

Applications of DFT (see Girvin and Yang):

- **structural determination**: the external potential is

$$v_{\text{ext}}(\vec{x}) = - \sum_l \frac{z_l e^2}{|\vec{x} - \vec{R}_l|}$$

The total energy is

$$E_{\text{tot}}[\{\vec{R}_l\}, n] = E_{\text{jel}}[n] + \int d^3x n(\vec{x}) v_{\text{ext}}(\vec{x}) + \sum_{l \neq l'} \frac{z_l z_{l'} e^2}{|\vec{R}_l - \vec{R}_{l'}|}$$

Given $\{\vec{R}_l\}$, extremize $E_{\text{tot}}[\{\vec{R}_l\}, n(\vec{x})]$ wrt $n(\vec{x})$ to obtain an energy $\Phi(\{\vec{R}_l\})$. Then minimize wrt nuclear positions $\{\vec{R}_l\}$. Typically use pbc, large xtal unit cell.

- **cohesive energy**: $E_{\text{coh}} = E_{\text{crystal}} - E_{\text{atomic}}$ is the crystalline binding energy (when $E_{\text{coh}} < 0$)
- **elastic constants**: vary $\Phi(\{\vec{R}_l\})$ wrt nuclear positions
- **phase diagram under pressure**: At $T=0$, $G = H = E + pV$
Including pV term, obtain G at finite pressure.

Lecture 9 (Feb. 2): Linear response theory

Response functions of jellium system to an external

potential: expand $E_{\text{jel}}[n_0 + \delta n]$ about uniform density n_0 :

$$E[n_0 + \delta n] = E_{jel}[n_0] + \frac{1}{2} \int d^3x \int d^3x' \left. \frac{\delta^2 E_{jel}[n]}{\delta n(\vec{x}) \delta n(\vec{x}')} \right|_{n_0} \delta n(\vec{x}) \delta n(\vec{x}') + \int d^3x (n_0 + \delta n(\vec{x})) v_{ext}(\vec{x}) + \dots$$

Thus,

$$\frac{\delta E[n]}{\delta n(\vec{x})} = v_{ext}(\vec{x}) + \int d^3x' \chi^{-1}(\vec{x}, \vec{x}') \delta n(\vec{x}') \equiv 0$$

where

$$\chi^{-1}(\vec{x}, \vec{x}') \equiv \left. \frac{\delta^2 E_{jel}[n]}{\delta n(\vec{x}) \delta n(\vec{x}')} \right|_{n_0}$$

is the inverse density susceptibility. We define the susceptibility $\chi(\vec{r}, \vec{r}')$ according to \rightarrow like $\sum_j \chi^{-1}_{ij} \chi_{jk} = \delta_{ik}$

$$\int d\vec{r}' \chi^{-1}(\vec{r}, \vec{r}') \chi(\vec{r}', \vec{r}'') = \delta(\vec{r} - \vec{r}'')$$

We may now write

\swarrow an external potential results in a density response

$$\delta n(\vec{x}) = - \int d^3x' \chi(\vec{x}, \vec{x}') \vec{v}_{ext}(\vec{x}')$$

Due to translation invariance, we must have

$$\chi(\vec{x}, \vec{x}') = \chi(\vec{x} - \vec{x}') \quad \Rightarrow \quad \hat{\chi}(\vec{q}) = \int d^3r \chi(\vec{r}) e^{-i\vec{q} \cdot \vec{r}}$$

