Assignment 12

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PC2135
Thermodynamics and Statistical Mechanics

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Problem 1

[**20 pts**] Consider a system of spin-1/2 free fermions. In the absence of a magnetic field, the energy of each spin component ranges from $\varepsilon = 0$ to $\varepsilon = W$, with density of states $g(\varepsilon)$ per spin component. In the presence of a magnetic field B, spin-up states receive an additional energy $-\mu_B B$ and spin-down states receive $+\mu_B B$. The magnetization is $M = N_\uparrow - N_\downarrow$, with total $N = N_\uparrow + N_\downarrow$ fixed. We work in the regime $\mu_B B, kT \ll \varepsilon_F, W - \varepsilon_F$.

(1) (2 pts) For $T = 0$, show that

$$N_\uparrow = \int_{-\mu_B B}^{\varepsilon_F(\mu_B B)} \mathrm{d}\varepsilon\ g(\varepsilon + \mu_B B), \quad N_\downarrow = \int_{\mu_B B}^{\varepsilon_F(\mu_B B)} \mathrm{d}\varepsilon\ g(\varepsilon - \mu_B B) \tag{1}$$

(2) (3 pts) Write $\varepsilon_F(\mu_B B) = \varepsilon_F + \sum_{n=1}^{\infty} \frac{\varepsilon_F^{(n)}}{n!}(\mu_B B)^n$. Expand to order $\mu_B B$ and show $\varepsilon_F^{(1)} = 0$.

(3) (4 pts) Calculate M to order $\mu_B B$. Show that the spin susceptibility $\chi \equiv \lim_{\mu_B B \to 0} M/B = 2\mu_B g(\varepsilon_F)$.

(4) (4 pts) At finite T, the particle numbers become

$$N_\uparrow = \int_{-\mu_B B}^{D+\mu_B B} \mathrm{d}\varepsilon\ g(\varepsilon + \mu_B B) n_F(\varepsilon), \quad N_\downarrow = \int_{\mu_B B}^{D-\mu_B B} \mathrm{d}\varepsilon\ g(\varepsilon - \mu_B B) n_F(\varepsilon) \tag{2}$$

where $D = W$ is the band cutoff and $n_F(\varepsilon) = 1/\left(e^{\beta(\varepsilon-\mu)} + 1\right)$. Let $N_0(\varepsilon) = \int_0^\varepsilon \mathrm{d}\varepsilon' g(\varepsilon')$ denote the cumulative single-spin DOS. Show that, up to errors exponentially small in $\varepsilon_F/(kT)$ and $(W - \varepsilon_F)/(kT)$,

$$N_\uparrow = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{N_0^{(n)}(\mu)}{m!(n-m)!} (kT)^{n-m} (\mu_B B)^m I_{n-m} \tag{3}$$

$$N_\downarrow = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{N_0^{(n)}(\mu)}{m!(n-m)!} (kT)^{n-m} (-\mu_B B)^m I_{n-m} \tag{4}$$

where $N_0^{(n)}(\mu) = \mathrm{d}^n N_0 / \mathrm{d}\varepsilon^n \mid_{\varepsilon=\mu}$ and $I_k = \int_{-\infty}^{\infty} x^k e^x/(e^x+1)^2\, \mathrm{d}x$.

(5) (3 pts) Writing $\mu = \varepsilon_F + \mu_{1,0} kT + \mu_{0,1}\mu_B B + \mu_{2,0}(kT)^2 + \mu_{1,1}(kT)(\mu_B B) + \mu_{0,2}(\mu_B B)^2 + \ldots$, use $N = N_\uparrow + N_\downarrow$ to show

$$\mu_{1,0} = \mu_{0,1} = \mu_{1,1} = 0, \quad \mu_{2,0} = -\frac{\pi^2 g'(\varepsilon_F)}{6 g(\varepsilon_F)}, \quad \mu_{0,2} = -\frac{g'(\varepsilon_F)}{2 g(\varepsilon_F)} \tag{5}$$

