Physics 127c: Statistical Mechanics

Weakly Interacting Fermi Gas

Unlike the Boson case, there is usually no *qualitative* change in behavior going from the noninteracting to the weakly interacting Fermi gas for *repulsive* interactions. For example the excitation spectrum for *adding* a particle of momentum $\hbar\mathbf{k}$ with $|\mathbf{k}| > k_F$ or for *removing* a particle with $|\mathbf{k}| < k_F$ creating a "hole" has the same qualitative form

$$\varepsilon_{\mathbf{k}} - \mu = \hbar v_F \, |k - k_F| \tag{1}$$

with μ the chemical potential or Fermi energy and k_F the Fermi wave vector (which can be shown to *unchanged* by the interactions—Luttinger's theorem). Here v_F is called the Fermi velocity

$$v_F = \left.\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k}\right|_{k=k_F} \tag{2}$$

and defines the spectrum. The *value* of v_F is altered by interactions. The familiar spectrum leads to the usual temperature dependences at low temperature, e.g. specific heat $C \propto T$, susceptibility χ independent of temperature.

Furthermore, since there is no qualitative change of behavior, unlike for the Boson case (where the canonical transformation was necessary) quantitative results can be calculated using perturbation theory.

When are the interactions weak? For a short range pair interaction potential this is small potential or low density. On the other hand for a Coulomb interaction, as for the electron gas, interactions are weak compared with the kinetic terms at *high* density

The Electron Gas

We write the interaction potential as

$$u(r) = \frac{e^2}{r}; \qquad \tilde{u}(q) = \frac{4\pi e^2}{q^2}, \tag{3}$$

where e is the electron charge in CGS units, and $e^2 = q_e^2/4\pi\varepsilon_0$ with q_e the electron charge in SI units.

An estimate of the interaction energy per particle is

$$\frac{V}{N} \sim \frac{e^2}{2r_0}, \tag{4}$$

with r_0 a measure of the interelectron spacing given by

$$\frac{4}{3}\pi r_0^3 = \frac{\Omega}{N}, \tag{5}$$

i.e. a sphere of radius r_0 contains on average one electron.

Since k_F is related to N by the usual counting of states

$$2.\frac{\Omega}{(2\pi)^3}\frac{4}{3}\pi k_F^3 = N \tag{6}$$

we have

$$k_F r_0 = \left(\frac{9\pi}{4}\right)^{1/3} \simeq 1.9192\ldots. \tag{7}$$

It is conventional to write r_0 in terms of the Bohr radius $a_0 = \hbar^2/me^2$

$$r_0 = r_s a_0 \tag{8}$$

and r_s the interelectron spacing in units of a_0 is the dimensionless measure of the density of the electron gas.

The estimate of the potential energy becomes

$$\frac{V}{N} \sim \frac{e^2}{2a_0}\frac{1}{r_s}. \tag{9}$$

The total kinetic energy is

$$\frac{E_{\text{kin}}}{N} = \frac{3}{5}\varepsilon_F^2 = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} = \frac{e^2}{2a_0}\frac{3}{5}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s^2} \simeq \frac{e^2}{2a_0}\frac{2.21}{r_s^2}. \tag{10}$$

Thus the potential energy is relatively small for small r_s, i.e. large density. For typical metals $2 \lesssim r_s \lesssim 6$ (e.g. for sodium $r_s \simeq 4$) and so the interactions are not weak.

Perturbation Theory

Potential Energy

The ground state energy correction to lowest order in the interactions is given by the expectation value of the potential energy in the *noninteracting* ground state. In conventional wavefunction notation we would just write the wavefunction as an antisymmetrized product (Slater determinant) of single particle wavefunctions (functions of coordinate and spin)

$$\psi_N(\mathbf{r}_1, \ldots \mathbf{r}_N; \sigma_1 \ldots \sigma_N) = \mathcal{A}\prod_{i=1}^{N}\chi_i(\mathbf{r}_i; \sigma_i), \tag{11}$$

with $\mathcal{A}$ the antisymmetrization operator (giving the Slater determinant form).

In chemistry, where we are dealing with electrons in an external potential as in the trapped Bose gases, the best single particle states χ_i would be found self consistently by minimizing the resulting energy expression.