We then have $\delta \hat{n}(\vec{q}) = -\hat{\chi}(\vec{q}) \hat{v}_{ext}(\vec{q})$. Now

$$\chi^{-1}(\vec{x}, \vec{x}') = \chi_0^{-1}(\vec{x}, \vec{x}') + \chi_H^{-1}(x, x') + \chi_{xc}^{-1}(\vec{x}, \vec{x}')$$

where

$$\chi_H^{-1}(\vec{x}, \vec{x}') = \left. \frac{\delta^2 E_H[n]}{\delta n(\vec{x}) \delta n(\vec{x}')} \right|_{n_0} = \frac{e^2}{|\vec{x} - \vec{x}'|}$$

and

$$\chi_{xc}^{-1}(\vec{x}, \vec{x}') = \left. \frac{\delta^2 E_{xc}[n]}{\delta n(\vec{x}) \delta n(\vec{x}')} \right|_{n_0}$$

and

$$\chi_0^{-1}(\vec{x}, \vec{x}') = \left. \frac{\delta^2 T_S[n]}{\delta n(\vec{x}) \delta n(\vec{x}')} \right|_{n_0}$$

Later on we shall derive

$$\chi_0^{-1}(\vec{x}, \vec{x}') = \frac{1}{V} \sum_{\vec{q}} \hat{\chi}_0^{-1}(\vec{q}) e^{i\vec{q} \cdot (\vec{x} - \vec{x}')}$$

$$\hat{\chi}_0(\vec{q}, T) = 2 \int_{\hat{\Omega}} \frac{d^d k}{(2\pi)^d} \frac{f^0(\vec{k} + \vec{q}) - f^0(\vec{k})}{\epsilon_0(\vec{k}) - \epsilon_0(\vec{k} + \vec{q})}$$

where $\epsilon_0(\vec{k}) = \hbar^2 \vec{k}^2 / 2m$ and $f^0(\vec{k}) = \left[\exp\left(\frac{\epsilon_0(\vec{k}) - \mu}{k_B T}\right) + 1 \right]^{-1}$.

At $T=0$, $f^0(\vec{k}) = \Theta(k_F - k)$ and in $d=3$ dimensions

$$\hat{\chi}_0(\vec{q}, T=0) = g(\varepsilon_F) L(q/2k_F)$$

where $g(\varepsilon_F) = mk_F/\pi^2\hbar^2$ with $k_F = (3\pi^2n)^{1/3}$, and

$$L(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|$$

is the Lindhard function. For translationally invariant systems, we have

$$\begin{aligned} \hat{\chi}^{-1}(\vec{q}) &= \hat{\chi}_0^{-1}(\vec{q}) + \frac{4\pi e^2}{\vec{q}^2} + \hat{\chi}_{xc}^{-1}(\vec{q}) \\ &\equiv \frac{4\pi e^2}{\vec{q}^2} + \hat{\Pi}^{-1}(\vec{q}) \end{aligned}$$

where the inverse polarization function is

$$\hat{\Pi}^{-1}(\vec{q}) = \hat{\chi}_0^{-1}(\vec{q}) + \hat{\chi}_{xc}^{-1}(\vec{q})$$

Static screening: We saw above how the linear response to an external potential $v_{\text{ext}}(\vec{x})$ is a density perturbation $\delta n(\vec{q}) = -\hat{\chi}(\vec{q}) \hat{v}_{\text{ext}}(\vec{q})$. This means that the potential is **screened**, and the effective potential experienced by an electron at \vec{x} is

$$v_{\text{scr}}(\vec{x}) = v_{\text{ext}}(\vec{x}) + \int d^3x' \frac{e^2}{|\vec{x}-\vec{x}'|} \delta n(\vec{x}')$$

Taking the Fourier transform,

$$\begin{aligned}\hat{v}_{scr}(\vec{q}) &= \hat{v}_{ext}(\vec{q}) - \frac{4\pi e^2}{q^2} \hat{\chi}(\vec{q}) \hat{v}_{ext}(\vec{q}) \\ &= \hat{v}_{ext}(\vec{q}) / \hat{\epsilon}(\vec{q})\end{aligned}$$

where

static dielectric function

$$\hat{\epsilon}^{-1}(\vec{q}) = 1 - \frac{4\pi e^2}{q^2} \hat{\chi}(\vec{q}) = \frac{1}{1 + \frac{4\pi e^2}{q^2} \hat{\Pi}(\vec{q})}$$

and thus

$$\hat{\epsilon}(\vec{q}) = 1 + \frac{4\pi e^2}{q^2} \hat{\Pi}(\vec{q})$$

Recall the definition of the polarization function $\hat{\Pi}(\vec{q})$:

$$\frac{1}{\hat{\Pi}(\vec{q})} = \frac{1}{\hat{\chi}_0(\vec{q})} + \frac{1}{\hat{\chi}_{xc}(\vec{q})}$$

