldsymbol{k}\boldsymbol{x}}$, for $\boldsymbol{k} \in \mathbb{R}^n$, and the associated transforms

$$\begin{aligned} \tilde{\psi}(\boldsymbol{k}) &:= \langle \boldsymbol{k}|\psi\rangle = (2\pi)^{-n/2} \int e^{-i\boldsymbol{k}\boldsymbol{x}} \psi(\boldsymbol{x}) \,\mathrm{d}^n\boldsymbol{x}, \\ \psi(\boldsymbol{x}) &:= \langle \boldsymbol{x}|\psi\rangle = (2\pi)^{-n/2} \int e^{i\boldsymbol{k}\boldsymbol{x}} \tilde{\psi}(\boldsymbol{k}) \,\mathrm{d}^n\boldsymbol{k}. \end{aligned} \tag{A.21}$$

A.2.1 Fourier transforms in finite regions

The Fourier basis for functions on $\mathbb{R}^n$ is continuous, which, as discussed above, comes with technical difficulties. Things are much easier for spaces of functions in finite regions.

Concretely, choose some length L and consider the box $B = [-L/2, L/2]^n$ with side length L centered at the origin. Let $L^2(B)$ be the space of functions defined on the region B with cyclic boundary conditions (i.e. functions take the same values on opposite faces of the box) and with inner products given by integrals over B only:

$$\langle \phi|\psi\rangle = \int_B \bar{\phi}(x)\psi(x) \,\mathrm{d}^n\boldsymbol{x}.$$

A plane wave $e^{i\boldsymbol{k}\boldsymbol{x}}$ complies with the boundary conditions if and only if every component k_i of the wave vector is an integer multiple of $\frac{2\pi}{L}$. Indeed, the discrete set of functions

$$\phi_{\boldsymbol{k}}(\boldsymbol{x}) := \frac{1}{L^{n/2}} e^{i\boldsymbol{k}\boldsymbol{x}}, \qquad k \in \frac{2\pi}{L}\mathbb{Z}^n,$$

forms an ONB for $L^2(B)$ and the formulas for the Fourier transform become

$$\begin{aligned} \tilde{\psi}(\boldsymbol{k}) &= \frac{1}{L^{n/2}} \int_B e^{-i\boldsymbol{k}\boldsymbol{x}} \psi(\boldsymbol{x}) \,\mathrm{d}^n\boldsymbol{x}, \\ \psi(\boldsymbol{x}) &= \frac{1}{L^{n/2}} \sum_{\boldsymbol{k}\in\frac{2\pi}{L}\mathbb{Z}^n} \tilde{\psi}(\boldsymbol{k}) e^{i\boldsymbol{k}\boldsymbol{x}}. \end{aligned} \tag{A.22}$$

Comparison with (A.21) shows that, formally, the transition between a finite and an unbounded volume Fourier transform is facilitated by the substitution

$$\frac{1}{\pi^{n/2}} \int_{\mathbb{R}^n} \mathrm{d}^n\boldsymbol{k} \quad \leftrightarrow \quad \frac{1}{L^{n/2}} \sum_{\boldsymbol{k}\in\frac{2\pi}{L}\mathbb{Z}^n} \tag{A.23}$$

Note the asymmetry in (A.22): Fourier transformation takes the compact domain B to the discrete domain $\frac{2\pi}{L}\mathbb{Z}^n$. We can of course reverse the interpretation of the two functions in (A.22). The formula then says that functions $\psi(\boldsymbol{x})$ defined on a lattice $\mathbb{Z}^n \frac{2\pi}{L}$ can be expanded in terms of plane waves $\phi_{\boldsymbol{k}}(\boldsymbol{x}) = \frac{1}{L^{n/2}} e^{-i\boldsymbol{k}\boldsymbol{x}}$ with wave vectors $\boldsymbol{k} \in B$. In this context, B is sometimes called the *Brillouin zone* and $\boldsymbol{k}$ the *crystal momentum* or *quasi-momentum*.

Of course, the universe isn't actually a finite box with cyclic boundary conditions... ...but we may as well pretend it were! Physics is local, so we can assume that all phenomena we are interested in take place in some box that is sufficiently large that the boundary does not affect the predictions we extract from the theory.

A.2.2 Translation symmetry

Fourier transforms are intimately connected to translation symmetry. Let $T_{\boldsymbol{a}}$ be the translation operator that shifts functions along the vector $\boldsymbol{a}$

$$(T_{\boldsymbol{a}}\psi)(\boldsymbol{x}) = \psi(\boldsymbol{x}-\boldsymbol{a}).$$

The Fourier basis diagonalizes translations:

$$\langle \boldsymbol{x}|T_{\boldsymbol{a}}|\phi_{\boldsymbol{k}}\rangle = e^{i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{a})} = e^{-i\boldsymbol{k}\boldsymbol{a}}\langle \boldsymbol{x}|\phi_{\boldsymbol{k}}\rangle \qquad \Rightarrow \qquad T_{\boldsymbol{a}} = \int e^{-i\boldsymbol{k}\boldsymbol{a}}|\phi_{\boldsymbol{k}}\rangle\langle\phi_{\boldsymbol{k}}|\,\mathrm{d}^n\boldsymbol{k}.$$

It is the unique common eigenbasis of all $T_{\boldsymbol{a}}$ (why?). Therefore, if A is any operator that commutes with translations

$$[T_{\boldsymbol{a}}, A] = 0 \qquad \forall\, \boldsymbol{a}, \tag{A.24}$$

then T must be diagonal in the Fourier basis, too. Explicitly, (A.24) implies that A is fully specified by its "first column"

$$f(\boldsymbol{z}) := \langle \delta_{\boldsymbol{z}}|A|\delta_0\rangle$$

in the sense that

$$\langle \delta_{\boldsymbol{x}}|A|\delta_{\boldsymbol{y}}\rangle = \langle \delta_{\boldsymbol{x}}|AT_{\boldsymbol{y}}T_{-\boldsymbol{y}}|\delta_{\boldsymbol{y}}\rangle = \langle \delta_{\boldsymbol{x}}|T_{\boldsymbol{y}}A|\delta_0\rangle = \langle \delta_{\boldsymbol{x}-\boldsymbol{y}}|A|\delta_0\rangle = f(\boldsymbol{x}-\boldsymbol{y}).$$

It then follows that the eigenvalues of A are proportional to the Fourier transform of f:

$$\begin{aligned}\langle \delta_{\boldsymbol{x}}|A|\phi_{\boldsymbol{k}}\rangle &= (2\pi)^{-n/2}\int \langle \delta_{\boldsymbol{x}}|A|\delta_{\boldsymbol{y}}\rangle e^{i\boldsymbol{k}\boldsymbol{y}}\,\mathrm{d}^n\boldsymbol{y} \\ &= e^{i\boldsymbol{k}\boldsymbol{x}}(2\pi)^{-n/2}\int f(\boldsymbol{x}-\boldsymbol{y})e^{-i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{y})}\,\mathrm{d}^n\boldsymbol{y} = (2\pi)^{n/2}\tilde{f}(\boldsymbol{k})\,\langle \delta_{\boldsymbol{x}}|\phi_k\rangle\end{aligned}$$

so that, summarizing,

$$A = (2\pi)^{n/2}\int \tilde{f}(\boldsymbol{k})\,|\phi_{\boldsymbol{k}}\rangle\langle\phi_{\boldsymbol{k}}|\,\mathrm{d}^n\boldsymbol{k}. \tag{A.25}$$

A.2.3 Fourier transform for functions depending on space and time

Common notation and sign conventions slightly differ when one coordinate has the interpretation of a time. Write $x = (t, \boldsymbol{x}) \in \mathbb{R}^n$, with t the "temporal" coordinate and $\boldsymbol{x} \in \mathbb{R}^{n-1}$ the "spatial" ones. Wave vectors are denoted by $k = (\omega, \boldsymbol{k})$. To compute inner products, we use the Minkowski form

$$\langle p, x\rangle = \omega t - \boldsymbol{k}\boldsymbol{x},$$

which (at least in the case of $n = 4$) determines the space-time metric in relativity. The commonly used basis of plane waves is

$$\phi_k(x) = (2\pi)^{-n/2}e^{-i\langle p,x\rangle} = (2\pi)^{-n/2}e^{-i\omega t+\boldsymbol{k}\boldsymbol{x}}$$

so that the forward and inverse Fourier transform are, respectively,

$$\begin{aligned}\tilde{\psi}(\omega,\boldsymbol{k}) &= (2\pi)^{-n/2}\int e^{i\omega t-i\boldsymbol{k}\boldsymbol{x}}\psi(t,\boldsymbol{x})\,\mathrm{d}t\,\mathrm{d}^n\boldsymbol{x}, \\ \psi(t,\boldsymbol{x}) &= (2\pi)^{-n/2}\int e^{-i\omega t+i\boldsymbol{k}\boldsymbol{x}}\tilde{\psi}(\omega,\boldsymbol{k})\,\mathrm{d}\omega\,\mathrm{d}^n\boldsymbol{k}.\end{aligned} \tag{A.26}$$

This convention extends to the case $n = 1$. That is, if a function ψ depends only on time, then its FT is taken to be $\tilde{\psi}(\omega) = \frac{1}{\sqrt{2\pi}}\int e^{i\omega t}\psi(t)\mathrm{d}t$, whereas if the single parameter is interpreted as a spatial coordinate or a generic parameter, then $\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}}\int e^{-ikx}\psi(x)\mathrm{d}x$.

A.2.4 Finite Fourier transform

Occasionally, we'll come across the finite Fourier transform. It is defined for functions $\psi : \mathbb{Z}_N \to \mathbb{C}$, where $\mathbb{Z}_N = \{0, \ldots, N-1\}$ with arithmetic done modulo N. The standard basis on this space is given by delta functions $\delta_x(y) = \delta_{xy}$ so that

$$|\psi\rangle = \sum_{x \in \mathbb{Z}_N} \psi(x) |\delta_x\rangle.$$

The Fourier basis is

$$|\phi_k\rangle = \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{Z}_N} e^{ikx} |\delta_x\rangle, \qquad k \in \frac{2\pi}{N} \mathbb{Z}_N.$$

The Fourier transform and its inverse thus take the form

$$\tilde{\psi}(k) = \langle \phi_k | \psi \rangle = \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{Z}_N} e^{-ikx} \psi(x), \quad \psi(x) = \langle \delta_x | \psi \rangle = \frac{1}{\sqrt{N}} \sum_{k \in \frac{2\pi}{N} \mathbb{Z}_N} e^{ikx} \tilde{\psi}(k).$$

The theory developed above can be easily translated to the finite case.

A.3 Some concrete systems

A.3.1 A single harmonic oscillator

Classical Hamiltonian mechanics

Let's first retrace the solution of a harmonic oscillator

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2.$$

in *classical* mechanics. Choose problem-adapted units for length and momentum:

$$\tilde{X} = \sqrt{\frac{m\omega}{\hbar}}X, \qquad \tilde{P} = \sqrt{\frac{1}{m\hbar\omega}}P \quad \Rightarrow \quad H = \frac{1}{2}\hbar\omega(\tilde{P}^2 + \tilde{X}^2).$$

Wait, what's $\hbar$ doing in a classical calculation? Well, it's convenient to work with dimensionless quantities $\tilde{X}, \tilde{P}$. But then $XP/(\tilde{X}\tilde{P})$ is a constant having the dimension of an action. There's no preferred scale of action in classical mechanics – but $\hbar$ does the job and facilitates the later transition to QM.

Next, introduce complex coordinates

$$a := \frac{1}{\sqrt{2}}(\tilde{X} + i\tilde{P}) \quad \Rightarrow \quad a^\dagger = \frac{1}{\sqrt{2}}(\tilde{X} - i\tilde{P}),$$

where we use the "dagger" superscript to denote complex conjugation. These complex coordinates may not have a direct physical interpretation, but they are easy to work with and we can recover the original position and momentum coordinates as

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}(a), \quad P = -i\sqrt{\frac{m\hbar\omega}{2}}(a - a^\dagger) = \sqrt{2m\hbar\omega}\,\mathrm{Im}(a).$$

The Poisson bracket $\{X, P\} = 1$ implies

$$\{a, a^\dagger\} = \frac{1}{2}\big(-i\{\tilde{X}, \tilde{P}\} + i\{\tilde{P}, \tilde{X}\}\big) = \frac{1}{i\hbar},$$

so the coordinate change $(X, P) \to (a, a^\dagger)$ is canonical up to the factor $1/(i\hbar)$. The Hamilton function reads in complex coordinates

$$H = \frac{1}{2}\hbar\omega(aa^\dagger + a^\dagger a) = \hbar\omega|a|^2. \tag{A.27}$$

and the equations of motion are (using standard properties of Poisson brackets)

$$\partial_t a = \{a, H\} = \hbar\omega\{a, a^\dagger a\} = \hbar\omega(a^\dagger\{a, a\} + \{a, a^\dagger\}a) = -i\omega a,$$

solved by $a(t) = a(0)e^{-i\omega t}$.

