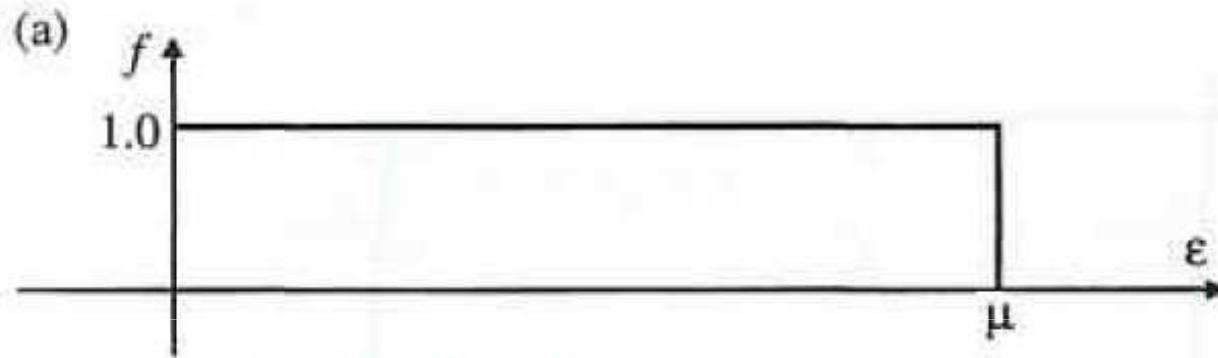


Distribuição de Fermi-Dirac

- Distribuição de férmions com energia ε :
$$f_D(\varepsilon, T, \mu) = \frac{1}{(e^{(\varepsilon-\mu)/k_B T} + 1)}$$



Ocupação média de um estado de energia ε em um gás de férmions conectados a um reservatório térmico de temperatura T e potencial químico μ .
(ensemble grand-canônico)

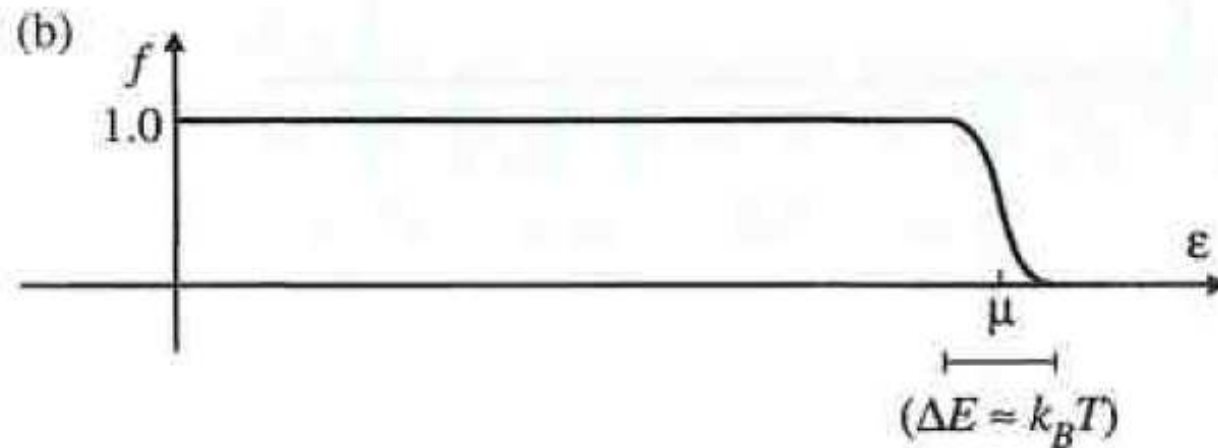


Fig. 1.7 The Fermi-Dirac distribution function at $T = 0$ and at a finite temperature $T \ll E_F/k_B$.

Potencial químico a T=0

- Número de férmions **fixo** (ensemble canônico): $N = \int_0^{\infty} \rho_{3D}(\varepsilon) f_D(\varepsilon, T, \mu) d\varepsilon$

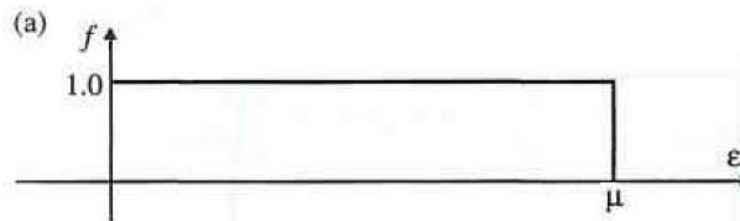
$$N = \frac{V_{\mathbf{r}}}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \int_0^{\infty} \frac{\varepsilon^{\frac{1}{2}}}{(e^{(\varepsilon-\mu)/k_B T} + 1)} d\varepsilon$$

