Supplement: Sommerfeld expansion (19 May)

Recall non-rel. Fermion gas

$$\langle N\rangle_F \propto \int_0^\infty F(E)\sqrt{E}\, dE$$

$$\langle E\rangle_F \propto \int_0^\infty E\, F(E)\sqrt{E}\, dE$$

Go beyond approximating $F(E)$ as step function

$\rightarrow$ Low-temp. heat capacity

$\rightarrow$ Chemical potential $\mu(T)$ approaches classical limit

Streamline notation

$$\langle N\rangle_F = \int_0^\infty g(E)\, F(E)\, dE$$

$$g(E) = g_0\sqrt{E} = V\frac{\sqrt{2m^3}}{\pi^2\hbar^3}\sqrt{E}$$

$\llcorner$ density of states

$g(E)$ is # of single-particle energy levels per unit energy

$F(E) = \dfrac{1}{e^{\beta(E-\mu)}+1}$ is occupation prob.

$T>0 \rightarrow$ particles occupy $E>E_F$ (exp. suppressed prob.)

$\rightarrow$ unoccupied $E<E_F$

Recall $\mu = E \longleftrightarrow F(E)=\frac{1}{2}$

Will see $\mu(T>0) < E_F = \mu(T=0)$

$$\frac{\langle N\rangle_F}{g_0} = \int_0^\infty E^{1/2}F(E)\,dE = \underbrace{\frac{2}{3}E^{3/2}F(E)\Big|_0^\infty}_{0} - \frac{2}{3}\int_0^\infty E^{3/2}\left(\frac{dF}{dE}\right)dE$$