In a homogeneous fermion gas the χ_i remain spin up or down plane wave states, and the wavefunction reduces to the noninteracting one. Thus

$$E - E_0 = \frac{1}{2\Omega}\left\langle \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \tilde{u}(\mathbf{q}) a^+_{\mathbf{k}+\mathbf{q},\sigma} a^+_{\mathbf{k}'-\mathbf{q},\sigma'} a_{\mathbf{k}',\sigma'} a_{\mathbf{k},\sigma} \right\rangle_0 . \tag{12}$$

In the noninteracting ground state the four particle expectation value factorizes into the product of the nonzero pairwise averages, and as you proved in Homework 1

$$\left\langle a^+_{\mathbf{k}+\mathbf{q},\sigma} a^+_{\mathbf{k}'-\mathbf{q},\sigma'} a_{\mathbf{k}',\sigma'} a_{\mathbf{k},\sigma} \right\rangle_0 = \left\langle a^+_{\mathbf{k}+\mathbf{q},\sigma} a_{\mathbf{k},\sigma} \right\rangle_0 \left\langle a^+_{\mathbf{k}'-\mathbf{q},\sigma'} a_{\mathbf{k}',\sigma'} \right\rangle_0 - \left\langle a^+_{\mathbf{k}+\mathbf{q},\sigma} a_{\mathbf{k}',\sigma'} \right\rangle_0 \left\langle a^+_{\mathbf{k}'-\mathbf{q},\sigma'} a_{\mathbf{k},\sigma} \right\rangle_0 \tag{13a}$$

$$= n_{\mathbf{k},\sigma} n_{\mathbf{k}',\sigma'} \delta_{\mathbf{q},0} - n_{\mathbf{k}+\mathbf{q},\sigma} n_{\mathbf{k},\sigma} \delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}} \delta_{\sigma\sigma'} \tag{13b}$$

where the minus sign for the second term comes because we have changed the order of the middle pair of Fermi operators (remember the *anti*commutation rules!), and $n_{\mathbf{k},\sigma}$ is the noninteracting ground state occupation number

$$n_{\mathbf{k},\sigma} = \begin{cases} 1 & \text{for } k < k_F \\ 0 & \text{for } k > k_F \end{cases} . \tag{14}$$

This gives

$$E - E_0 = \frac{1}{2\Omega}\left[\tilde{u}(0)\left(\sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma}\right)^2 - \sum_{\mathbf{k},\mathbf{q},\sigma} \tilde{u}(\mathbf{q}) n_{\mathbf{k}+\mathbf{q},\sigma} n_{\mathbf{k},\sigma}\right]. \tag{15}$$

The first term in Eq. (15) can be written as $\frac{1}{2}N^2\tilde{u}(0)/\Omega$ and is just the mean potential interaction between all the particles. In this context it is known as the Hartree term. You might have expected this to be the complete result since we are just using the noninteracting wavefunction, and indeed this would be the case for distinguishable particles. The second term arises from the antisymmetrization of the wavefunction, and is known as the exchange or Foch term. Together we have *Hartree-Foch* theory.

Radial Distribution Function

The Foch term can be understood better by remembering the result for the potential energy from our study of the classical interacting gas. For a pairwise interaction the potential energy just depends on the pair correlation function, conveniently expressed in terms of the radial distribution function $g(r)$

$$\langle V\rangle = \frac{1}{2}\frac{N^2}{\Omega}\int u(r)g(r)d^3r = \frac{1}{2}\frac{N^2}{\Omega^2}\sum_{\mathbf{q}} \tilde{u}(\mathbf{q})g(-\mathbf{q}). \tag{16}$$

The radial distribution function $g(\mathbf{r})$ is proportional to the probability of finding a particle at $\mathbf{r}$ given that there is one at the origin. It is normalized so that $g(r \to \infty) = 1$. Also, remember the convention for Fourier transforms I am using

$$f(\mathbf{r}) = \sum_{\mathbf{q}} \tilde{f}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}} \tag{17}$$

$$\tilde{f}(\mathbf{q}) = \frac{1}{\Omega}\int f(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}} \tag{18}$$

where at the end of the calculation we evaluate the wavevector sum as

$$\sum_{\mathbf{q}} \ldots \to \frac{\Omega}{(2\pi)^3}\int d^3q \ldots. \tag{19}$$

