**Hartree-Fock**

**Pairing Theory**

Now we’d like to work out a theory for the energy spectrum, and condensate fraction, etc. We’ll ignore the internal d.o.f. of the atoms (like the nuclear/atomic electronic excitations), because the KE/PE of/between the atoms themselves is largest. Our first attempt will presume a pair-wise interaction. We can definitely assert that an electron gas, say, would interact in pairs. But here we’re dealing with an intricate situation where each particle has internal d.o.f. which complicate things. This makes it a multi-body interaction. For consider two molecules next to each other interacting with some potential V. Now if I bring a third molecule nearby, it will influence the positions of the electrons on the other two molecules, and thus change their interaction, and so the interaction between particle 1 and 2 would depend on the position of particle 3, etc. This would not happen if I replaced the molecules with protons, say. Thus the true interaction is more than simply pair-wise. But as long as it’s unlikely that more than two particles should be in close proximity at any given time, pairing theory ought to be decent. This would restrict its applicability to low density/high T. But this assumption isn’t valid in a liquid and it is now known that the theory gives terrible quantitative predictions for quantum fluids. Nonetheless many of its qualitative predictions are valid, its ideas are influential and its predictions are actually successfull in superconductivity. So…

**Rough Overview**

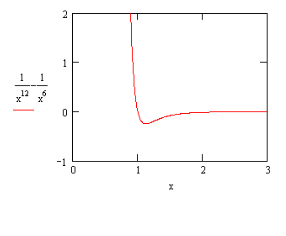
In the pairing theory, H is written as H = H0 + V2, where H0 is the usual KE term, and V2 the interaction potential. The typical H is:



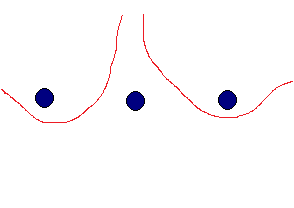
where we use the Leonard Jones potential.



ε ~ 10kB is the maximum well depth, and σ is the hard core radius, where the potential rises steeply. Note that the potential is repulsive in the short range and attractive in the long range. The r-6 term comes from Van der Waals forces, but the repulsive part is probably not r-12 and this approximation was chosen for mathematical convenience. The typical form of the potential is shown below,



The condensate fraction would form a rough lattice with each atom in the condensate situated at the minima of the net potential set up by its nearest neighbors (of course there would be more than 2 in a 3D structure). For instance,



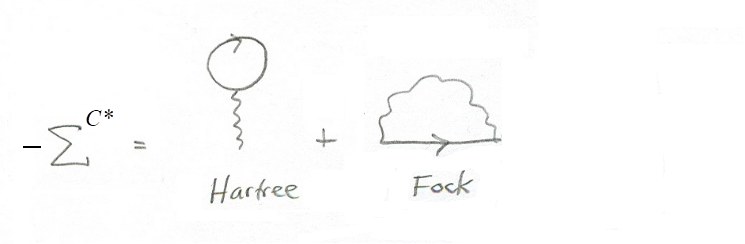
Thus, at low enough T, we expect each atom would settle into the n.n. V2(r) local minimum, and be in a bound state of sorts. The KE would likely be the zero point KE of a particle in a box. This model seems to agree fairly well with experiment. Excitations of the condensate could take the form of particle-in-box excitations, as well as collective excitations like density waves.

**Going to 2nd quantized form**

All operators are expanded in the basis set of H0. Note that we would want to know the thermodynamic properties of the fluid and so as usual we will, to facilitate calculating thermally averaged properties, subtract off the chemical potential from the single particle excitation energies. And also note that just because we have bosons doesn’t mean there isn’t a chemical potential. So we have,



The first thing to do is to look at the Hartree-Fock approximation to the self-energy, and see if it can produce the characteristic excitation spectrum. I guess these would be single particle excitations still, but it’s possible that the energy spectrum is modified by the interaction so that the low k part of the ε(k) is linear, and not parabolic? So consider:



This is (remember we’re spinless here, and can see Feynman rules for, say, interacting electrons – though we have spinless bosons here, or go back to Stat Mech folder and look up GF’s):



where n0 = N/V. So there we go. BTW, the expectation of the interaction potential energy expection <PE> can be simply expressed in terms of ΣHF. And since we said that <PE>/N ≈ -22kB(1) in the condensate, calculating <PE> would be another good check. We’ll go about this backwards. So at a certain temperature we can say that there are: n(εk2) particles with momentum k2, and n(εk1) particles with momentum k1. Each of these particles will interact via V2, and will form a pair wavefunction, Ψk1k2. The subscripts indicate that the unperturbed wavefunction would be [exp(i**k**1∙**r**1)exp(i**k**2∙**r**2)]. i.e.,



The potential energy of this pair would be:



But if we want the thermal expectation of the energy, then we have to sum over the occupation numbers of the single particle states themselves. So we’ll have to first order:



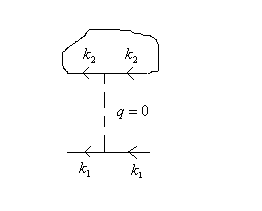
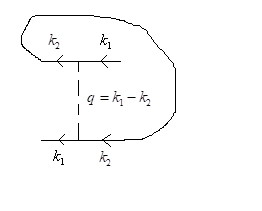
and in last we go to c.o.m. coordinates. Then,



(and in last line can switch k´-k to k-k´ cause integral should be real again) A problem with the formula is that it overcounts the self-interacting terms, but this can perhaps be put into the chemical potential. And we can write this as:



But there’s a big problem; since V2(q) doesn’t exist, thanks to the divergence of V(r) at r = 0, we can’t evaluate these diagrams. However we can relate them in a plausible way to the T matrix (I would suppose that a more formal argument could be made relating what we’re about to get with an exact sum of a certain subset of diagrams). To facilitate this reformulation let’s interpret the diagrams as scattering processes. Consider two Feynman diagrams, Hartree and Exchange.

From left to right (well that’s how i like to read it), the Hartree diagram depicts a particle (1) traveling along at k1 and another, (2) traveling with k2. They interact via V(q=0) term. Since q=0 there is no momentum exchange so they emerge with the same momenta as initially. The Xchange diagram depicts (1) traveling with momentum k1 interacting with (2) traveling at k2 again. But this time the exchange is q = k1 – k2. So (1) emerges with momentum k2, and (2) emerges with momentum k1. So the particles switch places in effect and that’s probably why its called the exchange diagram. Such scattering processes can be described by the T-matrix. The first would be Tk1,k1 and the second Tk1,k2. But Tkk’ is defined for when particles scatter into states with the same energy. Unfortunately, k1 and k2 above need not be restricted to this constant-energy surface. So we should switch to the COM view. The COM/relative momenta are:



Then the incoming/outgoing momenta, will be



If we’re traveling along in the COM frame, then the Hartree diagram describes forward scattering:



And in the X diagram we’ll see the process whereby



which is backward scattering. So this would suggest making the replacements,



So we’d say, evaluating ξ on shell because I guess we must have the momenta matching the energies, for the T-matrix:



Recall our result for T is:



This should be modified by replacing m with the reduced mass, μ = mm/(m+m) = m/2. Also, the Fourier transform of V is obtained by evaluating between Fourier states |k>F = eikx, whereas our T matrix here is evaluated between free states normalized to |k> = eikx/(2π)3/2 = |k>F/(2π)3/2. So, the T matrix evaluated between Fourier states would be (2π)3 times our expression above. So making these adjustments, we’ve got:



For the Tkk term we’d set θ = 0, and for the T-k,k term we’d set θ = 180. So,



Calculating the phase shifts merely entails solving for the eigenstates of V2, which can be done in principle, just as was done for the Hydrogen atom. But regardless, this is found to be a poor approximation. Perhaps it would describe the higher temperature regions better.