Finite temperature (Sommerfeld) expansions in general & for energy, free energy & entropy of indep. e^- systems

We are interested in expanding about $T=0$ integrals like

$$G(T) = \int dk \; g(\varepsilon_k)\, f_\beta(\varepsilon_k)$$

where g is some smooth function

and

$$f_\beta(\varepsilon) = \frac{1}{1+e^{\beta(\varepsilon-\mu)}} \quad , \quad \beta = 1/T$$

μ chosen to fix N

$$\left.\frac{\partial f}{\partial \beta}\right|_\mu = -\frac{e^{\beta(\varepsilon-\mu)}}{\left(1+e^{\beta(\varepsilon-\mu)}\right)^2}(\varepsilon-\mu)$$

$$= \frac{-(\varepsilon-\mu)}{\left(e^{\frac{\beta}{2}(\varepsilon-\mu)}+e^{-\frac{\beta}{2}(\varepsilon-\mu)}\right)^2}$$

clearly symmetric denominator

Also, $\dfrac{\partial}{\partial\beta} = -T^2\dfrac{\partial}{\partial T}$ is a useful rule.

OK:

$$\frac{\partial G}{\partial T} = \int dk \; g(\varepsilon_k)\, \frac{\partial f(\varepsilon_k)}{\partial T}$$

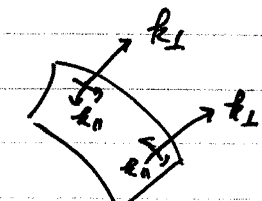
$$= -T^{-2}\int dk \; g(\varepsilon_k)\, \frac{\partial f}{\partial \beta}$$

$$= +\frac{1}{T^2}\int dk \; g(\varepsilon_k)\, \frac{(\varepsilon_k-\mu)}{\left(e^{x/2}+e^{-x/2}\right)^2} \qquad x \equiv \beta(\varepsilon-\mu)$$

We can change integral dk to over $k_\perp$ to constant energy surface & $k_\parallel$ in the surface:

$\varepsilon_k = \varepsilon_{k_\perp}$ clearly

$$\frac{\partial G}{\partial T} = +\frac{1}{T^2}\int dk_\parallel\, dk_\perp \; g(\varepsilon_{k_\perp})\, \frac{(\varepsilon_{k_\perp}-\mu)}{\left(e^{x/2}+e^{-x/2}\right)^2}$$



$$= +\frac{1}{T^2}\int \frac{d\varepsilon\, dk_\parallel}{|\nabla\varepsilon|}\, g(\varepsilon)\, \frac{(\varepsilon-\mu)}{\left(e^{x/2}+e^{-x/2}\right)^2} \qquad \left|\frac{\partial\varepsilon}{\partial k}\right| dk_\perp = d\varepsilon$$

For each $k_{\|}$, we can do $\int d\varepsilon$ integral: change variables to $x = \beta(\varepsilon - \mu) = \frac{\varepsilon - \mu}{T}$, $\varepsilon = \mu + xT$

$$\frac{\partial G}{\partial T} = +\frac{1}{T^2}\int dx \cdot T \cdot dk_{\|}\, \frac{g(\mu + Tx)}{|\nabla \varepsilon(\mu + Tx)|} \frac{T \cdot x}{(e^{x/2} + e^{-x/2})^2}$$

$$= +\int dx\, dk_{\|}\, \frac{g(\mu + Tx)}{|\nabla \varepsilon|}\, x \Big/ (\qquad)^2$$

Taylor expanding $\frac{g}{\nabla \varepsilon}$ about $x = 0$ & using symmetry of denominator & its rapid decay gives a series of form (integrand is positive)

$$\frac{\partial G}{\partial T} = T\, 2c_1 + T^3 c_3 \cdot 4 + O(T^5)$$

where c_1, c_2 are some constants depending on μ & other things but not T.

So for fixed μ, we get

$$\boxed{G(T, \mu) = G(0, \mu) + c_1 T^2 + c_3 T^4 + O(T^6)}$$

Power series in T^2!

Now μ is not free but must determine N fixed:

$$N(\mu, T) = N(\mu, 0) + n_1^{(\mu)} T^2 + n_3^{(\mu)} T^4 + O(T^6)$$
$$= N_0 \quad \text{for all } T$$

If we write a series for $\mu(T)$, it is easy to see that

$$\mu(T) = \mu(0) + m_2 T^2 + m_4 T^4 + O(T^6)$$

as well.

So, for fixed N, we also have

$$\boxed{G(T, N) = G(0, N) + c_1' T^2 + c_4' T^4 + O(T^6)}$$

For example, the energy has $g(\mathcal{E}) = \mathcal{E}$ & has such a series.

What of the entropy? ($k_B = 1$ in our units)

$$S = -\int dk \left[f(\varepsilon_k) \ln f(\varepsilon_k) + (1 - f(\varepsilon_k)) \ln (1 - f(\varepsilon_k)) \right]$$

is the entropy for any distribution $f(\varepsilon_k)$. Why? It gives us the Fermi-Dirac!