(6) (4 pts) Show that, up to order $(kT)^2$, the spin susceptibility is

$$\chi = 2\mu_B g(\varepsilon_F) + \frac{(\pi kT)^2}{3} \mu_B \left[g''(\varepsilon_F) - \frac{(g'(\varepsilon_F))^2}{g(\varepsilon_F)} \right] \tag{6}$$

Solution

Part (1): T = 0 occupation numbers

At $T=0$, a state is filled if and only if its total single-particle energy lies below $\varepsilon_{F(\mu_B B)}$. For spin-up fermions, a bare-band state at energy ξ has total energy $\xi-\mu_B B$; the filled condition $\xi-\mu_B B<\varepsilon_F$ means $\xi<\varepsilon_F+\mu_B B$. Substituting $\xi=\varepsilon+\mu_B B$:

$$N_\uparrow=\int_0^{\varepsilon_F+\mu_B B}\mathrm{d}\xi\ g(\xi)=\int_{-\mu_B B}^{\varepsilon_F(\mu_B B)}\mathrm{d}\varepsilon\ g(\varepsilon+\mu_B B) \tag{7}$$

For spin-down, the total energy is $\xi+\mu_B B<\varepsilon_F$, so $\xi<\varepsilon_F-\mu_B B$. Substituting $\xi=\varepsilon-\mu_B B$:

$$N_\downarrow=\int_0^{\varepsilon_F-\mu_B B}\mathrm{d}\xi\ g(\xi)=\int_{\mu_B B}^{\varepsilon_F(\mu_B B)}\mathrm{d}\varepsilon\ g(\varepsilon-\mu_B B) \tag{8}$$

Part (2): First-order correction to ε_F vanishes

After the substitution in Part (1), $N_\uparrow=\int_0^{\varepsilon_F+\mu_B B}g(\xi)\,\mathrm{d}\xi$ and $N_\downarrow=\int_0^{\varepsilon_F-\mu_B B}g(\xi)\,\mathrm{d}\xi$. Write $\varepsilon_{F(\mu_B B)}=\varepsilon_F+\varepsilon_F^{(1)}\mu_B B+O\big((\mu_B B)^2\big)$. Then to order $\mu_B B$:

$$\begin{aligned}N&=N_\uparrow+N_\downarrow\\&=\int_0^{\varepsilon_F+\left(\varepsilon_F^{(1)}+1\right)\mu_B B}g\,\mathrm{d}\xi+\int_0^{\varepsilon_F+\left(\varepsilon_F^{(1)}-1\right)\mu_B B}g\,\mathrm{d}\xi+O\Big(\big(\mu_B B\big)^2\Big)\\&=2\int_0^{\varepsilon_F}g\,\mathrm{d}\xi+2g(\varepsilon_F)\varepsilon_F^{(1)}\mu_B B+O\Big(\big(\mu_B B\big)^2\Big)\end{aligned} \tag{9}$$

Since $N=2\int_0^{\varepsilon_F}g(\varepsilon)\,\mathrm{d}\varepsilon$ is fixed, the coefficient of $\mu_B B$ must vanish. Since $g(\varepsilon_F)>0$:

$$\varepsilon_F^{(1)}=0 \tag{10}$$

Part (3): Pauli susceptibility

Using $\varepsilon_F^{(1)}=0$, the expressions for $N_\uparrow$ and $N_\downarrow$ to first order in $\mu_B B$ become

$$\begin{aligned}N_\uparrow&=\int_0^{\varepsilon_F+\mu_B B}g(\xi)\,\mathrm{d}\xi=N_0(\varepsilon_F)+g(\varepsilon_F)\mu_B B+O\Big(\big(\mu_B B\big)^2\Big)\\N_\downarrow&=\int_0^{\varepsilon_F-\mu_B B}g(\xi)\,\mathrm{d}\xi=N_0(\varepsilon_F)-g(\varepsilon_F)\mu_B B+O\Big(\big(\mu_B B\big)^2\Big)\end{aligned} \tag{11}$$

The magnetization is $M=N_\uparrow-N_\downarrow=2g(\varepsilon_F)\mu_B B+O\Big(\big(\mu_B B\big)^3\Big)$, so

$$\chi=\lim_{\mu_B B\to 0}\frac{M}{B}=2\mu_B g(\varepsilon_F) \tag{12}$$

This is the Pauli susceptibility: at zero temperature the magnetic response is set entirely by the density of states at the Fermi level. Filled bands contribute nothing because every filled spin-up state is paired with a filled spin-down state.

