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Exercise 1: The Hubbard model (Oral)

We consider fermions on a lattice. A single particle localized at the i-th lattice site is described by the wave-function $\phi_{i,\sigma}(\mathbf{r}) = \chi_\sigma \phi_i(\mathbf{r})$ with $\phi_i(\mathbf{r}) = \phi(\mathbf{r} - \mathbf{r}_i)$ and spinor χ_σ, where $\sigma \in \{\uparrow, \downarrow\}$ and $\mathbf{r}_i$ is the center position of the i-th lattice site. A general many-body Hamiltonian $H = T + V$, consisting of the spin-independent single-particle operator $T = \sum_{\alpha=1}^{N} t_\alpha$ and the two-particle operator $V = \frac{1}{2}\sum_{\alpha\neq\beta} v(\mathbf{r}_\alpha - \mathbf{r}_\beta)$, can be represented in the basis $\{\phi_{i,\sigma}\}$ by

$$H = \sum_{i,j}\sum_{\sigma} t_{ij}\, c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{1}{2}\sum_{i,j,k,l}\sum_{\sigma,\sigma'} V_{ijkl}\, c^\dagger_{i,\sigma} c^\dagger_{j,\sigma'} c_{l,\sigma'} c_{k,\sigma},$$

where we defined the matrix elements $t_{ij} = \langle i|T|j\rangle$ and $V_{ijkl} = \langle ij|V|kl\rangle$. Assuming that the overlap of the wave functions $\phi_i(\mathbf{r})$ from different lattice sites is very small, we can apply the following approximation:

$$t_{ij} = \begin{cases} w & \text{for } i = j, \\ -t & \text{for } i \text{ and } j \text{ neighboring}, \\ 0 & \text{otherwise}, \end{cases}$$

as well as

$$V_{ijkl} = U\delta_{ij}\delta_{il}\delta_{jk} \qquad \text{with} \qquad U = \int \mathrm{d}^3x \int \mathrm{d}^3y\, |\phi_i(\mathbf{x})|^2\, v(\mathbf{x},\mathbf{y})\, |\phi_i(\mathbf{y})|^2 .$$

a) Determine the matrix elements U for a contact interaction

$$v(\mathbf{r}_\alpha - \mathbf{r}_\beta) = \lambda\delta(\mathbf{r}_\alpha - \mathbf{r}_\beta)$$

between fermions. To this end, consider a lattice with lattice constant a and assume that the wave function $\phi(\mathbf{r})$ is well approximated by the ground state wave function of a harmonic oscillator $\phi(\mathbf{r}) = \frac{1}{\Delta^{3/2}\pi^{3/4}} \exp\left[-\mathbf{r}^2/(2\Delta^2)\right]$. Why is it a good approximation?

b) Why do we write w, but $-t$ (i.e. with a minus)? What is the physical meaning of the two parameters?

c) Next, determine the ground state of a one dimensional lattice at half filling, i.e., with one particle per lattice site on average. First, consider the case $U = 0$. Then the ground state is given by the Fermi sea. Calculate the ground state energy in this case. For small interactions $U \ll t$, the ground state is still given by the Fermi sea. Derive corrections to the ground-state energy within first order perturbation theory.

Note: Here, "half filling" means, that there is one particle per lattice site. The "full filling" would mean that there are two particles per lattice site.

d) Consider now the case of $t = 0$. What is the ground state in this regime and what is the ground state energy? This ground state is called Mott insulator. Why is the ground state degenerate? What is the energy gap separating the Mott insulator state from excited states with one doubly occupied site. To derive leading corrections to the ground state energy, we could consider the perturbation theory for $t \ll U$. Sketch the derivation and estimate the leading corrections to the energy.

What could we conclude from above analysis about a phase transition between a metal for small interactions and an insulator for large interactions?

Exercise 2: The pair correlation function of a Fermi Sea (Written, 4pts)

Consider the gas of N identical fermions with spin 1/2. The fermions are free and non-interacting. The pair correlation function describes the relative probability of finding an electron at the position $\mathbf{r}'$ in the spin state s', when we know that the second electron is at the position $\mathbf{r}$ in the spin state s. The pair correlation function $g_{ss'}(\mathbf{r} - \mathbf{r}')$ is defined as

$$\left(\frac{n}{2}\right)^2 g_{ss'}(\mathbf{r} - \mathbf{r}') = \left\langle \Phi_0 \middle| \Psi_s^\dagger(\mathbf{r}) \Psi_{s'}^\dagger(\mathbf{r}') \Psi_{s'}(\mathbf{r}') \Psi_s(\mathbf{r}) \middle| \Phi_0 \right\rangle . \tag{1}$$

Where $|\phi_0\rangle$ is the ground state of fermions is the Fermi sea with a total density $n = n_\uparrow + n_\downarrow$ and therefore $n_\uparrow = n_\downarrow = n/2$.

a) Express the field operators in the natural basis, i.e.,

$$\Psi_s(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} c_{\mathbf{p}s}, \tag{2}$$

where $c_{\mathbf{k}s}^\dagger$ and $c_{\mathbf{k},s}$ are the creation and annihilation operators, respectively. Then, expectation values of the form

$$\left\langle \Phi_0 \middle| c_{\mathbf{p}s}^\dagger c_{\mathbf{q}s}^\dagger c_{\mathbf{q}'s'} c_{\mathbf{p}'s'} \middle| \Phi_0 \right\rangle . \tag{3}$$

occur. Compute these expectation values explicitly. What conditions on p, p', q, q' and s, s' have to be satisfied so that the amplitudes are nonzero?

b) Next, consider the case $s \neq s'$ and use the above result to calculate explicitly the pair correlation function.

c) Now, consider the interesting case of $s = s'$ and determine the pair-correlation function. Sketch the result.

d) Show that the size of the dip in the correlation function corresponds to the displacement of one electron.