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Problem 1: Fermions on a Ladder (Oral)

> **Learning objective**
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> The goal in this problem is to become familiar with basis transformations in the formalism of second quantization. As an example, you will study the transition between real space and momentum space and therefore learn how to diagonalize a lattice Hamiltonian by means of a Fourier transform.
> You will need the acquired skills in Problem 2 below.

Consider a ladder (two parallel chains labeled a and b) with Hamiltonian

$$H = -t \sum_{i=1}^{L} (a_i^\dagger a_{i+1} + b_i^\dagger b_{i+1} + \text{h.c.}) - t_\perp \sum_{i=1}^{L} (a_i^\dagger b_i + b_i^\dagger a_i) + U \sum_{i=1}^{L} n_i^a n_i^b \,. \tag{1}$$

Here, a_i and b_i are fermionic operators of two modes located at position i (for example, two spin states of a fermion, see Problem 2), t is the hopping amplitude for the intra-chain hopping, while $t_\perp$ is the hopping amplitude for the inter-chain hopping. The last term ($n_i^x = x_i^\dagger x_i$ with $x = a, b$) accounts for the interaction between adjacent fermions on the two chains. Assume that each chain of the ladder has L sites and that the lattice spacing on each chain is d. Further assume that the ladder has periodic boundary conditions (i.e., $i + 1 = 1$ for $i = L$).

a) First, introduce the operators

$$\tilde{a}_k = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ikdj} a_j \,, \qquad \tilde{b}_k = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ikdj} b_j \,, \tag{2}$$

and show that this transformation is canonical, that is, show that the new operators still obey canonical anticommutation relations. What are the allowed values for k?

b) Consider the case where $t_\perp = 0$ and transform the Hamiltonian (1) into momentum space. Can you infer the spectrum from your result (no calculation needed)?

c) Finally, let $U = 0$ and $t_\perp \neq 0$. Calculate the spectrum $E_k^\pm$ of (1) using the Fourier transform (2).

Hint: Bring the Hamiltonian into the form

$$H = \sum_k \begin{pmatrix} \tilde{a}_k^\dagger & \tilde{b}_k^\dagger \end{pmatrix} \mathcal{H}_k \begin{pmatrix} \tilde{a}_k \\ \tilde{b}_k \end{pmatrix} \,, \tag{3}$$

where $\mathcal{H}_k$ is a Hermitian 2×2-matrix.
The spectrum can then be obtained by diagonalizing this matrix (why?).

Problem 2: The Fermi-Hubbard Model (Oral)

Learning objective

This problem studies the Fermi-Hubbard model, describing interacting fermions on a lattice. It demonstrates a very important application of many-body theory in quantum mechanics within the framework of second quantization. Despite its simple Hamiltonian, the Fermi-Hubbard model features rich physics and is subject to ongoing research both experimentally and theoretically. Among others, it is of particular interest as a model for high-temperature superconductivity (where BCS theory does not apply, cf. Problem 3 below).

Here we study N interacting spin-$1/2$ fermions in a deep lattice. This many-body system ($N \gg 1$) is well described by the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow}\,, \tag{4}$$

where $c^\dagger_{i,\sigma}, c_{i,\sigma}$ are the creation and annihilation operators of fermions with spin $\sigma \in \{\uparrow, \downarrow\}$ localized on lattice site i.

The first term of the Hamiltonian describes the kinetic energy of fermions hopping from lattice site j to lattice site i (thereby gaining energy t). The sum is restricted to nearest-neighbor sites of the D-dimensional lattice, indicated by $\langle i, j \rangle$. The second term of the Hamiltonian accounts for the interaction of two fermions with opposite spin: It describes the cost in energy ($U > 0$) to put two fermions with opposite spin on the same lattice site. The interaction is on-site (restricted to one lattice site) due to the localization of the fermions in the deep lattice.

In the following, we derive the ground state of this system at half-filling in the limits $t = 0$ and $U = 0$. “Half-filling” means that there is exactly one fermion per lattice site (in a completely filled lattice, there are *two* particles of opposite spin per site). For simplicity, we consider a $D = 1$-dimensional lattice of L sites with lattice constant a and periodic boundary conditions.

a) First, consider the case $U = 0$ where the ground state is given by a Fermi sea and calculate the ground state energy (assume $N = L \gg 1$ to simplify your result).
Derive the first-order correction to the ground state energy for small interactions $0 < U \ll t$.

b) Now consider the case where $t = 0$ and $U > 0$. Determine the ground state(s) in this regime and calculate the ground state energy.

The ground state manifold describes a *Mott insulator* and is highly degenerate (why?). What is the energy gap that separates the ground states from the first excited states with one doubly occupied site?

To derive leading corrections to the ground state energy, we use (degenerate) perturbation theory for $t \ll U$. Sketch the derivation and estimate the leading corrections to the energy.

Hint: Show that the first-order contribution vanishes and derive an upper bound for the matrix elements of the second-order correction (diagonalization of the matrix is not required).

c) Explain why your results suggest a phase transition between a metallic (conducting) phase for small interactions ($U \ll t$) and an insulating phase for large interactions ($U \gg t$).

Problem 3: The BCS Ground State (Written)

> **Learning objective**
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> The BCS theory describes conventional superconductors. Here you study the BCS ground state wavefunction as an example for a *quasiparticle vacuum*, i.e., the ground state of a non-interacting fermionic theory. This problem also serves as exercise for calculations in the formalism of second quantization.

We consider the famous BCS state (named after J. Bardeen, L. N. Cooper, J. R. Schrieffer)

$$|\Omega\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \right) |0\rangle \ , \tag{5}$$

where $u_{\mathbf{k}}, v_{\mathbf{k}} \in \mathbb{C}$ with $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ and the fermionic operator $c^\dagger_{\mathbf{k},\sigma}$ creates a fermion with momentum $\mathbf{k}$ and spin $\sigma \in \{\uparrow, \downarrow\}$. The product runs over the Brillouin zone of the lattice (which we do not specify here).

a) Show that the BCS state $|\Omega\rangle$ is normalized.

b) Evaluate $\langle\Omega| c^\dagger_{\mathbf{q},\uparrow} c^\dagger_{-\mathbf{q},\downarrow} |\Omega\rangle$ and $\langle\Omega| c^\dagger_{\mathbf{q},\sigma} c_{\mathbf{q},\sigma} |\Omega\rangle$ for a given wave vector $\mathbf{q}$.

c) Introduce the new *quasiparticle* operators $\alpha_{\mathbf{k},\sigma}$ via

$$\alpha_{\mathbf{k},\uparrow} = u_{\mathbf{k}} c_{\mathbf{k},\uparrow} - v_{\mathbf{k}} c^\dagger_{-\mathbf{k},\downarrow} \quad \text{and} \quad \alpha_{-\mathbf{k},\downarrow} = u_{\mathbf{k}} c_{-\mathbf{k},\downarrow} + v_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow} \,. \tag{6}$$

   Prove that these operators obey fermionic anticommutation relations.
   Show that $\alpha_{\mathbf{k},\sigma} |\Omega\rangle = 0$ for all $\mathbf{k}$ and σ and write down a Hamiltonian for which $|\Omega\rangle$ is the ground state (the *quasiparticle vacuum*).

d) What choice of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ makes $|\Omega\rangle$ the ground state of free fermions (with eigenmodes $c_{\mathbf{k},\sigma}$)? In this case, what does $\alpha^\dagger_{\mathbf{k},\sigma}$ describe for $|\mathbf{k}| \lessgtr k_F$ where k_F denotes the Fermi wave vector?