Quantum mechanics

Now assume that the X, P are not classical phase space coordinates, but instead position and momentum operators on $L^2(\mathbb{R})$. Replacing Poisson brackets $\{\cdot,\cdot\}$ by commutators $\frac{1}{i\hbar}[\cdot,\cdot]$ and complex conjugates by Hermitian conjugates, the above derivation goes through verbatim for the quantum case, up until Eq. (A.27). There, the fact that the $a_i^\dagger, a_i$ do not

commute means that we cannot simplify $\frac{1}{2}(a_i^\dagger a_i + a_i a_i^\dagger)$ as $|a_i|^2$. Using the commutation relations of the ladder operators instead, the Hamiltonian becomes

$$H = \hbar\omega\frac{1}{2}(a^\dagger a + aa^\dagger) = \hbar\omega\Big(a^\dagger a + \frac{1}{2}\Big).$$

Momentarily switching back to the position-space representation of the operators, one can easily see that there is a unique ground state $|0\rangle$, with wave function $\langle\tilde{x}|0\rangle = \pi^{-1/4}e^{-\tilde{x}^2/2}$. From the commutation relations of the ladder operators, it then follows that with

$$|n\rangle := \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle,$$

the set $\{|n\rangle\}_{n\geq 0}$ forms an ONB of the Hilbert space. It is indeed the eigenbasis of H:

$$a|n\rangle = \sqrt{n}|n-1\rangle \quad \Rightarrow \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad \Rightarrow \quad H|n\rangle = \hbar\omega\Big(n+\frac{1}{2}\Big)|n\rangle.$$

A.3.2 Normal modes

Classical Hamiltonian mechanics

In classical mechanics, consider the Hamilton function

$$H = \sum_k \frac{P_k^2}{2m} + \frac{1}{2}\sum_{kl} V_{kl}X_kX_l,$$

where the potential is given in terms of some coupling matrix $V = (V_{kl})$. Without loss of generality (why?), we can assume that V is symmetric and thus there exists an orthogonal O that diagonalizes V:

$$(OO^t)_{kl} = \delta_{kl}, \qquad (OVO^t)_{kl} = \delta_{kl}\lambda_k.$$

Instead of with the eigenvalues λ_k directly, we'll work with $\omega_k := \sqrt{\frac{\lambda_k}{m}}$. (The energy of the system is bounded below only if all $\lambda_k \geq 0$. Only this case is physically interesting, so don't worry about imaginary ω_k). The rows of O form an ortho-normal basis called the *normal modes* of the interaction. Expressing position and momentum in this basis gives the *normal coordinates*

$$\phi_k = \sum_l O_{kl}X_l, \quad \pi_k = \sum_l O_{kl}P_l \qquad \Rightarrow \qquad X_l = \sum_k O_{kl}\phi_k, \quad P_l = \sum_k O_{kl}\pi_k.$$

This transformation is canonical:

$$\{\phi_k, \pi_l\} = \sum_{ij} O_{ki}O_{jl}\underbrace{\{X_i, P_j\}}_{\delta_{ij}} = (OO^t)_{kl} = \delta_{kl}, \qquad \{\pi_k, \pi_l\} = \{\phi_k, \phi_l\} = 0.$$

Plugging in, the Hamiltonian decouples

$$H = \sum_k \Big(\frac{1}{2m}\pi_k^2 + \frac{1}{2}m\omega_k^2\phi_k^2\Big).$$

Each summand can now be treated as in Sec. A.3.1:

$$a_k := \sqrt{\frac{m\omega_k}{2\hbar}}\phi_k + i\sqrt{\frac{1}{2m\hbar\omega_k}}\pi_k \quad \Rightarrow \quad H = \sum_k \hbar\omega_k|a_k|^2,$$

solved by $a_k(t) = a_k(0)e^{-i\omega_k t}$. The transformation back to the original coordinates reads

$$X_l(t) = \sqrt{\frac{\hbar}{m}} \sum_k \frac{1}{\sqrt{2\omega_k}} (a_k e^{-i\omega_k t} O_{kl} + a_k^\dagger e^{i\omega_k t} O_{kl}),$$
$$P_l(t) = -i\sqrt{m\hbar} \sum_k \sqrt{\frac{\omega_k}{2}} (a_k e^{-i\omega_k t} O_{kl} - a_k^\dagger e^{i\omega_k t} O_{kl}).$$

In words, the configuration $X(t)$ of the particles is a linear combination of the normal modes, with the coefficients oscillating with the *eigenfrequencies* ω_k.

Some remarks:

- Even though V is real, it is sometimes convenient to choose the normal modes to be a set of complex eigenvectors. The most important example are translation-invariant couplings V, which are diagonal by suitable complex exponentials (Sec. A.2). The calculations above can be easily adapted to this case.
- With a bit more effort, one can see that *any* Hamiltonian that is (*i*) a quadratic expression in position and momenta and (*ii*) has a lower bound on the ground state energy can be diagonalized in a related way by a canonical change of coordinates. Check out *Williamson's Theorem* for details.

Quantum mechanics

As was done in the $n = 1$ case of Sec. A.3.1, assume now that the X_i, P_i are position and momentum operators on $L^2(\mathbb{R}^n)$. Then, again, the above applies verbatim to the quantum case, except that the Hamiltonian reads

$$H = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right).$$

In terms of normal coordinates

$$\sqrt{\frac{m\omega_k}{\hbar}} \phi_k |\tilde{\boldsymbol{x}}\rangle = \tilde{x}_k |\tilde{\boldsymbol{x}}\rangle,$$

the ground state wave function is

$$\langle \tilde{\boldsymbol{x}}|0\rangle = \prod_{i=1}^n \pi^{-1/4} e^{-\tilde{x}_i^2/2} = (4\pi)^{-n/4} e^{-\|\tilde{\boldsymbol{x}}\|^2/2}$$

and the eigenbasis arises from laddering (don't confuse the quantum numbers n_i with the number of n of degrees of freedom)

$$|n_1, \dots\rangle = \prod_i \frac{1}{\sqrt{n_i!}} (a_i^\dagger)^{n_i} |0\rangle \quad \Rightarrow \quad H|n_1, \dots\rangle = \sum_k \left(\hbar\omega_k n_k + \frac{1}{2}\right). \tag{A.28}$$

In principle, it is possible to work out the wave function $\langle \boldsymbol{x}|n_1, \dots\rangle$ in terms of the original coordinates. But this gets ugly pretty quickly, so one usually tries to extract physical predictions without having to go there.

A.3.3 Central potentials

For some constant κ, consider the Hamiltonian

$$H = \frac{\boldsymbol{P}^2}{2m} - \frac{\kappa}{\|\boldsymbol{X}\|}.$$

Because the Hamiltonian is rotationally invariant, we can find joint eigenvectors

$$\begin{aligned} H|E,l,m\rangle &= E|E,l,m\rangle, \\ L^2|E,l,m\rangle &= \hbar^2 l(l+1)|E,l,m\rangle, \\ L_z|E,l,m\rangle &= \hbar m|E,l,m\rangle. \end{aligned}$$

Negative energy solutions correspond to bound states. These energies are quantized:

$$E_n = -\frac{E_I}{n^2}, \qquad n \in \mathbb{N}, \qquad E_I = \frac{m\kappa^2}{2\hbar^2} \quad \text{(ionization energy)}.$$

The angular momentum quantum number l takes integer values between 0 and $n-1$ (as always, the magnetic quantum number m is an integer between $-l$ and l). In spherical coordinates, the eigenfunctions are of the form

$$\langle \boldsymbol{x}|n,l,m\rangle = Y_l^m(\theta,\phi)\, e^{-\frac{r}{a_0 n}} y_{nl}(r/a_0), \qquad a_0 = \frac{\hbar^2}{m\kappa} \quad \text{(Bohr radius)}$$

where $Y_l^m(\theta,\phi)$ are the spherical harmonics, and y_{nl} a polynomial of degree $n-1$ that one can explicitly work out in terms of generalized Laguerre polynomials. (Though roundabout nobody is thrilled by the prospect of "working things out in terms of generalized Laguerre polynomials" – and fortunately, one can often invoke more elegant arguments so that one doesn't have to).

Hydrogen atom, fine structure constant

The Hamiltonian for the electron of a hydrogen atom corresponds to $m = m_e$ (electron mass) and $\kappa = \frac{e^2}{4\pi\epsilon_0 r}$ (Coulomb repulsion). For atomic problems, it makes sense to express quantities in the natural units that can be formed by combining the constants $\hbar, m, c$, and the *fine structure constant*

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \simeq \frac{1}{137}.$$

In particular, the natural scales are mc^2 for energy; mc for momentum; $\frac{\hbar}{mc}$ for length; and $\frac{\hbar}{mc^2}$ for time.

Then the factor in front of the potential term reads $\kappa = \hbar c\alpha$, and we get $a_0 = \frac{\hbar}{mc}\frac{1}{\alpha}$ (Bohr radius), and $E_I = mc^2\frac{\alpha^2}{2}$ (ionization energy of hydrogen).

A.3.4 Fermionic oscillator

Let a be such that $a, a^\dagger$ fulfill the *canonical anti-commutation relations* (CAR)

$$[a, a^\dagger]_+ = 1, \quad [a,a]_+ = 2a^2 = 0, \quad [a^\dagger, a^\dagger]_+ = 2(a^\dagger)^2 = 0. \tag{A.29}$$

The Fermionic number operator $N = a^\dagger a$ is a projection:

$$N^2 = a^\dagger a a^\dagger a = a^\dagger(1 - a^\dagger a)a = N - (a^\dagger)^2 a^2 = N.$$

It follows that the Fermnionic occupation numbers can only be 0 and 1. Likewise,

$$aa^\dagger = 1 - a^\dagger a = 1 - N \tag{A.30}$$

is the complementary projection.

As in the Bosonic case, the Hamiltonian $H = \hbar\omega N$ gives rise to the Heisenberg-picture time evolution $a(t) = e^{-i\omega t}a(0)$. To see this, plug the expression into the Heisenberg equation of motion $i\hbar\partial_t a(t) = [a(t), H]$ and use

$$[a, a^\dagger a]_- = aa^\dagger a - a^\dagger aa = a(a^\dagger a) = a(1 - aa^\dagger) = a.$$

Using (A.30)

$$H' := H - \frac{\hbar\omega}{2}\mathbb{1} = \frac{\hbar\omega}{2}(a^\dagger a - aa^\dagger),$$

so the right hand side generates the same time evolution.

The simplest representation of the Fermionic oscillator is on $\mathcal{H} = \mathbb{C}^2$, with

$$a^\dagger = \frac{1}{2}(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \Rightarrow \quad a = \frac{1}{2}(\sigma_x - i\sigma_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Then the occupation number operator and the occupation number basis is

$$N = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and the Hamiltonian

$$H' = \frac{\hbar\omega}{2}\sigma_z = \frac{\hbar\omega}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

A.4 Perturbation theory

A.4.1 Fermi's golden rule

Here's the problem we want to solve. Consider a quantum system that starts in some *initial state* $|\psi(t = 0)\rangle = |i\rangle$. Choose a projection operator P_F onto a set of *final states* orthogonal to the initial state $P_F|i\rangle = 0$. The goal is to estimate the probability

$$P_{i\to F}(t) = \langle\psi(t)|P_F|\psi(t)\rangle$$

of finding the system in one of the final states when measured at time t.

We consider the situation where the Hamiltonian is of the form $H = H_0 + \lambda V$, where H_0 is sufficiently simple that the stationary Schrödinger equation can be solved

$$H_0|f\rangle = E_f|f\rangle,$$

and where λV is a "small" perturbation.

As is standard in perturbation theory, we assume (without much in the way of proof) that one can expand

$$|\psi(t)\rangle = \sum_{s=0}^{\infty} \lambda^s |\psi_s(t)\rangle$$

as a power series in λ and that low orders give meaningful answers. Separating the Schrödinger equation

$$i\hbar\partial_t\Big(\sum_s \lambda^s|\psi_s\rangle\Big) = (H_0 + \lambda V)\Big(\sum_s \lambda^s|\psi_s\rangle\Big)$$

by degrees of λ gives

$$\begin{aligned} i\hbar\partial_t|\psi_0\rangle &= H_0|\psi_0\rangle && \text{0th order} \\ i\hbar\partial_t|\psi_1\rangle &= H_0|\psi_1\rangle + V|\psi_0\rangle && \text{1st order} \\ &\vdots && \vdots \end{aligned}$$

With initial condition $|\psi(t=0)\rangle = |i\rangle$, the zeroth-order equation is solved by

$$|\psi_0(t)\rangle = e^{\frac{t}{i\hbar}E_i}|i\rangle.$$

Plugging this into the first-order one and projecting onto an eigenstate $|f\rangle$ gives

$$i\hbar\partial_t\langle f|\psi_1(t)\rangle = E_f\langle f|\psi_1(t)\rangle + e^{\frac{t}{i\hbar}E_i}\langle f|V|i\rangle$$

which is solved by

$$\langle f|\psi_1(t)\rangle = \langle f|V|i\rangle\frac{1-e^{\frac{1}{i\hbar}(E_i-E_f)t}}{E_f-E_i}e^{\frac{1}{i\hbar}E_f t} \qquad \text{for} \qquad E_f \neq E_i, \tag{A.31}$$

$$\langle f|\psi_1(t)\rangle = \langle f|V|i\rangle\frac{t}{i\hbar}e^{\frac{1}{i\hbar}E_f t} \qquad \text{for} \qquad E_f = E_i, f \neq i. \tag{A.32}$$

Using L'Hôspital's rule, one verifies that (A.31) tends to (A.32) for $E_f \to E_i$. In this sense, it suffices to work with (A.31) alone. Its square is

$$|\langle f|\psi(t)\rangle|^2 = 4|\langle f|V|i\rangle|^2\frac{\sin^2((E_i-E_f)\frac{t}{2\hbar})}{(E_i-E_f)^2} \qquad (i \neq f).$$

With $\epsilon = (E_f - E_i)$, $\tau = \frac{t}{2\hbar}$, the fraction is $\sin^2(\epsilon\tau)/\epsilon^2$, the square of the "sinc function" (Fig. A.2). It has a central peak of height τ, zeroes at $\epsilon = \pm\frac{\pi}{\tau}$, and shows oscillations of quadratically decreasing amplitude for $\epsilon \to \pm\infty$. It is known (by the Dirichlet integral) that the area under the curve is $\tau\pi$. Therefore, the family of functions $f_\tau(\epsilon) := \frac{1}{\pi\tau}\sin^2(\epsilon\tau)/\epsilon^2$, converges to a δ-function centered at 0 as $\tau \to \infty$.

Qualitatively, we can now describe which parameters enter the probability $P_{i\to F}(t)$. By the above, only states $|f\rangle$ with energy E_f in the range $E_i \pm \frac{2\pi\hbar}{t}$ pick up significant weight. For such states, the modulus squared is proportional to t and the squared coupling coefficient $|\langle f|V|i\rangle|^2$.