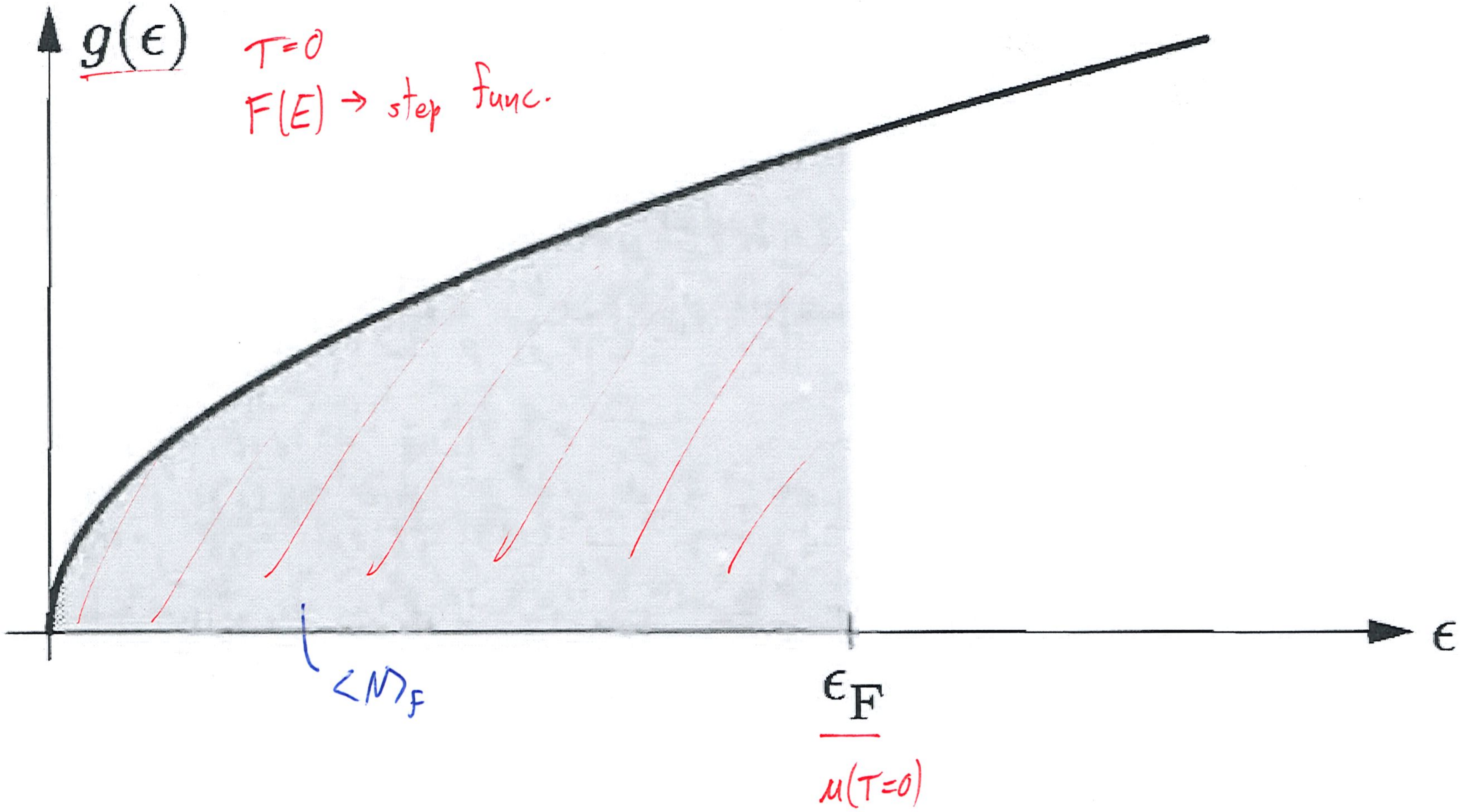
$u = F(E)$

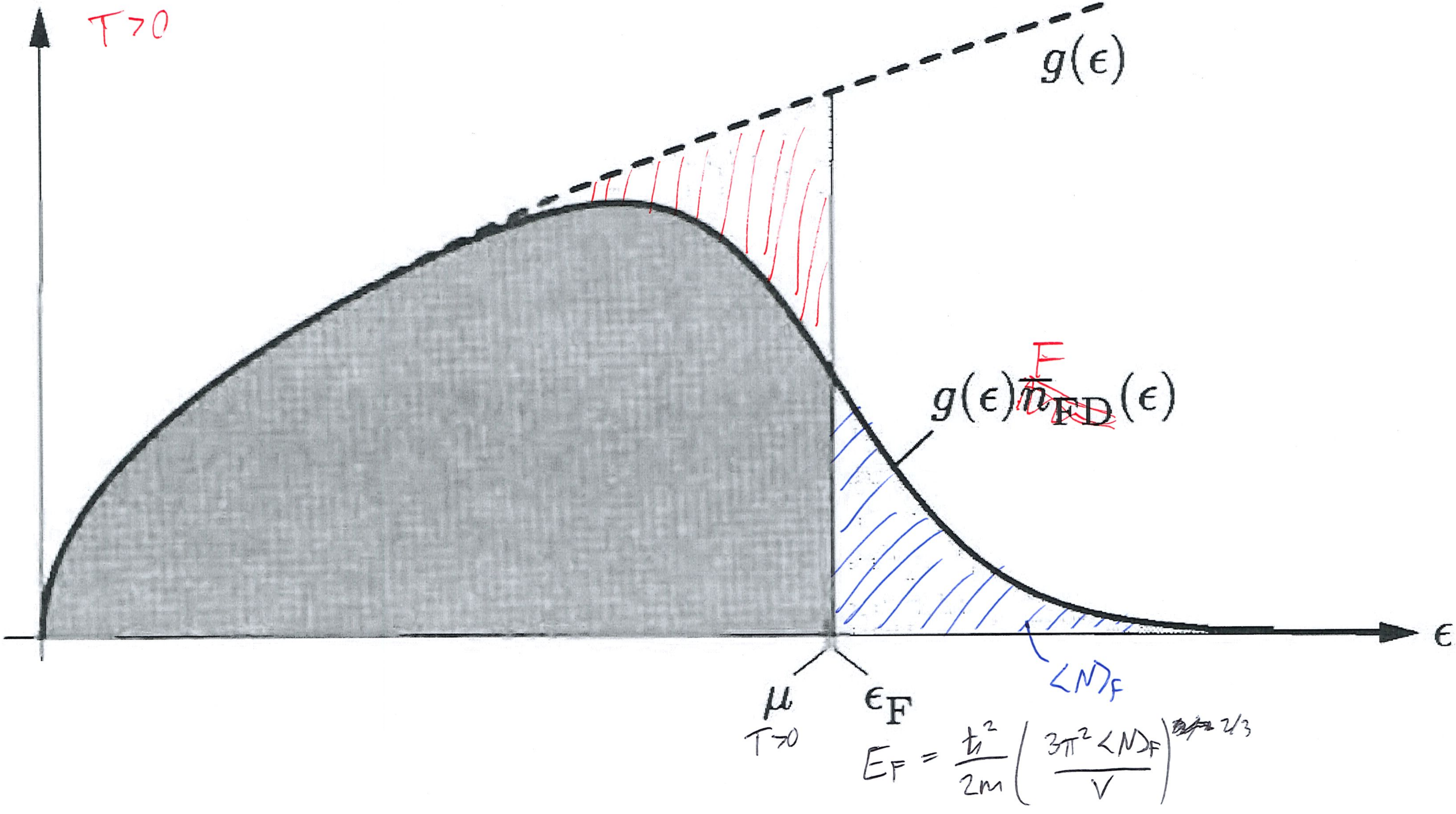
$dv = E^{1/2}\,dE$

$v = \frac{2}{3}E^{3/2}$

$x = \beta(E-\mu)$ $\quad E-\mu = \frac{x}{\beta} = xT$

$$-\frac{d}{dE}\left(e^{\beta(E-\mu)}+1\right)^{-1} = \frac{\beta\, e^{\beta(E-\mu)}}{\left(e^{\beta(E-\mu)}+1\right)^2} = \frac{\beta\, e^x}{\left(e^x+1\right)^2}$$


$g(\epsilon)$
$T=0$
$F(E) \rightarrow$ step func.
$\langle N \rangle_F$
ϵ_F
$\mu(T=0)$
ϵ



$E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2\langle N\rangle_F}{V}\right)^{2/3}$

$$\frac{\langle N\rangle_F}{g_0} = \frac{2}{3}\int_0^\infty \frac{e^x}{(e^x+1)^2} E^{3/2}\, d(\beta E) = \frac{2}{3}\int_{-\beta\mu}^\infty \frac{e^x}{(e^x+1)^2} \underline{E^{3/2}}\, dx$$

sharply peaked around $x=0$
$E=\mu$

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When $x \ll -1$ $\quad \frac{e^x}{(e^x+1)^2} \approx \frac{e^x}{1} \ll 1$

$x \gg 1$ $\quad \frac{e^x}{(e^x+1)^2} \approx \frac{e^x}{e^{2x}} = \frac{1}{e^x} \ll 1$

Peak allows approximations

1) Extend $\int_{-\beta\mu}^{\infty} \to \int_{-\infty}^{\infty}$ since $\mu > 0$ for low-T