OK. So suppose we approximate $\hat{\Pi}(\vec{q}) \approx \hat{\Pi}(0) \equiv Q^2/4\pi e^2$, where Q has dimensions of L^{-1} . Then we have

$$\epsilon(\vec{q}) \approx 1 + \frac{Q^2}{q^2}$$

and hence for $v_{ext}(\vec{x}) = -Ze^2/|\vec{x}|$ we have

$$\hat{v}_{scr}(\vec{q}) = -\frac{4\pi Ze^2}{q^2 + Q^2}$$

Transforming back to real space,

$$v_{\text{ext}}(r) = -\frac{Ze^2}{r} e^{-Qr}$$

which is a Yukawa potential. The total number of screening electrons is

$$\begin{aligned} \delta N &= \int d^3x \delta n(\vec{x}) = \lim_{\vec{q} \rightarrow 0} \delta \hat{n}(\vec{q}) = \lim_{\vec{q} \rightarrow 0} \left\{ -\hat{\chi}(\vec{q}) \hat{v}_{\text{ext}}(\vec{q}) \right\} \\ &= \lim_{\vec{q} \rightarrow 0} \left\{ \frac{Z}{1 + \frac{\vec{q}^2}{4\pi e^2 \hat{\Pi}(\vec{q})}} \right\} \end{aligned}$$

Therefore, if $\vec{q}^2 / \hat{\Pi}(\vec{q}) \rightarrow 0$ as $\vec{q} \rightarrow 0$, we have $\delta N = Z$, corresponding to perfect screening.

Approximations to $\hat{\Pi}(\vec{q})$:

Thus far we have been pushing around our ignorance and giving it different names, ultimately coalescing in the unknown polarization function $\hat{\Pi}(\vec{q})$. Two commonly invoked approximate forms:

- Lindhard approximation:

Here we set $\hat{\chi}_{xc}(\vec{q}) \rightarrow \infty$, in which case

$$\hat{\Pi}(\vec{q}) \approx \hat{\chi}_o(\vec{q}) \equiv \hat{\Pi}_L(\vec{q})$$

Then

$$\hat{\chi}(\vec{q}) \approx \hat{\chi}_L(\vec{q}) \equiv \frac{\hat{\chi}_0(\vec{q})}{1 + \frac{4\pi e^2}{\vec{q}^2} \hat{\chi}_0(\vec{q})}$$

$$\hat{\epsilon}(\vec{q}) \approx \hat{\epsilon}_L(\vec{q}) \equiv 1 + \frac{4\pi e^2}{\vec{q}^2} \hat{\Pi}_L(\vec{q})$$

In the $\vec{q} \rightarrow 0$ limit, from our earlier expression for $\hat{\chi}_0(\vec{q})$ one computes $\hat{\chi}_0(\vec{q}) = g(\epsilon_F) + \mathcal{O}(\vec{q}^2)$, which entails perfect screening. But when the full \vec{q} -dependence is accounted for, one obtains not a Yukawa form for $\hat{v}_{scr}(r)$, but rather

$$v_{scr}^L(r) \propto \frac{\cos(2k_F r)}{r^3}$$

at long distances. This arises from the logarithmic singularity in the Lindhard function $L(q/2k_F)$ at $q=2k_F$, which is a consequence of the sharpness of the Fermi surface.