Part (4): Finite-temperature double expansion

Since $-\mathrm{d}n_F/\mathrm{d}\varepsilon$ is sharply peaked at $\varepsilon=\mu$ with width $\sim kT$, and both μ and $W-\mu$ are $\gg kT$, extending the integration limits to $(-\infty,+\infty)$ introduces only exponentially small errors. Write $g(\varepsilon+\mu_B B)=\mathrm{d}N_0(\varepsilon+\mu_B B)/\mathrm{d}\varepsilon$ and integrate by parts (boundary terms vanish since $N_0(-\infty+\mu_B B)=0$ and $n_{F(+\infty)}=0$):

$$N_\uparrow = \int_{-\infty}^{\infty} g(\varepsilon + \mu_B B) n_{F(\varepsilon)}\, \mathrm{d}\varepsilon = -\int_{-\infty}^{\infty} N_0(\varepsilon + \mu_B B) \frac{\mathrm{d}n_F}{\mathrm{d}\varepsilon}\, \mathrm{d}\varepsilon \tag{13}$$

Now expand $N_0(\varepsilon + \mu_B B) = N_0(\mu + (\varepsilon - \mu + \mu_B B))$ as a Taylor series around μ:

$$N_0(\varepsilon + \mu_B B) = \sum_{n=0}^{\infty} \frac{N_0^{(n)}(\mu)}{n!} (\varepsilon - \mu + \mu_B B)^n = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{N_0^{(n)}(\mu)}{m!(n-m)!} (\varepsilon - \mu)^{n-m} (\mu_B B)^m \tag{14}$$

Substituting $x = (\varepsilon - \mu)/(kT)$, so $\varepsilon - \mu = kTx$ and $-\mathrm{d}n_F/\mathrm{d}\varepsilon = (1/(kT))e^x/(e^x+1)^2$:

$$N_\uparrow = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{N_0^{(n)}(\mu)}{m!(n-m)!} (kT)^{n-m} (\mu_B B)^m \int_{-\infty}^{\infty} x^{n-m} \frac{e^x}{(e^x+1)^2}\, \mathrm{d}x \tag{15}$$

which is the stated result with $I_k = \int_{-\infty}^{\infty} x^k e^x/(e^x+1)^2\, \mathrm{d}x$. The derivation for $N_\downarrow$ is identical with $\mu_B B \to -\mu_B B$.

Since $e^x/(e^x+1)^2$ is an even function of x (verifiable via $x \to -x$), $I_k = 0$ for all odd k. The nonzero values needed here are:

$$I_0 = 1, \quad I_2 = \frac{\pi^2}{3} \tag{16}$$

Part (5): Chemical potential expansion

$N = N_\uparrow + N_\downarrow$ receives contributions only from even m (odd-m terms cancel) and only from even $n - m$ (since $I_k = 0$ for odd k), so only even n survives. The leading terms are:

$$N = 2N_0(\mu) + g'(\mu)\left[(kT)^2 \frac{\pi^2}{3} + (\mu_B B)^2\right] + O(\text{4th order}) \tag{17}$$

The $n = 0$ term gives $2N_0(\mu)$; the two $n = 2$ contributions (m=0 and m=2) give $g'(\mu)\left[(kT)^2\frac{\pi^2}{3} + (\mu_B B)^2\right]$. Expanding $N_0(\mu) = N_0(\varepsilon_F) + g(\varepsilon_F)(\mu - \varepsilon_F) + \frac{1}{2}g'(\varepsilon_F)(\mu - \varepsilon_F)^2 + \ldots$ and setting $N = 2N_0(\varepsilon_F)$ at each order:

- **Order kT and $\mu_B B$:** $2g(\varepsilon_F)\mu_{1,0} = 0$ and $2g(\varepsilon_F)\mu_{0,1} = 0$, so $\mu_{1,0} = \mu_{0,1} = 0$.
- **Order $(kT)^2$:** $2g(\varepsilon_F)\mu_{2,0} + g'(\varepsilon_F)\frac{\pi^2}{3} = 0$, so
$$\mu_{2,0} = -\frac{\pi^2 g'(\varepsilon_F)}{6g(\varepsilon_F)} \tag{18}$$
- **Order $(kT)(\mu_B B)$:** all cross terms vanish (since $\mu_{1,0} = \mu_{0,1} = 0$), so $\mu_{1,1} = 0$.
- **Order $(\mu_B B)^2$:** $2g(\varepsilon_F)\mu_{0,2} + g'(\varepsilon_F) = 0$, so
$$\mu_{0,2} = -\frac{g'(\varepsilon_F)}{2g(\varepsilon_F)} \tag{19}$$

Part (6): Finite-temperature susceptibility

$M = N_\uparrow - N_\downarrow$ picks up only odd-m terms. Combined with $I_k = 0$ for odd k, only odd n contributes. In the limit $\mu_B B \to 0$, the two relevant terms are:

$$\begin{aligned}\frac{M}{\mu_B B} &= 2N_0^{(1)}(\mu)I_0 + 2\frac{N_0^{(3)}(\mu)}{2!}(kT)^2 I_2 + O(T^4) \\ &= 2g(\mu) + g''(\mu)\frac{\pi^2(kT)^2}{3} + O(T^4)\end{aligned} \tag{20}$$

Using Equation 18, $g(\mu) = g(\varepsilon_F) - \frac{\pi^2 (g'(\varepsilon_F))^2}{6g(\varepsilon_F)}(kT)^2 + O(T^4)$:

$$\frac{M}{\mu_B B} = 2g(\varepsilon_F) + (kT)^2 \left[-\frac{\pi^2 (g'(\varepsilon_F))^2}{3g(\varepsilon_F)} + \frac{\pi^2 g''(\varepsilon_F)}{3} \right] + O(T^4) \tag{21}$$

$$\chi = \frac{M}{B} = 2\mu_B g(\varepsilon_F) + \frac{(\pi kT)^2}{3}\mu_B \left[g''(\varepsilon_F) - \frac{(g'(\varepsilon_F))^2}{g(\varepsilon_F)} \right] \tag{22}$$

The first term is the $T = 0$ Pauli susceptibility Equation 12. The correction is second order in temperature and depends on the curvature and slope of the DOS at ε_F: a steeply rising DOS ($g' > 0$) suppresses χ at finite T because the shift $\mu_{2,0} < 0$ pulls μ into a region of lower DOS.

Problem 2

[**20 pts**] A Weyl semimetal has 2 species of Weyl fermions. For a given species and momentum $\boldsymbol{k}$ with $k \equiv |\boldsymbol{k}|$, there are 2 single-particle states with energies $+v_F k$ and $-v_F k$. The sample has N atoms in volume $V = L^3$. There are also Debye phonons with speed v_s. We ignore interactions and take the cutoff $\Lambda \to \infty$.

(1) (3 pts) What is the total electron density of states $g(\varepsilon)$?

(2) (7 pts) For $\varepsilon_F > 0$, calculate the heat capacities $C_F = a_F T^{\alpha_F}$ and $C_s = a_s T^{\alpha_s}$ contributed by electrons and phonons respectively in the low-temperature limit $kT \ll \varepsilon_F$ and $T \ll T_D$.