2) Expand
$$E^{3/2} \approx \mu^{3/2} + (E-\mu)\frac{\partial}{\partial E}E^{3/2}\Big|_{E=\mu} + \frac{1}{2}(E-\mu)^2\frac{\partial^2}{\partial E^2}E^{3/2}\Big|_{E=\mu}$$
$$= \mu^{3/2} + \frac{3}{2}(E-\mu)\mu^{1/2} + \frac{3}{8}(E-\mu)^2\mu^{-1/2}$$
$$= \mu^{3/2} + \frac{3}{2}xT\mu^{1/2} + \frac{3}{8}(xT)^2\mu^{-1/2}$$

low-T Sommerfeld expansion

Now have sum of simpler integrals

$$\frac{\langle N\rangle_F}{g_0} \approx \frac{2}{3}\mu^{3/2}\cancelto{1}{I_0} + T\mu^{1/2}\cancelto{0}{I_1} + \frac{T^2}{4\mu^{1/2}} I_2$$

$$I_0 = \int_{-\infty}^{\infty}\frac{e^x}{(e^x+1)^2}dx = \int_{-\infty}^{\infty}\frac{-dF}{dE}dE = -F(E)\Big|_{-\infty}^{\infty} = -0+1 = 1$$

$$I_1 = \int_{-\infty}^{\infty}\frac{xe^x}{(e^x+1)^2}dx = \int_{-\infty}^{\infty}\frac{xe^x}{(e^x+1)(e^x+1)}dx = \int_{-\infty}^{\infty}\frac{x}{(e^x+1)(1+e^{-x})}dx = 0$$

$$I_2 = \int_{-\infty}^{\infty}\frac{x^2e^x}{(e^x+1)^2}dx = 2\int_0^{\infty}\frac{x^2e^x}{(e^x+1)^2}dx = \cancelto{0}{\frac{-2x^2}{e^x+1}}\Big|_0^{\infty} + 2\int_0^{\infty}\frac{2x}{e^x+1}dx$$
$$= 4\left(1-\frac{1}{2}\right)\Gamma(2)\zeta(2)$$
$$= \pi^2/3$$

