Advanced Quantum Theory
WS 15/16

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Problem Set 8 (due Monday, 07.12.2015 in the lecture)

Questions

(Q1) What is ferromagnetism and what has the Heisenberg exchange operator to do with it?

(Q2) Why can it be advantageous to introduce creation and annihilation operators for holes (i.e., "defect electrons") instead of describing the electrons?

(Q3) How would the part of a second-quantized electron-hole Hamiltonian look that describes the transition of an electron from the valence to the conduction band (or *vice versa*)?

(8.1) Constructing a spin algebra *(2 points)*

$\hat{a}^\dagger_\pm$ and $\hat{a}_\pm$ create and annihilate a fermion of spin 1/2 at a given lattice site, respectively. Using (anti-) commutator relations, show that $\hat{s}_x$, $\hat{s}_y$, $\hat{s}_z$ defined via

$$\hat{s}_\pm = \hat{s}_x \pm \mathrm{i}\hat{s}_y = \hbar \hat{a}^\dagger_\pm \hat{a}_\mp$$

together with

$$\hat{s}_z = \frac{\hbar}{2}(\hat{n}_+ - \hat{n}_-), \qquad \hat{n}_\pm = \hat{a}^\dagger_\pm \hat{a}_\pm$$

satisfy indeed the angular momentum relations

$$[\hat{s}_x, \hat{s}_y] = -\frac{\hbar}{\mathrm{i}}\hat{s}_z \qquad \text{(and cyclic)},$$

as claimed in the lecture.

(8.2) Heisenberg exchange operator I *(2 points)*

Show that

$$\hat{H}^{\mathrm{A}}_{\mathrm{int}} = \frac{1}{2}\sum_{n_1 \neq n_2}\sum_{m_1 m_2} \hat{a}^\dagger_{n_1 m_1}\hat{a}^\dagger_{n_2 m_2} K_{n_1 n_2} \hat{a}_{n_1 m_2}\hat{a}_{n_2 m_1}$$

can indeed be written as

$$\hat{H}^{\mathrm{A}}_{\mathrm{int}} = -\sum_{n_1 \neq n_2} K_{n_1 n_2}\left(\frac{1}{\hbar^2}\hat{\mathbf{s}}_{n_1}\cdot\hat{\mathbf{s}}_{n_2} + \frac{1}{4}\hat{1}\right),$$

as claimed in the lecture.

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(8.3) HEISENBERG EXCHANGE OPERATOR II *(3 points)*

First, show that $\hat{H}^{\mathrm{A}}_{\mathrm{int}}$ can be written exclusively in terms of the spin-1/2 ladder operators (and unity):

$$\hat{H}^{\mathrm{A}}_{\mathrm{int}} = -\sum_{n_1 \neq n_2} K_{n_1 n_2} \left(\frac{1}{\hbar^4} \hat{s}_{n_1+}\hat{s}_{n_1-}\hat{s}_{n_2+}\hat{s}_{n_2-} - \right.$$
$$\left. + \frac{1}{2\hbar^2} \left(\hat{s}_{n_1+}\hat{s}_{n_2-} + \hat{s}_{n_1-}\hat{s}_{n_2+} - \hat{s}_{n_1+}\hat{s}_{n_1-} - \hat{s}_{n_2+}\hat{s}_{n_2-} \right) + \frac{1}{8}\hat{1} \right).$$

Second, show that the state $|- - - - - - \cdots\rangle$ (meaning "spins down at all lattice sites") is an eigenstate of $\hat{H}^{\mathrm{A}}_{\mathrm{int}}$ and determine its eigenenergy.

Useful: For any given lattice site $\hat{s}_-\hat{s}_+ + \hat{s}_+\hat{s}_- = \hbar^2\hat{1}$ (why?) and $\hat{s}_- \left|-\right\rangle = 0$.

(8.4) HARTREE-FOCK DERIVED IN SECOND QUANTIZATION *(3 points)*

Starting from the general, second-quantized Hamiltonian (see lecture notes, section 4.6)

$$\hat{H} = \sum_{kk'} \hat{a}^\dagger_k \hat{a}_{k'} \int \mathrm{d}x\, \varphi^*_k(x) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \right) \varphi_{k'}(x)$$
$$+ \frac{1}{2} \sum_{kk'll'} \hat{a}^\dagger_k \hat{a}^\dagger_{k'} \hat{a}_{l'} \hat{a}_l \int \mathrm{d}x \int \mathrm{d}x'\, \varphi^*_k(x)\varphi^*_{k'}(x') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \varphi_{l'}(x')\varphi_l(x),$$

show that

$$E[\Phi] = \langle \Phi^- | \hat{H} \left| \Phi^- \right\rangle$$
$$= \sum_{j=1}^{N} \int \mathrm{d}x\, \varphi^*_{k_j}(x) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \right) \varphi_{k_j}(x)$$
$$+ \frac{1}{2} \sum_{i,j} \int \mathrm{d}x \int \mathrm{d}x'\, \varphi^*_{k_j}(x)\varphi^*_{k_i}(x') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \varphi_{k_i}(x')\varphi_{k_j}(x)$$
$$- \frac{1}{2} \sum_{i,j} \int \mathrm{d}x \int \mathrm{d}x'\, \varphi^*_{k_j}(x)\varphi^*_{k_i}(x') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \varphi_{k_j}(x')\varphi_{k_i}(x),$$

where $|\Phi^-\rangle = \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\ldots\hat{a}^\dagger_{k_N}|0\rangle = \left|k_1k_2\ldots k_N^-\right\rangle$ is a general, antisymmetrized many-body state.

* Show that $\frac{\delta E}{\delta \varphi^*_{k_l}} = 0$ then yields the Hartree-Fock equations.