To get a more quantitative statement, let $\rho(f)$ be a measure such that

$$P_F = \int_F |f\rangle\langle f|\rho(f)\,\mathrm{d}f.$$

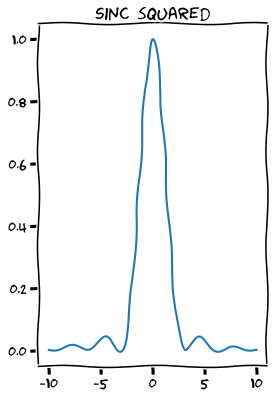


Figure A.2: Squared sinc function $\sin^2(\epsilon\tau)/\epsilon^2$. x axis in units of τ, y axis in units of $\frac{1}{\tau}$.

In other words, $\rho(f)$ is the "density of states", in the sense of Sec. A.1.7. Then

$$\langle\psi(t)|P_F|\psi(t)\rangle = \int_F |\langle f|\psi(t)\rangle|^2 \rho(f)\,\mathrm{d}f = \int_F 4|\langle f|V|i\rangle|^2 \frac{\sin^2\left((E_i-E_f)\frac{t}{2\hbar}\right)}{(E_i-E_f)^2}\rho(f)\,\mathrm{d}f.$$

Given the discussion above, optimistically,

$$\langle\psi(t)|P_F|\psi(t)\rangle \simeq t\,\frac{2\pi}{\hbar}\int_F |\langle f|V|i\rangle|^2\,\delta(E_i-E_f)\rho(f)\,\mathrm{d}f =: t\,\Gamma. \tag{A.33}$$

Let's suspend disbelief for a while and take (A.33) at face value. It is called *Fermi's Golden Rule*: The probability $P_{i\to F}(t)$ increases linearly, with slope Γ proportional to the squared coupling and the density of states, integrated over all final states with the right energy.

The "$\simeq$"–step in (A.33) involved quite the leap of faith. The squared-sinc-construction gives a delta function only in the limit of large times, but first-order perturbation theory is valid, at most, at short times. It's unclear whether there's an intermediate regime where both approximations simultaneously hold. Also, if the spectrum is discrete, the density of states $\rho(f)$ is itself a sum of delta functions (Sec. A.1.7), so that the integral has no obvious meaning. The cleanest (but not only) way around this issue is to restrict attention to energies E_i that lie in the continuous part of the spectrum of H_0. This frequently involves letting the "quantization region" L^3 go to ∞ (c.f. Sec. A.2). One could analyze the conditions for (A.33) to hold more carefully – but this is rarely done in practice. Experience has shown that the "golden" rule gives the right answer more often than one could have hoped, hence the moniker.

Appendix B

Miscellaneous Integrals

B.1 Gaussian and Fresnel integrals

Starting point is the famous formula due to Gauss

$$\int_{-\infty}^{\infty} e^{-x^2}\,\mathrm{d}x = \sqrt{\pi},$$

which can be obtained by evaluating its square in polar coordinates.

From there, we one finds the general form

$$\int_{-\infty}^{\infty} e^{-\alpha x^2+\beta x+\gamma}\,\mathrm{d}x = \sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}+\gamma} \tag{B.1}$$

which holds for all complex α, β, γ such that the integral converges: either $\mathrm{Re}[\alpha] > 0$; or $\mathrm{Re}[\alpha] = 0$ and $\mathrm{Re}[\beta] = 0$ (though in the latter case, the integral is not absolutely convergent, so it should be handled with care). In the formula, $\sqrt{\pi/\alpha}$ is the *principal square root*, defined to be the unique root with argument in $(-\pi, \pi]$. For real α, β, γ's, the above can be proven by completing the square and using the substitution rule. For complex coefficients, one has to use a suitable contour integration. The special case $\alpha = \mp i$ and $\beta = \gamma = 0$ is the complex asymptotic *Fresnel integral*

$$\int_{-\infty}^{\infty} e^{\pm i x^2}\,\mathrm{d}x = \sqrt{\pi} e^{\pm i\pi/4}. \tag{B.2}$$

The Gaussian integral (B.1) is taken over the entire real real line $x \to \pm\infty$, but in fact, is already close to its asymptotic value if the limits of the integral are large compared to $\sqrt{|\alpha|}$. This is obvious if α has a large real part (because the absolute value of the integrand is decaying with $e^{-\mathrm{Re}\,\alpha x^2}$). Imaginary parts of α also aid convergence, but for a more subtle reason: They cause the integrand to oscillate rapidly for large arguments, so that its contributions to the integral tend to cancel.

To visualize this effect, consider the non-asymptotic real Fresnel integrals

$$C(x) := \int_0^x \cos(t^2)\,\mathrm{d}t, \qquad S(x) := \int_0^x \sin(t^2)\,\mathrm{d}t.$$

Separating real and imaginary parts in (B.2) gives

$$\lim_{x\to\infty} C(x) = \lim_{x\to\infty} S(x) = \sqrt{\frac{\pi}{8}}. \tag{B.3}$$

Their convergence is shown in (Fig. B.1).

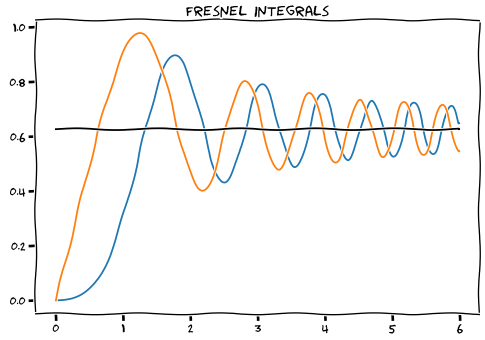


Figure B.1: The Fresnel integrals $C(x)$ (orange) and $S(s)$ (blue). The integral quickly converges towards its asymptotic value $\sqrt{\pi/8}$ (black line), with contributions of larger arguments canceling to the oscillating behavior of the integrand.

B.2 Some Fourier transforms

Rotationally invariant functions

Let $V(\boldsymbol{x}) = V(\|x\|)$ be a rotationally-invariant function in $\mathbb{R}^3$. Its Fourier transform $\tilde{V}(\boldsymbol{k})$ is computed most easily in the coordinate system $(r, \mu = \cos\theta, \phi)$ where (r, θ, ϕ) are spherical coordinates with polar vector parallel to $\boldsymbol{k}$. The volume element is

$$r^2 \sin\theta \, \mathrm{d}r \, \mathrm{d}\theta \, \mathrm{d}\phi = r^2 \, \mathrm{d}r \, \mathrm{d}\mu \, \mathrm{d}\phi \tag{B.4}$$

so that the Fourier transform

$$\begin{aligned}
\tilde{V}(\boldsymbol{k}) &= (2\pi)^{-3/2} \int e^{-i\boldsymbol{k}\boldsymbol{x}} V(r) \, \mathrm{d}^3\boldsymbol{x} \\
&= (2\pi)^{-1/2} \int_0^\infty \mathrm{d}r \, r^2 \, V(r) \int_{-1}^1 \mathrm{d}\mu \, e^{-ikr\mu} \\
&= (2\pi)^{-1/2} \int_0^\infty \mathrm{d}r \, r^2 V(r) \left[\frac{e^{-ikr\mu}}{-ikr} \right]_{\mu=-1}^1 \\
&= \frac{i}{(2\pi)^{1/2} k} \int_0^\infty \mathrm{d}r \, r V(r) \left(e^{-ikr} - e^{ikr} \right) \qquad \text{(B.5)} \\
&= \sqrt{\frac{2}{\pi}} \frac{1}{k} \int_0^\infty r V(r) \sin(kr) \, \mathrm{d}r \qquad \text{(B.6)}
\end{aligned}$$

reduces to a one-dimensional integral.

Appendix C

Function spaces and distributions

In this chapter, we take a more pedantic look at the function spaces that occur in QM. For simplicity of presentation, we'll mainly restrict attention to the one-dimensional case.

C.1 Square-integrable functions

What mathematical properties should a "wave function" $\psi : \mathbb{R} \to \mathbb{C}$ for a particle in one dimension have?

First, according to the Born interpretation, $p(x) := |\psi(x)|^2$ is the probability density describing the distribution of position measurement outcomes. For this interpretation to make sense, $\int |\psi(x)|^2 \, \mathrm{d}x$ must equal 1.

Next, physical predictions depend on ψ only through integrals. Integrals stay the same if the value of the integrand is changed on a set of measure zero. Therefore, two functions that agree *almost everywhere* (i.e. everywhere except on a set of measure zero) define the same physical state and should therefore be identified. For any function $\psi : \mathbb{R} \to \mathbb{C}$, write $[\psi]$ for the set of functions that agree with ψ almost everywhere.

These two conditions suggest that wave functions should belong to the space

$$L^2(\mathbb{R}) = \left\{ [\psi] \,\middle|\, \psi : \mathbb{R} \to \mathbb{C}, \int |\psi(x)|^2 \, \mathrm{d}x < \infty \right\}$$

of equivalence classes of *square-integrable* functions.[1] This is indeed the standard choice.

In practice, the identification of functions agreeing almost everywhere is usually left implicit. That is, $L^2(\mathbb{R})$ is called "the space of square-integrable functions" instead of the more precise "space of equivalence classes of square-integrable functions", and one writes $\psi \in L^2(\mathbb{R})$ as a short-hand for $[\psi] \in L^2(\mathbb{R})$. We will also follow this convention.

The *Cauchy-Schwarz inequality* says that

$$\left| \int \psi(x)^* \phi(x) \, \mathrm{d}x \right| \leq \left| \int \psi(x)^* \psi(x) \, \mathrm{d}x \right|^{1/2} \left| \int \phi(x)^* \phi(x) \, \mathrm{d}x \right|^{1/2}, \tag{C.1}$$

so that

$$\langle \psi | \phi \rangle := \int \psi(x)^* \phi(x) \, \mathrm{d}x$$

[1] See any textbook on analysis, e.g. Folland's *Modern analysis*, Chapter 2 for more details on integration theory. Just two comments on terminology: (1) All integrals in the theory of function spaces are to be understood in the sense of Lebesgue. (2) A function f is *integrable* if the integral $\int f$ exists *and* is finite. (So, counter-intuitively, "f is integrable" and "the integral of f exists" are different statements!)

is well-defined as a sesquilinear form $L^2(\mathbb{R}) \to \mathbb{C}$.

Remarks on the use of equivalence classes

Identifying functions that lead to the same physical predictions makes sense. Let's reiterate, though, that consequently elements of $L^2(\mathbb{R})$ aren't strictly speaking functions, but rather *equivalence classes* of functions. In particular, "the value $\psi(x)$" of an element $[\psi] \in L^2(\mathbb{R})$ at a point x is *not* a well-defined concept! This might be surprising, because in practice, we work with point-wise values $\psi(x)$ all the time. We get away with this because either: (1) We use $\psi(x)$ in a context (e.g. under an integral) where it does not matter which representative of the equivalence class has been chosen. Or, (2), there is an (implicit) convention that fixes a representative. For example, it is easy to see that every equivalence class contains at most one continuous function (Fig. **??**). Thus, if we agree to use continuous representatives whenever possible, there is no ambiguity for such classes.

The identification also makes the mathematical theory cleaner. For example, for a function $\psi : \mathbb{R} \to \mathbb{C}$, the integral $\|[\psi]\|^2 := \int |\psi(x)|^2 \, \mathrm{d}x$ vanishes if and only if ψ is supported on a set of measure zero, i.e. iff $[\psi] = [0]$. The implication $\|[\psi]\| = 0 \Rightarrow [\psi] = 0$ is part of the mathematical definition of a *norm*. It is frequently invoked in physics arguments: For example, in the algebraic treatment of the harmonic oscillator, one typically shows that $\|a|0\rangle\| = 0$ and concludes that $a|0\rangle = 0$, i.e. that the attempt to construct a negative-energy eigenstate by laddering leads to the 0 function.

C.1.1 Why go beyond L^2?

The choice of $L^2(\mathbb{R}^n)$ as the space of wave functions was physically well-motivated. But it turns out that for the purpose of doing some calculations, it is "too small", while for others, "too large".

Too small: $L^2(\mathbb{R})$ does not contain the eigenfunctions of some important operators. The eigenfunctions of the momentum operator are plane waves, which have norm ∞, and therefore do not belong to L^2. The eigenfunctions of the position operator are supported only on one single point. As elements of L^2, they are therefore equivalent to the function that is identically 0.

Too large: $L^2(\mathbb{R})$ contains elements for which important operators are undefined. For example, there are classes $[\psi] \in L^2(\mathbb{R})$ that do not contain any continuous representative, in which case the action of the momentum operator is not well-defined. For an example involving the position operator, take the function

$$\psi(x) = \frac{1}{\sqrt{\pi}(x+i)}. \tag{C.2}$$

Then

$$\int |\psi(x)|^2 \, \mathrm{d}x = \frac{1}{\pi} \int \frac{1}{x^2+1} \, \mathrm{d}x = \frac{1}{\pi} \left[\arctan(x)\right]_{-\infty}^{\infty} = 1,$$

so $\psi \in L^2(\mathbb{R})$. But (by comparison with $\int_a^\infty 1/x \, \mathrm{d}x = \infty$), one can easily see that the integral $\langle\psi|X^k|\psi\rangle = \int \frac{x^k}{x^2+1} \, \mathrm{d}x$ is infinite for even $k \in \mathbb{N}$ and undefined for odd $k \in \mathbb{N}$. In particular, $\|X\psi\|^2 = \langle\psi|X^2|\psi\rangle = \infty$, implying that $X\psi \notin L^2(\mathbb{R})$.

Figure C.1: *Rigged Hilbert spaces* are "rigged" in the sense of "fully equipped" (like Imperator Furiosa's *War Rig*, pictured above), not in the sense of "manipulated with the goal to deceive", like a loaded die. (OK, *maayybe* I was just looking for an excuse to include that picture in my lecture notes).

Discussion

Do these issues mean that $L^2(\mathbb{R})$ is not an appropriate mathematical model for the space of wave functions? Arguably not!

For the eigenfunction examples, note that infinitely extended or infinitely concentrated states are unphysical, so we cannot complain that the space $L^2(\mathbb{R})$, designed to model physical wave functions, does not contain them.

