PHYSICS 210A : EQUILIBRIUM STATISTICAL PHYSICS
HW ASSIGNMENT #5 SOLUTIONS

(1) Consider a two-dimensional gas of fermions which obey the dispersion relation

$$\varepsilon(\boldsymbol{k}) = \varepsilon_0 \Big((k_x^2 + k_y^2)\, a^2 + \tfrac{1}{2}(k_x^4 + k_y^4)\, a^4 \Big) \ .$$

Sketch, on the same plot, the Fermi surfaces for $\varepsilon_{\rm F} = 0.1\,\varepsilon_0$, $\varepsilon_{\rm F} = \varepsilon_0$, and $\varepsilon_{\rm F} = 10\,\varepsilon_0$.

`Solution`:

It is convenient to adimensionalize, writing

$$x \equiv k_x a \quad , \quad y \equiv k_y a \quad , \quad \nu \equiv \frac{\varepsilon}{\varepsilon_0} \ .$$

Then the equation for the Fermi surface becomes

$$x^2 + y^2 + \tfrac{1}{2}x^4 + \tfrac{1}{2}y^4 = \nu \ .$$

In other words, we are interested in the *level sets* of the function $\nu(x,y) \equiv x^2+y^2+\frac{1}{2}x^4+\frac{1}{2}y^4$. When ν is small, we can ignore the quartic terms, and we have an isotropic dispersion, with $\nu = x^2 + y^2$. *I.e.* we can write $x = \nu^{1/2}\cos\theta$ and $y = \nu^{1/2}\sin\theta$. The quartic terms give a contribution of order ν^4, which is vanishingly small compared with the quadratic term in the $\nu \to 0$ limit. When $\nu \sim \mathcal{O}(1)$, the quadratic and quartic terms in the dispersion are of the same order of magnitude, and the continuous $\mathsf{O}(2)$ symmetry, namely the symmetry under rotation by any angle, is replaced by a discrete symmetry group, which is the group of the square, known as C_{4v} in group theory parlance. This group has eight elements:

$$\big\{ E \ , \ R \ , \ R^2 \ , \ R^3 \ , \ \sigma \ , \ \sigma R \ , \ \sigma R^2 \ , \ \sigma R^3 \big\}$$

Here R is the operation of counterclockwise rotation by 90°, sending $(x\,,\,y)$ to $(-y\,,\,x)$, and σ is reflection in the y-axis, which sends $(x\,,\,y)$ to $(-x\,,\,y)$. One can check that the function $\nu(x,y)$ is invariant under any of these eight operations from C_{4v}.

Explicitly, we can set $y = 0$ and solve the resulting quadratic equation in x^2 to obtain the maximum value of x, which we call $a(\nu)$. One finds

$$\tfrac{1}{2}x^4 + x^2 - \nu = 0 \qquad \Longrightarrow \qquad a = \sqrt{\sqrt{1+2\nu} - 1} \ .$$

So long as $x \in \{-a, a\}$, we can solve for $y(x)$:

$$y(x) = \pm\sqrt{\sqrt{1 + 2\nu - 2x^2 - x^4} - 1} \ .$$

A sketch of the level sets, showing the evolution from an isotropic (*i.e.* circular) Fermi surface at small ν, to surfaces with discrete symmetries, is shown in fig. 1.

(2) Using noninteracting quantum statistics for fermions, answer the following:

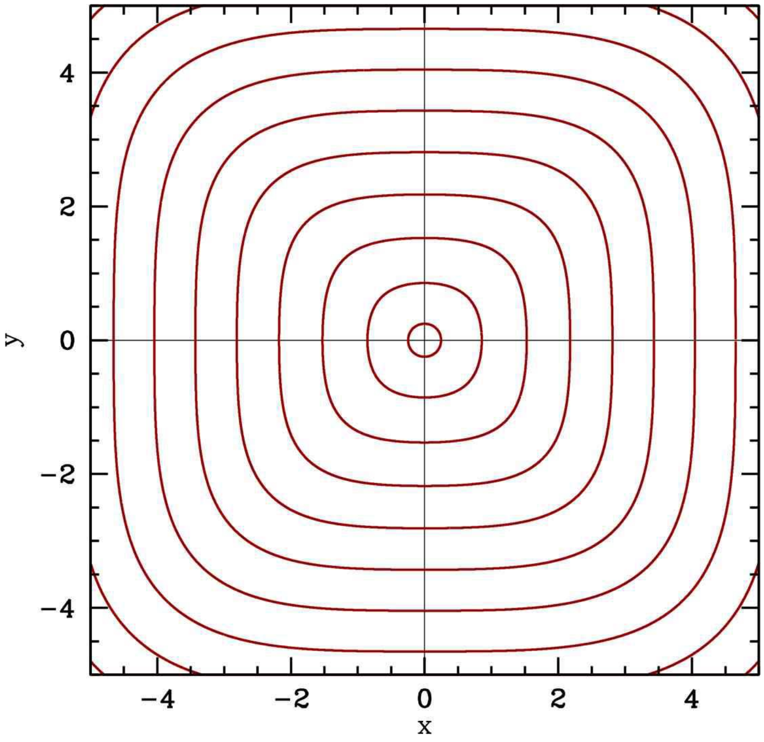

Figure 1: Level sets of the function $\nu(x,y) = x^2 + y^2 + \frac{1}{2}x^4 + \frac{1}{2}y^4$ for $\nu = (\frac{1}{2}n)^4$, with positive integer n.

