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Fermions in a slab

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Abstract

The specific heat is computed for an ensemble of fermions confined to a slab.

An ensemble of N identical fermions, each of mass m, is confined to a rectangular box of area A and thickness d. The single-particle wavefunctions along the z-direction perpendicular to the slab are proportional to $\sin(\pi nz/d)$, for $n = 1, 2, ...$, so that the single-particle energies are given by

$$\varepsilon_n(k) = \hbar^2 k^2/2m + \varepsilon_0 n^2 \quad , \tag{1}$$

where $\mathbf{k}$ is the (continuous) in-plane wavevector and $\varepsilon_0 = \pi^2\hbar^2/2md^2$. The number of particles is given by

$$N = g\frac{A}{(2\pi)^2}\int d\mathbf{k}\sum_{n=1}^{\infty}\frac{1}{\exp\left[\varepsilon_n(k)-\mu\right]\beta+1} \quad , \tag{2}$$

where g is the spin degeneracy, μ is the chemical potential and $\beta = 1/T$ is the inverse of the temperature. We assume that

$$\beta\varepsilon_0 \ll 1 \quad , \tag{3}$$

so that we may replace the summation over n in (2) by an integral, according to the formula

$$\sum_a^b f(n) = \int_{a-1/2}^{b+1/2} dn\cdot f(n) - \frac{1}{24}f'(n)\,\Big|_{a-1/2}^{b+1/2} \quad . \tag{4}$$

For the Fermi distribution in (2) this formula reads

$$\sum_{n=1}^{\infty} f(n) = \frac{1}{2}\int_{-\infty}^{+\infty} dn\cdot f(n) - \frac{1}{2}f(0) \quad , \tag{5}$$

so that (2) becomes

$$N = g\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[\int_0^\infty d\varepsilon\cdot\frac{\varepsilon^{1/2}}{\exp(\varepsilon-\mu)\beta+1} - \frac{\sqrt{\varepsilon_0}}{2}\int_0^\infty d\varepsilon\cdot\frac{1}{\exp(\varepsilon-\mu)\beta+1}\right] \quad , \tag{6}$$

where the volume $V = Ad$; it contains the bulk contribution and a small correction term in $\sqrt{\varepsilon_0}$, due to the finite size of the sample. Estimating the Fermi integrals by

$$\int_0^\infty d\varepsilon\cdot f(\varepsilon)\cdot\frac{1}{\exp(\varepsilon-\mu)\beta+1} = \int_0^\mu d\varepsilon\cdot f(\varepsilon) + \frac{\pi^2 T^2}{6}f'(\mu) + ... \quad , \tag{7}$$

valid for $\mu\beta \gg 1$, we get

$$N = g\frac{V}{6\pi^2}\left(\frac{2mT}{\hbar^2}\right)^{3/2}(\ln z)^{3/2}\left[1+\frac{\pi^2}{8}\frac{1}{(\ln z)^2}-\frac{3}{4}\sqrt{\varepsilon_0\beta}\frac{1}{(\ln z)^{1/2}}\right] \quad , \tag{8}$$

where the fugacity $z = \exp(\mu\beta)$ has been introduced. We introduce the Fermi energy $\varepsilon_F = \hbar^2 k_F^2/2m$, where the Fermi wavevector k_F is given by $N = gVk_F^3/6\pi^2$, and obtain from (8)

$$\ln z = (\beta\varepsilon_F)\left[1-\frac{\pi^2}{12}\frac{1}{(\beta\varepsilon_F)^2}\right]\left\{1+\frac{1}{2}\sqrt{\varepsilon_0/\varepsilon_F}\left[1+\frac{\pi^2}{12}\frac{1}{(\beta\varepsilon_F)^2}\right]\right\} \quad , \tag{9}$$

for $\beta\varepsilon_F \gg 1$.

By similar calculations we obtain the energy of the ensemble as being given by

$$\beta E = g\frac{V}{10\pi^2}\left(\frac{2mT}{\hbar^2}\right)^{3/2}(\ln z)^{5/2}\cdot$$
$$\cdot\left\{1+\frac{5\pi^2}{8}\frac{1}{(\ln z)^2}-\frac{5}{8}\sqrt{\varepsilon_0\beta}\frac{1}{(\ln z)^{1/2}}\left[1+\frac{\pi^2}{3}\frac{1}{(\ln z)^2}\right]\right\} \quad , \tag{10}$$

whence, using (8) and (9), we get

$$E/N = \frac{3}{5}\varepsilon_F+\frac{3}{8}\sqrt{\varepsilon_0\varepsilon_F}+\frac{\pi^2}{4}\left(1-\frac{1}{4}\sqrt{\varepsilon_0/\varepsilon_F}\right)\frac{T^2}{\varepsilon_F} \quad , \tag{11}$$

and the specific heat

$$c = \frac{\pi^2}{2}\left(1-\frac{1}{4}\sqrt{\varepsilon_0/\varepsilon_F}\right)\frac{T}{\varepsilon_F} \quad . \tag{12}$$

The grand-canonical potential $\Omega = -pV = -(1/\beta)\ln Q$, where p is the pressure and Q is the grand-partition function, is given by

$$\beta\Omega = -g\frac{A}{(2\pi)^2}\int d\mathbf{k}\sum_{n=1}^{\infty}\ln\left\{1+\exp\left[\mu-\varepsilon_n(k)\right]\beta\right\} \quad , \tag{13}$$

and, by similar manipulations, we obtain

$$\Omega = -\frac{2}{3}E+g\frac{A}{12\pi}\frac{m}{\hbar^2}\int_0^{\infty}d\varepsilon\cdot\frac{\varepsilon}{\exp(\varepsilon-\mu)\beta+1} \quad . \tag{14}$$

On the other hand, by using (13) and (14), we obtain the entropy

$$S = \beta^2\frac{\partial\Omega}{\partial\beta} = \frac{5}{3}\beta E - N\ln z - g\frac{A}{12\pi}\frac{m}{\hbar^2}\beta\int_0^{\infty}d\varepsilon\cdot\frac{\varepsilon}{\exp(\varepsilon-\mu)\beta+1} \quad , \tag{15}$$

and we can check easily that $S \sim T$ for $T \to 0$; whence the specific heat given by (12) represents both the specific heat at constant volume and the specific heat at constant pressure.

Introducing the inter-particle distance a by $V = Na^3$, we have $\varepsilon_F = \left(\hbar^2/2ma^2\right)\left(6\pi^2/g\right)^{2/3}$ and $\varepsilon_0/\varepsilon_F = \left(\pi g/6\right)^{2/3}\left(a/d\right)^2$, so that (12) becomes

$$c = \frac{ma^2}{\hbar^2}\left[\left(\pi g/6\right)^{2/3} - \frac{1}{4}\frac{a}{d}\left(\pi g/6\right)\right]T \quad , \tag{16}$$

and one can see easily that the correction term is that of a two-dimensional ensemble of fermions; indeed, in this case we have

$$c = \frac{\pi^2}{3}\frac{T}{\varepsilon_F} = \frac{ma^2}{\hbar^2}\left(\pi g/6\right)T \quad , \tag{17}$$

where $\varepsilon_F = \left(\hbar^2/ma^2\right)\left(2\pi/g\right)$ and $A = Na^2$.

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