

Quantum Mechanics II

Exercise 6: Second quantization. N -body problems.

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1. Express two-particle operator $\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} \hat{f}^{(2)}(x_\alpha; x_\beta)$ in terms of creation and annihilation operators for the case of bosons as well as fermions.

Reminder: $\sum_{\alpha=1}^N |i\rangle_\alpha \langle j|_\alpha = a_i^\dagger a_j$.

2. Show that the number operator $\hat{N} = \sum_i \hat{a}_i^\dagger \hat{a}_i$ (for bosons and fermions) commutes with the Hamiltonian

$$\hat{H} = \sum_{ij} \hat{a}_i^\dagger \langle i|T|j\rangle \hat{a}_j + \frac{1}{2} \sum_{ijkm} \hat{a}_i^\dagger \hat{a}_j^\dagger \langle ij|V|km\rangle \hat{a}_m \hat{a}_k.$$

3. Is the sum of ionization energies found by Hartree approximation equal to the total energy (binding energy of atom)?
4. Beryllium atom ($Z = 4$)

- a) Find the fundamental state of the neutral atom (write down the state using Slater determinant).
- b) Write down Hartree-Fock equations taking into account only kinetic energy of electrons and Coulomb's interaction. Explicit the exchange and coulomb's terms. How many independent equations exist for the fundamental state?
- c) Show that Hartree-Fock equations depend only on the radial coordinate.

Reminder:

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{l=0}^{\infty} \frac{r_m^l}{r_M^l} P_l(\cos \theta),$$

where $r_m = \min(|\mathbf{r}|, |\mathbf{r}'|)$, $r_M = \max(|\mathbf{r}|, |\mathbf{r}'|)$, and the angle between \mathbf{r} and \mathbf{r}' is denoted as θ . Functions $P_l(x)$ obey

$$\int_{-1}^1 P_l(x) dx = 2\delta_{0l}.$$

- d) Discuss qualitatively the neutral Be atom in an excited state.