**Feynman Approach**

**Beyond pairing theory (sort of)**

Mahan says that we cannot really treat liquid Helium with pair-wise interactions, like we have in the previous two files. I suppose since 4He is a composite atom with internal charge, the interaction potential energy between two such atoms doesn’t depend solely on themselves, because if we place a third such atom nearby, then the internal charge distributions (nucleus + electrons) of the first two He’s will change. And so the interaction potential energy between any two He’s depends, in principle, on the positions of all the other He’s. Only if the liquid were dilute in some sense would we be able to effectively use a pair-wise approximation. So since we’re not doing so well with the pairing theory, we’ll attempt to directly describe the many-body GS wavefunction and eventually the low-lying excited states. Seems we’ll still be implicitly presuming the interactions are pairwise so…..? Maybe problem is just that the interaction potential energy is strong, not weak, and so nothing we’ve done so far has tackled this problem head on.

**Static Fluid Ground State**

So we’re basically going to just guess a form for the ground state wavefunction, and excited states. We could use a variational method to refine this approach. So from the partition function we’d expect that the probability for a particle to be at location r is proportional to exp(-βE(r)). If we’re dealing with a (stationary) bound state then, the main contribution to the energy is V(r), and so we’d expect that the density, classically, would look like ρ(r) ≈ exp(-βV(r)) (very succesfull Percus-Yevick eqn). This is the Jastrow approach. So we postulate a wavefunction form like:



where LN is a normalization constant. It satisfies symmetry under exchange. A slightly different form would be necessary I suppose for fermions to make it AS under exchange. What is u(r)? We’ll specialize to N = 2 and find out. So let’s consider a two particle system so that u(r) describes correlations only between two particles. Then in our two particle system, the Jastrow wavefunction is:



Note the similarity with the WKB approximation form. Starting with the two-particle Schrodinger equation, going to COM coordinates, factoring out the spherical harmonics part, etc., we eventually get (see QM folder)…for the radial part of the Schrodinger equation:



Filling in our ansatz,



We expect u(r) to be sharply diverging for small r because Ψ0(r) must vanish for small r since the particles certainly can’t be on top of each other (because the Lennard Jones potential is strongly repulsive at short distances, not because they can’t be in principle). The first derivative squared is the dominant term for small r [can check by saying u = r-p and seeing which terms have largest p values]. So ignoring the rest we come to, for small r:



We choose the – sign so Ψ converges (to zero). So this is the approximate short range form of u(r). Using the small r part of the L-J potential as an example, the repulsive part is V(r) = ε(σ/r)12, and we’d have,



This is practically identical to results for the Jastrow wavefunction determined by previous workers. What they did was to assume that the L-J potential was simply a hard wall potential. Then they parameterized Ψ0(r1,r2) simply by assuming the form above, [with a power law u(r)] and minimized the GS energy in that form (keeping all the terms in H). The long range behavior of u(r) was investigated by some. They showed that the long range form of u(r) would look like



This is the long range form assumed by the many-body wavefunction of coupled HO (it is?). And we would presume to have such an entity in our GS b/c of the acoustic spectrum we see in the neutron scattering experiments. So overall,



and now we have taken into account the hard wall repulsion behavior (small r form of u) and collective mode behavior (large r form of u) into our Ψ0.

**Static Fluid GS Prediction of nk, <KE>, <PE>**

We can setup the density matrix thing (recall the many-body correlations file in QM folder/Identical Particles):



The single particle correlation function would be:



where we use the fact that u(ri – rj) = u(rj – ri). It is clear, FWIW, that f(r1|r´1) is symmetric w/r to interchange of r1 and r´1. The two particle probability density function is:



So, FWIW,



These aren’t necessarily the easiest formulas to work with though. It’s seems easier to work directly from the wavefunction. One easy thing to calculate is the momentum expectation.



Let’s evaluate that derivative. So,



Now



Therefore,



And we’ll observe that the total momentum operator annihilates the wavefunction,



And so we get zero momentum expectation.



Now let’s look at the kinetic energy.



Continuing,



Now from the many-body correlations file (QM), we have:



(where n0 = N/V) Filling this in,



g, just like u, should be a function of |**r**j – **r**m|, so we can say:



We can go to center mass coordinates, R = (r1 + r2)/2, r = r1 – r2 and get:



and so the KE per particle would be:



(Mahan gets half this….hmmmmmm) We also have the potential energy per particle (on average), from the many body correlations file in QM folder.



We can also get the momentum distribution nk. We’ll recall from the many body correlations file, that:



where,



I would like to see how one actually does these integrals. Might have to do a mean field approximation…? Anyway, we can use u(r) to get R(r), and then calculate the momentum distribution function n(k). The experimental and theoretical results are shown below. The non-diverging solid line didn’t use uℓ(r). If you do try to include long range order by adding in the uℓ term you get the diverging line. So note how n(k) blows up for small k when there are long range correlations.