Comparing with Eq. () we can introduce the spin dependent radial distribution function $g_{\sigma\sigma'}$ and write

$$\tilde{g}(\mathbf{q}) = \frac{1}{4}\sum_{\sigma\sigma'} \tilde{g}_{\sigma\sigma'}(\mathbf{q}) \tag{20}$$

with

$$\tilde{g}_{\sigma\sigma'}(\mathbf{q}) = \frac{\Omega}{(N/2)^2}\left\langle \sum_{\mathbf{k},\mathbf{k}'} a^+_{\mathbf{k}-\mathbf{q},\sigma} a^+_{\mathbf{k}'+\mathbf{q},\sigma'} a_{\mathbf{k}',\sigma'} a_{\mathbf{k},\sigma}\right\rangle_0, \tag{21}$$

or Fourier transforming

$$g_{\sigma\sigma'}(R) = \frac{1}{(N/2)^2}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}}\left\langle \sum_{\mathbf{k},\mathbf{k}'} a^+_{\mathbf{k}-\mathbf{q},\sigma} a^+_{\mathbf{k}'+\mathbf{q},\sigma'} a_{\mathbf{k}',\sigma'} a_{\mathbf{k},\sigma}\right\rangle_0. \tag{22}$$

Using the same factorization procedure gives (writing the last term in terms of $\mathbf{k}$, $\mathbf{k}'$ rather than $\mathbf{k}$, $\mathbf{q}$)

$$g_{\sigma\sigma'}(R) = \frac{4}{N^2}\left[\left(\sum_{\mathbf{k}} n_{\mathbf{k},\sigma}\right)\left(\sum_{\mathbf{k}'} n_{\mathbf{k}',\sigma'}\right) - \delta_{\sigma\sigma'}\sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}} n_{\mathbf{k}',\sigma} n_{\mathbf{k},\sigma}\right]. \tag{23}$$

This can be written in terms of the real function $\phi(\mathbf{R})$

$$\phi(\mathbf{R}) = \frac{2}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} n_{\mathbf{k}\sigma}. \tag{24}$$

as

$$g_{\sigma\sigma'} = 1 - \delta_{\sigma\sigma'}\phi^2(\mathbf{R}). \tag{25}$$

The function ϕ is easily evaluated, since $n_{\mathbf{k}\sigma}$ is 1 for $k < k_F$ and 0 for $k > k_F$ as

$$\phi(\mathbf{R}) = \frac{2}{n}\int_0^{k_F} \frac{4\pi k^2 dk}{(2\pi)^3}\frac{1}{2}\int_{-1}^{1} d(\cos\theta)e^{ikR\cos\theta} \tag{26}$$

$$= \frac{3}{(k_F r)^3}\int_0^{k_F r} dy\, y \sin y \tag{27}$$

(writing the density n in terms of k_F and introducing $y = k_F r$), or

$$\phi(\mathbf{R}) = \frac{3}{(k_F r)^3}\left[\sin(k_F r) - (k_F r)\cos(k_F r)\right]. \tag{28}$$

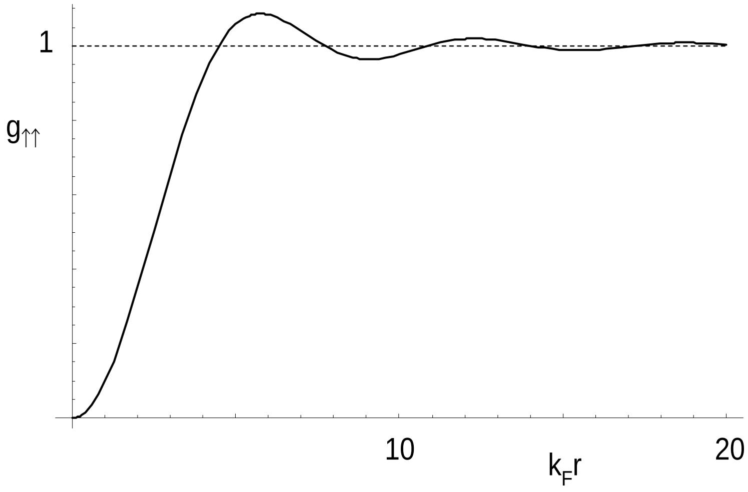

Figure 1: Radial distribution function for parallel spin fermions plotted from Eqs. (25) and (28).

