University of Regensburg, Physics Department SS 2006

Assignments to Condensed Matter Theory I
Sheet 10

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sheet online: http://www-MCG.uni-R.de/teaching/

Problem set: Electron-Electron Interaction

10.1. Occupation number representation

Let us consider a fermionic system with two single particle states $|\phi_1\rangle$ and $|\phi_2\rangle$ that span the (two-dimensional) single particle Hilbert space.

(a) Which dimension has the two-particle Hilbert space? Which dimension has the Fock space? Write down the form of the basis of the Fock space explicitly as Slater determinants of the states ϕ_1, ϕ_2 and in the occupation number representation.

(b) Calculate in this basis the matrix representation of the creation and annihilation operators c_i, $c_i^\dagger$ $(i = 1, 2)$ and also of the occupation operators $n_i = c_i^\dagger c_i$

(c) Calculate the anticommutator relations

$$[c_i, c_j]_+ = [c_i^\dagger, c_j^\dagger]_+ = 0\,; \quad [c_i, c_j^\dagger]_+ = \delta_{ij}$$

explicitly using matrix multiplication of the matrices calculated at point (b).

(d) Consider an Hamilton operator

$$H = T + V$$

where T is a single particle operator and V a two particle one. With respect to the single particle basis $|\phi_i\rangle$ the matrix elements are:

$$\langle\phi_i|T|\phi_i\rangle = \epsilon\,; \quad \langle\phi_i|T|\phi_j\rangle = t \text{ for } i \neq j$$
$${}^{(1)}\langle\phi_1|^{(2)}\langle\phi_2|V|\phi_2\rangle^{(2)}|\phi_1\rangle^{(1)} = U\,; \quad {}^{(1)}\langle\phi_1|^{(2)}\langle\phi_2|V|\phi_1\rangle^{(2)}|\phi_2\rangle^{(1)} = J$$

where the notation is such that, *e.g.*:

$${}^{(1)}\langle\phi_1|^{(2)}\langle\phi_2|V|\phi_1\rangle^{(2)}|\phi_2\rangle^{(1)} \equiv \frac{1}{V^2}\int \mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2\phi_1^*(\mathbf{r}_1)\phi_2^*(\mathbf{r}_2)V(\mathbf{r}_1,\mathbf{r}_2)\phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)$$

Write the operator H in second quantization and in the matrix representation (starting from the single particle basis introduced). Calculate the eigenvalues and eigenvectors for H.

(e) Again, write H in second quantization, but this time as a single particle basis use the eigenvectors of T. Which is the connection between this creation and annihilation operators and the ones considered in the points (a)-(d)? Is this a unitary transformation?

10.2. Wick's theorem

(a) Show that, for a system of non-interacting fermions described by the Hamiltonian in the eigenvalue basis

$$H = \sum_\alpha \epsilon_\alpha c^\dagger_\alpha c_\alpha,$$

the following relation for the many-body grancanonical expectation values holds:

$$\langle c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} c_{\alpha_3} c_{\alpha_4} \rangle = \langle c^\dagger_{\alpha_1} c_{\alpha_4} \rangle \langle c^\dagger_{\alpha_2} c_{\alpha_3} \rangle \delta_{\alpha_1\alpha_4} \delta_{\alpha_2\alpha_3} - \langle c^\dagger_{\alpha_1} c_{\alpha_3} \rangle \langle c^\dagger_{\alpha_2} c_{\alpha_4} \rangle \delta_{\alpha_1\alpha_3} \delta_{\alpha_2\alpha_4},$$

where

$$\langle c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} c_{\alpha_3} c_{\alpha_4} \rangle \equiv \frac{1}{Z} \mathrm{Tr} \left\{ c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} c_{\alpha_3} c_{\alpha_4} \exp[-\beta(H - \mu N)] \right\}$$

and Z is the grancanonical partition function. The trace is taken over the full Fock space.

(b) Derive from point (a) that, for non-interacting fermions, in every other given single particle basis $\{|n\rangle\}$ the following relation holds:

$$\langle c^\dagger_{n_1} c^\dagger_{n_2} c_{n_3} c_{n_4} \rangle = \langle c^\dagger_{n_1} c_{n_4} \rangle \langle c^\dagger_{n_2} c_{n_3} \rangle - \langle c^\dagger_{n_1} c_{n_3} \rangle \langle c^\dagger_{n_2} c_{n_4} \rangle.$$

Note that this is valid even if in this basis the Hamiltonian

$$H = \sum_{n,m} t_{nm} c^\dagger_n c_m$$

would contain non-diagonal terms t_{nm} for $n \neq m$.

Hint: Diagonalize first H using a unitary transformation $c_n = \sum_\alpha u_{n\alpha} c_\alpha$. Apply then the equation proved in point (a). Finally perform the canonical transformation in the opposite direction.

10.3. [Kür] Model of two interacting particles in 1D

Let us consider two interacting particles to model a helium atom in 1D. In properly chosen dimensionless coordinates, write the first quantization Hamiltonian as:

$$H = -\frac{d^2}{dx_1^2} - 2V(|x_1|) - \frac{d^2}{dx_2^2} - 2V(|x_2|) + V(|x_1 - x_2|)$$

where

$$V(x) = \frac{2}{x + \delta}$$

is the "truncated" one dimensional Coulomb potential. The factor of two in the single particle potential is due to the double positive charge of the "Helium" nucleus.

(a) Calculate the Hamiltonian in second quantization in the form:

$$H = \sum_{i,\sigma} \epsilon_i c^\dagger_{i\sigma} c_{i\sigma} + \frac{1}{2} \sum_{i_1 i_2 i_3 i_4, \sigma\sigma'} u_{i_1 i_2 i_3 i_4} c^\dagger_{i_1\sigma} c^\dagger_{i_2\sigma'} c_{i_3\sigma'} c_{i_4\sigma}$$

relative to the basis $|i\rangle$ of the eigenvectors of the single particle Hamiltonian. The single particle eigenfunctions $\phi_i(x) = \langle x|i\rangle$ fulfill the Schrödinger equation:

$$\left(-\frac{d^2}{dx^2} - 2V(|x|)\right)\phi_i(x) = \epsilon_i \phi_i(x).$$

In other words you have to calculate the eigenvalues ϵ_i and the Coulomb matrix elements u for $i, i_l \in \{1, 2\}$ numerically.

`Hint:` For the numerical calculation discretize the space $x \to x_n$ with $n = 1, \ldots, N$. Now the wave-function is a vector since $\phi(x) \to \phi(x_n)$. The discrete version of the derivative now reads $\phi'(x_n) = (\phi(x_{n+1}) - \phi(x_{n+1}))/(x_{n+1} - x_n)$. Work out analogously the second derivative and, finally, remember that the potential operator acts locally $(V\phi)(x) = V(x)\phi(x)$. Put all together and you have transformed the single particle Schrödinger equation into an algebraic equation that can be solved numerically.

(b) Calculate the lowest energy two-particle eigenstates exactly and in Hartree-Fock approximation under the assumption that you can consider only the lowest single particle quantum number (that is $i, i_l \in \{1, 2\}$). Treat separately the singlet- (antiparallel spins, "ortho-helium") and the triplet-case (total spin 1, "para-helium").