Our calculations show that it diverges at k = 0, but it can’t really of course. This is just an indication of the presence of the condensate. In any event, we do have a pretty good prediction of nk. By consequence, we have a good prediction of KE since we can get <KE> from nk. What about the PE? We could calculate that from our wavefunction but he doesn’t do this. I assume it is good. So the next question is, how do we interpret our results. What is the physical picture we put on it? Recall the values for KE ~ 15K, and PE ~ -22K that were asserted at the top of the file.

We can put a physical picture to the situation. Say the condensate looked something like a cubic crystal structure, with each atom situated at the minimum of the others potential wells. Then each atom would have 6 n.n. And since each well has a depth of -10K energy. Those 6 bonds would amount to -60K energy. But each bond shares its energy with 2 atoms, so per atom we have -30K. That’s a little high, but in the ball park. It turns out the g(r) calculated above (but not actually) suggest the atoms are much further apart, and that the lattice is more like each atom having 8 n.n. situated further away, with an average potential energy between each of about 5K.

The next question is, ‘where is the KE of approximately 10K coming from?’. He says it’s coming from particle-in-a-box like fluctuations of the molecules about their equilibrium positions. He observes that the first peak in g(r) - the two particle distribution function - has a peak around 0.4nm. So each particle lives in a box about 0.4nm wide, tall, deep. If you calculate the GS KE of a 4He particle in such a box, (basically 3·k2/2m, where k = π/a, and 3 comes from 3 dimensions) then the KE comes out to be around 15K, which is about right. So the average KE simply comes from the zero point motion of the particles inside the potential wells that they sit in. This is the zero point energy that they talk about. And remember this is the zero point energy of the condensate, mostly (as these measurements are done at T = 1K, in which case the condensate predominates over the normal liquid).

**Low lying excited states: Biji - Feynman Theory**

Now we’d like to try to find a way to fit the excitation spectrum. So we need excited states (with momentum k, and I think k would have to be non-zero). We will asume that the excited states still have the long range order that the GS has, and so will only need minor modifications. From neutron scattering experiments, the energy excitation spectrum can be plotted (see phenomenology file), and the observed low lying excitations are suspected to be acoustic waves. We saw in the Bogoliubov file that in the weak interaction limit, these were given by,



where,



where nk is the FT of the density operator/function. And so we’ll go with this ansatz here too. Could write this in operator way as:



Don’t think these excited states are actually orthogonal. I do think they are to order 1/N or something though. Close enough I guess. Anyway let’s find the normalization constant,



The guy in brackets isn’t a trivial evaluation because Ψ0 has r dependence too. But this is at least a thing – it’s in fact the structure factor (see Quantum Mechanics/Identical Particles/Many Body Correlations file). Well, it’s the structure factor if we can exclude the k = 0 term, and I think we can, since setting k = 0 would just return to us the ground state again. So we can say:



And so,



Remember Sk describes fluctuations in the density, and is related to the two-particle density function.

**Static Fluid GS Prediction of <P>, <E>**

And now that we’ve got the normalization, we can calculate the expectation of the momentum.



And then with the normalization of Ψ0,k­, we have:



This makes sense as we know acoustic wave quanta characterized by wavelength λ = 2π/k, carry momentum k. Now let’s consider the energy. I’m going to do this in an operatory way. And we’re going to try to write the energy in terms of the GS energy and terms involving S(k).



Mahan says that in the first term, we can say 0|Ψ0> = E0, the ground state energy. And then [H,n] = [KE + V,n] = [KE,n] since V and n are just position operators. So then we’d have:



But I’m not sure that we can say 0|Ψ0> = E0|Ψ0>, as |Ψ0> isn’t an exact eigenstate. Maybe it is ‘to O(1/N)’ or something. Could say that the presence of the n\*knk operator, since it oscillates rapidly in position space, will wash out the integral, unless k = 0, in which case nk = 1, and we would be left with <Ψ0|H|Ψ0> = E0, where E0 would be the energy expectation of the ground state. Oh, well he says we’re constructing the excited states from the exact GS |Ψ0>, of which our |Ψ0> in the previous section was just an approximation. So in that case I guess we do get E0. Anyway, now we have to work out that commutator. Gonna follow Mahan and do this in position space,



Now what? Filling this back in,



where in last line we IBP. Now we’ll take the gradient of the that stuff in the second term. Note that if index i = j, then e-i**k**·(**r**\_i – **r**\_j) → 1, and the derivative is zero.