$u = x^2$

$v = \frac{-1}{e^x+1} \qquad dv = \frac{e^x}{(e^x+1)^2}dx$

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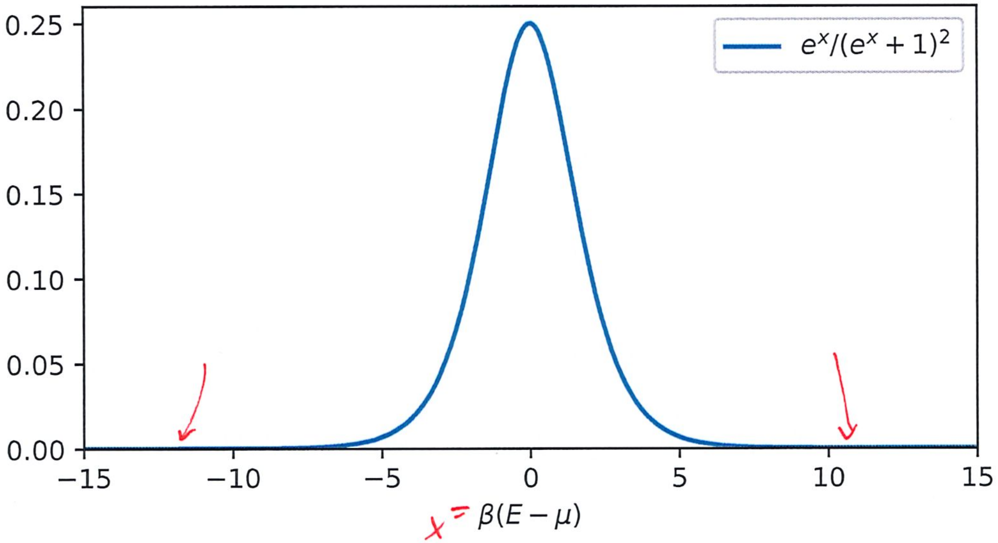0.25
0.20
0.15
0.10
0.05
0.00
−15
−10
−5
0
5
10
15
$e^x/(e^x+1)^2$
x = $\beta(E-\mu)$

$$\langle N \rangle_F \approx g_0 \left[\frac{2}{3} \mu^{3/2} + \frac{\pi^2 T^2}{12 \mu^{1/2}} \right]$$

Connect to $E_F = \mu(T=0) = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 \langle N \rangle_F}{V} \right)^{2/3}$

$$E_F^{3/2} = \frac{3\hbar^3 \pi^2}{2\sqrt{2m^3}} \left(\frac{1}{V} \right) \langle N \rangle_F = \frac{3}{2} \frac{\langle N \rangle_F}{g_0}$$

$$g_0 = \frac{3}{2} \frac{\langle N \rangle_F}{E_F^{3/2}}$$

$$\cancel{\langle N \rangle}_F \approx \cancel{\langle N \rangle}_F \left(\frac{\mu}{E_F} \right)^{3/2} + \frac{\pi^2 T^2 \cancel{\langle N \rangle}_F}{8 E_F^{3/2} \mu^{1/2}}$$

$$\frac{\mu}{E_F} \approx \left(1 - \frac{\pi^2 T^2}{8 E_F^{3/2} \mu^{1/2}} \right)^{2/3} \approx 1 - \frac{\pi^2}{12} \left(\frac{T}{E_F} \right)^2$$

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Low-T $\rightarrow E_F \approx \mu$

$$\mu(T>0) \approx E_F - \frac{\pi^2}{12} \left(\frac{T^2}{E_F} \right)$$

confirms $\mu < E_F$
for low $T > 0$ ✓

Very similar result for $\frac{\langle E \rangle_F}{g_0} = \int_0^\infty E^{3/2} F(E)\, dE$

$$\approx \frac{2}{5} \int_{-\infty}^{\infty} \frac{e^x}{(e^x+1)^2} E^{5/2}\, dx$$

$$\approx \frac{2}{5} \mu^{5/2} \underset{\downarrow 1}{\cancel{I_0}} + T \mu^{3/2} \underset{\downarrow 0}{\cancel{I_1}} + \frac{3}{4} T^2 \mu^{1/2} \underset{\downarrow \pi^2/3}{\cancel{I_2}}$$

$$\langle E \rangle_F \approx g_0 \left[\frac{2}{5} \mu^{5/2} + \frac{1}{4} \pi^2 T^2 \mu^{1/2} \right]$$

$$= \frac{3}{5} \frac{\langle N \rangle_F \mu^{5/2}}{E_F^{3/2}} + \frac{3}{8} \langle N \rangle_F \pi^2 T^2 \frac{\mu^{1/2}}{E_F^{3/2}}$$