Now let's look at the function ψ defined in (C.2). The fact that $X\psi \notin L^2(\mathbb{R})$ does not mean that position measurements aren't well-defined. To the contrary, $p(x) = |\psi(x)|^2 = \frac{1}{\pi(x^2+1)}$ is a perfectly good probability density describing position measurement outcomes. It's just that none of the *moments* $\langle X^k \rangle$ (including the expectation value, $k = 1$) exist and are finite. But nobody ever promised us that all probability distributions can be characterized via moments, so there is no fundamental issue with this. Likewise, any $\psi \in L^2(\mathbb{R})$, even if it exhibits discontinuities, has a Fourier transform $\tilde{\psi}$, and thus a probability density $p(\hbar k) = |\tilde{\psi}(k)|^2$ over momentum measurement outcomes.

However, the discussion does suggest that for the purpose of doing calculations, it would be good to identify a "sandwich of spaces"

$$\Phi \subset L^2(\mathbb{R}) \subset \Phi', \tag{C.3}$$

where Φ is "sufficiently small" that all relevant operators are well-defined on it, and Φ' is "large enough" that it contains a complete set of eigenvectors for all relevant operators.

As we'll see, the spaces Φ and Φ' are usually constructed together. Elements of Φ are called *test functions* and those of Φ' *distributions*. Constellations as in (C.3) are studied as *Gelfand triples* or *rigged Hilbert spaces* (Fig. C.1)).

Which spaces of functions are the best choice for Φ, Φ' depends on the problem one wants to solve. An important set for quantum mechanics is *Schwartz space* (after Laurent Schwartz, not to be confused with Hermann Schwarz of Cauchy-Schwarz-inequality fame) for Φ and the associated space of *tempered distributions* for Φ'. We'll look at this case next, and briefly sketch the general theory in Sec. C.3.

> ***Remark***. The *domain* D of a function f is the set of mathematical objects on which f is defined. One equivalently says that "f is a function on D"... ...except in the theory of Hilbert spaces. We have seen above that P and X are not defined on certain elements of the Hilbert space $L^2(\mathbb{R})$ – their domains $D(P), D(X)$ are strictly smaller. But one still says that "X is the position operator on $L^2(\mathbb{R})$". In general, if T is any linear operator whose domain $D(T)$ is dense in a

Hilbert space $\mathcal{H}$, it is customary in functional analysis to call T a *linear operator on* $\mathcal{H}$. (Of course, physicists don't worry about such details at all).

C.2 Distributions

C.2.1 Schwartz space

The most important set of test functions Φ in QM is *Schwartz space* $\mathcal{S}$, the "smooth functions whose derivatives vanish rapidly":

$$\mathcal{S} = \Big\{ \phi \in C^\infty(\mathbb{R}) \,\Big|\, \forall \alpha, \beta \in \mathbb{N}_0 : \sup_x |x^\alpha \partial_x^\beta \phi(x)| < \infty \Big\}. \tag{C.4}$$

The condition $\phi \in C^\infty(\mathbb{R})$ means that elements of Schwartz space are infinitely differentiable; while the second condition says that ϕ and its derivatives vanish faster than any polynomial function as $|x| \to \infty$. It follows that $\mathcal{S}$ is invariant under P and X. It is also easy to see that any square-integrable function can be arbitrarily-well approximated by Schwartz-class functions, i.e. for every $\psi \in L^2(\mathbb{R})$ and every $\epsilon > 0$, there exists a $\phi \in \mathcal{S}$ such that $\|\psi - \phi\| \leq \epsilon$. (Technically: $\mathcal{S}$ is *dense* in $L^2(\mathbb{R})$ w.r.t. norm topology).

This already solves half of our problems: Because well-behaved functions are dense, there is little loss of generality in assuming that any wave function of physical interest lies in $\mathcal{S}$. One can then apply X and P without any issue.

C.2.2 Tempered distributions

Constructing the space that contains the generalized eigenvectors requires us to to take a little detour: We will first have to study *linear functionals* $\mathcal{S} \to \mathbb{C}$.

A function $u : \mathbb{R} \to \mathbb{C}$ is *locally integrable* if for any compact set $K \subset \mathbb{R}$,

$$\int_K |u(x)| \, \mathrm{d}x < \infty.$$

For example, continuous functions are locally integrable, whereas $1/x$ isn't (e.g. $\int_0^1 |\frac{1}{x}| \, \mathrm{d}x = \infty$). Now, for any locally integrable function u that grows at most polynomially as $|x| \to \infty$, and for any $l \in \mathbb{N}_0$, define a functional $T_{D^l u} : \mathcal{S} \to \mathbb{C}$ by

$$T_{D^l u}(\phi) := \int u(x)(-\partial_x)^l \phi(x) \, \mathrm{d}x. \tag{C.5}$$

(The notation $D^l u$ will be explained below). Then $T_{D^l u}$ is well-defined as a linear functional $\mathcal{S} \to \mathbb{C}$. That's because $\phi \in \mathcal{S}$ implies that $\partial_x^l \phi \in \mathcal{S}$ as well; local integrability of u and continuity of $\partial_x^l \phi$ implies that the integrand is locally integrable; and finally fact that $\partial_x^l \phi$ vanishes faster than any polynomial, together with the matching growth restriction on u, means that the integral remains finite as $|x| \to \infty$. A functional of this form is called a *tempered distribution*, and the space of all tempered distributions is denoted by $\mathcal{S}'$.

In contrast, note that $T_{D^l u}$ is rarely well-defined as a functional on $L^2(\mathbb{R})$. For one, elements $\psi \in L^2(\mathbb{R})$ aren't in general differentiable, and even if they are, they generally vanish too slowly for the integral to converge. So we see that $\mathcal{S}$, on account of being *smaller* than $L^2(\mathbb{R})$, allows for a *larger* set of linear functionals! Recall that we're out to find a set larger than $L^2(\mathbb{R})$, so this seems like a promising direction to explore. Let's look at some examples.

Plane waves: $T_{e^{ikx}}$ defines a linear functional on Schwartz space, but, because e^{ikx} is not normalizable, not on $L^2(\mathbb{R})$.

Delta functional: Let $\theta(x)$ be the step function that is 0 for $x < 0$ and 1 for $x \geq 0$. Then, using integration by parts,

$$T_{D\theta(x)}(\phi) = -\int \theta(x)\partial_x\phi(x)\,\mathrm{d}x = -\int_0^\infty \partial_x\phi(x)\,\mathrm{d}x = \phi(0). \tag{C.6}$$

The operation only makes sense for functions ϕ that are differentiable at 0 – so certainly for elements of $\mathcal{S}$, but not necessarily elements of $L^2(\mathbb{R})$.

"Bra vectors": For every $\psi \in L^2(\mathbb{R})$, the "bra" $\phi \mapsto \langle\psi|\phi\rangle = T_{\psi^*}$ defines a tempered distribution. (Indeed, every square-integrable function is also locally integrable. That's an easy consequence of the Cauchy-Schwarz inequality).

The principal value is important in the theory of partial differential equations, where one often wants to associate a distribution with the function $u(x) = \frac{1}{x}$ in some way. Unfortunately, $\frac{1}{x}$ is not locally integrable, and indeed, $\int \frac{\phi(x)}{x}\,\mathrm{d}x$ does not in general exist. But as we'll see, the *principal value*

$$\mathrm{pv}\left(\frac{1}{x}\right)(\phi) := \lim_{\epsilon\to 0^+}\int_{\mathbb{R}\setminus(-\epsilon,\epsilon)} \frac{\phi(x)}{x}\,\mathrm{d}x \tag{C.7}$$

is finite for all $\phi \in \mathcal{S}$ and, what is more, is given by the tempered distribution $T_{D\log|x|}(\phi)$. To see that this makes sense, we first need to convince ourselves that $\log|x|$, even though it diverges as $x \to 0$, is locally integrable. This follows from the fact that the anti-derivative of $\log|x|$ is $F(x) = x\log|x| - x + C$, which remains finite at the singularity: $\lim_{x\to 0} F(x) = C$. Therefore, $T_{D\log|x|}$ is indeed a tempered distribution. It remains to be shown that it evaluates to the principal value:

$$\begin{aligned}
T_{D\log|x|}(\phi) &= -\int \log|x|\,\phi'(x)\,\mathrm{d}x \\
&= \lim_{\epsilon\to 0^+}\left(-\int_{-\infty}^{-\epsilon}\log(-x)\,\phi'(x)\,\mathrm{d}x - \int_\epsilon^\infty \log x\,\phi'(x)\,\mathrm{d}x\right) \\
&= \lim_{\epsilon\to 0^+}\left(\int_{-\infty}^{-\epsilon}\frac{\phi(x)}{x}\,\mathrm{d}x - \phi(-\epsilon)\log\epsilon + \int_\epsilon^\infty \frac{\phi(x)}{x}\,\mathrm{d}x + \phi(\epsilon)\log\epsilon\right) \\
&= \mathrm{pv}\left(\frac{1}{x}\right)(\phi) + \lim_{\epsilon\to 0^+}\log(\epsilon)(\phi(\epsilon) - \phi(-\epsilon)) \\
&= \mathrm{pv}\left(\frac{1}{x}\right)(\phi) + 2\phi'(0)\underbrace{\lim_{\epsilon\to 0^+}\epsilon\log(\epsilon)}_{=0} = \mathrm{pv}\left(\frac{1}{x}\right)(\phi).
\end{aligned}$$

Powers of $1/r$ in higher dimensions: In contrast to the previous example, $u(\boldsymbol{x}) = \|\boldsymbol{x}\|^{-k}$ *is* locally integrable as a function on $\mathbb{R}^n$, as long as $n > k$. This can be seen by switching to n-dimensional spherical coordinates, where the volume element is proportional to r^{n-1}, which lifts the singularity at 0. The definition (C.5) is easily adapted to higher dimensions, and integrating against such a u thus defines a tempered distribution. Unsurprisingly, the case $k = 1, n = 3$ is important due to its relation to the Coulomb and the gravitational potential.

Regular distributions

Distributions of the form T_u (i.e. those that can be expressed without differentiating the argument before integrating) are called *regular*. For regular distributions, it is common

to use the same symbol for both the distribution $\mathcal{S} \to \mathbb{C}$ and for the function $\mathbb{R} \to \mathbb{C}$ defining it:

$$T(\phi) = \int T(x)\phi(x)\,\mathrm{d}x. \tag{C.8}$$

You might complain that such an overloading of notation is not a nice thing to do. And you'd be right. But things are about to get worse. Such a convention is even used for non-regular distributions!

Consider e.g. the delta distribution $\delta(\phi) = \phi(0)$ discussed above. It is not regular. (Because a hypothetical function giving rise to it would have to be zero everywhere except at $x = 0$ – but an integral over a function supported on only one point is zero). But, in analogy to (C.8), one still writes

$$\delta(\phi) = \int \delta(x)\phi(x)\,\mathrm{dx}.$$

The r.h.s. is *not* an integral and $\delta(x)$ *not* a function – the entire r.h.s. is to be read as an elaborate notation for $\delta(\phi)$. Whether this convention is genius (because it allows practitioners to work with distributions without having to learn the abstract theory) or horrific (because the *one* job of mathematics is to be rigorous and not to pretend that objects exist when in fact they don't) is a question that may be controversially debated.

C.2.3 Operations on distributions

Our goal is still to find generalized eigenvectors for X and P. These will turn out to be distributions. For that to even make sense, we have to define what it means for an operator to act on distributions.

Let A be any operator that maps $\mathcal{S}$ to $\mathcal{S}$. There is a unique operator A^t, the *transpose* of A, such that, for $\phi, \psi \in \mathcal{S}$,

$$\int (A\psi)(x)\phi(x)\,\mathrm{d}x = \int \psi(x)(A^t\phi)(x)\,\mathrm{d}x.$$

(This is the bilinear analogue of the definition of the adjoint for sesquilinear inner products). It directly follows that for regular distributions with $u \in \mathcal{S}$, $T_{Au}(\phi) = T_u(A^t\phi)$. Using the notation in (C.8), this means

$$(AT)(\phi) = T(A^t\phi). \tag{C.9}$$

We take Eq. (C.9) as the general definition for the action of an operator on distributions. In words: Operations on distributions are defined by shifting them onto the argument.

Derivatives of distributions

The most important application is the *differentiation operator* $(D\phi)(x) = \partial_x\phi(x)$. By partial integration, $D^t = -D$ from which we get

$$(DT_u)(\phi) = \int u(x)(-\partial_x^l)\phi(x)\,\mathrm{d}x = T_{Du}(\phi)$$

and, more generally, $D^l T_u = T_{D^l u}$ (which justifies the notation $D^l u$, as promised).

With these conventions in place, we can explain the notion of "derivative in the sense of distribution" that you will likely have come across before. Take for example the step

function θ. Seen as a function $\mathbb{R} \to \mathbb{C}$, it is not differentiable, due to the discontinuity at 0. But the distribution T_θ does have a derivative: $DT_\theta = \delta$, as computed in (C.6). Identifying θ with T_θ, this fact is often expressed as "$\partial_x \theta(x) = \delta(x)$ in the sense of distribution". Note that every locally integrable function is infinitely differentiable in the sense of distribution (by virtue of the elements of the test function space $\mathcal{S}$ having this property).

As an application, let's derive a famous identity that expresses the principal value in terms of a "side limit of a deformed version of $1/x$", namely

$$\lim_{\epsilon \to 0^+} \frac{1}{x \pm i\epsilon} = \mathrm{pv}\left(\frac{1}{x}\right) \mp i\pi\delta. \tag{C.10}$$

First, recall that the principal complex logarithm

$$\mathrm{Log}(x + iy) = \log \sqrt{x^2 + y^2} + i \arctan \frac{x}{y}$$

is an analytic continuation of the logarithm to the complex numbers, except for a branch cut on the negative real axis (Fig. **??**). It follows that

$$\lim_{\epsilon \to 0^+} \mathrm{Log}(x \pm i\epsilon) = \log |x| \mp i\pi\theta(x)$$

which immediately implies (C.10) by differentiating both sides in the sense of distribution.