(a) For ideal Fermi gases in $d = 1$, 2, and 3 dimensions, compute at $T = 0$ the average energy per particle E/N in terms of the Fermi energy $\varepsilon_{\rm F}$.

(b) Using the Sommerfeld expansion, compute the heat capacity for a two-dimensional electron gas, to lowest nontrivial order in the temperature T.

Solution :

(a) The number of particles is

$$N = \mathsf{g}\,V\!\int\!\frac{d^d\!k}{(2\pi)^d}\,\Theta(k_{\rm F} - k) = V \cdot \frac{\mathsf{g}\,\Omega_d}{(2\pi)^d}\,\frac{k_{\rm F}^d}{d}\ ,$$

where g is the internal degeneracy and Ω_d is the surface area of a sphere in d dimensions. The total energy is

$$E = \mathsf{g}\,V\!\int\!\frac{d^d\!k}{(2\pi)^d}\,\frac{\hbar^2 k^2}{2m}\,\Theta(k_{\rm F} - k) = V \cdot \frac{\mathsf{g}\,\Omega_d}{(2\pi)^d}\,\frac{k_{\rm F}^d}{d+2} \cdot \frac{\hbar^2 k_{\rm F}^2}{2m}\ .$$

Therefore,

$$\frac{E}{N} = \frac{d}{d+2}\,\varepsilon_{\rm F}\ .$$

(b) In the notes we obtained the result

$$\frac{E}{V} = \int\limits_{-\infty}^{\varepsilon_F} d\varepsilon\, g(\varepsilon)\,\varepsilon + \frac{\pi^2}{6}\,(k_B T)^2\, g(\varepsilon_F) + \mathcal{O}(T^4)\;.$$

This entails a heat capacity of $C_{V,N} = V \cdot \frac{1}{3}\pi^2 k_B\, g(\varepsilon_F) \cdot k_B T$. The density of states at the Fermi level, $g(\varepsilon_F)$, is easily found to be

$$g(\varepsilon_F) = \frac{d}{2} \cdot \frac{n}{\varepsilon_F}\;.$$

Thus,

$$C_{V,N} = N \cdot \frac{d\,\pi^2}{6}\, k_B \cdot \left(\frac{k_B T}{\varepsilon_F}\right)\,,$$

a form which is valid in any spatial dimension d.

(3) Consider a three-dimensional Fermi gas of $S = \frac{1}{2}$ particles obeying the dispersion relation $\varepsilon(\boldsymbol{k}) = A\,|\boldsymbol{k}|^4$.

(a) Compute the density of states $g(\varepsilon)$.

(b) Compute the molar heat capacity.

(c) Compute the lowest order nontrivial temperature dependence for $\mu(T)$ at low temperatures. *I.e.* compute the $\mathcal{O}(T^2)$ term in $\mu(T)$.

Solution :

(a) The density of states in $d = 3$ (g $= 2S + 1 = 2$) is given by

$$g(\varepsilon) = \frac{1}{\pi^2}\int\limits_0^\infty dk\, k^2\, \delta\big(\varepsilon - \varepsilon(k)\big) = \frac{1}{\pi^2}\, k^2(\varepsilon)\, \frac{dk}{d\varepsilon}\bigg|_{k=(\varepsilon/A)^{1/4}} = \frac{\varepsilon^{-1/4}}{4\pi^2 A^{3/4}}\;.$$

(b) The molar heat capacity is

$$c_V = \frac{\pi^2}{3n}\, R\, g(\varepsilon_F)\, k_B T = \frac{\pi^2 R}{4} \cdot \frac{k_B T}{\varepsilon_F}\,,$$

where $\varepsilon_F = \hbar^2 k_F^2/2m$ can be expressed in terms of the density using $k_F = (3\pi^2 n)^{1/3}$, which is valid for any isotropic dispersion in $d = 3$. In deriving this formula we had to express the density n, which enters in the denominator in the above expression, in terms of ε_F. But this is easy:

$$n = \int\limits_0^{\varepsilon_F} d\varepsilon\; g(\varepsilon) = \frac{1}{3\pi^2}\left(\frac{\varepsilon_F}{A}\right)^{3/4}\;.$$

