Lecture 4:

Last time, we showed that the structure function is defined in terms of the radial distribution function:

\[ S(r) = 1 + \rho \int g(r) e^{i \mathbf{k} \cdot \mathbf{r}} \, d^{3}r, \]

with \( g(r) \) the RDF. \( g(r) \) tells you the probability of finding a particle at \( r \) given there is one at the origin. See Pages 115-116 for pictures of \( g(r) \) in solids, liquids, etc. A few materials of note are as follows:

a) **Liquid Crystals**: Smectic ordering breaks both rotational and translational order. Nematic just involves rotational symmetry breaking. \( \theta \theta \theta \theta \theta (s) : \theta \theta \theta \theta \theta (N) \).

b) **Glasses**: Cool a liquid quickly. For window glass, the atoms get stuck in a glassy phase for a rate of 10 K/s. Ni requires a cool rate of 10^7 K/s. The density as well as the viscosity increase.
\[ \eta \propto e^{\frac{C}{\tau^\alpha}} \] Exponential growth of the viscosity.

C.) Quasi-crystals. Crystals with 3-fold and 5-fold symmetry.

Algi6Muy was the first material. The order involves a quasi-periodic tiling. Two periods with the period irrational: \( f(x) = \cos x + 80.3\pi x \). The ratio is \( \sqrt{5} \).

1-d tiling.

\[ x_n = n + x + \frac{1}{2} |n + \beta| \]

\( \alpha \) arbitrary #.

\[ x_{n+1} = x_n \]

Let \( x_0 = L \), \( x_1 = LS \), \( x_2 = LSL \), \( x_3 = LSLLS \), ...

All the S's never touch. The pattern is not periodic.

So here we have 2 separations. Let's call them L and S. The sequence will be of the Fibonacci type.

\[ x_{n+1} = x_n x_{n-1} \]

2-D: Penrose tiling

\[ \frac{1}{\sqrt{5}} \]

Join together only when arrows match.
2.) Free Electrons:

\[ H = \sum \mathbf{p}_i^2 / 2m. \]

\[ \mathbf{k} = \frac{2\pi}{L} (l_x, l_y, l_z) \Rightarrow \Delta k = \frac{2\pi}{L} \]

\( k_x, k_y, k_z \) are integers.

\[ \epsilon_{k} = \frac{(kL)^2}{2m}. \]

\[ \psi(k) = \sqrt{V} (p^2 + L). \Rightarrow \psi_k = e^{ikx} / \sqrt{V} \]

\( (2\pi/L)^3 = \text{volume of each k-point} \)

\[ p = k_x k_y k_z. \]

A.) Number of Particles

\[ N(T=0) = 2 \sum_{F} \Theta(p_F - p) \]

\[ \sum_{F} \Rightarrow V \int \frac{d^3 P}{(2\pi)^3} \]

\[ \Rightarrow N(T=0) = 2V \frac{4\pi}{(2\pi)^3} \int_{0}^{p_F} p^2 dp \]

\[ \Rightarrow n_e = \frac{N}{V} = \frac{p_F^3}{3\pi^2 \hbar^3}. \]
\[ 1 = \frac{4\pi r_e^3 n_e}{3} \]

def. of re.

\[ \Rightarrow \quad r_e^3 = \frac{3}{4\pi} \frac{3\pi^2 \chi^3}{r_e^3} \]

\[ \Rightarrow \quad r_e = 1.92 \chi / P_e. \]

We can define a dimensionless spacing

\[ r_s = \frac{r_e}{a_0} = 1.92 \frac{\varepsilon}{k^2} \frac{m_e^2}{2} \]

What does this mean? Let's rewrite it noting that in a.u. P \sim X/\Lambda \sim X/r_e.

\[ r_s = r_e = \frac{r_e^2 \cdot m_e^2}{a_0 \cdot k^2} \]

\[ = \frac{\varepsilon^2 / r_e}{K \cdot E.} \]

\( r_s \) denotes the strength of the potential relative to the kinetic energy of the electron.

<table>
<thead>
<tr>
<th>( r_s )</th>
<th>Li</th>
<th>Na</th>
<th>K</th>
<th>Rb</th>
<th>Cs</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r_s )</td>
<td>3.25</td>
<td>3.93</td>
<td>4.86</td>
<td>5.2</td>
<td>5.62</td>
</tr>
</tbody>
</table>

\( \varepsilon \) is the most correlated metal.
Chemical potential: \( \mu_0 = \frac{P_F^2}{2m} = 3.1 \text{eV} \) for Na.

Grand-State energy

\[
E = 2 \sum_P \varepsilon_P
\]

\[
= \frac{2V}{(2\pi \hbar)^3} \int P_F^4 \frac{dp}{2m}
\]

\[
= \frac{2V}{(2\pi \hbar)^3} \frac{P_F^5}{10m}
\]

Note \( V = N \frac{3\pi^2 k^3}{P_F^3} \), \( \mu_0 = \frac{P_F^2}{2m} \).

\[
\Rightarrow E = \frac{3}{5} N \mu_0
\]

Pressure:

\[
\frac{\partial E}{\partial V}_{T,N} = -2 \frac{3N \mu_0}{(2V)^{5/3}}
\]

\( \mu_0 < \frac{P_F^2}{2m} \) but \( P_F < V^{1/3} \).

\( \Rightarrow \mu_0 \sim V^{-2/3} \)

\( \Rightarrow \frac{\partial \mu_0}{\partial V} = -\frac{2}{3} \frac{\mu_0}{V} \).