Generalized eigenvectors

We say that a distribution T is a *generalized eigenvector* of an operator $A : \mathcal{S} \to \mathcal{S}$ if

$$A\,T = \lambda\,T.$$

Plane waves are therefore eigenvectors of the differentiation operator D or the momentum operator $P = -iD$:

$$D\,T_{e^{ikx}} = T_{\partial_x e^{ikx}} = T_{ike^{ikx}} = ik\,T_{e^{ikx}}, \qquad P\,T_{e^{ikx}} = k\,T_{e^{ikx}}.$$

Likewise, if $\delta_a = \partial_x \theta(x - a) : \phi \mapsto \phi(a)$ is the delta distribution at $a \in \mathbb{R}$, then

$$(X\,\delta_a)(\phi) = \delta_a(X\phi) = a\phi(a) = a\,\delta_a(\pi) \quad \Rightarrow \quad X\,\delta_a = a\,\delta_a.$$

So, with all these preparations in the bag, it was pretty easy to identify the generalized eigenvectors!

Interface conditions for piece-wise continuous potentials. In one dimension, the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x) - E\right)\psi(x) = 0 \tag{C.11}$$

is an ordinary differential equation. The Picard-Lindelöf theorem says that if V is Lipschitz continuous, then the ODE can be solved.

A staple of introductory QM lectures are potentials that are only piece-wise continuous. In this case, there aren't necessarily solutions to (C.11) in the ordinary sense. Here, we'll work out under which conditions one can stitch piece-wise solutions together to get a generalized eigenvector of the Hamiltonian.

We treat the case where (C.11) has ordinary solutions $\psi_-(x)$ on $(-\infty, 0)$ and $\psi_+(x)$ on $(0, \infty)$. Assume that both solutions and their first derivatives are continuous and bounded around 0, and can thus be extended to 0. We also require that V is bounded around 0. Then

$$\psi(x) := \begin{cases} \psi_-(x) & x \leq 0, \\ \psi_+(x) & x > 0 \end{cases}$$

is a generalized eigenvector if and only if, for all test functions ϕ,

$$\int_{-\infty}^{\infty} \phi(x) \left(-\frac{\hbar^2}{2m} \partial_x^2 + V(x) - E \right) \psi(x) \, \mathrm{d}x = 0.$$

Because ψ is an ordinary solution away from zero, the integral is equal to

$$\lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} \phi(x) \left(\frac{-\hbar^2}{2m} \partial_x^2 + V(x) - E \right) \psi(x) \, \mathrm{d}x = \frac{-\hbar^2}{2m} \lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} \phi(x) \partial_x^2 \psi(x) \, \mathrm{d}x,$$

where we have used that $(V(x) - E)$ does not contribute to the integral in the limit, as ϕ, ψ, and V are bounded around 0. Integrating by parts,

$$\begin{aligned} \lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} \phi(x) \psi''(x) \, \mathrm{d}x =& \phi(0) \big(\psi'_+(0) - \psi'_-(0) \big) - \lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} \phi'(x) \psi'(x) \, \mathrm{d}x \\ =& \phi(0) \big(\psi'_+(0) - \psi'_-(0) \big) - \phi'(0) \big(\psi_+(0) - \psi_-(0) \big), \end{aligned}$$

which vanishes for all ϕ if and only if the *interface conditions*

$$\psi_+(0) = \psi_-(0) \quad \text{and} \quad \psi'_+(0) = \psi'_-(0) \tag{C.12}$$

are met. Notably, these do not imply that ψ is twice differentiable, which would be required for ordinary solutions to (C.11).

Fourier transforms of tempered distributions

Because the Fourier transform exchanges X and P, the characterization (C.4) of $\mathcal{S}$, and hence the space itself, is invariant under Fourier transforms. Applying the general scheme (C.9), the Fourier transform of a tempered distribution T is $(\mathcal{F}T) : \phi \mapsto T(\mathcal{F}^t \phi)$.

To get more explicit formulas, first note that $\mathcal{F}^t = \mathcal{F}$:

$$\int (\mathcal{F}\psi)(k) \phi(k) \, \mathrm{d}k = \frac{1}{\sqrt{2\pi}} \int \int e^{-ikx} \psi(x) \phi(k) \, \mathrm{d}x \, \mathrm{d}k = \int \psi(x) (\mathcal{F}\phi)(x) \, \mathrm{d}x.$$

Thus, using the shorthand "tilde notation" for the Fourier transform,

$$\tilde{T}(\phi) = T(\tilde{\phi}).$$

Delta distribution. For δ, compute

$$\tilde{\delta}(\phi) = \delta(\tilde{\phi}) = \tilde{\phi}(0) = \int \frac{1}{\sqrt{2\pi}} \phi(x) \, \mathrm{d}x = T_{\frac{1}{\sqrt{2\pi}}}(\phi), \tag{C.13}$$

that is, the FT of δ is a regular distribution, arising from the constant function

$$\tilde{\delta}(k) = \frac{1}{\sqrt{2\pi}}. \tag{C.14}$$

One could be tempted to use the following formal calculation to arrive at the same conclusion:

$$\hat{\delta}(k) = \text{“}\frac{1}{\sqrt{2\pi}}\int e^{-ikx}\delta(x)\,\mathrm{d}x\text{”} = \frac{1}{\sqrt{2\pi}}.$$

But, unlike, (C.13), this is *not* a rigorous argument given our development of the theory so far! That's because we have defined $\delta(\phi)$ only for $\phi \in \mathcal{S}$, but e^{-ikx} is most definitely not an element of Schwartz space. The integral is therefore only heuristically defined. One can sometimes make sense of products of distributions – but the issue is subtle and we will not pursue it here.

Constant functions. The constant function $\underline{1}(x) = 1$ does not have a Fourier transform in the ordinary sense. For one, the integral $(2\pi)^{-1}\int \mathrm{d}x$ that would define $\tilde{\underline{1}}(0)$ is infinite. However, because $T_{\underline{1}}$ defines a tempered distribution, it does have a FT. Slightly abusing language once again, we call it the FT of $\underline{1}$ (in the sense of distribution).

We can find it by expressing $\mathcal{F}^{-1}$ in terms of $\mathcal{F}$ and applying it to (C.14). To this end, let Π be the *parity operator*, which mirrors functions about the origin: $(\Pi\phi)(x) = \phi(-x)$. Then it is easy to see that $\mathcal{F}^\dagger = \Pi\mathcal{F}^t$ and hence unitarity of $\mathcal{F}$ implies

$$(\Pi\mathcal{F})\mathcal{F} = \mathcal{F}^\dagger\mathcal{F} = \mathbb{1} \quad \Rightarrow \quad \mathcal{F}^{-1} = \Pi\mathcal{F}. \tag{C.15}$$

Applying this to (C.14) gives

$$\mathcal{F}\left(\underline{1}\right) = \sqrt{2\pi}\delta.$$

The principal value. From an easy contour integration, the FT of $1/(x+i\epsilon)$ is

$$\frac{1}{\sqrt{2\pi}}\int \frac{1}{x+i\epsilon}e^{-ikx}\,\mathrm{d}x = -i\sqrt{2\pi}e^{-\epsilon k}\theta(k) \to -i\sqrt{2\pi}\theta(k) \qquad (\epsilon \to 0^+).$$

Using (C.10), we then find that the FT of the principal value is a regular distribution:

$$\begin{aligned}\big(\mathcal{F}\ \mathrm{pv}(1/x)\big)(k) &= \lim_{\epsilon\to 0^+}\mathcal{F}\left(\frac{1}{x+i\epsilon}\right)(k) + i\pi\mathcal{F}(\delta)(k) \\ &= i\sqrt{\frac{\pi}{2}}\left(-2\theta(k)+1\right) = -i\sqrt{\frac{\pi}{2}}\,\mathrm{sign}(k).\end{aligned} \tag{C.16}$$

Combining this result with (C.15) gives further transforms of common distributions:

$$\left(\mathcal{F}\,\mathrm{sign}\right)(k) = i\sqrt{\frac{2}{\pi}}\,\mathrm{pv}(1/k) \tag{C.17}$$

$$\left(\mathcal{F}\theta\right)(k) = \frac{1}{2}\mathcal{F}\left(\mathrm{sign}+1\right)(k) = i\frac{1}{\sqrt{2\pi}}\left(\mathrm{pv}(1/k) - i\pi\delta\right). \tag{C.18}$$

Coulomb and Yukawa potentials. Up to constants, the Coulomb potential is $u(\boldsymbol{x}) = -\frac{1}{\|\boldsymbol{x}\|}$ in $\mathbb{R}^3$. Just like the constant function treated above, it does not have an ordinary Fourier transform. For example, $\tilde{u}(0)$ would be given by

$$-(2\pi)^{-3/2}\int \frac{1}{\|\boldsymbol{x}\|}\,\mathrm{d}^3\boldsymbol{x} = -2(2\pi)^{-1/2}\int r\,\mathrm{d}r = -\infty. \tag{C.19}$$

But as discussed in Sec. C.2.2, $u(\boldsymbol{x})$ defines a regular distribution whose Fourier transform turns out to be regular again, given by

$$\tilde{u}(\boldsymbol{k}) = -\sqrt{\frac{2}{\pi}}\frac{1}{\|\boldsymbol{k}\|^2}. \tag{C.20}$$

Here's how to find (C.20). Express

$$T_u(\tilde{\phi}) = -\int \frac{\tilde{\phi}(\boldsymbol{k})}{\|\boldsymbol{k}\|}\,\mathrm{d}^3\boldsymbol{k} = -\lim_{s\to 0^+}\int \frac{e^{-s\|\boldsymbol{k}\|}}{\|\boldsymbol{k}\|}\tilde{\phi}(\boldsymbol{k})\,\mathrm{d}^3\boldsymbol{k}. \tag{C.21}$$

as a limit of integrals involving the "regularizing" factor $e^{-s\|\boldsymbol{k}\|}$.

This is valid, because the integral, interpreted as a function of $s \in [0,\infty)$, is continuous at 0. In fact, it is even differentiable:

$$-\partial_s|_0 \int \frac{e^{-s\|\boldsymbol{k}\|}}{\|\boldsymbol{k}\|}\tilde{\phi}(\boldsymbol{k})\,\mathrm{d}^3\boldsymbol{k} = \int \tilde{\phi}(\boldsymbol{k})\,\mathrm{d}^3\boldsymbol{k}, \tag{C.22}$$

which is finite for $\tilde{\phi} \in \mathcal{S}$. (Note that the same regularization does *not* work for the integral in (C.19), which formally corresponds to the case $\tilde{\phi}(\boldsymbol{k}) = 1$. Of course, the constant function is not an element of Schwartz space, and indeed, this choice would cause (C.22) to diverge).

Plugging in the definition of the FT and exchanging integrals,

$$T_u(\tilde{\phi}) = \lim_{s\to 0}\int \left(-(2\pi)^{-3/2}\int \frac{e^{-s\|\boldsymbol{k}\|}}{\|\boldsymbol{k}\|}e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\phi(\boldsymbol{x})\mathrm{d}^3\boldsymbol{k}\right)\mathrm{d}^3\boldsymbol{x}.$$

The expression in parentheses is the FT of

$$V(\boldsymbol{x}) = -\frac{1}{\|\boldsymbol{x}\|}e^{-s\|\boldsymbol{x}\|}$$

which, up to constants, is known as the *Yukawa potential*. Its Fourier transform follows from the general formula (B.5) for rotationally-invariant functions in terms of $k = \|\boldsymbol{k}\|$:

$$\tilde{V}(\boldsymbol{k}) = \frac{i}{(2\pi)^{1/2}k}\int_0^\infty \left(e^{-sr-ikr} - e^{-sr+ikr}\right)\mathrm{d}r.$$

The one-dimensional integral can immediately be solved as

$$-\left[\frac{e^{r(-s-ik)}}{-s-ik}\right]_0^\infty + \left[\frac{e^{r(-s+ik)}}{-s+ik}\right]_0^\infty = -\frac{1}{-s-ik} + \frac{1}{-s+ik} = -\frac{2ik}{s^2+k^2}.$$

Collecting constants, we get the FT of the Yukawa potential, which gives (C.20) as $s \to 0$:

$$\tilde{V}(\boldsymbol{k}) = -\sqrt{\frac{2}{\pi}}\frac{1}{s^2+k^2}. \tag{C.23}$$

Products and tensor products

If T is a tempered distribution, and v a smooth function that grows at most polynomially as $|x| \to \infty$, then the product vT between v and T is the tempered distribution

$$vT : \phi \mapsto T(v\phi). \tag{C.24}$$

The product between a smooth function and a distribution behaves mostly like the product between functions. In particular, if $T = T_u$ is regular, then $vT_u = T_{uv}$.

However, one cannot extend (C.24) to products between arbitrary distributions, while retaining the basic properties of "multiplication". For example

$$\begin{aligned} & \delta\, x = 0 && \text{by (C.24)} \\ \Rightarrow \quad & (\delta\, x)\,\mathrm{pv}(1/x) = 0\,\mathrm{pv}(1/x) = 0 && \text{by above and (C.24)} \end{aligned}$$

$$\begin{aligned} & x\,\mathrm{pv}(1/x) = 1 && \text{by (C.24)} \\ \Rightarrow \quad & \delta\,(x\,\mathrm{pv}(1/x)) = \delta\, 1 = \delta && \text{by above and (C.24)} \end{aligned}$$

so there is no associative way to assign a meaning to "$\delta\, x\,\mathrm{pv}(1/x)$".

Tensor products between distributions are perfectly well-defined, though. If S, T are distributions, then $S \otimes T$ is the bilinear form that sends $\phi, \psi \in \mathcal{S}$ to $S(\phi)T(\psi)$.

Using the fictional function notation $T(x)$ for distributions T (as in (C.8)), the situation can be summarized as: "$T(x)S(x)$ makes no sense, but $T(x)S(y)$ is unremarkable – just integrate against *two* test functions".

