University of Regensburg Summer Term 2014

Quantum Theory of Condensed Matter I

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Sheet 8

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1. Wick's theorem

1. Show that, for a system of non-interacting fermions described by the Hamiltonian in the energy basis

$$\hat{H} = \sum_{\alpha} \epsilon_\alpha \hat{c}^\dagger_\alpha \hat{c}_\alpha \left(= \sum_{i=1}^{N} \hat{h}_i \right)$$

the following relation for the many-body grandcanonical expectation value holds:

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

where

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

and Z is the grandcanonical partition function. The trace is taken over the full Fock space. Hint: Consider the use of the eigenbasis of $\hat{h}$. **(2 Points)**

2. Derive from 1.1 that, for noninteracting fermions, in every other given single particle basis $\{|n\rangle\}$ the following relation holds:

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

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

$$\hat{H} = \sum_{n,m} h_{nm} \hat{c}^\dagger_n \hat{c}_m$$

would contain non-diagonal terms, h_{nm} for $n \neq m$. Hint: Diagonalize H first, using a unitary transformation $\hat{c}_n = \sum_\alpha u_{n\alpha} \hat{c}_\alpha$. Apply the equation proven in 1.1. Finally perform the canonical transformation in the reverse direction. **(2 Points)**

2. Spectrum of a many-body Hamiltonian

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

1. Consider the Hamilton operator

$$\hat{H} = \hat{T} + \hat{V}\,,$$

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

$$\langle \phi_i | \,\hat{T}\, |\phi_i\rangle = \epsilon\,, \quad \langle \phi_i | \,\hat{T}\, |\phi_j\rangle = t \text{ for } i \neq j$$
$$\langle \phi_1, \phi_2 | \,\hat{V}\, |\phi_1, \phi_2\rangle = U\,, \quad \langle \phi_1, \phi_2 | \,\hat{V}\, |\phi_2, \phi_1\rangle = J$$

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

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

Remember that in second quantization a single and two particle operators are respectively written as:

$$\hat{T} = \sum_{\lambda,\mu} c_\lambda^\dagger \langle \phi_\lambda | \hat{T} | \phi_\mu \rangle c_\mu \, , \quad \hat{V} = \frac{1}{2} \sum_{\lambda\mu\lambda'\mu'} c_\lambda^\dagger c_\mu^\dagger \langle \phi_\lambda, \phi_\mu | \hat{V} | \phi_{\lambda'}, \phi_{\mu'} \rangle c_{\mu'} c_{\lambda'} \, ,$$

where $|\phi_\lambda\rangle$ represent a generic single particle basis and $c_\lambda^\dagger$ the corresponding creation operator. Write the operator $\hat{H}$ in second quantization and in the matrix representation (starting from the single particle basis introduced). Calculate the eigenvalues and eigenvectors for $\hat{H}$. **(2 Points)**

2. **(Oral)** Again, write $\hat{H}$ in second quantization, but this time as a single particle basis use the eigenvectors of $\hat{T}$. Compute explicitly the matrix that connects the many-body basis generated in point 2.1 and the one obtained from the eigenstates of $\hat{T}$. Finally, extend the result to the general case of an arbitrary number of orbitals, by proving the following relation:

$$\langle \{n_\alpha\} | \{n_\ell\} \rangle = \det \left(M_{\{n_\alpha\},\{n_\ell\}} \right)$$

where $\{n_\alpha\}$ ($\{n_\ell\}$) is a string of (0 or 1) occupation numbers in the single particle basis labeled by the quantum number α (ℓ), $M_{\alpha\ell}$ is the unitary matrix connecting the two single particle bases and $M_{\{n_\alpha\},\{n_\ell\}}$ indicates the sub-matrix obtained extracting only the elements of M for which $n_\alpha = n_\ell = 1$.

Frohes Schaffen!