(3) (3 pts) For $\varepsilon_F = 0$, what is the chemical potential at temperature $T > 0$? Argue from the shape of the Fermi-Dirac distribution.

(4) (7 pts) For $\varepsilon_F = 0$, calculate $C_F = a_F T^{\alpha_F}$ and $C_s = a_s T^{\alpha_s}$ in the low-temperature limit $T \ll T_D$.

Solution

Part (1): Density of states

Each of the 2 species has 2 energy branches: $\varepsilon = +v_F k$ (positive branch) and $\varepsilon = -v_F k$ (negative branch). For states on the positive branch with energy in $[\varepsilon, \varepsilon + \mathrm{d}\varepsilon]$ at $\varepsilon > 0$: $k = \varepsilon / v_F$, so

$$g_+(\varepsilon) = 2 \cdot \frac{V}{(2\pi)^3} \cdot 4\pi k^2 \frac{\mathrm{d}k}{\mathrm{d}\varepsilon} = 2 \cdot \frac{V}{2\pi^2} \cdot \frac{\varepsilon^2}{v_F^3} = \frac{V\varepsilon^2}{\pi^2 v_F^3}, \quad \varepsilon > 0 \tag{23}$$

where the factor 2 counts the two species. By the same counting, negative-branch states at energy $\varepsilon < 0$ have $k = |\varepsilon|/v_F$, giving $g_-(\varepsilon) = V\varepsilon^2/(pi^2 v_F^3)$ for $\varepsilon < 0$ (since $|\varepsilon|^2 = \varepsilon^2$). The full density of states is:

$$g(\varepsilon) = \frac{V\varepsilon^2}{\pi^2 v_F^3} \tag{24}$$

This is quadratic in energy, reflecting the linear 3D dispersion.

Part (2): Heat capacity at $\varepsilon_F > 0$

Electrons. For $kT \ll \varepsilon_F$, the Sommerfeld expansion gives the leading electronic heat capacity:

$$C_F = \frac{\pi^2}{3} k^2 g(\varepsilon_F) T = \frac{\pi^2}{3} k^2 \cdot \frac{V\varepsilon_F^2}{\pi^2 v_F^3} T = \frac{k^2 V \varepsilon_F^2}{3 v_F^3} T \tag{25}$$

So $\alpha_F = 1$ and $a_F = k^2 V \varepsilon_F^2 / (3 v_F^3)$. This is the standard result for any metal with a well-defined Fermi surface; the Weyl linear dispersion enters through $g(\varepsilon_F) = V\varepsilon_F^2/(pi^2 v_F^3)$.

Phonons. For $T \ll T_D$, the Debye model gives the low-temperature heat capacity exactly as for an ordinary solid:

$$C_s = \frac{12\pi^4}{5} Nk \left(\frac{T}{T_D}\right)^3 \tag{26}$$

So $\alpha_s = 3$ and $a_s = 12\pi^4 Nk / (5T_D^3)$.

At low enough T, the electronic T term dominates over the phonon T^3 term, as in ordinary metals.

Part (3): Chemical potential at $\varepsilon_F = 0$

The Fermi-Dirac distribution at chemical potential μ satisfies

$$n_{F(\varepsilon;\mu)} + n_{F(-\varepsilon;\mu)} = \frac{1}{e^{\beta(\varepsilon-\mu)}+1} + \frac{1}{e^{\beta(-\varepsilon-\mu)}+1} = 1 \quad \leftrightarrow \quad e^{-\beta\mu} = e^{\beta\mu} \tag{27}$$

so the identity $n_{F(\varepsilon;\mu)} + n_{F(-\varepsilon;\mu)} = 1$ holds for all ε if and only if $\mu = 0$.

At charge neutrality ($\varepsilon_F = 0$), the number of excited electrons (states with $\varepsilon > 0$ that become occupied at finite T) must equal the number of holes (states with $\varepsilon < 0$ that become unoccupied). With $\mu = 0$, $n_{F(\varepsilon;0)} = 1 - n_{F(-\varepsilon;0)}$ for every ε, so these two counts are exactly equal for any DOS satisfying $g(-\varepsilon) = g(\varepsilon)$, which holds here. This is particle-hole symmetry.