A propose bilinear forms. Take any distribution K on test functions on $\mathbb{R}^2$, not necessarily a tensor product. If ϕ, ψ are test functions on $\mathbb{R}$, then *their* tensor product $(\phi \otimes \psi)(x, y) = \phi(x)\psi(y)$ can be paired with K. This way, K, too, defines a bilinear form:

$$\phi, \psi \mapsto K(\phi \otimes \psi) \quad \text{also written as} \quad K(\phi \otimes \psi) = \int K(x, y)\phi(x)\psi(y)\,\mathrm{d}x\,\mathrm{d}y.$$

One says that K is the *integral kernel* of the bilinear map.

This definition can be extended straight-forwardly to multilinear or sesquilinear functions. The sesquilinear case is frequently used in quantum mechanics – c.f. Eq. (A.20).

C.3 Topological aspects, more pedantry, and generalizations

Our definition of tempered distributions in Eq. (C.5) was *constructive*: We showed how to build distributions concretely given a function u and derivatives ∂_x^l. The mathematical theory is usually formulated *axiomatically*. Distributions are defined indirectly, as linear functionals on test function spaces, subject to some abstract properties. These properties are phrased in the language of point set topology. In this section, we briefly introduce this more abstract point of view.

Topological spaces

Consider a set X. A *topology* on X is a rule that allows us to decide when a sequence $x_k : \mathbb{N} \to X$ converges to an element $x \in X$.

As a first example, assume that X is a vector space equipped with a norm $\|\cdot\|$. This covers an extremely wide range of spaces, from $X = \mathbb{R}$, the real numbers with norm $\|x\| = |x|$ the absolute value, to $X = L^2(\mathbb{R})$ with norm $\|x\| = \langle x|x\rangle^{1/2}$ derived from the inner product. We say that a sequence x_k *converges in norm topology* to x,

$$x_k \to x, \qquad \text{if} \qquad \lim_{k\to\infty} \|x_k - x\| = 0. \tag{C.25}$$

We'll use these concepts to give very general definitions of *continuity* and *completeness*.

Figure C.2: *Sequence continuity* is equivalent to the more familiar "ϵ-δ-definition" of continuity for functions $f : \mathbb{R} \to \mathbb{R}$. It is more general, though, and can also be applied to spaces whose topologies do not derive from a distance measure.

Continuity

A function f between two topological spaces is *continuous* if it maps convergent sequences to convergent sequences (Fig. C.2), i.e. if

$$x_k \to x \qquad \Rightarrow \qquad f(x_k) \to f(x).$$

Example (important!): *If $\psi \in L^2(\mathbb{R})$, then the linear functional $\langle\psi|$ is continuous.*
The proof reduces to the Cauchy-Schwarz inequality. If $\lim_{k\to\infty} \|\phi_k - \phi\| = 0$, then

$$\big|\langle\psi|\phi_k\rangle - \langle\psi|\phi\rangle\big| = \big|\langle\psi|(|\phi_k\rangle - |\phi\rangle)\big| \leq \|\psi\|^{1/2} \big\|\phi_k - \phi\big\|^{1/2} \to 0 \quad (k \to \infty).$$

Completeness and Hilbert spaces

Now for *completeness*. A sequence x_k is *Cauchy* if "its elements eventually become arbitrarily close" in the sense that

$$\forall\, \epsilon > 0,\ \exists\, n \in \mathbb{N} \text{ such that } \forall\, k, l > n, \text{ it holds that } \|x_k - x_l\| \leq \epsilon.$$

A space X is *complete* if every Cauchy sequence converges to an element of X.

As an example of a Cauchy sequence, let x_k be the approximation of $\sqrt{2}$ to k decimal places. This example shows that the rational numbers are not complete: There is no $q \in \mathbb{Q}$ such that $x_k \to q$ (for then q would have to equal $\sqrt{2}$, which, famously, is not rational).

In the mathematical literature, a *Hilbert space* is defined as a

- complex vector space,
- with a sesquilinear inner product $\langle\cdot|\cdot\rangle$,
- that is *complete* with respect to the norm derived from the inner product.

The final condition is often glossed over in physics presentations. It is important, though. For one, it means that series like

$$|\psi(t)\rangle = \sum_{k=0}^{\infty} \frac{1}{k!}(itH)^k|\psi(0)\rangle := \lim_{K\to\infty} \sum_{k=0}^{K} \frac{1}{k!}(itH)^k|\psi(0)\rangle,$$

used ubiquitously, are actually well-defined. Another reason is that the equivalence of "kets" and "bras" requires this property: The set of continuous linear functionals on a Hilbert space $\mathcal{H}$ is denoted by $\mathcal{H}'$. If $|\psi\rangle \in \mathcal{H}$, then we've shown above that $\langle\psi|$ is continuous, i.e. an element of $\mathcal{H}'$. The *Riesz representation theorem* says that the converse is also true: Every continuous linear functional of a Hilbert space is given by some "bra vector".

One can show that $L^2(\mathbb{R})$ is complete, i.e. actually a Hilbert space.

Contrast this with Schwartz space $\mathcal{S}$. It, too is a complex vector space with the same sesquilinear inner product as $L^2(\mathbb{R})$. But it is not complete in norm topology and hence no Hilbert space. The argument works just like the $\sqrt{2}$-example above. Because $\mathcal{S}$ is dense in $L^2(\mathbb{R})$, for every $\psi \in L^2(\mathbb{R})$, there exists a sequence $\phi_k : \mathbb{N} \to \mathcal{S}$ converging to ψ in norm. Thus, if $\psi \notin \mathcal{S}$, the sequence ϕ_k has no limit point in $\mathcal{S}$.

Topology on Schwartz space

Return to Schwartz space $\mathcal{S}$. Because it is a subspace of $L^2(\mathbb{R})$, we can use the norm topology also for $\mathcal{S}$. However, there's a second, important, topology on that space. For $\alpha, \beta \in \mathbb{N}_0$, define the (semi)-norms

$$\|\phi\|_{\alpha,\beta} := \sup_{x\in\mathbb{R}} |X^\alpha \partial_\beta \psi(x)|.$$

A sequence $\phi_k : \mathbb{N} \to \mathcal{S}$ converges with respect to this family of semi-norms,

$$\phi_k \underset{\mathcal{S}}{\to} \phi, \qquad \text{if} \qquad \lim_{k\to\infty} \|\phi - \phi_k\|_{\alpha,\beta} = 0 \quad \forall \alpha, \beta \in \mathbb{N}_0. \tag{C.26}$$

To avoid confusion, we'll write $\phi_k \underset{L^2}{\to} \phi$ if we mean convergence with respect to the Hilbert space norm. It is easy to see that $\phi_k \underset{\mathcal{S}}{\to} \phi$ implies $\phi_k \underset{L^2}{\to} \phi$, but not the other way round. One says that the topology (C.26) is *finer* than norm topology.

There's a non-trivial *regularity theorem* (Reed-Simon, Thm. V.10), which states that the constructive definition (C.5) of tempered distribution characterizes exactly the space of linear functionals on Schwartz space that is continuous in the sense of (C.26).

Generalizations

The topological formulation above is the basis of generalizations. The common recipe is to choose a test function space Φ (often norm-dense in $L^2(\mathbb{R})$), endow it with a finer topology, and then consider the continuous dual Φ'.

The most important choice is to take Φ to be the space of *bump functions* $C_c^\infty(\mathbb{R})$: smooth functions with compact support. "Compact support" means that these functions are identically zero for $|x|$ large enough. (It is not obvious that one can define functions that transition smoothly from being identically zero in some region to being non-zero in other regions, but such functions do exist). In the context of distributions, the space of bump functions is usually denoted by $\mathcal{D}$.

Recall that Schwartz functions vanish faster than any polynomial, and thus integrals against locally integrable functions $u(x)$ that grow at most polynomially are finite. Because bump functions vanish identically for large x, integrals against *any* locally integrable u are well-defined. This suggests, correctly, that the space of distributions $\mathcal{D}'$ is even larger than the space of tempered distributions $\mathcal{S}'$.

The structure of $\mathcal{D}'$ is somewhat more complicated than was the case for $\mathcal{S}'$. We will not discuss it here, but, for completeness, give the topology from which it derives. It is defined in terms of the (semi-)norms

$$\|\phi\|_{K,\alpha} := \sup_{x\in K} |\partial_x^\alpha \phi(x)|$$

indexed by compact subsets $K \subset \mathbb{R}$ and a number $n \in \mathbb{N}_0$, in the same way as (C.26):

$$\phi_k \underset{\mathcal{D}}{\to} \phi \qquad \text{if} \qquad \lim_{k\to\infty} \|\phi - \phi_k\|_{K,\alpha} = 0 \quad \forall \alpha, K.$$

Because elements of $\mathcal{D}$ are smooth, distributions in $\mathcal{D}'$ are arbitrarily often differentiable. However, the space $\mathcal{D}$ is easily seen not be be invariant under Fourier transforms, so the Fourier transform is not defined on $\mathcal{D}'$. This is the reason the space plays a less prominent role in quantum theory.

Terminology

The word "distributions" used without qualification is most likely to refer to $\mathcal{D}'$, but can also mean a general continuous dual space Φ', and may *also* refer to tempered distributions $\mathcal{S}'$, depending on context. Making matters worse, $\mathcal{S}$ is always called "Schwartz space", but the name "Schwartz" is also associated with the general mathematical theory of distributions and in particular also with $\mathcal{D}'$. "Tempered distributions" always means $\mathcal{S}'$, at least.

Lastly, if a science professor answers an inquiry about a questionable derivation by claiming that it is to be understood "in the sense of distribution", they likely mean neither $\mathcal{D}'$ nor Φ' nor $\mathcal{S}'$. Instead, they are probably vaguely aware of the fact that what they are doing isn't quite rigorous, but are optimistic that a smart mathematician could figure it out, and in any case, want to get through their lecture with their dignity intact and have found that "distribution" is a fully general incantation that reliably suppresses follow-up questions.

Needless to say, *I* would never engage in such tactics.

Appendix D

Green's functions

D.1 Introduction

In this chapter, we are interested in the affine equation

$$Lu = f \tag{D.1}$$

for u, given L and f. We'll restrict attention to the most important special case, where L is a translation-invariant differential operator on $\mathbb{R}^n$.

> **Example: The damped harmonic oscillator.** Newton's equation for the position $u(t)$ of a particle subject to a driving force $mf(t)$, viscous damping coefficient $(m\gamma)/2$, and undamped eigenfrequency ω_0 is
>
> $$\left(\partial_t^2 + 2\gamma\partial_t + \omega_0^2\right) u = f.$$
>
> The problem is to find $u(t)$ given $f(t)$ and the boundary condition $u(-\infty) = 0$.

Now here's the basic idea: Formally, $f(x) = \int f(x')\delta(x - x')\,\mathrm{d}x'$ is a superposition of "delta impulses". Thus, if we could work out how the system reacts to a delta impuls, we should be able to solve the general problem by linearity. Exploiting translational invariance, we may even get away treating just the case of $f(x) = \delta(x)$.

This indeed works out. Assume we can find a G such that

$$LG = \delta. \tag{D.2}$$

Then defining u to be a superposition of shifted solutions $G(x - x')$, weighted by $f(x)$,

$$u(x) = \int G(x - x')f(x')\,\mathrm{d}^n x'. \tag{D.3}$$

we get a solution of $Lu = f$, as anticipated:

$$(Lu)(x) = \int (LG)(x - x')f(x')\,\mathrm{d}^n x' = \int \delta(x - x')f(x')\,\mathrm{d}^n x' = f(x).$$

Some terminology: G is *the Green's function of* L.[1] The expression (D.3) for u is known as the *convolution* $G \star f$ of G and f.

[1] Yes, it's "the Green's function of L", not "the Green function of L" as would be more in line with the standard naming convention in mathematics (or, I guess, English grammar).

Technically, (D.2) should be interpreted in the language of Chapter C. One assumes (often implicitly) that f is an element of some space Φ of test functions. Then a Green's function G is a distribution in Φ' and $LG = \delta$ is to be understood in the sense of distribution.

If h is a solution to the *homogeneous* equation $Lh = 0$, then G is a Green's function if and only if $G + h$ is one. Thus G is unique if and only if L is invertible, in which case $G(x - x') = \langle x|L^{-1}|x'\rangle$ gives the matrix element of the inverse. Else, one can find an entire affine space worth of Green's functions (just as there's an entire affine space of solutions to $Lu = f$). Typically, physically motivated boundary conditions are used to select a particular one.

Elementary examples

The simplest example is $L = \partial_t$. The general solution to $Lu = f$ is, of course, the integral

$$u(t) = \int_a^t f(t')\,\mathrm{d}t'.$$

Because ∂_t is not invertible on the space of all differentiable functions, there is an ambiguity in the solution, represented by a. Fixing a amounts to choosing the boundary condition $u(a) = 0$. In these notes, we only treat the translationally-invariant theory, so we will restrict attention to the choices $a = \pm\infty$. For $a = -\infty$,

$$u(t) = \int_{-\infty}^t f(t')\,\mathrm{d}t' = \int \theta(t - t')f(t')\,\mathrm{d}t'.$$

The Green's function G^+ of ∂_t under the boundary condition $u(-\infty) = 0$ is therefore the step function θ. And indeed, by Sec. C.2.3, $\partial_t\theta(t) = \delta(t)$ holds in the sense of distribution, so that the step function fulfills (D.2).

An analogous calculation for $a = +\infty$ leads to $G^-(t) = -\theta(-t)$. Because the solutions $u(t)$ constructed using G^+ only depend on the $u(t')$ for $t' \leq t$, one usually calls G^+ a *retarded Green's function* and, likewise, G^- an *advanced Green's function*. Their difference $h(t) := G^+(t) - G^-(t) = 1$ is a solution of the homogeneous equation $\partial_t h(t) = 0$, consistent with our reasoning above.

