

**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)

$\hat{a}_\pm^\dagger$  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

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

together with

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

satisfy indeed the angular momentum relations

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

as claimed in the lecture.

(8.2) HEISENBERG EXCHANGE OPERATOR I (2 points)

Show that

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

can indeed be written as

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

as claimed in the lecture.

*cont'd overleaf*

## (8.3) HEISENBERG EXCHANGE OPERATOR II

(3 points)

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

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

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

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

## (8.4) HARTREE-FOCK DERIVED IN SECOND QUANTIZATION

(3 points)

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

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

show that

$$\begin{aligned} E[\Phi] &= \langle \Phi^- | \hat{H} | \Phi^- \rangle \\ &= \sum_{j=1}^N \int dx \varphi_{k_j}^*(x) \left( -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \varphi_{k_j}(x) \\ &\quad + \frac{1}{2} \sum_{ij} \int dx \int dx' \varphi_{k_j}^*(x) \varphi_{k_i}^*(x') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \varphi_{k_i}(x') \varphi_{k_j}(x) \\ &\quad - \frac{1}{2} \sum_{ij} \int dx \int dx' \varphi_{k_j}^*(x) \varphi_{k_i}^*(x') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \varphi_{k_j}(x') \varphi_{k_i}(x), \end{aligned}$$

where  $|\Phi^- \rangle = \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \dots \hat{a}_{k_N}^\dagger |0\rangle = |k_1 k_2 \dots k_N^- \rangle$  is a general, antisymmetrized many-body state.

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