

Übungen zur Computational Nanoscience

– Blatt 12 –

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Aufgabe 1) Creation and annihilation operators

Proof the following relations for the fermionic creation $\hat{a}_i^\dagger$ and annihilation $\hat{a}_i$ operators and the particle number operator $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$:

- $\hat{n}_i^2 = \hat{n}_i$
- $\hat{a}_i \hat{n}_i = \hat{a}_i$
- $\hat{a}_i^\dagger \hat{n}_i = 0$
- $\hat{n}_i \hat{a}_i = 0$
- $\hat{n}_i \hat{a}_i^\dagger = \hat{a}_i^\dagger$

Aufgabe 2) Matrix elements

Calculate the matrix element of bosonic and fermionic operators over the vacuum state $|0\rangle$

$$\langle 0 | \hat{a}_i \hat{a}_j \hat{a}_k^\dagger \hat{a}_m^\dagger | 0 \rangle$$

Aufgabe 3) Coulomb Interaction

Using the general representation of the two-particle interaction in the field operators:

$$H_{int} = \frac{1}{2} \int d^3r d^3r' \hat{\Psi}(\vec{r})^\dagger \hat{\Psi}(\vec{r}')^\dagger U(\vec{r} - \vec{r}') \hat{\Psi}(\vec{r}') \hat{\Psi}(\vec{r}).$$

show that the Coulomb interaction $U = \frac{1}{|\vec{r} - \vec{r}'|}$ (in a.u.) for spinless fermions has the following form in impulse $\vec{k}$ -space:

$$H_{int} = \frac{1}{2V} \sum_{\vec{k}, \vec{k}', \vec{q}} U_{\vec{q}} \hat{a}_{\vec{k}+\vec{q}}^\dagger \hat{a}_{\vec{k}'}^\dagger \hat{a}_{\vec{k}'} \hat{a}_{\vec{k}-\vec{q}}$$