Advanced Quantum Theory

WS 13/14

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Problem Set 5 (due Monday, 18.11.2013 in the lecture)

Questions

(Q1) Why need wavefunctions of identical particles either be symmetric or antisymmetric?

(Q2) How does the "exchange interaction energy" $K_{n\ell}$ in the He-example of the lecture arise? Give a simple physical argument why $K_{n\ell} > 0$.

(5.1) spin *(4 points)*

(i) Consider two spin-1/2 particles. Show explicitly that the total spin is 0 for the singlet-state $(|+-\rangle - |-+\rangle)/\sqrt{2}$ and 1 for the triplet-states $|++\rangle$, $(|+-\rangle + |-+\rangle)/\sqrt{2}$, and $|--\rangle$.

(ii) Show that

$$\hat{P}_1 = \frac{3}{4} + \frac{1}{\hbar^2}\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2$$

projects onto the triplet sub-space.

(5.2) total orbital momentum *(4 points)*

Consider the total orbital angular momentum of the two electrons in He,

$$\hat{\boldsymbol{L}} = \hat{\boldsymbol{l}}_1 + \hat{\boldsymbol{l}}_2.$$

Show that L and M_L are "good quantum numbers" (spin-orbit coupling neglected).
Hint: Show that

$$\left[\hat{\boldsymbol{L}}, \frac{1}{|\hat{\boldsymbol{r}}_1 - \hat{\boldsymbol{r}}_2|}\right] = \mathbf{0},$$

i.e., any component of $\hat{\boldsymbol{L}}$ commutes with $\frac{1}{|\hat{\boldsymbol{r}}_1 - \hat{\boldsymbol{r}}_2|}$.

*Why is this sufficient to prove that L and M_L are "good quantum numbers"?

(5.3) correction due to finite nuclear mass *(2 points)*

The He atom is actually a three-body problem:

$$\hat{H} = \frac{\hat{\boldsymbol{p}}_{\mathrm{n}}^2}{2M} + \frac{\hat{\boldsymbol{p}}_1^2}{2m} + \frac{\hat{\boldsymbol{p}}_2^2}{2m} + \hat{V}(|\hat{\boldsymbol{r}}_1 - \hat{\boldsymbol{R}}|, |\hat{\boldsymbol{r}}_2 - \hat{\boldsymbol{R}}|, |\hat{\boldsymbol{r}}_1 - \hat{\boldsymbol{r}}_2|)$$

with $\hat{\boldsymbol{p}}_{\mathrm{n}}$ the momentum of the nucleus, $\hat{\boldsymbol{p}}_i$, $i = 1, 2$ the momenta of the electrons, $\hat{\boldsymbol{R}}$ the position of the nucleus, $\hat{\boldsymbol{r}}_i$ the positions of the electrons, and M (m) the mass of the nucleus (an electron). $\hat{V}$ collects all potential terms (attraction between electrons and nucleus and repulsion between the electrons).

Write down the Hamiltonian in center-of-mass and relative electron-electron and electron-nucleus coordinates. Write the Hamiltonian as the infinite-nuclear-mass Hamiltonian plus corrections.