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Note: For this discussion and on pages 252 - 259, the interaction is attractive, which means $\lambda<0$ with our original definition. Some of the equations in 252+ assume $|\lambda|$ is used $\Rightarrow$ be careful of the signs.

- Also, on 259, the dimensionless variable is $\tilde{\lambda}' \equiv m\lambda \frac{\pi}{2\epsilon_F} = \frac{m\lambda}{\rho}$ (and not $\tilde{\lambda}$, which has dimensions) for $g=2$ (which we assumed).

- We found that there are two regions at a given density, depending on the strength of the coupling. Or, at fixed coupling, there are two regions of density:

$$\boxed{\frac{m\lambda}{\rho} > \frac{\pi^2}{2} \Rightarrow \text{solution with } z = \frac{E_2}{2\epsilon_F} < 0}$$

$$\boxed{0 < \frac{m\lambda}{\rho} < \frac{\pi^2}{2} \Rightarrow \text{solution with } 0 < z < 1}$$

- The analog to Cooper pairing near the Fermi surface in three dimensions is the second (high density) case.
  - The high density limit is also where we thought our perturbative calculation should be good, so we'll focus on that region.

- Since $z<1$, we can define Δ by (and δ)

$$\boxed{E_2 = 2\epsilon_F - \Delta} \quad \text{or} \quad \boxed{\Delta = 2\epsilon_F(1-z) \equiv 2\epsilon_F\,\delta}$$

$\Rightarrow \Delta$ is like the binding energy of the pair of opposite momentum states.

- Note that Δ is independent of the momenta of those states.

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In the weak coupling/high density limit, $z \to 1$ so $\delta \to 0$ and we can expand the transcendental equation (using Mathematica):

$$\boxed{\frac{\pi^2 \sqrt{z}}{\lambda'} - \ln\left[\frac{1+\sqrt{z}}{1-\sqrt{z}}\right] = 0} \Rightarrow \boxed{\frac{\pi^2}{|\lambda'|} + \ln\frac{\delta}{4} = \delta\left(\frac{1}{2} - \frac{\pi^2}{2\lambda'}\right) + O(\delta^2)}$$

- Keeping only the leading δ dependence (drop linear and higher)

$$\Rightarrow \frac{\delta}{4} \doteq e^{-\pi^2/|\lambda'|} \quad \text{or} \quad \boxed{\Delta = 8\epsilon_F\, e^{-\pi^2 \hbar^2 / m|\lambda|}}$$

- So the energy shift of a pair with relative momentum k is

$$\boxed{\Delta E = E_2 - 2\epsilon_k^0 = 2(\epsilon_F - \epsilon_k^0) - \Delta}$$

which is negative everywhere and independent of L.

- Δ has an essential singularity in the coupling constant so it has no Taylor series about $|\lambda| = 0$
  $\Rightarrow$ cannot be obtained from finite-order perturbation theory.

- We should repeat the analysis for center-of-mass momentum $P_{cm} \neq 0$, since the result in the medium will depend on P_{cm} (since the Fermi sea defines a rest frame!).
  - In free space, $E = B_2 + P_{cm}^2/4m$, so $P_{cm} \neq 0$ always increases the energy. We'll assume here that back-to-back ($P_{cm} = 0$) is also favored in the medium.
    [You check $P_{cm} \neq 0$ in PS#2!]

- So we've learned that the particles like to pair up, at least if considered 2 at a time. How do we deal with the many-body problem?

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- A good place to start is a variational calculation, because at worst we overestimate the true groundstate energy.

- In PS#1, you did a variational estimate of the energy of this system by calculating

$$\boxed{E_{HF} = E^{(0)} + E^{(1)} = \langle F|\hat{H}|F\rangle}$$

where

$$\boxed{\hat{H} = \sum_{k\alpha} \frac{k^2}{2m} a^\dagger_{k\alpha} a_{k\alpha} - \frac{|\lambda|}{2L} \sum_{kpq} \sum_{\alpha_1\alpha_2} a^\dagger_{k+q\,\alpha_1} a^\dagger_{p-q\,\alpha_2} a_{p\alpha_2} a_{k\alpha_1}}$$

and the variational trial state is $|F\rangle$, which is a Fermi sea filled up to k_F:

$$\boxed{|F\rangle = \prod_{k\alpha}^{k<k_F} a^\dagger_{k\alpha}|0\rangle} \quad \text{with } |0\rangle \text{ the vacuum}$$

and $\boxed{\rho = \frac{g k_F}{\pi} \to \frac{2k_F}{\pi}}$ for $g=2$ (which we assume here).

- Recall that we found

$$\boxed{\begin{aligned} E^{(0)} = \langle F|\hat{H}_0|F\rangle &= \frac{1}{2m}\sum_{k\alpha} k^2 \langle F|\hat{n}_{k\alpha}|F\rangle \\ &= \frac{1}{2m}\sum_\alpha \frac{L}{(2\pi)}\int_{-\infty}^{\infty} dk\, k^2 \theta(k_F - k) \\ &= \frac{1}{2m}\,\overset{g}{2}\,\frac{L}{2\pi}\,2\cdot\frac{k_F^3}{3} = \frac{\pi^2}{24}\frac{\rho^3}{m}L = \left(\frac{\pi^2}{24}\frac{\rho^2}{m}\right)N \end{aligned}}$$

for the kinetic energy

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and for the HF piece  :

$$\boxed{\begin{aligned} E^{(1)} = \langle F|\hat{H}_1|F\rangle &= -\frac{|\lambda|}{2L}\sum_{kpq}\sum_{\alpha_1\alpha_2}\langle F|a^\dagger_{k+q,\alpha_1}\, a^\dagger_{p-q\,\alpha_2}\, a_{p\alpha_2}\, a_{k\alpha_1}|F\rangle \\ &= -N\left(\frac{|\lambda|}{2}\rho - \frac{1}{g}\frac{|\lambda|}{2}\rho\right) \longrightarrow -\frac{|\lambda|}{4}\rho N \end{aligned}}$$