We just found $\mu^{5/2} = E_F^{5/2} \left(1 - \frac{\pi^2 T^2}{12 E_F^2} \right)^{5/2} \approx E_F^{5/2} - \frac{5}{24} \pi^2 T^2 E_F^{1/2}$

page

$$\langle E \rangle_F = \frac{3}{5}\langle N \rangle_F E_F - \frac{1}{8}\langle N\rangle_F \pi^2 \frac{T^2}{E_F} + \frac{3}{8}\langle N\rangle_F \pi^2 \frac{T^2}{E_F} + \mathcal{O}(T^4)$$

$$= \frac{3}{5}\langle N\rangle_F E_F + \frac{\pi^2}{4}\langle N\rangle_F \frac{T^2}{E_F} + \mathcal{O}(T^4)$$

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Heat capacity $c_V = \frac{\partial}{\partial T}\langle E\rangle_F \Big|_{N,V} \approx \frac{\pi^2}{2}\frac{\langle N\rangle_F}{E_F} T$ ✓

$$a = \frac{\pi^2}{2}\frac{\langle N\rangle_F}{\boxed{E_F}}$$

Finally consider higher $T \sim E_F$

Sommerfeld expansions above (powers of $\frac{T}{E_F} \ll 1$) may not converge

Need numerical solution of

$$\langle \cancel{N} \rangle_F = g_0 \int_0^\infty \frac{\sqrt{E}}{e^{\beta(E-\mu)}+1}\, dE = \frac{3}{2}\frac{\cancel{\langle N\rangle_F}}{E_F^{3/2}} \int_0^\infty \frac{\sqrt{E}}{e^{\beta(E-\mu)}+1}\, dE$$

Use dim'less ratio $x = \frac{E}{T}$ $\quad E = xT$

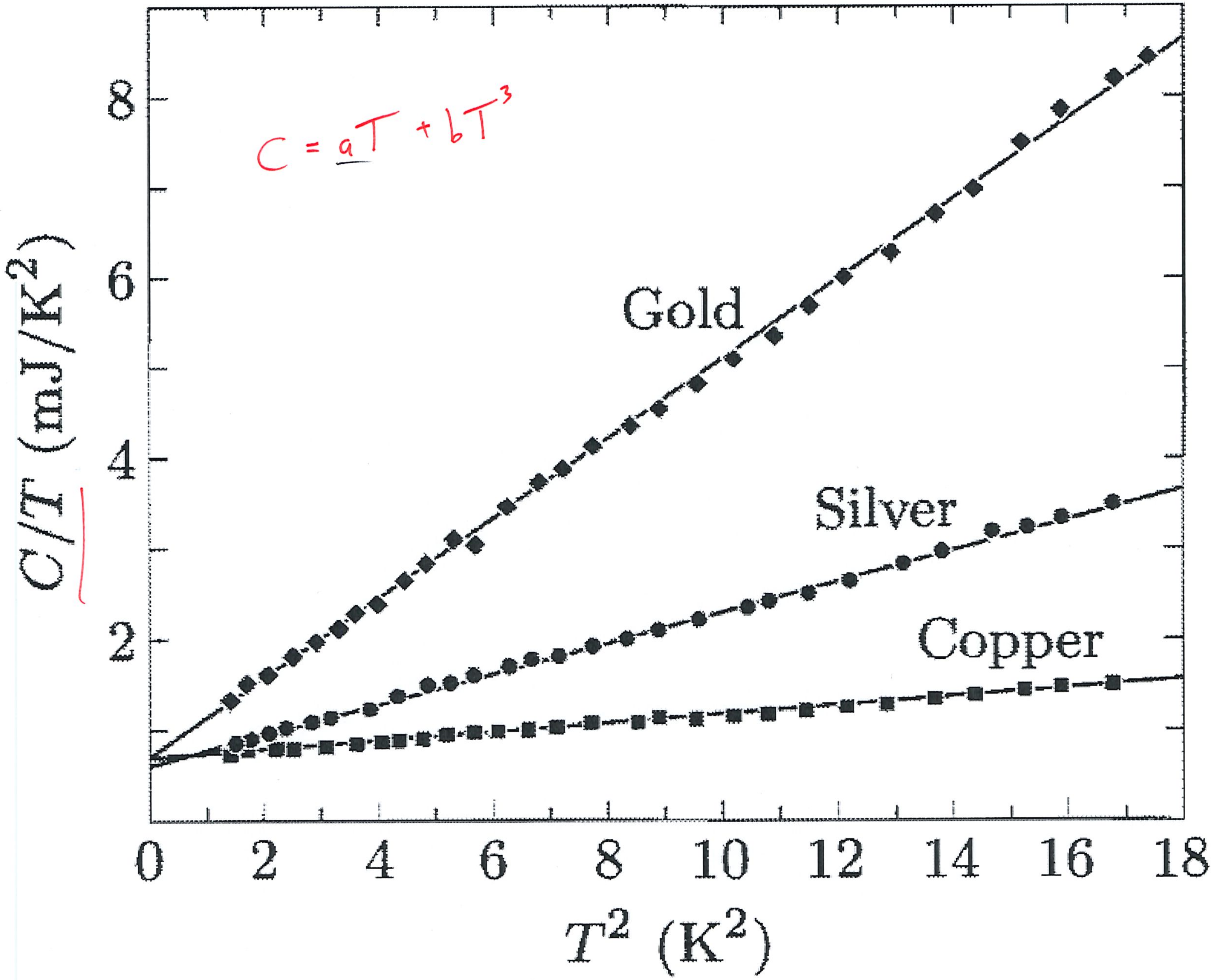
$$1 \overset{?}{=} \frac{3}{2}\underbrace{\left(\frac{T}{E_F}\right)}_{t}^{3/2} \int_0^\infty \frac{\sqrt{x}}{e^x e^{-\mu/T}+1}\, dx = \frac{3}{2} t^{3/2} \int_0^\infty \frac{\sqrt{x}\, e^{-x}}{e^{-c/t} + \underbrace{e^{-x}}_{\text{small as } x\to\infty}}\, dx$$