- A T=0, temos:

$$N = \frac{V_{\mathbf{r}}}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \int_0^{\mu(0)} \varepsilon^{\frac{1}{2}} d\varepsilon = \frac{V_{\mathbf{r}}}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \frac{2}{3} [\mu(0)]^{\frac{3}{2}}$$

Invertendo e solando o potencial químico, obtemos:

$$\mu(T=0) = (3\pi^2)^{\frac{2}{3}} \left(\frac{\hbar^2}{2m^*} \right) n^{\frac{2}{3}} = \varepsilon_F$$



Potencial químico a $T \neq 0$

- Número de elétrons:
$$N = \int_0^\infty \rho_{3D}(\varepsilon) f_D(\varepsilon, T, \mu) d\varepsilon$$
$$N = \frac{V_r}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \int_0^\infty \frac{\varepsilon^{\frac{1}{2}}}{(e^{(\varepsilon-\mu)/k_B T} + 1)} d\varepsilon$$

- Temos que resolver a integral e inverter para obter $\mu(T)$. Como?

- Usamos a **expansão de Sommerfeld** (1927):

$$\int_0^\infty \frac{x^j}{(e^{(x-x_0)} + 1)} dx \approx \frac{x_0^{j+1}}{j+1} \left(1 + \frac{\pi^2 j(j+1)}{6x_0^2} + \mathcal{O}(x_0^{-4}) \right)$$

- Para $j=1/2$ e $x=\varepsilon/k_B T$, $x_0=\mu/k_B T$, temos (Tarefa de hoje!):

$$\int_0^\infty \frac{\varepsilon^{\frac{1}{2}}}{(e^{(\varepsilon-\mu)/k_B T} + 1)} d\varepsilon \approx \frac{2\mu^{\frac{3}{2}}}{3} \left(1 + \frac{\pi^2 (k_B T)^2}{8\mu^2} \right)$$

Potencial químico a $T \neq 0$

- Substituindo e tomando o limite $\mu \gg k_B T$, temos (Tarefa de hoje):

$$\mu \approx \varepsilon_F \left(1 - \frac{\pi^2 (k_B T)^2}{12 \mu^2} \right)$$

- Um último passo: substituir recursivamente μ por ε_F no lado direito:

$$\mu \approx \varepsilon_F - \frac{\pi^2 (k_B T)^2}{12 \varepsilon_F} + \dots$$

- Logo, a primeira correção devido à temperatura é da ordem de $(k_B T)^2 / \varepsilon_F$:

$$\mu(T) \approx \mu(0) - \frac{\pi^2 (k_B T)^2}{12 \varepsilon_F} + \dots$$

Energia do gás de elétrons a T=0

- Densidade de energia interna do gás: $u(T) = \frac{1}{V_{\mathbf{r}}} \int_0^{\infty} \rho_{3D}(\varepsilon) f_D(\varepsilon, T, \mu) \varepsilon d\varepsilon$

$$u(T) = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \int_0^{\infty} \frac{\varepsilon^{\frac{3}{2}}}{(e^{(\varepsilon-\mu)/k_B T} + 1)} d\varepsilon$$

- À T=0, temos: $u(0) = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \int_0^{\varepsilon_F} \varepsilon^{\frac{3}{2}} d\varepsilon = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \frac{2}{5} \varepsilon_F^{\frac{5}{2}}$

- Usando a definição de ε_F : $\left[\frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} = \frac{3}{2} n \varepsilon_F^{-\frac{3}{2}} \right]$

$$u(0) = \frac{3}{2} n \varepsilon_F^{-3/2} \frac{2}{5} \varepsilon_F^{5/2} \quad \rightarrow \quad \boxed{u(0) = \frac{3}{5} n \varepsilon_F} \quad \left(u(0) = \frac{E}{V_{\mathbf{r}}} \right)$$

Energia do gás de elétrons a $T \neq 0$

- Densidade de energia interna do gás: $u(T) = \frac{1}{V_{\mathbf{r}}} \int_0^{\infty} \rho_{3D}(\varepsilon) f_D(\varepsilon, T, \mu) \varepsilon d\varepsilon$

$$u(T) = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \int_0^{\infty} \frac{\varepsilon^{\frac{3}{2}}}{(e^{(\varepsilon-\mu)/k_B T} + 1)} d\varepsilon \quad \left[\frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} = \frac{3}{2} n \varepsilon_F^{-\frac{3}{2}} \right]$$