For another example, take a quick look at $L = \partial_t^2$. Because $\delta(t)t = 0$ as distributions,

$$\partial_t^2(t\theta(t)) = \partial_t\big(t\delta(t) + \theta(t)\big) = \partial_t\theta(t) = \delta(t),$$

which shows that $G^+(t) = t\theta(t)$ is a (retarded) Green's function for ∂_t^2. Other solutions are

$$G^-(t) = -t\theta(-t), \qquad G = \frac{1}{2}G^- + \frac{1}{2}G^+ = \frac{1}{2}|x|.$$

D.2 Green's functions from Fourier transforms

Fourier transforms turn derivatives into multiplications. Thus, for every differential operator L with constant coefficients, the equation $Lu = f$ is equivalent to an equation

$$P(k)\tilde{u}(k) = \tilde{f}(k) \tag{D.4}$$

involving a polynomial multiplication operator $P(k)$ and the Fourier transforms of the functions. Formally, (D.4) is trivial to solve:

$$\tilde{u}(k) = \frac{\tilde{f}(k)}{P(k)} \quad \Rightarrow \quad u(x) = (2\pi)^{-n/2} \int e^{ikx} \frac{\tilde{f}(k)}{P(k)} \, \mathrm{d}^n k. \tag{D.5}$$

Likewise, the Fourier transform of the defining equation $LG = \delta$ for Green's function is

$$P\tilde{G} = (2\pi)^{-n/2} \, \underline{1}, \tag{D.6}$$

which has the formal solution

$$\tilde{G}(k) = (2\pi)^{-n/2} \frac{1}{P(k)} \quad \Rightarrow \quad G(x) = (2\pi)^{-n} \int e^{ikx} \frac{1}{P(k)} \, \mathrm{d}^n k. \tag{D.7}$$

The trouble is, of course, that if P has real zeros, the integrals in Eqs. (D.5, D.7) might not exist. In the next sections, we'll go through a variety of methods for anyway extracting solutions by modifying these equations.

> The problem of characterizing all $\tilde{G} \in \Phi'$ that satisfy (D.6) is known as the "problem of division" in the theory of distributions. In the univariate case, $n = 1$, it is fairly easy to solve (we'll introduce all necessary ingredients in Sec. D.2.3). Essentially, this case is simple because univariate polynomials have finitely many roots. If P has continuous sets of zeros, the problem can become very complicated, though.

D.2.1 Direct integration

No real zeros

The easiest case is the one where $P(k)$ has no real roots. Then L is invertible (at least as long as one assumes that u has a Fourier transform). Therefore, there is a unique Green's function. It is given by (D.7), which is absolutely integrable for all x.

As an example, let's treat the damped harmonic oscillator with strictly positive viscous damping coefficient, $\gamma > 0$. It corresponds to

$$L = \partial_t^2 + 2\gamma\partial_t + \omega_0^2 \quad \Rightarrow \quad P = -\omega^2 - 2i\gamma\omega + \omega_0^2.$$

The polynomial factorizes as

$$P = -(\omega - \omega_+)(\omega - \omega_-), \qquad \omega_\pm = i\gamma \pm \sqrt{\omega_0^2 - \gamma^2}.$$

Thus (employing the sign convention for the FT of time variables, as in (A.26)),

$$G(t) = -\frac{1}{2\pi} \int \frac{e^{-i\omega t}}{(\omega - \omega_+)(\omega - \omega_-)} \mathrm{d}\omega.$$

A simple exercise in contour integration gives

$$G(t) = i\theta(t) e^{-\gamma t} \left(-\frac{1}{\omega_+ - \omega_-} e^{i\sqrt{\omega_0^2 - \gamma^2}\, t} + \frac{1}{\omega_+ - \omega_-} e^{-i\sqrt{\omega_0^2 - \gamma^2}\, t} \right).$$

Since we're done integrating in Fourier space, we can re-use the letter ω, defining it to be $\sqrt{|\omega_0^2 - \gamma^2|}$. Then the above may be simplified (using l'Hôpital for the equality case) to

$$G(t) = \theta(t) \frac{e^{-\gamma t}}{\omega} \begin{cases} \sin(\omega t) & \omega_0 > \gamma \\ e^{-\gamma t} t & \omega_0 = \gamma \\ \sinh(\omega t) & \omega_0 < \gamma \end{cases}. \tag{D.8}$$

Locally integrable case

Even if $P(k)$ does have real roots, (D.7) might be locally integrable and thus well-defined as a distribution (c.f. Sec. C.2.2). The most important example is the Laplace operator $L = -\Delta = -\sum_{i=1}^{3} \partial_{x_i}$. Then $P(\boldsymbol{k}) = \|\boldsymbol{k}\|^2$, and, by (C.20),

$$G(\boldsymbol{x}) = (2\pi)^{3/2}\, \mathcal{F}^{-1}\left(\frac{1}{\|\boldsymbol{k}\|^2}\right)(\boldsymbol{x}) = \frac{1}{4\pi}\frac{1}{\|\boldsymbol{x}\|} \tag{D.9}$$

is a Green's function. (As the homogeneous equation $-\Delta h = 0$ has plenty of solutions, G is far from unique).

D.2.2 Complex integration

Univariate case

Given a univariate polynomial $P(\omega)$, choose a deformation γ of the real axis in the complex plane that avoids the zeros of P and consider the complex integral

$$G_\gamma(t) := \frac{1}{2\pi}\int_\gamma \frac{e^{-i\omega t}}{P(\omega)}\,\mathrm{d}\omega. \tag{D.10}$$

The good news is that the integral now exists. The bad news is that it is not clear any more that it has anything to do with Green's functions. But actually, it does! Applying L,

$$LG_\gamma(t) = \frac{1}{2\pi}\int_\gamma P(\omega)\frac{e^{-i\omega t}}{P(\omega)}\,\mathrm{d}\omega = \frac{1}{2\pi}\int_\gamma e^{-i\omega t}\,\mathrm{d}\omega = \frac{1}{2\pi}\int e^{-i\omega t}\,\mathrm{d}\omega = \delta(t).$$

The cool trick that makes this calculation work is that after multiplying with $P(\omega)$, the integrand is an entire function, so we can move the integration path right back to the real line without changing the value of the integral.

For the same reason, two paths γ, γ' will lead to the same Green's function if they can be deformed into each other without crossing a pole. In general, however, G_γ does depend on the choice of γ.

"Infinitesimal" deformations

There's a variant of this constructing that can be interpreted as "shifting the roots of P away from the real axis" instead of "deforming the integration path to avoid the roots".

Write the complex ω's on the path γ as $\omega = u + iv(u)$. Then

$$\frac{1}{2\pi}\int_\gamma \frac{e^{-i\omega t}}{P(\omega)}\,\mathrm{d}\omega = \frac{1}{2\pi}\int e^{v(u)t}\frac{e^{-iut}}{P(u+iv(u))}\,\mathrm{d}u.$$

If there are no zeros between γ and the real line, the integral does not change under the substitution $v(u) \mapsto \epsilon v(u)$ for $1 \le \epsilon < 0$. In particular, by continuity of the exponential,

$$\frac{1}{2\pi}\lim_{\epsilon\to 0^+}\int e^{\epsilon v(u)t}\frac{e^{-iut}}{P(u+i\epsilon v(u))}\,\mathrm{d}u = \frac{1}{2\pi}\lim_{\epsilon\to 0^+}\int \frac{e^{-iut}}{P(u+i\epsilon v(u))}\,\mathrm{d}u.$$

In the common special case where $v(u)$ is constant, the limit is typically written as

$$G^{\pm}(t) = \frac{1}{2\pi}\int \frac{e^{-i\omega t}}{P(\omega \pm i0)}\,\mathrm{d}\omega, \tag{D.11}$$

with the sign depending on $\operatorname{sgn} v$. (This construction should remind you of the formula (C.10), expressing the principal value as the "side limit" $1/(x \pm i0)$). Of course, $\omega \mapsto P(\omega \pm i\epsilon)$ is a polynomial whose roots are shifted by $\mp i\epsilon$ compared to the ones of P.

Multivariate case

We can reduce the problem for arbitrary n to the $n = 1$-case. While the technique works in general, it is particularly natural if one of the variables is distinguished in some way. In physics applications, this is typically the time. With this in mind, we'll use $x = (t, \boldsymbol{x})$ for the arguments of u, f, G, and $k = (\omega, \boldsymbol{k})$ for the arguments of Fourier transforms.

Define $p_{\boldsymbol{k}}(\omega) = P(\omega, \boldsymbol{k})$. Then $p_{\boldsymbol{k}}$ is a univariate polynomial, and we can just repeat the $n = 1$-construction from above, but in a $\boldsymbol{k}$-dependent way. That is to say, choose deformations $\gamma_{\boldsymbol{k}}$ avoiding the zeros of $p_{\boldsymbol{k}}$ and define

$$G_\gamma(x) := \int \left(\int_{\gamma_{\boldsymbol{k}}} \frac{e^{-i\omega t}}{p_{\boldsymbol{k}}(\omega)} \, \mathrm{d}\omega \right) e^{i\boldsymbol{k}\boldsymbol{x}} \, \mathrm{d}^{n-1}\boldsymbol{k}. \tag{D.12}$$

The proof that G_γ is a Green's function works exactly as in the univariate case.

Example: The Klein-Gordon equation

The Klein-Gordon equation $L = \partial_t^2 - \sum_{i=1}^3 \partial_{x_i}^2 + m^2$ corresponds to the polynomial

$$P = -\omega^2 + \sum_{i=1}^{3} k_i^2 + m^2 = -(\omega - \omega_k)(\omega + \omega_k), \quad \omega_k = \sqrt{m^2 + \|\boldsymbol{k}\|^2}. \tag{D.13}$$

There are three natural choices for deformations $\gamma_{\boldsymbol{k}}$ avoiding the poles. The simplest ones are $\gamma_{\boldsymbol{k}}^{\pm}$: straight lines parallel to the real axis with imaginary parts $\pm\epsilon$. From the discussion above, the integral does not depend on the value of $\epsilon > 0$. The third contour is $\gamma_{\boldsymbol{k}}^F$, which moves around $-\omega_k$ in the lower half-plane and around $+\omega_k$ in the upper half-plane (the superscript "F" is for Feynman; see Fig. **??**).

Let's look at $G^+(x) = G_{\gamma^+}(x)$. The frequency integral can be evaluated exactly as in the damped harmonic oscillator example above, leading to

$$2\pi i \theta(t) \frac{e^{-i\omega_k t} - e^{i\omega_k t}}{2\omega_k}$$

so that the full integral is

$$G^+(x) = i\theta(t) \int \frac{1}{2\omega_k} \left(e^{-i\omega_k t} - e^{+i\omega_k t} \right) e^{-i\boldsymbol{k}\boldsymbol{x}} \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}.$$

The $\boldsymbol{k}$-integral can be expressed in terms of Bessel functions (but the result isn't pretty). In any case, the θ term means that the convolutions $u = G^+ \star f$ only depend on $f(t, \boldsymbol{x})$ for $t \leq 0$. We have thus constructed a retarded Green's function.

D.2.3 Using the principal value

One can generalize the principal value (Sec. C.2.2) to find Green's functions. We'll outline how one can use this approach to construct *all* Green's functions for a given one-dimensional problem.

Start with $L = \partial_t$. A Green's function is a solution to

$$\omega \tilde{G}(\omega) = \frac{i}{\sqrt{2\pi}}. \tag{D.14}$$

Thus we're looking for distributions $\tilde{G}$ "proportional to $1/\omega$". That was exactly our motivation for introducing the principal value in Eq. (C.7). And indeed,

$$\left(\omega \operatorname{pv}\left(\frac{1}{\omega}\right)\right)(\tilde{f}) = \lim_{\epsilon \to 0^+} \int_{|\omega| \geq \epsilon} \omega \frac{1}{\omega} \tilde{f}(\omega)\, \mathrm{d}\omega = \int 1\, \tilde{f}(\omega)\, \mathrm{d}\omega \quad \Rightarrow \quad \omega \operatorname{pv}\left(\frac{1}{\omega}\right) = 1.$$

Using that $\omega\delta(\omega) = 0$, an affine space of solutions to (D.14) is given by

$$\tilde{G}_\lambda(\omega) = \frac{i}{\sqrt{2\pi}} \operatorname{pv}\left(\frac{1}{\omega}\right) + \lambda\delta(\omega),$$

and one can show that these are all. An inverse Fourier transform gives

$$G_\lambda(t) = \frac{1}{2}\operatorname{sign}(t) + \frac{\lambda}{\sqrt{2\pi}}$$

Choosing $\lambda = \pm\sqrt{\frac{\pi}{2}}$, we recover the retarded/advanced Green's functions $G^\pm$ found before in Sec. D.1.

Let's now sketch how to generalize this construction to solve $P\tilde{G} = (2\pi)^{-1/2}$ for a general polynomial P.

First assume that all real roots of P are simple, i.e. that

$$P(\omega) = Q(\omega) \prod_{l=1}^{d} (\omega - a_l)$$

where Q is a polynomial with only complex roots and the a_l are distinct real numbers. Define

$$\tilde{G}(\tilde{f}) = \frac{1}{\sqrt{2\pi}} P \int \frac{\tilde{f}(\omega)}{P(\omega)}\, \mathrm{d}\omega,$$

where the symbol $P\int$ denotes the *principal value integral* that is computed by approaching each of the singularities a_l symmetrically, the same way integration around 0 is handled in $\operatorname{pv}(1/\omega)$. The proof that $\tilde{G}$ is indeed a Green's function then works as the one for $\operatorname{pv}(1/\omega)$ given above. The ambiguity in defining $\tilde{G}$ corresponds to adding multiples of delta distributions supported on the real zeros of P:

$$\tilde{G} \mapsto \tilde{G} + \sum_{i=1}^{l} \lambda_l \delta_{a_l}.$$

It remains to treat roots with higher multiplicity. Here, we only discuss the case $P(\omega) = -\omega^2$; the general case works similarly. The trick is to write

$$-\frac{1}{\omega^2} = \partial_\omega \frac{1}{\omega}.$$

But we already know how to associate a distribution with $1/\omega$ (the principal value) and how to differentiate distributions (by differentiating minus the test function). Indeed, with

$$\tilde{G} = \frac{1}{\sqrt{2\pi}}\, D \operatorname{pv}(1/\omega)$$

we get

$$\begin{aligned}(-\omega^2)\tilde{G}(\tilde{f}) &= \frac{1}{\sqrt{2\pi}}\, P\int \frac{1}{\omega}(-\partial_\omega)(-\omega^2\phi(\omega))\,\mathrm{d}\omega \\ &= \frac{1}{\sqrt{2\pi}}\, P\int \frac{1}{\omega}(2\omega\phi(\omega)+\omega^2\partial_\omega\phi(\omega))\,\mathrm{d}\omega \\ &= \frac{1}{\sqrt{2\pi}}\left(2\int \phi(\omega)\,\mathrm{d}\omega - \int \phi(\omega)\,\mathrm{d}\omega\right) = \int \frac{1}{\sqrt{2\pi}}\phi(\omega)\,\mathrm{d}\omega.\end{aligned}$$

One may verify that the ambiguity is given by

$$\tilde{G} \mapsto \tilde{G} + \lambda_1\delta + \lambda_2\delta'.$$

D.3 Resolvents

Given a linear operator L on a Hilbert space $\mathcal{H}$, the function that maps complex numbers z to the operator

$$R(z;L) := (z\mathbb{1} - L)^{-1},$$

is called the *resolvent* of L. (Warning: Some authors use the sign convention $(L-z\mathbb{1})^{-1}$!). From the discussion in Sec. D.1, it is clear that if $(L-z)$ is invertible, its Green's function is

$$G(z;\boldsymbol{x}) = -\langle 0|R(z;L)|\boldsymbol{x}\rangle.$$

We'll see that even if $(L-z)$ is not invertible, suitable limits in z make sense as distributions and define Green's functions.

