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8.512 Theory of Solids II  
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## 8.512 Theory of Solids

### Problem Set 7

Due April 13, 2004

1. Show that within the Heitler-London approximation for two hydrogen-like atoms located at  $R_a$  and  $R_b$ , the singlet and triplet variational energies are given by

$$E_{s,t} = E_a + E_b + \frac{V \pm I}{I \pm l^2}$$

where  $l = \int d\mathbf{r} \phi_a^*(\mathbf{r}) \phi_b^*(\mathbf{r})$  is the overlap integral,

$$V = \int d\mathbf{r}_1, d\mathbf{r}_2 |\phi_a(\mathbf{r}_1) \phi_b(\mathbf{r}_2)|^2 (\Delta H)$$

and  $I$  is the exchange integral

$$I = \int d\mathbf{r}, d\mathbf{r}_2, \phi_a^*(\mathbf{r}_1) \phi_b^*(\mathbf{r}_2) \phi_b(\mathbf{r}_1) \phi_a(\mathbf{r}_2) (\Delta H)$$

where

$$\Delta H = \frac{e^2}{R_{ab}} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2a}} .$$

2. Problem 5, p.723 from Ashcroft and Mermin

#### 5. Anisotropic Heisenberg Model

Consider the anisotropic Heisenberg spin Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} [J_z(\mathbf{R} - \mathbf{R}') \mathbf{S}_z(\mathbf{R}) \mathbf{S}_z(\mathbf{R}') + J(\mathbf{R} - \mathbf{R}') \mathbf{S}_\perp(\mathbf{R}) \cdot \mathbf{S}_\perp(\mathbf{R}')] \quad (33.71)$$

with  $J_z(\mathbf{R} - \mathbf{R}') > J(\mathbf{R} - \mathbf{R}') > 0$ .

- (a) Show that the ground state (33.5) and one-spin-wave states (33.23) remain eigenstates of  $\mathcal{H}$ , but that the spin wave excitation energies are raised by

$$S \sum_{\mathbf{R}} [J_z(\mathbf{R}) - J_z(\mathbf{R}')] . \quad (33.72)$$

- (b) Show that the low-temperature spontaneous magnetization now deviates from saturation only exponentially in  $-1/T$ .
- (c) Show that the argument on page 708, that there can be no spontaneous magnetization in two dimensions, no longer works.