- Thomas-Fermi (TF) approximation:

Here we ignore the \vec{q} -dependence of $\hat{\chi}_0(\vec{q})$ and take

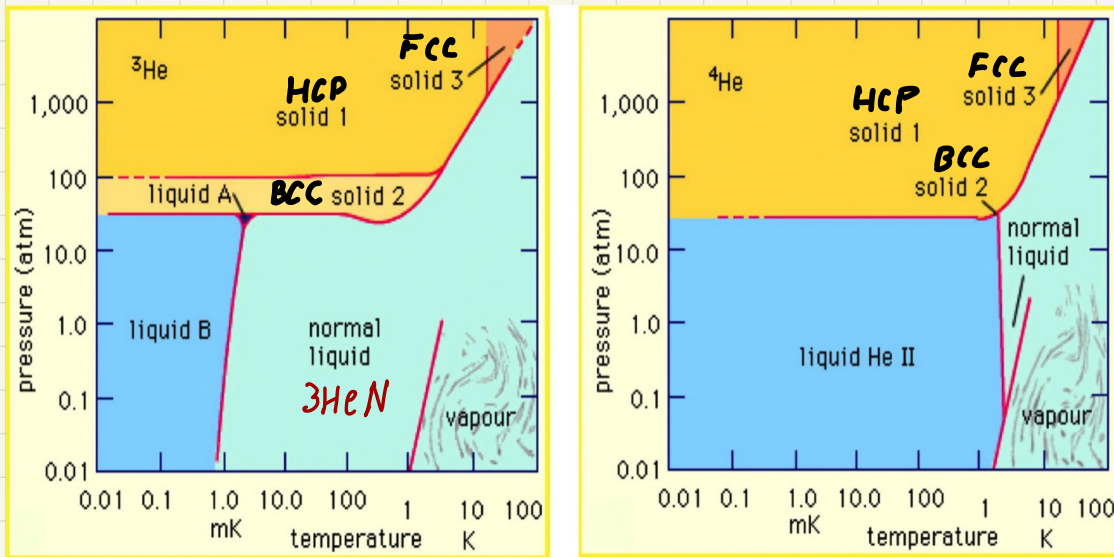
$$\hat{\Pi}_L(q) \approx \hat{\chi}_0(0) = g(\epsilon_F) = \frac{Q_{TF}^2}{4\pi e^2}$$

Thus $Q_{TF} = (4\pi e^2 g(\epsilon_F))^{1/2}$ is the TF screening wavenumber, and $\hat{\epsilon}_{TF}(\vec{q}) = 1 + Q_{TF}^2/\vec{q}^2$, resulting in a screened potential of the Yukawa form, viz.

$$\hat{v}_{scr}(r) = -\frac{Ze^2}{r} e^{-Q_{TF} r}$$

- Landau Fermi liquid theory

${}^3\text{He} = 2p^+ + n + 2e^-$, an $I = \frac{1}{2}$ fermion (at sufficiently low energy scales). Compare phase diagrams of ${}^3\text{He}$ and ${}^4\text{He}$ (a boson):



${}^3\text{He A}$ and ${}^3\text{He B}$ are superfluid phases differing in the symmetry of their order parameters. ${}^3\text{HeN}$ is a normal fluid which behaves much as a degenerate Fermi gas, but in which interaction effects play an important role: there is a linear in T specific heat $c_v(T) \propto T$ and a Pauli-like magnetic susceptibility $\chi(T) \propto T^0$ (i.e. constant). Because $m_3 = 5.01 \times 10^{-24} \text{ g} \approx 6000 m_e$, and its typical density is $n = 1.64 \times 10^{22} \text{ cm}^{-3}$, one has

$$T_F({}^3\text{HeN}) = \frac{\hbar^2}{2m_3 k_B} (3\pi^2 n)^{2/3} = 4.97 \text{ K}$$

Compare $T_F(\text{Cu}) \approx 81,000 \text{ K}$ and $T_F(\text{Al}) \approx 135,000 \text{ K}$.

