**Ground State Energy**

We’d like to calculate the GS energy of a Jelly metal [note we could get things like the T = 0 pressure, compressibility, etc., with this information]. And we’d like to do this perturbatively, as was argued we could, in the case of a high density electron ‘gas’. Now we can calculate the self energy of interacting particles, but it is a mistake to treat the system as simply being composed of renormalized particles interacting with each other – that would be ignoring the collective excitations for example. So we cannot simply find the self-energy of the particles, their new ε(k) distribution, and add up to the Fermi level to calculate the GS energy. We could just use good old fashioned Perturbation Theory from QM 1. We would say, e.g.,



where V1 would be the interaction of the Hamiltonian, below:



and the wavefunctions |ψn(0)> would just be:



where npσ is the set of occupation numbers for all states pσ. So this would run over all states where npσ can be 0 or 1, subject to the restriction that the number of particles adds up to N. This calculation could be kind of cumbersome though. Thankfully, it turns out there *is* a way to get the total ground state energy from the single particle self-energy. Seitz’s theorem relates the ground state energy to the chemical potential. μ is the energy it takes to add or remove an electron from the material (at constant entropy and no work done). So at T = 0 [where don’t have to worry about entropy and we’ll just presume no work function]



and N the number of electrons. Now let’s consider that:



where GS is the ground state energy per electron. This is Seitz’s theorem,



Now at T = 0, μ is the energy of a particle at the Fermi surface. Recalling the structure of the electron GF:



the energy (minus the chemical potential), k would be given by the solution:



To first order, the solution would be:



I think Luttinger’s theorem is that this is exact at the Fermi surface, for the e-e interaction. So we’d have:



and therefore,



So the procedure is to solve for μ(kF) via kF2/2m + Σ(kF,0). And then for via μ = ∂(n)/∂n.

Might throw in the comment that at least to second order, we can calculate EGS like we did in the SCHF, whereby we add up all the kinetic energies and potential (self) energies (divided by two since each electron carries half the potential energy of any given pair) of the electron gas, up to the Fermi level.



Not sure if we can do this to all orders in the self energy. But generally we’ll just take the safe route and do:



So proceeding…

**High Density Expansion of GS Energy**

So let’s start, and we’ll note that this will turn out to be a power series in terms of 1/rs. So this will work out to be a high density expansion, as befits the fact that the KE dominates for small rs…

**Kinetic Energy**

So we have:



This makes sense as it is in fact just the sum of all the kinetic energies of the particles, i.e.,



So so far we have (recall EF in terms of rs from the excitations file)



**Fock (Exchange) Potential Energy**

We have:



Filling this into our formula,



we have, noting F(1) = 1/2:



This matches what we found in previous Excitations file. In terms of ERy, this is:



The Fock contribution to the self-energy comes simply from calculating the average potential energy of electrons whose pair distribution function is given by the non-interacting many-body wavefunction. Recall we found the PE to be (in Quantum Mechanics/Identical Particles/many-body correlations file):



where n0 = N/V. But this was just for the two-particle potential. We have to include the background as well. So let’s consider the potential of the jelly interacting with the e-‘s. We have,



and so the energy per particle (e-) associated with this interaction is:



Now we’ll consider the energy associated with the jellium interacting with itself. This is:



Adding these all together we have,



And then recall we found (in the many-body correlations file)



And these relate to g via:



Plugging those guys in:



Plugging this into our formula, we have:



Apparently, this will indeed work out to:



So this is what the F term is calculating. We can interpret this as the energy of interaction between an electron and the ‘exchange hole’ that it carries with it. Anyway, with this and the same previous results we can estimate the total ground state energy to be:



So here we note the linear dependence on kF as opposed to the quadratic dependence from the KE. In terms of rs, we have so far:



**Correlation Potential Energy**

Now we’ll do the 2nd order terms. Our result has the appearance of a power series in 1/r and it turns out that this will indeed be the case. Moving on to the correlation energy, recall we found in the previous Excitations file, valid out to O(V2), that the total self-energy was given by:



We define the correlation part of the self-energy as all terms beyond the Fock contribution:



So just the correlation part would be:



If we use Seitz’s theorem to calculate the contribution of this part to the energy per particle, we find:

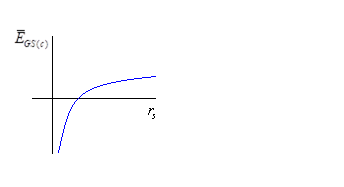


And all together, we have:



Bruekner and Gell-Man also obtained this series from Raleigh-Schrödinger perturbation theory.