These results show that $g_{\uparrow\downarrow} = g \downarrow\uparrow = 1$ as might be expected for the noninteracting wave function. However $g_{\uparrow\uparrow} = g_{\downarrow\downarrow}$ go to zero as $r \to 0$, and there is a "correlation hole" of radius $\sim k_F^{-1}$ because of the antisymmetrization of the wavefunction, the nonlocal ramification of the Pauli exclusion principle, see Fig. 1. Note that the recovery to $g_{\uparrow\uparrow} = g_{\downarrow\downarrow} = 1$ for $r \to \infty$ is oscillatory and with a power law tail

$$1 - g_{\uparrow\uparrow}(r \to \infty) \propto \frac{\cos(2k_F r)}{r^4}. \tag{29}$$

These slowly decaying oscillations, appearing here and in other quantities, and resulting from the sharp discontinuity at the Fermi surface are known as Friedel oscillations.

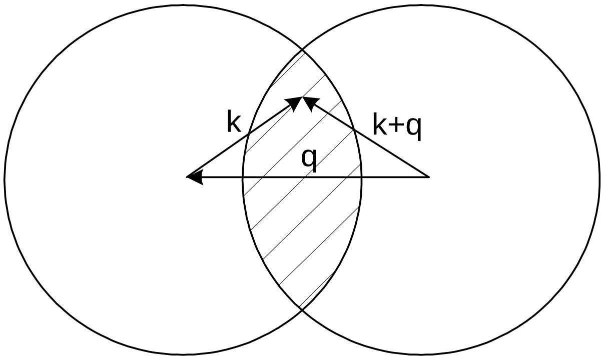

Figure 2: Shaded volume gives the integral in the Foch term of the ground state energy.

Potential Energy for the Electron Gas

For the electron gas with a uniform positive background (the jellium model) the first term in Eq. (15) is cancelled by the interaction with the positive background. This leaves the Foch term. There is a lowering of the energy because as we have seen from $g_{\uparrow\uparrow}$ like spins tend to stay apart, reducing the repulsive interaction.

To evaluate Eq. (15) or (**??**) we need to calculate

$$\sum_{\mathbf{k}} n_{\mathbf{k}+\mathbf{q},\sigma} n_{\mathbf{k},\sigma}. \tag{30}$$

This is easily evaluated geometrically, since the product $n_{\mathbf{k}+\mathbf{q}} n_{\mathbf{k}}$ is unity inside the intersection of the Fermi sea and a Fermi sea displaced by $-\mathbf{q}$ (shaded in Fig. (2)) and zero outside. The shaded volume is

$$2k_F^3 \int_{q/2k_F}^{1} \pi \sin^2\theta \, d(\cos\theta) = \frac{4}{3}\pi k_F^3 \left[1 - \frac{3}{2}\frac{q}{2k_F} + \frac{1}{2}\left(\frac{q}{2k_F}\right)^3 \right] \tag{31}$$

for $q < 2k_F$ and zero otherwise. Thus

$$\sum_{\mathbf{k}} n_{\mathbf{k}+\mathbf{q},\sigma} n_{\mathbf{k},\sigma} = \frac{\Omega}{(2\pi)^3}\frac{4}{3}\pi k_F^3 \left[1 - \frac{3}{2}\frac{q}{2k_F} + \frac{1}{2}\left(\frac{q}{2k_F}\right)^3 \right] \Theta(2k_F - 2k_F) \tag{32}$$

$$= \frac{N}{2}\left[1 - \frac{3}{2}\frac{q}{2k_F} + \frac{1}{2}\left(\frac{q}{2k_F}\right)^3 \right] \Theta(2k_F - q). \tag{33}$$

The Foch term to the perturbation of the energy is then

$$E - E_0 = \frac{-1}{2\Omega}\left(\frac{\Omega}{8\pi^3}\right) \int_0^{2k_F} 4\pi q^2 \frac{4\pi e^2}{q^2}\frac{N}{2}\left[1 - \frac{3}{2}\frac{q}{2k_F} + \frac{1}{2}\left(\frac{q}{2k_F}\right)^3 \right] dq. \tag{34}$$

$$= -\frac{Ne^2}{2}\frac{4k_F}{\pi}\int_0^1 dx[1 - \frac{3}{2}x + \frac{1}{2}x^3] - \frac{-Ne^2}{2}\frac{3k_F}{2\pi} \tag{35}$$

or in terms of r_s

$$E - E_0 = -\frac{Ne^2}{2\alpha_0}\frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s}. \tag{36}$$

This gives for the total energy

$$E = \frac{e^2}{2a_0}\left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \cdots\right] \tag{37}$$

where the kinetic energy is given by summing over the Fermi sphere in the usual way. Evaluating the higher order terms was a major focus of many in the early days of many body physics, using diagrammatic perturbation theory or other approaches.