Take $F - \mu N = E - TS - \mu N$ & optimize over occupancies only:

$$\delta F - \mu \delta N = 0 = \delta E - T \delta S - \mu \delta N = 0$$

$$\Rightarrow (\varepsilon - T \frac{\delta S}{\delta f} - \mu) \delta f = 0$$

$$\frac{\delta S}{\delta f} = -\ln f + \ln(1-f) = \ln(1/f - 1) \quad \text{so}$$

$$\varepsilon - T \ln(1/f - 1) - \mu = 0 \rightarrow \ln(\tfrac{1}{f} - 1) = \frac{\varepsilon - \mu}{T}$$

$$f = (1 + e^{\frac{\varepsilon - \mu}{T}})^{-1} \checkmark$$

The entropy is <u>not</u> of the $g(\varepsilon)$ form since its "g" depends of β & μ as well. But this is not so hard actually:

$$\frac{\partial S}{\partial T} = + \int dk \ln(\tfrac{1}{f} - 1) \frac{\partial f}{\partial T} = -\frac{1}{T^2} \int dk \ln(\tfrac{1}{f} - 1) \frac{\partial f}{\partial \beta}$$

We are interested in F-D distrib: plug in

$$\frac{\partial S}{\partial T} = -\frac{1}{T^2} \int dk \left(\frac{\varepsilon - \mu}{T}\right) \frac{\partial f}{\partial \beta} = -\frac{1}{T^3} \int dk (\varepsilon - \mu) \frac{\partial f}{\partial \beta}$$

<u>Now</u> it is in previous form!

$$\frac{\partial S}{\partial T} = \frac{1}{T^3} \int dk \frac{(\varepsilon - \mu)^2}{(e^{x/2} + e^{-x/2})^2} = \frac{1}{T^3} \int dx \int dk_{\parallel} \frac{T \cdot T^2 x^2}{(e^{x/2} + e^{-x/2})^2}$$

$$= a_0 + a_2 T^2 + a_4 T^4 + O(T^6)$$

Since $S(T=0) = 0$ we can solve quickly

$$\boxed{S(T) = s_1 T + s_3 T^3 + O(T^5)}$$

Let $E(T) = e_0 + e_2 T^2 + e_4 T^4 + O(T^6)$
then

$$F(T) = f_0 + f_2 T^2 + f_4 T^4 + O(T^6) = E - TS$$

where

$$f_0 = e_0$$
$$f_2 = e_2 - s_1$$
$$f_4 = e_4 - s_3 \quad \text{etc.}$$

One more thing: s_1 & e_2 are not independent!

Say we consider a first order change in $F(T,N)$

$$\delta F = \delta E - (\delta T) \cdot S - T \cdot \delta S$$
$$= [\delta E - T\delta S - \mu \delta N] - S \cdot \delta T + \mu \delta N$$

The term in bracket is zero for F.D. distrib! So we get the obvious $\delta F = -S\delta T + \mu \delta N$

For fixed N:

$$\left.\frac{\partial F}{\partial T}\right|_N = -S \qquad \text{(duh!)}$$

For <u>our form of S</u>, we see that

$$\frac{\partial S}{\partial T} = -\frac{1}{T^3}\int (\varepsilon - \mu)\frac{\partial f}{\partial \beta} dk = -\frac{1}{T^3}\int \varepsilon \frac{\partial f}{\partial \beta} dk$$

since N is fixed

$$= -\frac{1}{T^3}\frac{\partial}{\partial \beta} E = +\frac{1}{T}\frac{\partial E}{\partial T} \quad \therefore \quad \boxed{\frac{\partial S}{\partial T} = \frac{1}{T}\frac{\partial E}{\partial T}} \text{ for this entropy!}$$

applied about $T=0$, this says that

$$\boxed{s_1 = 2e_2}$$
$$3s_3 = 4e_4 \text{ etc.}$$

<u>$s_1 = 2e_2$ means $f_2 = -e_2$</u>

So we have the extra relation

$$\boxed{\frac{E(T)+F(T)}{2} = e_0 + \left(\frac{e_4+f_4}{2}\right)T^4 + O(T^6) \qquad e_0 = E(0) = F(0)}$$

A nice cancellation, but only true for our independent particle entropy & energy.

Works for any indep. particle case where

$$E = \int dk\ \varepsilon\, f(\varepsilon)$$

$$S = \int dk\ \mathrm{Func}(f(\varepsilon)) = \int dk\ h[f(\varepsilon)]$$

extremum of $F-\mu N$ says $\frac{\delta}{\delta f}(F-\mu N) = 0$

$$\varepsilon - \mu - T h'(f) = 0 \quad \Rightarrow \quad h'(f) = \frac{\varepsilon-\mu}{T}$$

is the optimal distrib.

Then $\frac{\partial S}{\partial T} = \int dk\ h'(f)\frac{\partial f}{\partial T}$

$$= \int dk \left(\frac{\varepsilon-\mu}{T}\right)\partial f/\partial T \quad \text{, fixed } N = \int dk \cdot f$$

$$= \frac{1}{T}\int dk\ \varepsilon\frac{\partial f}{\partial T}$$

$$= \frac{1}{T}\frac{\partial E}{\partial T} \quad ✓$$

Actually true in general!

$\left.\frac{\partial F}{\partial T}\right|_N = -S$ is true ; now $F = E - TS$

so $\frac{\partial E}{\partial T} - T\frac{\partial S}{\partial T} = 0$ needed

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