(c) We have

$$\delta\mu = -\frac{\pi^2}{6}\,(k_{\mathrm{B}}T)^2\,\frac{g'(\varepsilon_{\mathrm{F}})}{g(\varepsilon_{\mathrm{F}})} = \frac{\pi^2}{24}\cdot\frac{(k_{\mathrm{B}}T)^2}{\varepsilon_{\mathrm{F}}}\ .$$

Thus,

$$\mu(n,T) = \varepsilon_{\mathrm{F}}(n) + \frac{\pi^2}{24}\cdot\frac{(k_{\mathrm{B}}T)^2}{\varepsilon_{\mathrm{F}}(n)} + \mathcal{O}(T^4)\ ,$$

where $\varepsilon_{\mathrm{F}}(n) = \frac{\hbar^2}{2m}\,(3\pi^2 n)^{2/3}$.

(4) In an n-type semiconductor, the donor levels lie a distance Δ below the bottom of the conduction band. Suppose there are M such donor levels. Due to the fact that such donor levels are spatially localized, one can ignore the possibility of double occupancy. Thus, each donor level can be occupied by at most one electron, but of either spin polarization. Assume the conduction band dispersion is isotropic, given by $\varepsilon_{\boldsymbol{k}} = \hbar^2\boldsymbol{k}^2/2m^*$. (Set the conduction band minimum to $\varepsilon = 0$.)

(a) Assuming that the conduction band is very sparsely populated, find an expression for the conduction electron density $n_{\mathrm{c}}(T,\mu)$.

(b) Suppose there are N_{d} electrons sitting on the donor sites, *i.e.* N_{d} of the M donor levels are singly occupied. Find the entropy of these electrons.

(c) Find the chemical potential of the donor electrons.

(d) Use the fact that the donor electrons and the conduction band electrons are in thermal equilibrium to eliminate μ from the problem, and find the conduction electron density $n_{\mathrm{c}}(T)$ and the fraction $\nu_{\mathrm{d}}(T)$ of occupied donor sites. Assume that the donor concentration is ρ_{d}, and that all conduction electrons are due to singly ionized donors.

Solution :

(a) We have

$$n_{\mathrm{c}} = 2\int\frac{d^3\!k}{(2\pi)^d}\,\frac{1}{e^{\beta(\varepsilon_{\boldsymbol{k}}-\mu_{\mathrm{c}})}+1} \approx 2\lambda_{\mathrm{c}}^{-3}\,e^{\mu_{\mathrm{c}}/k_{\mathrm{B}}T}\ ,$$

where μ_{c} is the chemical potential and $\lambda_{\mathrm{c}} = (2\pi\hbar^2/m^* k_{\mathrm{B}}T)^{1/2}$ thermal de Broglie wavelength for the conduction electrons.

(b) We assume that each donor site can either be empty, or else occupied by an electron in one of two possible polarization states. We forbid double occupancy of the donors, due to the large Coulomb energy associated with such a state. The number of configurations for N_{d} occupied donor sites is then

$$\Omega(N_{\mathrm{d}},M) = 2^{N_{\mathrm{d}}}\binom{M}{N_{\mathrm{d}}}\ ,$$

and therefore

$$S_{\mathrm{d}} = k_{\mathrm{B}} \ln\!\left(\frac{2^{N_{\mathrm{d}}}\, M!}{N_{\mathrm{d}}!\,(M-N_{\mathrm{d}})!}\right) .$$

The free energy of the donor system is then

$$\begin{aligned} F(T,N_{\mathrm{d}},M) &= -N_{\mathrm{d}}\,\Delta - k_{\mathrm{B}}T\ln\!\left(\frac{2^{N_{\mathrm{d}}}\, M!}{N_{\mathrm{d}}!\,(M-N_{\mathrm{d}})!}\right) \\ &\approx -N_{\mathrm{d}}\,\Delta - N_{\mathrm{d}}\,k_{\mathrm{B}}T\ln 2 + Mk_{\mathrm{B}}T\left\{\frac{N_{\mathrm{d}}}{M}\ln\!\left(\frac{N_{\mathrm{d}}}{M}\right) + \left(\frac{M-N_{\mathrm{d}}}{M}\right)\ln\!\left(\frac{M-N_{\mathrm{d}}}{M}\right)\right\} , \end{aligned}$$

where we have invoked Stirling's approximation. The chemical potential for the donor level electrons, which we will need later, is then

$$\mu_{\mathrm{d}} = \left(\frac{\partial F}{\partial N_{\mathrm{d}}}\right)_{T,M} = -\Delta - k_{\mathrm{B}}T\ln 2 + k_{\mathrm{B}}T\ln\!\left(\frac{f_{\mathrm{d}}}{1-f_{\mathrm{d}}}\right) ,$$

where $f_{\mathrm{d}} = N_{\mathrm{d}}/M$ is the fraction of donor sites which are occupied.