We can also calculate the excitation energy $\bar{\varepsilon}_{\mathbf{k},\sigma}$ —the energy required to add an additional particle—within the same approximation:

$$\bar{\varepsilon}_{\mathbf{k},\sigma} = \frac{\partial E}{\partial n_{\mathbf{k},\sigma}} \simeq \varepsilon_k + \tilde{u}(0)\frac{1}{\Omega}\sum_{\mathbf{k}',\sigma'} n_{\mathbf{k}',\sigma'} - \frac{1}{\Omega}\sum_{\mathbf{k}'} \tilde{u}(\mathbf{k}-\mathbf{k}')n_{\mathbf{k}',\sigma} \tag{38}$$

with kinetic, Hartree and Foch terms. (Note in the later the interaction is only with the same spin particles—there is no spin sum in this term.). It turns out the for the Coulomb interaction, the last term gives a logarithmic singularity at $k = k_F$, so that $v_F = \partial\varepsilon_k/\partial k$ is infinite. This is an unphysical result, and results from the diverging potential at small q. In this limit we must take *screening* into account—an electron repels its neighbors via the Coulomb interaction giving an effective positive screening cloud, so that the inter-electron interaction is reduced. Using the Thomas-Fermi approximation, the same method we used in the calculation of white dwarf stars (see the Appendix below), leads to the replacement

$$\frac{4\pi e^2}{q^2} \to \frac{4\pi e^2}{q^2 + q_{TF}^2} \tag{39}$$

with the Thomas-Fermi wavevector given by

$$q_{TF}^2 = \frac{6\pi n e^2}{\varepsilon_F} = \frac{4}{\pi}k_F/a_0. \tag{40}$$

We can think of this as replacing the screening the $1/q^2$ potential with a dielectric constant

$$\tilde{u}_{eff}(\mathbf{q}) = \frac{4\pi e^2}{q^2\varepsilon(q)} \tag{41}$$

with the Thomas-Fermi approximation to the dielectric constant

$$\varepsilon_{TF}(q) = 1 + \frac{q_{TF}^2}{q^2}. \tag{42}$$

In real space this corresponds to a Yukawa potential

$$u_{eff}(r) = \frac{e^2}{r}e^{-q_{TF}r} \tag{43}$$

with an exponential decay at large separations. This screened potential leads to a finite Fermi velocity. The corresponding corrections to the ground state energy are in the $+\cdots$ in Eq. (37).

Diagrammatic Language

The approximation we have done can be expressed (if you like such things!) in diagrammatic language as shown in Fig. (3). The diagrams for the screening of the interaction (the last line of the figure) can be

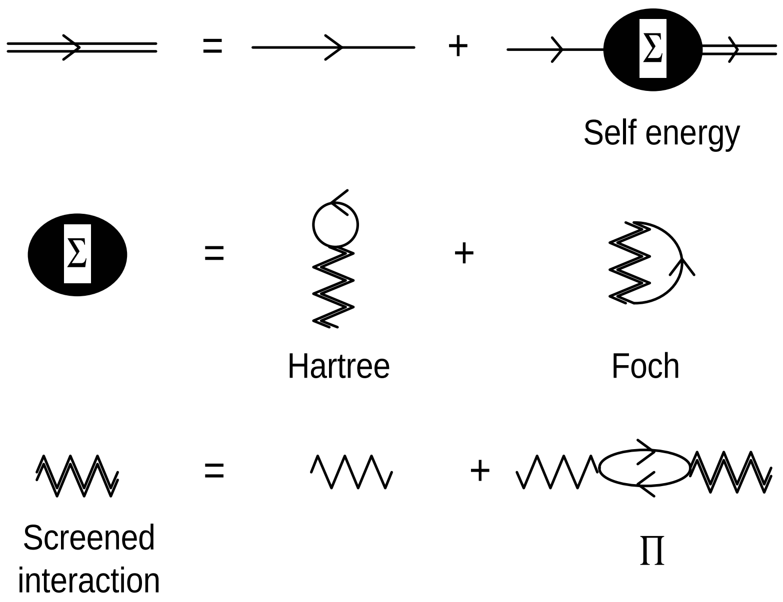

Figure 3: Diagrams for the Hartree-Foch calculation of the single particle propagator using the screened interaction, with the screening calculated to lowest order.

