

Advanced Quantum Mechanics

Exercise sheet 3

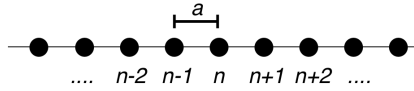
Winter term 2014/15

Homepage: <http://www.thp.uni-koeln.de/trebst/Lectures/2014-QM2.shtml>

Due date: Monday, **October 27th**, 2014 (10 am, i.e. before the lecture starts)

8. Tight-binding Hamiltonian (10 points)

Consider a one-dimensional lattice with lattice constant a and N lattice sites ($L = Na$):



Fermions can be created and annihilated on each site n with operators \mathbf{c}_n^\dagger and \mathbf{c}_n that fulfill $\{\mathbf{c}_n, \mathbf{c}_m^\dagger\} = \delta_{n,m}$ and $\{\mathbf{c}_n^\dagger, \mathbf{c}_m^\dagger\} = \{\mathbf{c}_n, \mathbf{c}_m\} = 0$. The tight-binding Hamiltonian describes the hopping of fermions between nearest-neighbour lattice sites with amplitude τ ,

$$\mathcal{H} = -\tau \sum_n \left(\mathbf{c}_{n+1}^\dagger \mathbf{c}_n + \mathbf{c}_n^\dagger \mathbf{c}_{n+1} \right) - \mu \sum_n \mathbf{c}_n^\dagger \mathbf{c}_n. \quad (1)$$

The sum is over all lattice sites n and the chemical potential is μ .

- a) Introduce fermionic operators in momentum space, $\mathbf{a}_k = \frac{1}{\sqrt{N}} \sum_n \mathbf{c}_n e^{ikx_n}$ and $\mathbf{a}_k^\dagger = \frac{1}{\sqrt{N}} \sum_n \mathbf{c}_n^\dagger e^{-ikx_n}$, with $x_n = na$. The momentum k is defined within the first Brillouin zone, $k = \frac{2\pi m}{Na}$, with $-N/2 < m \leq N/2$. Show that $\{\mathbf{a}_k, \mathbf{a}_p^\dagger\} = \delta_{k,p}$.
Hint: $\frac{1}{N} \sum_n e^{ikx_n} = \delta_{k,0}$ and $\sum_{k \in 1^{st} BZ} e^{ikx_n} = N\delta_{n,0}$.
- b) Rewrite the Hamiltonian using operators \mathbf{a}_k and \mathbf{a}_k^\dagger . Bring it to the form $\mathcal{H} = \sum_{k \in 1^{st} BZ} \epsilon(k) \mathbf{a}_k^\dagger \mathbf{a}_k$ and determine the energy dispersion $\epsilon(k)$.
- c) The particle counting operator at site n is given by $\mathbf{n}_n = \mathbf{c}_n^\dagger \mathbf{c}_n$. Consider the Heisenberg equation $\partial_t \mathbf{n}_n(t) = \frac{i}{\hbar} [\mathcal{H}, \mathbf{n}_n(t)]$ with the operator in the Heisenberg picture, $\mathbf{n}_n(t) = e^{i\mathcal{H}t/\hbar} \mathbf{n}_n e^{-i\mathcal{H}t/\hbar}$. Show that it takes the form $\partial_t \mathbf{n}_n(t) = \mathbf{J}_{n+1/2}(t) - \mathbf{J}_{n-1/2}(t)$ with the operator \mathbf{J}_l defined on a link between two lattice sites (l is half integer)

$$\mathbf{J}_l = -\frac{i\tau}{\hbar} (\mathbf{c}_{l+1/2}^\dagger \mathbf{c}_{l-1/2} - \mathbf{c}_{l-1/2}^\dagger \mathbf{c}_{l+1/2}). \quad (2)$$

Interpret this result! Evaluate the mean current

$$\frac{1}{N} \sum_l J_l = \frac{1}{L} \sum_{k \in 1^{st} BZ} v(k) \mathbf{a}_k^\dagger \mathbf{a}_k \quad (3)$$

and show that $v(k)$ is given by the group velocity $v(k) = \epsilon'(k)/\hbar$.

9. Spin operator in second quantization (10 points)

A single-particle operator \hat{O} in second quantization can be expressed as

$$\hat{O} = \sum_{\mu, \nu} \langle \mu | \hat{o} | \nu \rangle a_{\mu}^{\dagger} a_{\nu}$$

where μ and ν label a complete set of single particle states, a_{μ}^{\dagger} and a_{μ} are creation and annihilation operators with quantum number μ , and \hat{o} is the corresponding operator in its first-quantized form. In the following, we consider fermions with spin $S = 1/2$.

a) The Hamiltonian for a non-interacting N -particle system reads in first-quantized form

$$\mathcal{H} = \sum_{i=1}^N \left[-\frac{\nabla_i^2}{2m} + V(x_i) \right]$$

where i labels the particle number. Find the second-quantized expression for \mathcal{H} both in the real space basis $|\mathbf{x}, \sigma\rangle$ and the momentum space basis $|\mathbf{k}, \sigma\rangle$, where $\sigma = \uparrow, \downarrow$.

b) The spin-density operator of N localized spin- $\frac{1}{2}$ particles in first quantized form is given by

$$\mathbf{S}(x) = \sum_{j=1}^N \delta(x - x_j) \mathbf{S}_j \quad \text{with } \mathbf{S} = \frac{\boldsymbol{\sigma}}{2}$$

where $\boldsymbol{\sigma}$ is the vector of Pauli matrices. Find the second-quantized expression for the spin-density operator $\mathbf{S}(x)$ with respect to the real-space basis and the momentum space basis.

c) Show that the spin-spin interaction $\mathbf{S}_i \cdot \mathbf{S}_j$ can be written as a combination of a spin-exchange term $\sum_{\sigma, \sigma'} a_{i, \sigma}^{\dagger} a_{j, \sigma'}^{\dagger} a_{i, \sigma'} a_{j, \sigma}$ and a density-density interaction $\hat{n}_i \hat{n}_j$.
Hint: Make use of the following identity (proof it): $\boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$.