8.512 Theory of Solids II
Spring 2009

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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

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

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

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

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

$$\mathcal{H} = -\frac{1}{2} \sum_{RR'} \left[ J_z(\mathbf{R} - \mathbf{R}') S_z(\mathbf{R}) S_z(\mathbf{R}') + J(\mathbf{R} - \mathbf{R}') S_\perp(\mathbf{R}) \cdot S_\perp(\mathbf{R}') \right]$$

(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
\[ S \sum_R [J_z(R) - J_z(R)] \cdot (33.72) \]

(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.