What this means is that one begins to see a crossover to Curie behavior $\chi_c(T) = n\mu_3^2/k_B T$, with $\mu_3 = -1.16\mu_B$ is the ^3He magneton. For free fermions ($s=1/2$),

$$k_F = (3\pi^2 n)^{1/3}$$

$$C_V = \frac{1}{V} \left(\frac{\partial E}{\partial T} \right)_{N,V} = \frac{\pi^2}{3} g(\epsilon_F) k_B^2 T + \mathcal{O}(T^3)$$

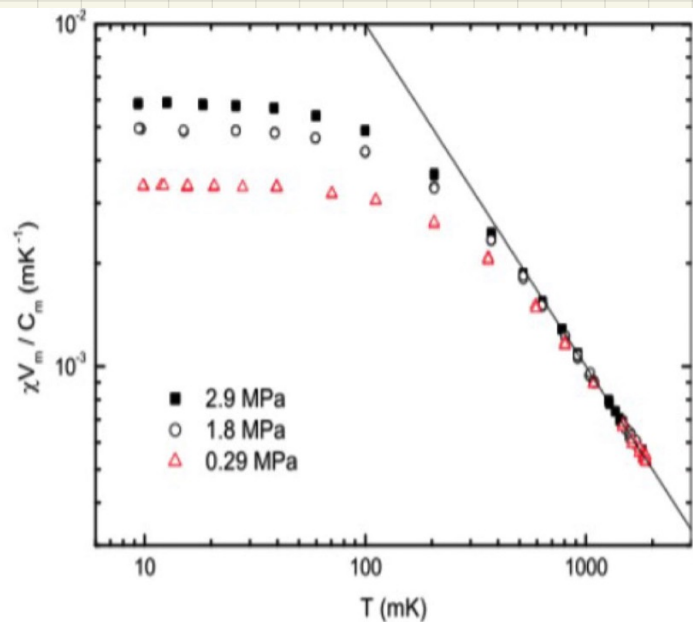
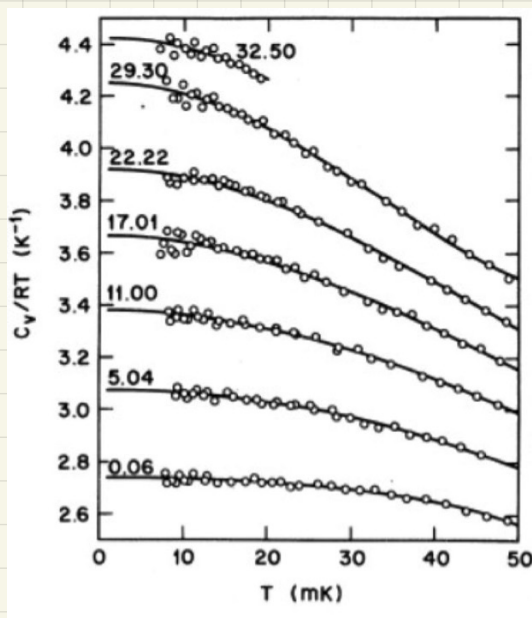
$$g(\epsilon_F) = mk_F / \pi^2 \hbar^2$$

$$\chi = \left(\frac{\partial M}{\partial H} \right)_{N,V} = \mu_0^2 g(\epsilon_F) + \mathcal{O}(T^2)$$

$$f(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1}$$

$$\kappa = n^{-2} \left(\frac{\partial n}{\partial \mu} \right)_T = n^{-2} g(\epsilon_F) + \mathcal{O}(T^2)$$

Let $c_V^0(T, n)$, $\chi^0(T, n)$, and $\kappa^0(T, n)$ be the IFG values. One finds that the ratios C_V/C_V^0 , χ/χ^0 , and κ/κ^0 for ^3HeN all tend to different values as $T \rightarrow 0$.



