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Advanced Quantum Mechanics

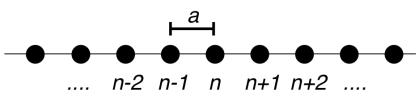
Exercise sheet 3

Winter term 2015/16

Homepage: http://www.thp.uni-koeln.de/trebst/Lectures/2015-QM2.shtml
Due date: Monday, **November 9th**, 2015 (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,

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

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)

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

Interpret this result! Evaluate the mean current

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

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

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

where μ and ν label a complete set of single particle states, $a^\dagger_\mu$ 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

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

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 $\sum_{\sigma,\sigma'} a^\dagger_{i,\sigma} a^\dagger_{j,\sigma'} a_{i,\sigma'} a_{j,\sigma}$ and a density-density interaction $\hat{n}_i \hat{n}_j$.
Hint: Make use of the following identity (proof it): $\boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$.