Therefore $\mu = 0$ for all T when $\varepsilon_F = 0$.

Part (4): Heat capacity at $\varepsilon_F = 0$

Electrons. With $\mu = 0$ and the DOS Equation 24, the energy of the electrons above the $T = 0$ ground state is:

$$\Delta U = \int_{-\infty}^{\infty} \varepsilon\ g(\varepsilon) n_{F(\varepsilon;0)}\,\mathrm{d}\varepsilon - \int_{-\infty}^{0} \varepsilon\ g(\varepsilon)\,\mathrm{d}\varepsilon \tag{28}$$

Split ΔU using particle-hole symmetry. For the negative-energy contribution, substitute $\varepsilon \to -\varepsilon$ and use $n_{F(-\varepsilon;0)} = 1 - n_{F(\varepsilon;0)}$:

$$\int_{-\infty}^{0} \varepsilon\ g(\varepsilon) n_{F(\varepsilon;0)}\,\mathrm{d}\varepsilon = -\int_{0}^{\infty} \varepsilon\ g(\varepsilon)\left[1 - n_{F(\varepsilon;0)}\right]\mathrm{d}\varepsilon \tag{29}$$

The ground-state subtraction $-\int_{\{-\infty\}}^{0} \varepsilon\ g(\varepsilon)\,\mathrm{d}\varepsilon = +\int_{0}^{\infty} \varepsilon\ g(\varepsilon)\,\mathrm{d}\varepsilon$ (since $\varepsilon < 0$ there). Combining:

$$\Delta U = 2\int_{0}^{\infty} \varepsilon\ g(\varepsilon) n_{F(\varepsilon;0)}\,\mathrm{d}\varepsilon = \frac{2V}{\pi^2 v_F^3}\int_{0}^{\infty} \frac{\varepsilon^3}{e^{\beta\varepsilon}+1}\,\mathrm{d}\varepsilon \tag{30}$$

Substitute $x = \beta\varepsilon = \varepsilon/(kT)$:

$$\Delta U = \frac{2V}{\pi^2 v_F^3}(kT)^4 \int_{0}^{\infty} \frac{x^3}{e^x+1}\,\mathrm{d}x = \frac{2V}{\pi^2 v_F^3}(kT)^4 \cdot \frac{7\pi^4}{120} = \frac{7\pi^2 V (kT)^4}{60 v_F^3} \tag{31}$$

where $\int_0^\infty x^3/(e^x+1)\,\mathrm{d}x = 7\pi^4/120$ is the standard Fermi integral. Differentiating:

$$C_F = \frac{\mathrm{d}(\Delta U)}{\mathrm{d}T} = \frac{7\pi^2 V k^4}{15 v_F^3} T^3 \tag{32}$$

So $\alpha_F = 3$ and $a_F = 7\pi^2 V k^4/(15 v_F^3)$.

At charge neutrality the Fermi surface has collapsed to a point. All thermal excitations involve states far from $\varepsilon = 0$ on the scale kT, so the energy integral runs over a wide range rather than being sharply Sommerfeld-expanded. The result $C_F \propto T^3$ is the same power law as phonons — both arise from massless linear dispersion. The prefactors differ: Weyl fermions carry a Fermi statistics factor $7\pi^4/120$ while phonons carry the Bose statistics factor $\pi^4/15$.

Phonons. The Debye result is unchanged:

$$C_s = \frac{12\pi^4}{5} Nk \left(\frac{T}{T_D}\right)^3, \quad \alpha_s = 3, \quad a_s = \frac{12\pi^4 Nk}{5 T_D^3} \tag{33}$$

Both contributions scale as T^3 at $\varepsilon_F = 0$. The total heat capacity is $(a_F + a_s)T^3$ and disentangling the two requires independent knowledge of v_F and v_s.