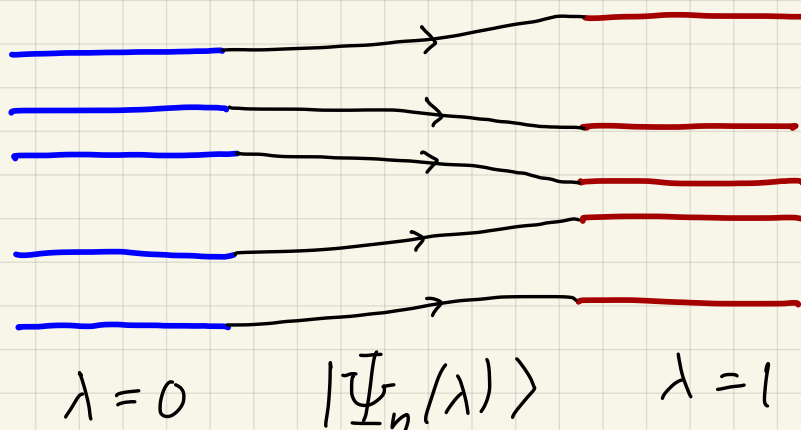
With only one adjustable parameter, m^* , it is impossible to bring these data into agreement. ^3HeN is not an ideal Fermi gas.

Theory of the normal Fermi liquid:

The core concept behind Landau's Fermi liquid theory is the notion of **adiabatic continuity**. Imagine a Hamiltonian

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_1$$

where \hat{H}_0 is a free particle (i.e. noninteracting) term and \hat{H}_1 is the interaction part. We're interested in the eigenspectrum of $\hat{H}(\lambda=1)$. Imagine starting at $t = -\infty$ with $\lambda(-\infty) = 0$, and adiabatically evolving to $t=0$ where $\lambda(0) = 1$. If there are no level crossings, then we have a 1:1 correspondence between states of the IFG ($\hat{H} = \hat{H}_0$) and the fully interacting system ($\hat{H} = \hat{H}_0 + \hat{H}_1$):



The IFG states are given by

$$N = \sum_{\mathbf{k}, \sigma} N_{\mathbf{k}\sigma}$$

$$|\Psi_0[\{N_{\mathbf{k}\sigma}\}]\rangle = \prod_{\mathbf{k}, \sigma} (c_{\mathbf{k}\sigma}^\dagger)^{N_{\mathbf{k}\sigma}} |0\rangle$$

with $N_{\mathbf{k}\sigma} \in \{0, 1\}$. Upon adiabatic evolution, the

interacting state energy is then a function of the occupancies :

$$E_0 = \sum_{k,\sigma} N_{k\sigma} \varepsilon_{k\sigma}^0, \quad E = E(\{N_{k\sigma}\})$$

More generally, we can consider the density matrix,

$$\hat{\rho}_0 = \bigotimes_{k,\sigma} \left[(1-n_{k\sigma}) |0\rangle\langle 0| + n_{k\sigma} \overbrace{c_{k\sigma}^\dagger |0\rangle\langle 0| c_{k\sigma}} \right]$$

where $n_{k\sigma} \in [0, 1] \forall k, \sigma$. In this case, $\{n_{k\sigma}\}$ may be considered a smooth distribution on k for each σ .

First law of thermodynamics: The entropy of the distribution is

$$\begin{aligned} S[\{n_{k\sigma}\}] &= -k_B \text{Tr} \hat{\rho}_0 \ln \hat{\rho}_0 \\ &= -k_B \sum_{k,\sigma} \left\{ n_{k\sigma} \ln n_{k\sigma} + (1-n_{k\sigma}) \ln (1-n_{k\sigma}) \right\} \end{aligned}$$

The first variation of S is then

$$\delta S = -k_B \sum_{k,\sigma} \ln \left(\frac{n_{k\sigma}}{1-n_{k\sigma}} \right) \delta n_{k\sigma}$$