(c) Invoking our results from part (a) and (b), and setting $\mu_{\mathrm{c}} = \mu_{\mathrm{d}} \equiv \mu$, we have

$$e^{\mu/k_{\mathrm{B}}T} = \tfrac{1}{2}\, n_{\mathrm{c}} \lambda_{\mathrm{c}}^3 = \tfrac{1}{2}\, e^{-\Delta/k_{\mathrm{B}}T}\,\frac{f_{\mathrm{d}}}{1-f_{\mathrm{d}}} ,$$

Thus,

$$\big(f_{\mathrm{d}}^{-1} - 1\big)\, n_{\mathrm{c}} = \lambda_{\mathrm{c}}^{-3}\, e^{-\Delta/k_{\mathrm{B}}T} .$$

Now suppose the donor site density is ρ_{d}. All the conduction electrons must come from ionized donor sites. The fraction of such sites is $1-f_{\mathrm{d}}$, hence $n_{\mathrm{c}} = (1-f_{\mathrm{d}})\,\rho_{\mathrm{d}}$. Therefore, we have

$$\frac{(1-f_{\mathrm{d}})^2}{f_{\mathrm{d}}} = \frac{e^{-\Delta/k_{\mathrm{B}}T}}{\rho_{\mathrm{d}}\lambda_{\mathrm{c}}^3} \equiv b(T) .$$

This yields a quadratic equation for $1-f_{\mathrm{d}}$, whose solution is

$$1 - f_{\mathrm{d}} = -\tfrac{1}{2}b + \sqrt{\tfrac{1}{4}b^2 + b} \qquad \Rightarrow \qquad n_{\mathrm{c}} = \left\{ -\tfrac{1}{2}b + \sqrt{\tfrac{1}{4}b^2 + b}\right\}\rho_{\mathrm{d}} .$$

Note that $f_{\mathrm{d}} \to 1$ as $b \to 0$. In this limit, which is achieved when $k_{\mathrm{B}}T \ll \Delta$, or when $\rho_{\mathrm{d}}\lambda_{\mathrm{c}}^3 \gg 1$, or by some combination of these two conditions, all the donor sites are occupied, and the conduction electron density is zero. It is energetically/entropically two costly for the donors to donate an electron to the conduction band. In the $T \to 0$ limit, we have $1 - f_{\mathrm{d}} \simeq \sqrt{b}$, hence the chemical potential becomes

$$\mu(T\to 0) = -\tfrac{1}{2}\Delta + k_{\mathrm{B}}T\ln\!\left[\tfrac{1}{2}\rho_{\mathrm{d}}\left(\frac{2\pi\hbar^2}{m^* k_{\mathrm{B}}T}\right)^{3/2}\right] ,$$

which ultimately ends up exactly halfway between the donor levels and the bottom of the conduction band.

This problem is very similar to the adsorption model considered in §4.9.3 of the Lecture Notes. There, we considered a surface of adsorption sites in equilibrium with a classical gas. The only difference here is that the adsorbate particles can exist in one of two energetically degenerate polarization states. One can also solve for the donor density in the grand canonical ensemble. The donors are independent, hence the partition function for the donor electrons is

$$\Xi_{\mathrm{d}} = \big(1 + 2\, e^{\mu/k_{\mathrm{B}}T}\, e^{\Delta/k_{\mathrm{B}}T}\big)^{M} \ .$$

Note the factor of two, due to the degeneracy of the spin polarization states. If we were to include the possibility of doubly occupied donors, we would have instead

$$\Xi_{\mathrm{d}} = \big(1 + 2\, e^{\mu/k_{\mathrm{B}}T}\, e^{\Delta/k_{\mathrm{B}}T} + e^{2\mu/k_{\mathrm{B}}T}\, e^{(2\Delta - U)/k_{\mathrm{B}}T}\big)^{M} \ ,$$

where the energy of the doubly occupied level is $-2\Delta + U$, with U being the Coulomb repulsion energy for two electrons to sit on the same localized donor site. Again, we have assumed U is much larger than every other energy scale in this problem, meaning we can ignore the possibility of double occupancy. The grand potential for the donor electrons is then $\Omega_{\mathrm{d}} = -k_{\mathrm{B}}T \ln \Xi_{\mathrm{d}}$, and so

$$f_{\mathrm{d}} = -\frac{1}{M}\left(\frac{\partial \Omega_{\mathrm{d}}}{\partial \mu}\right)_{T,M} = \frac{1}{\frac{1}{2} e^{-(\mu+\Delta)/k_{\mathrm{B}}T} + 1} \ ,$$

which recovers the result previously obtained in part (a).