Recalling the value of Lk = 1/√NS(k), we have:



Note all of the new physics is in the structure factor S(k) which we don’t exactly have an explicit expression for [but see Many-Body Correlations file…S(k) is roughly Fourier transform of two-particle probability density function f(r1-r2)). There is a theorem that S(k) ~ k for small k [see many-body correlations file for confirmation, but not explanation, alas]. And so the excitations we’ve constructed would seem to be consistent with acoustic waves. Now we can create compound, approximate, excited states. We construct this by simply piling Ak’s onto the GS.



like we did for the low temperature phase of the Ising Ferromagnet. We can think of these states as sort of basis states, or fundamental modes of excitations. We can pile more ‘boson’s into each mode, and write, for our low lying excitations the general expression:



This is supported by some work that the Feenberg guys did which produced the following results…



So the states are nearly normalized and nearly orthogonal – for large N. And we also have



So the energies add, like bosonic excitations. This suggests the obvious analogy Ak ~ ak†. To a degree this makes sense since formal manipulations with the operators would reproduce some of our results.



So we can approximately say that:



But he says not to push the analogy too far since different states are not quite orthogonal, though assuming they are might give you the leading contributions. Anyway, when we do calculate or experimentally determine S(k) and plot the single particle excitation spectrum, ω(k), we obtain the following.



Our result successfully produces the roton minimum, which is caused by a peak in S(k) around k = 2A. But we see that our result is about a factor of 2 too large. By the way, seems clear that low k excitations are acoustic waves, and high k excitations are particle-hole. But what is going on at the minimum? These are called roton excitations. Found an explanation from book by James Annet.

Diagram

Description automatically generated

We must press on…

**Improved Excitation Spectra**

…and include interactions between the approximate excited states. Our approximate states are not exact states of course, and so there will be residual interactions between them. He recommends looking for the details in Feenberg’s (1969) book, as he was the one to pioneer this method. In short, we will take the non-orthogonality of those states into account. This means that our excitations are not exact eigenstates, and so the residual interaction between these excitations gives them a self-energy of sorts. So we’ll try to calculate the self-energy of a single |k> excitation.



The first order Σ term is shown below. A state with one excitation, |k>, will interact with/split into a two excitation state |kʹ, k-kʹ> and then recombine into a the single particle |k> state. The bubble is |kʹ, k-kʹ> basically.



Note how momentum must be conserved. Using second order Brillioun-Wigner perturbation theory, the self energy for such a diagram is:



I imagine that we’re using H – E = T + V – E, instead of V alone because our approximate wavefunctions are not eigenstates of T, and so V is not the perturbation per se. Rather our Ψ’s are approximate eigenfunctions of H = T + V, and the ‘perturbation’ is H – E. Feenburg attempted an approximate solution for the spectrum (setting E = E0 + ω0(k) + Σ(k,E) = 0 and solving for E, I presume) by approximating H – E with H – E0 – ω0(k)



calculating the matrix elements, and solving, etc. When this is done numerically rather, the results for the excitation spectra compare quite well with experiment. They’re shown below.



These results, plus the previous ones are sufficient now to predict the various properties of system, such as superfluidity, etc. It is to these properties that we now turn.

**Moving Fluid Ground State**

Now let’s construct the wavefunctions applicable to a moving superfluid. We’ll start with the ground state again. It would stand to reason that the wavefunction would be given by translating the static ground state at rate **v**. So this would correspond to:



where, as we might expect, T is basically the translation operator:



We’ll note that Ψv is normalized, presuming Ψ0 is. The momentum expectation can be calculated. And we get, recalling that of course,





Therefore,



So the whole liquid is moving in unison with velocity **v**, as we’d expect. We can calculate the total energy too.



So we have:



where E0 is the stationary GS energy – which includes the PE – and εv = (1/2)mv2. So this choice does indeed describe a uniform flow of the particles.

**Low lying moving excited states**

Now we want to consider the excitation spectrum of the moving fluid. We do this by using Ψv­ as our superfluid GS. And the excited states will be the acoustic oscillations that we discussed before. I think that the excitations pump particles out of the superfluid state and into the normal fluid state? Is it true that the more excitations we have, the less superfluid condensate we have? So anyway, let’s construct a single excited state |k>.



This is normalized, presuming Ψv is, and it is. So now let’s look at its momentum.



So we have:



which has the natural interpretation of being an acoustic wave excitation within a moving fluid. Now consider the energy.



So we have:



And note the extra **k**∙**v** factor. This can be understood in that for low **k**, ω0(k) ≈ **k·v**s. And if we are moving at velocity **v**, then the total velocity is **vs** + **v**. And so the energy would change to ω0(k) → **k**·(**v**S + **v**)∙**k** = **k**·**v**s + **k**·**v** = ω0(k) + **k**·**v**. So since we’re moving, the energy of the acoustic wave is enhanced. I presume that if we have multiple excitations, we’ll have something like this?



where, just to emphasize, nk is telling us how many excitations of energy ω0(**k**) + **k**·**v** we have. It’s not the bose distribution function or anything.