expressed algebraically as

$$u_{\text{eff}}(q) = \frac{4\pi e^2}{q^2} + \frac{4\pi e^2}{q^2}\Pi(q)u_{\text{eff}}(q) \tag{44}$$

$$u_{\text{eff}}(q) = \frac{4\pi e^2}{q^2 + 4\pi e^2\left[-\Pi(q)\right]} \tag{45}$$

where $\Pi(q)$ is given (to lowest order) by the loop or "bubble" diagram, and corresponds to an approximate evaluation of the *polarizability* of the electron gas. Actually Π is frequency dependent (q represents $\mathbf{q}$, ω), and the full dielectric constant screening the interaction

$$\varepsilon(q) = 1 - \frac{4\pi e^2}{q^2}\Pi(q) \tag{46}$$

is also frequency dependent. In the static and long wavelength limit, the expression reduces to the Thomas-Fermi result. More generally we could use the expression for the bubble to give a better approximation to Π. This gives the *Lindhard* approximation to the dielectric constant. Using this interaction to evaluate the properties of the electron gas is known as the *Random Phase Approximation* or *RPA*.

Appendix: Thomas-Fermi Calculation of Dielectric Constant

The Thomas-Fermi approach balances the degeneracy pressure against the forces from the electrostatic potential in a local approximation: at each point the degeneracy pressure is calculated for a gas at the local density as for a homogeneous gas. We used this before in the physics of white dwarf stars in Lecture 17 of Ph127a and trapped-atom Bose systems in Lecture 7 this term.

Suppose that there is a net potential $V(\mathbf{r})$ acting on the electrons, coming from some fixed set of charges and the electrons themselves. The chemical potential must be constant, and is the sum of potential and kinetic terms

$$V(\mathbf{r}) + \varepsilon_F(n(\mathbf{r})) = \text{const}, \tag{47}$$

where n is the local electron density, $\varepsilon_F \propto k_F^2 \propto n^{2/3}$ is the local Fermi energy, and we are considering low temperatures $k_B T \ll \varepsilon_F$. To calculate the dielectric constant we assume a *small* external potential, and may then linearize Eq. (47)

$$\delta V(\mathbf{r}) + \frac{2}{3}\frac{\varepsilon_{F0}}{n_0}\delta n = 0, \tag{48}$$

with n_0, ε_{F0} the values without the perturbation.

The potential derives from the sum of external charges and $-e\delta n$ from the electrons

$$\nabla^2 \delta V = 4\pi(\rho_{ext} - e\delta n). \tag{49}$$

Equations (48) and (49) are easily solved by Fourier transforming

$$\delta\tilde{V}(\mathbf{q}) = -\frac{4\pi\tilde{\rho}_{ext}}{q^2 + q_{TF}^2}, \tag{50}$$

with the *Thomas-Fermi wave vector* given by

$$q_{TF}^2 = \frac{6\pi n_0 e^2}{\varepsilon_{F0}}. \tag{51}$$

The potential without the screening would be $\delta\tilde{V}_{ext} = -4\pi\rho_{ext}/q^2$ and so we may introduce the dielectric constant $\delta\tilde{V} = \delta\tilde{V}_{ext}/\varepsilon(\mathbf{q})$ with

$$\varepsilon(\mathbf{q}) = 1 + \frac{q_{TF}^2}{q^2}. \tag{52}$$

This is singular at small q due to the efficient screening at long wavelengths.

For the interaction between electrons, the "external" charge is provided by another electron. The effective interaction in the Thomas-Fermi approximation is

$$\tilde{u}(\mathbf{q}) = \frac{4\pi e^2}{q^2 + q_{TF}^2}, \qquad u(r) = \frac{e^2}{r}e^{-q_{TF}r}, \tag{53}$$

a *screened* potential finite as $q \to 0$ in Fourier representation, and a *Yukawa potential* decaying exponentially at large separations in real space.

The Thomas-Fermi wavevector is typically comparable to the inverse spacing for the electron gas in metals, although it actually scales as the inverse of the square root of the spacing

$$q_{TF} = \frac{4}{\pi}\left(k_F a_0^{-1}\right)^{1/2} \simeq \frac{1.5632}{r_s^{1/2}}\frac{1}{a_0}. \tag{54}$$

April 25, 2004