The particle number is

$$N[\{n_{k\sigma}\}] = \text{Tr} \left(\hat{\rho}_0 \underbrace{\sum_{k,\sigma} \hat{n}_{k\sigma}}_{\hat{N}} \right) = \sum_{k,\sigma} n_{k\sigma}$$

and therefore

$$\delta N = \sum_{\mathbf{k}, \sigma} \delta n_{\mathbf{k}\sigma}$$

Note that S and N are adiabatic invariants. But the energy E is not an adiabatic invariant. While

$$E_0 = \text{Tr}(\hat{\rho}_0 \hat{H}_0) = \sum_{\mathbf{k}, \sigma} n_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma}^0$$

the energy of the adiabatically evolved density matrix is written as a functional of the distributions $\{n_{\mathbf{k}\sigma}\}$, and

$$\delta E = \sum_{\mathbf{k}, \sigma} \tilde{\epsilon}_{\mathbf{k}\sigma} \delta n_{\mathbf{k}\sigma}, \quad \tilde{\epsilon}_{\mathbf{k}\sigma} = \frac{\delta E}{\delta n_{\mathbf{k}\sigma}}$$

The quantity $\tilde{\epsilon}_{\mathbf{k}\sigma}$ is thus both a function of (\mathbf{k}, σ) as well as a functional of the distributions $\{n_{\mathbf{k}\sigma}\}$.

We shall define

$$\frac{\delta \tilde{\epsilon}_{\mathbf{k}\sigma}}{\delta n_{\mathbf{k}'\sigma'}} = \frac{\delta^2 E}{\delta n_{\mathbf{k}\sigma} \delta n_{\mathbf{k}'\sigma'}} \equiv \frac{1}{V} \tilde{f}_{\mathbf{k}\sigma, \mathbf{k}'\sigma'}$$

Here $\tilde{f}_{\mathbf{k}\sigma, \mathbf{k}'\sigma'}$ has dimensions of energy \times volume, and is itself a functional of $\{n_{\mathbf{k}\sigma}\}$.

We're now ready to write the First Law:

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

Since the $\{\delta n_{\mathbf{k}\sigma}\}$ are all independent variations, we conclude

$$-k_B T \ln \left(\frac{n_{\mathbf{k}\sigma}}{1-n_{\mathbf{k}\sigma}} \right) = \tilde{\epsilon}_{\mathbf{k}\sigma} - \mu \Rightarrow n_{\mathbf{k}\sigma} = \frac{1}{e^{(\tilde{\epsilon}_{\mathbf{k}\sigma} - \mu)/k_B T} + 1}$$

This last expression is vastly more complex than it might first appear. Since $\tilde{\epsilon}_{\mathbf{k}\sigma}$ is itself a functional of the $\{n_{\mathbf{k}\sigma}\}$, this relation is in fact an implicit nonlinear equation for the individual occupations $n_{\mathbf{k}\sigma}$.

At $T=0$, though, we have

$$n_{\mathbf{k}\sigma}(T=0) = \Theta(\mu - \tilde{\epsilon}_{\mathbf{k}\sigma}) \equiv n_{\mathbf{k}\sigma}^0$$

In an isotropic system with no magnetic field, we have

$$n_{\mathbf{k}\sigma}^0 = \Theta(k_F - k)$$

with $k_F = (3\pi^2 n)^{1/3}$ as for the IFG.

We now define

$$\delta n_{\mathbf{k}\sigma} \equiv n_{\mathbf{k}\sigma} - n_{\mathbf{k}\sigma}^0$$

and write the energy E as

$$E[\delta n] = E_0 + \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}\sigma} \delta n_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{k}, \sigma} \sum_{\mathbf{k}', \sigma'} f_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} \delta n_{\mathbf{k}\sigma} \delta n_{\mathbf{k}'\sigma'} + \dots$$