Independent of their use for constructing Green's functions, resolvents play an important role in functional analysis. We'll have a brief look at general properties first, and work out some Green's functions in Sec. D.3.2.

D.3.1 Resolvents and the spectrum

Recall that if L is a finite-dimensional square matrix, then each of the following conditions are equivalent to z being an eigenvalue:

- $(z-L)$ is not injective,
- $(z-L)$ is not surjective,
- $\det(z-L) = 0$.

The final condition allows us to prove that over $\mathbb{C}$, every matrix has an eigenvalue. That's because the determinant is a polynomial, and thus, by the fundamental theorem of arithmetic, has a root over the complex number.

In infinite dimensions, the situation is more complicated. Injectivity and surjectivity of a linger map from a space to itself are no longer equivalent notions, and the definition of the determinant makes no sense in infinite dimensions. Still, the analysis of eigenvalues for linear operators, culminating in the *spectral theorem*, starts with a classification of how $(z-L)$ is or is not invertible.

Here's a summary of results. If L is a Hermitian operator, then every $z \in \mathbb{C}$ falls into one of three categories:

- $(z - L)$ fails to be injective.
  This happens iff z is a proper eigenvalue of L, i.e. iff there is a normalizable $|\psi\rangle \in \mathcal{H}$ such that $L|\psi\rangle = z|\psi\rangle$. The set of such z is called the *point spectrum* of L.

- $(z - L)$ is injective, but not surjective.
  This happens iff z is a generalized (but not a proper) eigenvalue of L, i.e. an eigenvalue associated with a non-normalizable distribution. In this case $(z - L)^{-1}$ is an unbounded operator on $\operatorname{range} L$, which turns out to be dense in $\mathcal{H}$. The set of such z is called the *continuous spectrum* of L.

- $(z - L)$ is both injective and surjective.
  This happens iff $(z-L)^{-1}$ is bounded. Because the spectrum of Hermitian operators is real, $\operatorname{Im} z \neq 0$ is sufficient for this case. These z form the *resolvent set* of L.

It also holds that $z \mapsto R(z; L)$ is an (operator-valued) analytic function on the resolvent set. This means one can use results from complex analysis, e.g.:

- The Taylor series of the resolvent converges. (This is almost as nice as it being a polynomial, and replaces the use of the fundamental theorem of arithmetic in the proof that every bounded operator has an eigenvalue).

- The residue theorem for contour integration applies, see Fig. **??**.

D.3.2 The resolvent of the Laplacian

Here, we compute the resolvent function for the Laplacian $-\sum_{i=1}^{n} \partial_{x_i}^2$ for $n = 1$ and $n = 3$.

The Laplacian in one dimension

Set $L = -\partial_x^2$. Compute, using principal square roots,

$$\begin{aligned} G(z, \boldsymbol{x}) &= -\langle 0|(z + \partial_x^2)^{-1}|x\rangle \\ &= \frac{-1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \, \frac{e^{ikx}}{z - k^2} \\ &= \frac{-1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \, \frac{e^{ikx}}{-(k + \sqrt{z})(k - \sqrt{z})}. \end{aligned}$$

Assuming $\operatorname{Im} z \neq 0$, the expression can be evaluated by contour integration. If $x \geq 0$, then e^{ikx} remains bounded when k takes values in the upper half-plane. The contour is then positively oriented and encloses a pole at $k = \pm\sqrt{z}$, where the sign is the one of $\operatorname{Im} z$. Thus,

$$G(z; x) = 2\pi i \operatorname{Res}(\pm\sqrt{z}) = i\frac{e^{\pm i\sqrt{z}x}}{\pm 2\sqrt{z}} = i\frac{e^{\pm i\sqrt{z}|x|}}{\pm 2\sqrt{z}}, \qquad \pm = \operatorname{sign} \operatorname{Im} z.$$

If $x < 0$, the contour needs to be closed in the lower half-plane, but a similar argument shows that the same end result holds in this case, too.

Now for real values of $z = u \in \mathbb{R}$. The spectrum of the Laplacian is $\mathbb{R}_{\geq 0}$ (associated with the distributions e^{ikx}, for $k = \sqrt{u}$). Therefore, if $u < 0$, it is an element of the resolvent set, where the $R(z)$ is analytic and hence continuous. We thus expect $G(u; x)$ to be independent of the particular limit taken. On the other hand, value $z = u \geq 0$ are part

of the spectrum, and limits $G(z \to u, x)$ might fail to exist or depend on the particular way the limit is taken. For concreteness, we evaluate two *side limits*

$$G^{\pm}(u;x) := \lim_{s\downarrow 0} G(u \pm is; x) = \begin{cases} \pm i\frac{e^{\pm i\sqrt{u}|x|}}{2\sqrt{u}} & u > 0 \\ \frac{e^{-\sqrt{|u|}|x|}}{2\sqrt{|u|}} & u < 0 \end{cases}.$$

The side limits $\lim_{s\downarrow 0} G(\pm is; x)$ at $u = 0$ do not converge. These results are compatible with our expectations.

The $G^{\pm}(u;x)$ are indeed Green's functions for $(u - \partial_x^2)$. We only need to verify this for $u > 0$, where we find

$$-\partial_x^2\Big(\pm i\frac{e^{\pm i\sqrt{u}|x|}}{2\sqrt{u}}\Big) = \frac{1}{2}\partial_x\big((\operatorname{sign} x)e^{\pm i\sqrt{u}|x|}\big) = \Big(\delta(x) \pm \frac{i\sqrt{u}}{2}\Big)e^{\pm i\sqrt{u}|x|}$$

$$\Rightarrow \quad (-\partial_x^2 - u)G^{\pm}(u;x) = \delta(x) \pm \frac{i\sqrt{u}}{2}e^{\pm i\sqrt{u}|x|} \mp \frac{i\sqrt{u}}{2}e^{\pm i\sqrt{u}|x|} = \delta(x).$$

The side limits don't converge if $u = 0$, but the limit of their mean does:

$$\lim_{u\downarrow 0}\frac{1}{2}(G^{+}(u,x) + G^{-}(u,x)) = \lim_{u\downarrow 0}\frac{1}{2}\frac{i}{2\sqrt{u}}2i\sin\big(\sqrt{u}|x|\big) = -\frac{1}{2}|x|,$$

which is a Green's function for $L = -\partial_x^2$, as already argued in Sec. D.1.

The Laplacian in three dimensions

Evaluate the inner product in spherical coordinates in Fourier space (compare Eq. (B.4)) to find

$$\begin{aligned} G(z,\boldsymbol{x}) &= -\langle 0|(z+\Delta)^{-1}|\boldsymbol{x}\rangle \\ &= \frac{-1}{(2\pi)^3}\int \mathrm{d}^3\boldsymbol{k}\,\frac{1}{z - \|\boldsymbol{k}\|^2}e^{i\boldsymbol{k}\boldsymbol{x}} \\ &= \frac{-1}{(2\pi)^2}\int_0^{\infty}\mathrm{d}k\,\frac{k^2}{z-k^2}\int_{-1}^{1}\mathrm{d}\mu\, e^{ikx\mu} \\ &= \frac{-1}{(2\pi)^2}\int_0^{\infty}\mathrm{d}k\,\frac{k^2}{z-k^2}\frac{e^{ikx} - e^{-ikx}}{ikx} \\ &= \frac{-1}{(2\pi)^2 ix}\int_{-\infty}^{\infty}\mathrm{d}k\,\frac{ke^{ikx}}{z-k^2} \\ &= \frac{-1}{(2\pi)^2 ix}\int_{-\infty}^{\infty}\mathrm{d}k\,\frac{ke^{ikx}}{-(k+\sqrt{z})(k-\sqrt{z})}. \end{aligned}$$

Arguing as in the one-dimensional case, a contour integration gives for $\operatorname{Im} z \neq 0$,

$$G(z;\boldsymbol{x}) = 2\pi i\operatorname{Res}\big(\pm\sqrt{z}\big) = \frac{-1}{2\pi x}\frac{(\pm\sqrt{z})e^{\pm i\sqrt{z}x}}{-2(\pm\sqrt{z})} = \frac{e^{\pm i\sqrt{z}x}}{4\pi x}, \qquad \pm = \operatorname{Im} z.$$

The side limits are

$$G^{\pm}(u;\boldsymbol{x}) = \lim_{s\downarrow 0}\frac{e^{\pm i\sqrt{u\pm is}x}}{4\pi x} = \frac{e^{\pm i\sqrt{u}x}}{4\pi x}.$$

Unike the one-dimensional case, the expression does make sense for $u =$, where we get $G^{\pm}(0;\boldsymbol{x}) = \frac{1}{4\pi x}$, as previously computed in Eq. (D.9).

D.4 Propagators

Consider again a differential operator L on functions of time t and space $\boldsymbol{x} \in \mathbb{R}^{n-1}$. There is a close connection between *inhomogeneous equations* we have considered so far and *homogeneous initial value problems*. For simplicity, we restrict attention to the case where L is of the form

$$L = \frac{1}{c}\partial_t - H, \tag{D.15}$$

for some constant c and where H acts only on the spatial degrees of freedom. Prime example is

$$L = i\hbar\partial_t + \frac{\hbar^2}{2m}\Delta - V,$$

so that $L\psi(t, \boldsymbol{x}) = 0$ is the Schrödinger equation.

Recall that the *inhomogeneous equation with causal boundary conditions* is

$$\begin{aligned} Lu(t, \boldsymbol{x}) &= f(t, \boldsymbol{x}), \\ \lim_{t' \to -\infty} u(t', \boldsymbol{x}) &= 0 \end{aligned}$$

As we have seen, if we have a Green's function

$$\begin{aligned} LG(t, \boldsymbol{x}) &= \delta(t)\delta(\boldsymbol{x}) \\ G(t', \boldsymbol{x}) &= 0 \qquad\qquad \text{for all } t' \leq 0, \end{aligned}$$

then a solution is given by

$$u(t, \boldsymbol{x}) = \int \mathrm{d}t' \int \mathrm{d}^{n-1}\boldsymbol{x}'\, G(t', \boldsymbol{x}')f(t', \boldsymbol{x}').$$

In contrast, the *homogeneous problem with initial value* $\phi(\boldsymbol{x})$ is

$$\begin{aligned} Lu(t, \boldsymbol{x}) &= 0, \\ u(s, \boldsymbol{x}) &= \phi(\boldsymbol{x}) \qquad\qquad \text{for some } s \in \mathbb{R}. \end{aligned}$$

A *propagator* for L is a distribution $K(t, \boldsymbol{x})$ satisfying

$$\begin{aligned} LK(t, \boldsymbol{x}) &= 0, \\ K(0, \boldsymbol{x}) &= \delta(\boldsymbol{x}). \end{aligned} \tag{D.16}$$

One immediately verifies that given K, the initial value problem is solved by

$$u(t, \boldsymbol{x}) = \int \mathrm{d}^{n-1}\boldsymbol{x}'\, K(t - t', \boldsymbol{x}')f(t', \boldsymbol{x}'). \tag{D.17}$$

For the first-order differential operator (D.15), the propagator is given by the "matrix elements" of e^{tcH}

$$K(t, \boldsymbol{x}) = \langle t, \boldsymbol{x}|e^{ctH}|0, 0\rangle.$$

(In QM, the exponential is of course known as the *time evolution* operator $U(t) = e^{\frac{t}{i\hbar}H}$).

After these preparations, we can now state an observation sometimes known as *Duhamel's principle*. It says that one can solve the inhomogeneous problem in terms of homogeneous ones, or, equivalently, one can obtain the Green's function G from the propagator K. For the latter point of of view, just set

$$G(t, \boldsymbol{x}) = c\theta(t)K(t, \boldsymbol{x}),$$

and verify, using (D.16),

$$\begin{aligned} LG(t, \boldsymbol{x}) &= \partial_t(\theta(t)K(t, \boldsymbol{x})) - cH\theta(t)K(t, \boldsymbol{x}) \\ &= \delta(t)K(t, \boldsymbol{x}) + \theta(t)\partial_t K(t, \boldsymbol{x}) - c\theta(t)HK(t, \boldsymbol{x}) \\ &= \delta(t)\delta(\boldsymbol{x}) + c\theta(t)LK(t, \boldsymbol{x}) \\ &= \delta(t)\delta(\boldsymbol{x}). \end{aligned}$$

D.5 Epilogue

Warning: The concepts treated in this section are used in sufficiently many fields (quantum physics, partial differential equations, functional analysis) and some of them (Green's functions, resolvents, propagators) are sufficiently strongly related that the terminology in the literature is a complete mess. Any one of the three terms might be used to refer to any one of the three concepts by various authors. Bottom line is that you have to be careful when combining results from different sources.