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## Problem 12.1: Interactions in first and second quantization

[**Written** | 6 pt(s)]

ID: ex_first_vs_second_quant_interaction:aqt2324

**Learning objective**

The second quantization is a formalism for simplifying many body problems of identical particles. Nevertheless, these problems can also be treated in first quantization. Since both formalisms are equivalent, they should yield the same result. In this problem you show this explicitly for the example of a two-particle interaction operator. While doing so, you might appreciate the simple notation in the second quantization formalism.

We consider three identical bosonic particles with the single particle wave functions $\phi_\alpha(x_i) = \langle x_i|\alpha\rangle$ of particle $i$ at position $x_i$. Furthermore, we only consider four orthonormal states $|\alpha\rangle$ with $\alpha \in \{1, 2, 3, 4\}$.

a) Write down the symmetrized and normalized wavefunctions in first quantization for: **2** pt(s)
(i) $\Psi(x_1, x_2, x_3)$ with one particle in each of the states $\alpha = 1, 2, 3$
(ii) $\varphi_1(x_1, x_2, x_3)$ with two particles in state $\alpha = 1$ and one particle in $\alpha = 2$ and
(iii) $\varphi_2(x_1, x_2, x_3)$ with one particle in each of the states $\alpha = 1, 2, 4$.

Now consider an interaction

$$V = \frac{1}{2}\sum_{i\neq j} V_{ij}\,, \tag{1}$$

where the entries of the symmetric two-particle interaction operators $V_{ij} = V_{ji}$ are given by

$$\langle\alpha\beta|\, V_{ij}\, |\gamma\delta\rangle = \int dx_i dx_j \phi^*_\alpha(x_i)\phi^*_\beta(x_j)V(x_i, x_j)\phi_\gamma(x_i)\phi_\delta(x_j) = V_{\alpha\beta,\gamma\delta}\,. \tag{2}$$

b) Calculate the interaction strength $\langle\Psi|\, V\, |\varphi\rangle$ in first quantization for $\varphi_1$ and $\varphi_2$. **2** pt(s)
**Hint:** Start by calculating $\langle\Psi|\, V_{12}\, |\varphi\rangle$.
How many terms are there in total and which of these terms are nonzero?

Now we introduce the second quantization. In this formalism the interaction can be written as

$$V = \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} V_{\alpha\beta,\gamma\delta}\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma\,, \tag{3}$$

where $a_\alpha$ ($a^\dagger_\alpha$) is the annihilation (creation) operator of a particle in the mode $\alpha$.

c) Write the states $\Psi$, $\varphi_1$ and $\varphi_2$ in second quantization and calculate the interaction strengths $\langle\Psi|\, V\, |\varphi\rangle$ in this formalism. **2** pt(s)

## Problem 12.2: The Fermi-Hubbard model

[**Oral** | 4 (+2 bonus) pt(s)]

ID: ex_fermi_hubbard:aqt2324

**Learning objective**

This problem studies the Fermi-Hubbard model describing interacting fermions in a lattice and gives a very important application of many-body theory in quantum mechanics in the framework of second quantization. Despite its simple Hamiltonian, it features rich physics and is subject to ongoing research both in experimental and theoretical physics. Among others, it is of particular interest as a model for high-temperature superconductivity.

In this problem, 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

$$H = -t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \, , \tag{4}$$

where $c^\dagger_{i,\sigma}, c_{i,\sigma}$ are the creation and annihilation operators of fermions with spin $\sigma$ localized at some lattice site with index $i$, respectively. The first term of the Hamiltonian refers to the kinetic energy and describes fermions hopping from lattice site $i$ to lattice site $j$ gaining energy $t$, the sum is restricted to nearest-neighbor sites, which is 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 following, determine the ground state of this system at half filling in the limits $t = 0$ and $U = 0$. Half filling means that there is one particle per lattice site, while full filling means that there are two particles per site. For simplicity, consider a one-dimensional lattice with lattice spacing $a$. You may assume periodic boundary conditions.

a) First, consider the case $U = 0$, where the ground state is given by the Fermi sea and calculate the ground state energy in this case. **2pt(s)**
**Hint:** Apply a basis transformation from the site basis to plain waves, i.e.

$$c_{i,\sigma} = \frac{1}{\sqrt{L}} \sum_k e^{-ikx_i} c_{k,\sigma}, \qquad c^\dagger_{i,\sigma} = \frac{1}{\sqrt{L}} \sum_k e^{ikx_i} c^\dagger_{k,\sigma}. \tag{5}$$

Note that this corresponds to Fourier transformation. Then, diagonalize the Hamiltonian in momentum space.

b) Now study the case where $t = 0$. What is the ground state in this regime and what is the ground state energy? The ground state is called Mott insulator and is highly degenerate (why?). What is the energy gap separating the Mott insulator state from the excited states with one doubly occupied site? **2pt(s)**

*c) Discuss your results in the context of a phase transition between a metal for small interactions and an insulator for large interactions. **+2pt(s)**

## Problem 12.3: The pair correlation function of a Fermi Sea [**Oral** | 6 pt(s)]

ID: ex_fermi_sea_correlation:aqt2324

**Learning objective**

In this problem, you apply your knowledge of calculating expectation values of fermionic operators in second quantization to determine the pair correlation function of non-interacting fermions in free space.

Consider a gas of $N$ identical non-interacting fermions with spin $1/2$ in free space. The pair correlation function $g_{\sigma\sigma'}(\boldsymbol{r}-\boldsymbol{r}')$ is defined as

$$g_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') = \left(\frac{2}{n}\right)^2 \langle\Phi_0|\, \Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})\,|\Phi_0\rangle\,, \tag{6}$$

where $|\Phi_0\rangle$ is the Fermi sea with a total density $n = n_\uparrow + n_\downarrow$ and $n_\uparrow = n_\downarrow$. The pair correlation function describes the conditional probability of finding an electron at the position $\mathbf{r}'$ in the spin state $\sigma'$, when we know that the second electron is at the position $\mathbf{r}$ in the spin state $\sigma$.

a) Express the field operators in the natural basis, that is, **2pt(s)**

$$\Psi_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\sum_{\boldsymbol{p}} e^{i\boldsymbol{p}\cdot\boldsymbol{r}} c_{\boldsymbol{p}\sigma}\,, \tag{7}$$

where $c^\dagger_{\mathbf{p}\sigma}$ and $c_{\mathbf{p}\sigma}$ are the creation and annihilation operators of a fermion with momentum $\mathbf{p}$ and spin $\sigma$, respectively. In the course of calculating the pair correlation function, expectation values of the form

$$\langle\Phi_0|\, c^\dagger_{\mathbf{p}\sigma}c^\dagger_{\mathbf{q}\sigma'}c_{\mathbf{q}'\sigma'}c_{\mathbf{p}'\sigma}\,|\Phi_0\rangle \tag{8}$$

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

b) Next, consider the case $\sigma \neq \sigma'$ and use the above results to calculate explicitly the pair correlation function. **2pt(s)**

c) Finally, consider the interesting case of $\sigma = \sigma'$ and determine the pair-correlation function. Sketch the result. **2pt(s)**