It turns out that we need go no farther than $\mathcal{O}(\delta n^2)$ to obtain the low- T thermodynamic properties of the Fermi liquid. Note $\epsilon_{\mathbf{k}\sigma} = (\delta E / \delta n_{\mathbf{k}\sigma})|_{\delta n=0}$, while

$$\tilde{\epsilon}_{\mathbf{k}\sigma} = \frac{\delta E}{\delta n_{\mathbf{k}\sigma}} = \epsilon_{\mathbf{k}\sigma} + \frac{1}{V} \sum_{\mathbf{k}', \sigma'} f_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'} + \dots$$

and hence

$$\epsilon_{\mathbf{k}\sigma} = \left. \frac{\delta E}{\delta n_{\mathbf{k}\sigma}} \right|_{\delta n=0}$$

$$\frac{1}{V} f_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} = \left. \frac{\delta \tilde{\epsilon}_{\mathbf{k}\sigma}}{\delta n_{\mathbf{k}'\sigma'}} \right|_{\delta n=0} = \left. \frac{\delta^2 E}{\delta n_{\mathbf{k}\sigma} \delta n_{\mathbf{k}'\sigma'}} \right|_{\delta n=0}$$

In isotropic systems,

$$\frac{1}{\hbar} \left. \frac{\partial \epsilon_{\mathbf{k}\sigma}}{\partial \mathbf{k}} \right|_{\mathbf{k}=k_F} = v_F \hat{\mathbf{k}}$$

with v_F the Fermi velocity. The Fermi energy is $\epsilon_F = \epsilon_{\mathbf{k}\sigma}|_{\mathbf{k}=k_F}$ and the DOS at the Fermi level is

$$g(\epsilon_F) = \sum_{\sigma} \int \frac{d^3 k}{(2\pi)^3} \delta(\epsilon_F - \epsilon_{\mathbf{k}\sigma}) = \frac{m^* k_F}{\pi^2 \hbar^2}$$

In systems with spin isotropy, we define

$$f_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} = f_{\mathbf{k}, \mathbf{k}'}^s + \sigma\sigma' f_{\mathbf{k}, \mathbf{k}'}^a$$

Thus,

$$f_{\mathbf{k}\uparrow, \mathbf{k}'\uparrow} = f_{\mathbf{k}\downarrow, \mathbf{k}'\downarrow} = f_{\mathbf{k}, \mathbf{k}'}^s + f_{\mathbf{k}, \mathbf{k}'}^a$$

$$f_{\mathbf{k}\uparrow, \mathbf{k}'\downarrow} = f_{\mathbf{k}\downarrow, \mathbf{k}'\uparrow} = f_{\mathbf{k}, \mathbf{k}'}^s - f_{\mathbf{k}, \mathbf{k}'}^a$$

Recall $[f_{\mathbf{k}\sigma, \mathbf{k}'\sigma'}] = E \cdot V$. Thus, multiplying by $g(\varepsilon_F)$, we obtain the dimensionless functions

$$F_{\mathbf{k}, \mathbf{k}'}^{s,a} \equiv g(\varepsilon_F) f_{\mathbf{k}, \mathbf{k}'}^{s,a}$$

$$F_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} \equiv g(\varepsilon_F) f_{\mathbf{k}\sigma, \mathbf{k}'\sigma'}$$

With \mathbf{k} and \mathbf{k}' both on the Fermi surface, i.e. $\mathbf{k} = k_F \hat{\mathbf{k}}$ and $\mathbf{k}' = k_F \hat{\mathbf{k}'}$, we may write

$$F_{k_F \hat{\mathbf{k}}, k_F \hat{\mathbf{k}'}}^{s,a} \equiv F^{s,a}(\vartheta_{\hat{\mathbf{k}}, \hat{\mathbf{k}'}}) \equiv \sum_{L=0}^{\infty} F_L^{s,a} P_L(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}'})$$

where $\vartheta_{\hat{\mathbf{k}}, \hat{\mathbf{k}'}} \equiv \cos^{-1}(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}'})$. From either function $F^{s,a}(\vartheta)$, we can obtain the coefficients $F_L^{s,a}$ by

$$F_L^{s,a} = \frac{2L+1}{4\pi} \int d\Omega F(\vartheta) P_L(\cos\vartheta)$$

where $d\Omega = \sin\vartheta d\vartheta d\phi$ is the differential solid angle.