Physics 223b: Problem Set 4
due 10am, February 21, 2014 in Prof. Balents' mailbox at the KITP

1. **Friedel Oscillations:** Consider a free electron gas (Sommerfeld model) confined in one direction by hard walls (infinite potential barriers) to $0 < x < L$, and infinite in the other two directions, taking $L \to \infty$ eventually. Express your answers below in terms of x and k_F.

   (a) Calculate the ground state charge density, $n(\mathbf{r})$, as a function of x. Hint: use the formula $n(\mathbf{r}) = \sum_j |\phi_j(\mathbf{r})|^2$, where j sums over occupied states with wavefunction $\phi_j(\mathbf{r})$.

   The wavefunctions factor into plane waves parallel to the walls, and standing waves, i.e. $\phi(\mathbf{r}) = \phi(x)e^{i(k_y y+k_z z)}$, with

$$\phi(x) = \sqrt{\frac{2}{L}} \sin k_x x, \tag{1}$$

   where $k_x = n\pi/L$. We must sum over all states with $|k| = \sqrt{k_x^2 + k_y^2 + k_z^2} < k_F$. As usual, taking periodic boundary condition in y and z and taking those distances to infinity, we have

$$n(x) = 2\int_{-\infty}^{\infty} \frac{dk_y dk_z}{(2\pi)^2} \sum_{k_x=n\pi/L} \frac{2}{L} \sin^2 k_x x \, \Theta(k_F - \sqrt{k_x^2 + k_y^2 + k_z^2}). \tag{2}$$

   The first factor of 2 is for spin degeneracy. Now we take the $L \to \infty$ limit. We have $\sum_{k_x=n\pi/L} \to \frac{L}{\pi}\int_0^\infty dk_x$. Defining $q = \sqrt{k_y^2 + k_z^2}$, using circular shells we have $\int dk_y dk_z = \int dq 2\pi q$ and hence

$$\begin{aligned} n(x) &= 2\frac{1}{(2\pi)^2}\frac{2}{L}\frac{L}{\pi}\int_0^\infty dq 2\pi q \int_0^\infty dk_x \sin^2 k_x x \, \Theta(k_F - \sqrt{k_x^2 + q^2}) \\ &= \frac{2}{\pi^2}\int_0^{k_F} dk_x \sin^2 k_x x \int_0^{\sqrt{k_F^2 - k_x^2}} dq\, q = \frac{1}{\pi^2}\int_0^{k_F} dk_x\, (k_F^2 - k_x^2)\sin^2 k_x x \\ &= \frac{k_F^3}{3\pi^2} + \frac{k_F \cos(2k_F x)}{4\pi^2 x^2} - \frac{\sin(2k_F x)}{8\pi^2 x^3}. \end{aligned} \tag{3}$$

   The last line is the answer. One check on the answer is that at $x \to \infty$, the density should approach the bulk value. This is just the $2(4/3\pi k_F^3)/(2\pi)^3 = k_F^3/(3\pi^2)$. This agrees with the first term of the above result.

   (b) Show that $n(x)$ vanishes as the wall at $x = 0$ is approached, and has an oscillatory part that decays as a power (what power?) of x into the bulk. These are called Friedel oscillations, and occur any time a metal is locally disturbed, by a surface, an impurity, etc. They can be measured using STM, and have numerous consequences for physical phenomena in metals.

   As $x = 0$ is approached, we need to just Taylor expand for $k_F x \ll 1$. There are numerous cancellations, leaving the leading behavior as

$$n(x) \sim \frac{2k_F^5}{15\pi^2}x^2, \tag{4}$$

for $k_F x \ll 1$. Into the bulk, i.e. for $k_F x \gg 1$, the leading oscillatory term is the cosine, which decays as $\sim 1/x^2$.

(c) How is the form of the Friedel oscillations changed for a one-dimensional electron gas ($k_y = k_z = 0$) with an end at $x = 0$?

In this case, we have no plane wave part parallel to the interface, so we just have

$$n(x) = 2 \sum_{k_x = n\pi/L} \frac{2}{L} \sin^2 k_x x \, \Theta(k_F - k_x). \tag{5}$$

Taking again the continuum limit, we obtain

$$\begin{aligned} n(x) &= 2\frac{L}{\pi}\frac{2}{L}\int_0^{k_F} dk_x \, \sin^2 k_x x \\ &= \frac{2k_F}{\pi} - \frac{\sin(2k_F x)}{\pi x}. \end{aligned} \tag{6}$$

We see that the envelope of the one-dimensional Friedel oscillations decays like $1/x$ rather than $1/x^2$ as in three dimensions.