Quantum Mechanics II

Exercise 4: Second quantization. N-body problems.

12 October 2016

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) commute 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. How many independent equations exist for the fundamental state? Explicit the exchange and coulomb's terms.

   c) Show that Hartree-Fock equations depend only on the radial coordinate. Clue:

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

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