$$\underline{c = \frac{\mu}{E_F}}$$

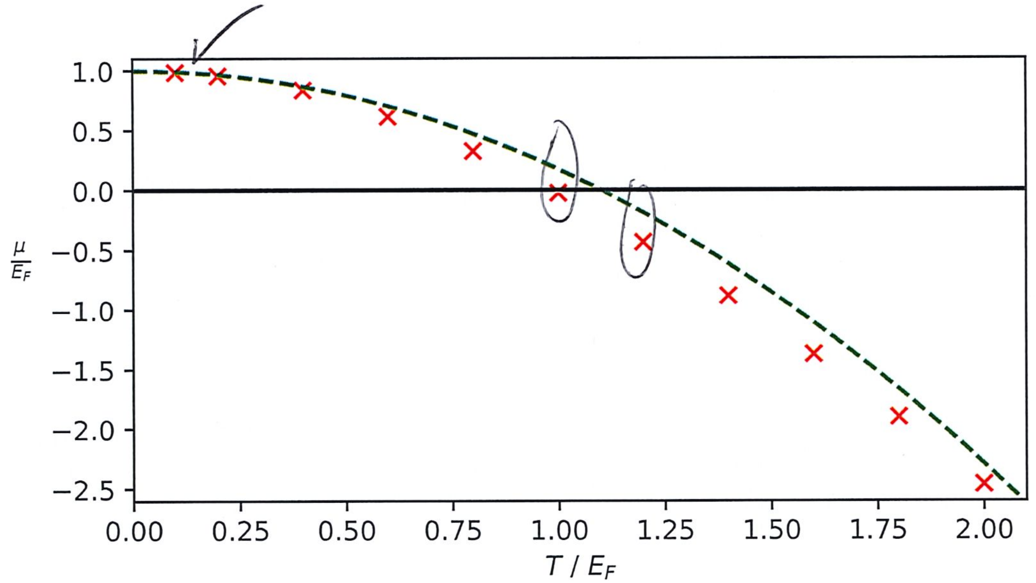
Fix t, numerically compute integral adjusting c to satisfy consistency condition

As T increases, μ becomes more negative

→ classical limit $-\mu \gg T \gg E_F$ ✓



$C = \underline{a}T + bT^3$


1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
$\frac{\mu}{E_F}$
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
T / E_F