A plot of ΣRc(k) shows that it goes infinitely negative at r = 0 (from the ln term), and increases thereafter until it crosses the rs-axis to become positive at r = 2.4 or so.



Now the correlation energy ought to always be negative according to general arguments – so our expression certainly isn’t valid around r = 2.4. Unfortunately, the region of metallic densities is 1.8 < rs < 6. So our expansion is good only up to rs ~ 2, just barely entering into the normal metallic density region, and nowhere near the low density region rs ~ 6. In actual fact, at low densities (large r), the electrons become localized and the self energy is markedly different than that given here. Wigner tried to make an interpolation scheme to correct this defect.

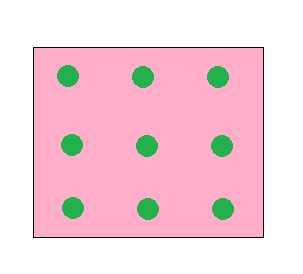
**Low density electrons (Wigner Lattice)**

Actual systems exist over a range of densities. In the previous sections we derived formulas for the correlation energy valid for high densities but we’d like the same for small densities as well. Unfortunately, it is high density at which the usual perturbative expansion is valid. And so to obtain the low density results, we need another perspective.

At very low density the potential energy becomes more important than the kinetic energy. And Wigner speculated that the electrons would become localized and form a regular lattice. But localization cannot occur until the zero point energy (the GS KE) is less than the potential energy.

One can investigate the feasibility of this scenario within the jelly model. The electron lattice would presumably be a close packed structure such as ccc, fcc, or hcp, in which electrons would vibrate around their equilibrium positions. There would be vibrational modes of electrons, and they would be at the plasma frequency. And these vibrational modes would give the 0-point energy. Really? Wouldn’t it just be ‘particle in a box’ energy within that volume? Well I guess we can’t have one electron oscillating back and forth by itself when it’s also interacting with other electrons. So they probably must oscillate together. Whatever.

So first we’ll note the GS of our ‘Wigner lattice’ is stable because displacing the electric charge jelly to the right some distance would just give rise to the plasma oscillation stuff.



I guess I won’t go through the calculation again, but in the metal-sheet dynamics file in the Electrodynamics folder we calculate the plasma oscillation frequency and found it to be:



Converting to ‘fake’ Gaussian units (ε0 = 1/4π), we have:



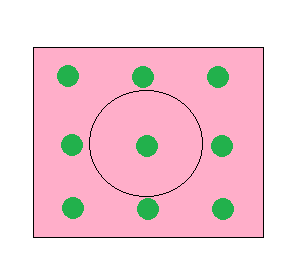
as previously stated. Now if we treat the system as a whole as a harmonic oscillator with this resonant frequency, then its H would be:



and so its ground state (kinetic) energy would just be:



Now Wigner calculated the potential energy in the following fashion. A Wigner-Seitz model was taken for each unit cell of the lattice. It is a sphere (pictured below) with radius rsa0, with the electron at the center. Each sphere has overall neutrality since the electron density and background density is the same. Outside the sphere, the electric field is zero and hence the spheres exert no forces on each other. Thus the potential energy of the solid is just the sum of the potential energies of the spheres themselves. There are two contributions – the interaction energy between the e- and jelly in the sphere, and the interaction between the jelly and itself.



The first term is (note e/r is the electron’s field, and n0e is the jelly charge density)



And the jelly-jelly term is, via similar procedure:



The total is:



This is what we will suppose the PE should go to in the large rs limit. And we’ll note that indeed the PE would dominate the KE in the large rs limit. So it seems a bound state structure is possible.

**Low Density – High Density EGS Interpolation**

So now then, we attempt to find what the Σc *should* be (I think this means basically what all the 2nd order and higher terms should come out to be). So we demand, in the large rs, low density limit…



in the low density limit. Nice thing about this is that it is always negative. He also (incorrectly because the limit includes a ln(r) term as we saw, not simply a constant term in the small r limit) estimated the high density limit to be:



and interpolated between these two values to obtain a simple formula for Ec in all ranges,



for a total result of:



and this works fairly well except for very small r where the ln(r) term he’s missing in that limit takes over.