Quantentheorie II

Prof. Milena Grifoni Dr. Andrea Donarini

Blatt 8

1. Occupation number representation

Let us consider a fermionic system with two single particle states $|\phi_1\rangle$ and $|\phi_2\rangle$ (for simplicity we neglect the spin degree of freedom) that span the (two-dimensional) *one*-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 wave functions $\phi_1(\mathbf{r})$, $\phi_2(\mathbf{r})$ and in the occupation number representation. (**2 Points**)

b) • Calculate, in the Fock basis, the matrix representation of the creation and annihilation operators c_i, $c_i^\dagger$ $(i = 1, 2)$ and also of the occupation operators $n_i = c_i^\dagger c_i$. *Hint*: Remember that, in the occupation representation, one state is unambiguously defined only when a precise ordering is given for the involved creation operators. (**3 Points**)

c) • Verify the anti-commutator 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). (**2 Points**)

d) • Consider a 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 $\hat{H}$. (**3 Points**)

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

Return the solution of the exercises marked with • by Monday 8th of December at 10:00.