8.512 Theory of Solids II
Spring 2009

**8.512 Theory of Solids II** **Problem Set 9** **Due April 22, 2009**

1. (a) We can include the effects of Coulomb repulsion by the following effective potential:

$$V(\omega) = V_p(\omega) + V_c(\omega)$$

where $V_p = -V_0$ for $|\omega| < \omega_D$ is the phonon mediated attraction and $N(0)V_c = \mu > 0$ for $|\omega| < E_F$ represents the Coulomb repulsion. Write down the self-consistent gap equation at finite temperature. Show that $\Delta(\xi)$ is frequency dependent even near $T_c$ so that the $T_c$ equation becomes

$$\Delta(\xi) = -N(0) \int d\xi' V(\xi - \xi') \Delta(\xi') \frac{1 - 2f(\xi')}{2\xi'} \tag{1}$$

This integral equation is difficult to solve analytically, but we may try the following approximate solution:

$$\begin{aligned} \Delta(\omega) &= \Delta_1, \ |\omega| < \omega_D \\ &= \Delta_2, \ |\omega| > \omega_D \end{aligned}$$

Now rewrite Eq.(1) as

$$\Delta(\xi) = -N(0) \int d\xi' V_p(\xi' - \xi) \Delta(\xi') \frac{1 - 2f(\xi')}{2\xi'} + A \tag{2}$$

where

$$A(\xi) = -N(0) \int d\xi' V_c(\xi' - \xi) \Delta(\xi') \frac{1 - 2f(\xi')}{2\xi'} \tag{3}$$

Convince yourself that $A(\xi)$ is a slowly varying function of $\xi$ for $\xi << E_F$, so that we may approximate $A(\xi)$ by $A(0)$ in Eq.(2). Produce an argument to show that in the region $\xi > \omega_D$ the first term in the R.H.S. of Eq.(2) is small compared with $A$ so that in fact $\Delta_2 \approx A(0)$. In the same spirit show that

$$\Delta_1 \sim N(0) V_0 \Delta_1 \ln \frac{\omega_D}{kT_c} + \Delta_2$$

Combining this with an equation for $\Delta_2$ using Eq.(3), show that the T$_c$ equation becomes

$$1 = \ln\left(\frac{\omega_D}{kT_c}\right)(N(0)V_0 - \mu^*) \tag{4}$$

where $\mu^* = \frac{\mu}{1+\mu\ln(E_F/\omega_D)}$. $\mu^* < \mu$ is called the renormalized Coulomb repulsion. It can be thought of as an effective repulsion with a cutoff at $\omega_D$ instead of $E_F$. Equation (4) shows that the condition for superconductivity is $N(0)V_0 > \mu^*$ and not $N(0)V_0 > \mu$. For screened Coulomb repulsion, estimate $\mu$ and $\mu^*$ for a typical metal.

(b) Upon isotope substituting $M \to M + \delta M$, how is the Debye frequency affected to leading order? Assuming that this is the only effect, how is $\delta T_c/T_c$ related to $\delta M/M$, (i) in the absence of Coulomb repulsion, and (ii) including Coulomb repulsion.

2. 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

$$E_{s,t} = E_a + E_b + \frac{V \pm I}{1 \pm l^2}$$

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

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

and $I$ is the exchange integral

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

where

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