\( \Rightarrow P = \frac{2}{5} \frac{N}{V} \mu_0 = \frac{2}{5} \text{ne} \mu_0 \).

This pressure is due entirely to Pauli exclusion.

B. Finite Temperature:

\[
f_P(\varepsilon) = \frac{\varepsilon - \mu}{e^\frac{\varepsilon - \mu}{kT} + 1}
\]

\( \Rightarrow f^l \) is peaked at \( \mu = 3 \).
\[ C_V = T \left( \frac{\partial S}{\partial T} \right)_V \] heat capacity.

Let's use the entropy from Stat. mech.

\[ S = k_B \ln W = k_B \sum_{\sigma} f_{\sigma} \ln f_{\sigma} + (1-f_{\sigma}) \ln (1-f_{\sigma}). \]

\[ \Rightarrow SS = -2k_B \sum_{\sigma} f_{\sigma} \ln f_{\sigma} / (1-f_{\sigma}). \]

\[ = 2V k_B \int \frac{d^3P}{(2\pi \hbar)^3} f_{\sigma} \left( \frac{\epsilon_{\sigma} - \mu}{k_B T} \right). \]

Density of states.

\[ N(\epsilon) = 2 \int \frac{d^3P}{(2\pi \hbar)^3} S(\epsilon - \epsilon_{\sigma}) \]

\[ = 2 \frac{4\pi}{(2\pi \hbar)^3} \int \frac{P^2 dP}{d\epsilon_{\sigma}} S(\epsilon - \epsilon_{\sigma}) d\epsilon_{\sigma} \]

\[ N(\epsilon_{\sigma}) = \frac{\epsilon_{\sigma}^3}{\pi^2 \hbar^3} \]

\[ \Rightarrow SS = \frac{V}{4} \int_0^\infty d\epsilon_{\sigma} f(\epsilon_{\sigma}) N(\epsilon_{\sigma}) (\epsilon_{\sigma} - \mu). \]

Let's consider \( I = \int_0^\infty d\epsilon f(\epsilon) h(\epsilon) \).

Integrate by parts.

\[ I = \int_0^\infty f(\epsilon) H(\epsilon) d\epsilon. \]

\[ H(\epsilon) = -\int_0^\epsilon h(x) dx. \]
\[ H(e) = H(m) + (e-m) \frac{\partial H}{\partial \epsilon} \bigg|_{\epsilon=m} + \frac{1}{2} (e-m)^2 \frac{\partial^2 H}{\partial \epsilon^2} \bigg|_{\epsilon=m} + \ldots \]

Here \( H = N(e)(e-m) \)

\[ L_j = - \int_0^\infty (e-m)^j f'(\epsilon) \, d\epsilon \]

\[ f' = \beta e^{\beta (e-m)} / (1 + e^{\beta (e-m)})^2. \]

\[ x = \beta (e-m) \implies dx = \beta \, de. \]

\[ \Rightarrow L_j = \frac{1}{\beta^j} \int_0^\infty x^j \frac{e^x}{(e^x+1)^2} \, dx. \]

The integrand is odd \( \Rightarrow \) only even \( j \)'s survive.

\[ L_0 = 1 \]

\[ L_2 = \frac{\pi^2}{3} (k_B T)^2. \]

\[ \vdots \]

\[ \Rightarrow I = H(m) - L_2 \frac{H''(m)}{2!} + \ldots \]

\[ = - \int_0^\infty h(e) + \frac{4}{3} \frac{\pi^2}{5} (k_B T)^2 h'(e) \, de. \]

\[ \Rightarrow \int_0^\infty \, d\epsilon \, Sf \, h(e) = \frac{\pi^2}{3} h'(e=m) \cdot k_B T \cdot eT. \]

\[ h = N(\epsilon)(e_p-\epsilon) \implies h'(e=m) = N(e=m) \]
\[ \Rightarrow SS = \frac{\pi^2}{3} k_B N(e_F) T S T. \]

\[ \Rightarrow CV = \frac{SS}{8T} = V \frac{\pi^2}{3} k_B^2 N(e_F) T. \]

\[ \Rightarrow CV = \frac{\pi^2}{3} k_B^2 \frac{3 \pi^2 k^3}{P_F^2} \frac{m^2 e_F}{\pi^2 k^3} T \]

\[ = \frac{\pi^2}{2} k_B \left( \frac{2m}{P_F^2} \right) \frac{K_0}{T} \]

\[ = \frac{\pi^2}{2} k_B T / T_F. \]

\[ \Rightarrow \text{only electrons within } T \text{ or } T_F \text{ contribute} \]

\[ \gamma \equiv \frac{CV}{T} = \frac{\pi^2 - 15}{2} \frac{\alpha T}{P_F^2} \]

<table>
<thead>
<tr>
<th></th>
<th>Li</th>
<th>Na</th>
<th>K</th>
<th>Rb</th>
<th>Cs</th>
<th>UBe_{13}</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \gamma )</td>
<td>1.65</td>
<td>1.38</td>
<td>2.08</td>
<td>2.63</td>
<td>3.97</td>
<td>14.00</td>
</tr>
</tbody>
</table>

\( \gamma \) is the Sommerfeld constant which is an indication of the mass. While, as expected, Cs has the largest value of \( \gamma \), UBe_{13} is the GOAT. (Sorry I am watching football)

UBe_{13} is a heavy-Fermion! Why are the electrons in UBe_{13} so heavy?

\[ = \text{Good thesis problem!} \]