- Expansão de Sommerfeld: $\int_0^{\infty} \frac{\varepsilon^{\frac{3}{2}}}{(e^{(\varepsilon-\mu)/k_B T} + 1)} d\varepsilon \approx \frac{2\mu^{\frac{5}{2}}}{5} \left(1 + \frac{5\pi^2 (k_B T)^2}{8\mu^2} \right)$

- Lembrando que temos que usar $\mu(T)$: $\mu^{\frac{5}{2}} \approx \varepsilon_F^{\frac{5}{2}} \left(1 - \frac{5}{2} \frac{\pi^2 (k_B T)^2}{12\varepsilon_F^2} \right)$

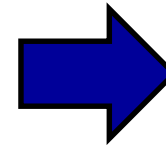
- Juntando tudo: $u(T) = \frac{3}{5} n \varepsilon_F \left(1 - \frac{5\pi^2 (k_B T)^2}{24\varepsilon_F^2} \right) \left(1 + \frac{5\pi^2 (k_B T)^2}{8\varepsilon_F^2} \right)$

$$u(T) \approx \frac{3}{5} n \varepsilon_F \left(1 + \frac{5\pi^2 (k_B T)^2}{12\varepsilon_F^2} + \mathcal{O}(k_B T)^4 \right)$$

Capacidade calorífica do gás de férmions

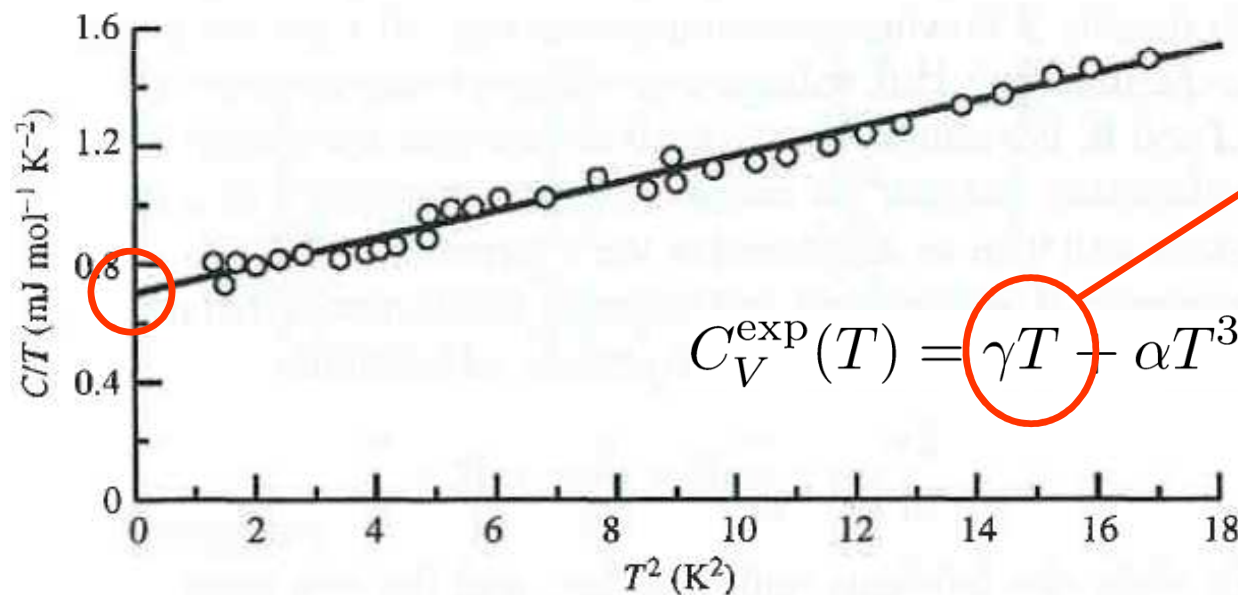
- Capacidade calorífica por volume: $C_V = \frac{\partial u}{\partial T}$

- No caso: $u(T) = \frac{3}{5}n\varepsilon_F + \frac{n\pi^2(k_B T)^2}{4\varepsilon_F}$



$$C_V^{\text{el}}(T) = \frac{n\pi^2 k_B}{2} \frac{T}{T_F}$$

- Comparação com experimento:



**Contribuição eletrônica
Linear com T !!**

Fig. 1.4 Plot of C_V/T versus T^2 for Cu; the intercept gives γ . (Data from W.S. Corak *et al.*, *Phys. Rev.* **98**, 1699 (1955).)