- We can also calculate the chemical potential from

$$\boxed{\mu = \left(\frac{\partial E}{\partial N}\right)_V = \frac{E}{N} + \rho\,\frac{\partial(E/N)}{\partial\rho} = \frac{\pi^2\rho^2}{8m} - \frac{|\lambda|\rho}{2}}$$

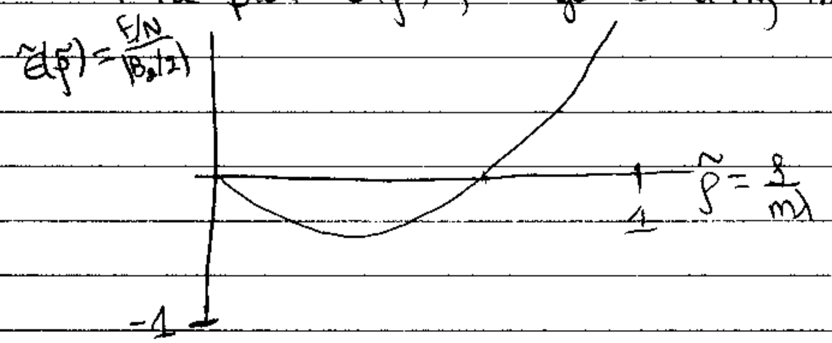
- Let's plot E/N vs. ρ in dimensionless variables.
  - In particular, $\boxed{1/\lambda' = \rho/m\lambda \equiv \tilde{\rho}}$ is dimensionless
  - Also, compare E/N to the energy/particle we expect at zero density, which is $\boxed{-|B_2|/2 = -m\lambda^2/8.}$

$$\Rightarrow \boxed{\tilde{\varepsilon}(\tilde{\rho}) \equiv \frac{(E/N)}{|B_2/2|} = \frac{\pi^2}{3}\tilde{\rho}^2 - 2\tilde{\rho}} \qquad \boxed{\tilde{\rho} \equiv \rho/m\lambda}$$

and

$$\boxed{\tilde{\mu}(\tilde{\rho}) \equiv \frac{\mu}{m\lambda^2} = \frac{\pi^2}{8}\tilde{\rho}^2 - \frac{1}{2}\tilde{\rho}}$$

- So for the real solution, we expect $\tilde{\varepsilon}(\tilde{\rho}\to 0) = -1$.
  - If we plot $\tilde{\varepsilon}(\tilde{\rho})$, we get something like



- Let's try a more general variational trial functional than $|F\rangle$.

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- We follow B, C, and S (Bardeen, Cooper, and Schrieffer) and use the BCS ansatz, which is motivated by our observation that $k\uparrow$ and $-k\downarrow$ states are energetically favored to pair up.

- So consider

$$\boxed{|BCS\rangle = \prod_k \left(u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\right)|0\rangle}$$

where the product is over all momenta (+ and −) but not spin (which is taken care of explicitly).

- The u_k's and v_k's are, in general, complex numbers which will be chosen to minimize $\langle BCS|\hat{H} - \mu\hat{N}|BCS\rangle$.
  - With no loss of generality we can take the u_k's to be real
  - We will assume the v_k's are real as well, although this can be shown from the minimalization.

- What about normalization $\langle BCS|BCS\rangle = 1$?

$$\boxed{\begin{aligned}\langle BCS|BCS\rangle &= \langle 0|\prod_{kk'}\left(u_{k'} + v_{k'} a_{-k'\downarrow} a_{k'\uparrow}\right)\left(u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\right)|0\rangle \\ &= \prod_k \left(u_k^2 + v_k^2\right)\end{aligned}}$$

so we take $\boxed{u_k^2 + v_k^2 = 1}$

Try arguing why we get $u_k^2 + v_k^2$.

[We can match up the corresponding k and k' $\Rightarrow$ one product $\prod_k$ of $(u_k + v_k a_\downarrow a_\uparrow)(u_k + v_k a^\dagger_\uparrow a^\dagger_\downarrow)$ terms, which commute with all other terms.

- since $a_\downarrow a_\uparrow a^\dagger_\uparrow a^\dagger_\downarrow|0\rangle = 1$ while $a_\downarrow a_\uparrow|0\rangle = \langle 0|a^\dagger_\uparrow a^\dagger_\downarrow = 0$, we don't get any cross terms, but only $u_k^2 + v_k^2$]

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- We can express $|BCS\rangle$ differently by writing out the product

$$\boxed{|BCS\rangle = (u_{k_1} + v_{k_1} a^\dagger_{k_1\uparrow} a^\dagger_{-k_1\downarrow})(u_{k_2} + v_{k_2} a^\dagger_{k_2\uparrow} a^\dagger_{-k_2\downarrow}) \cdots |0\rangle}$$

multiplying it out and then grouping all terms with 0, 2, 4, and so $a^\dagger$ operators.

- We also "factor out" the product of "0" operators:

$$\boxed{|BCS\rangle = \left(\prod_i u_{k_i}\right)\left[|0\rangle + \sum_k \frac{v_k}{u_k} a^\dagger_{k\uparrow} a^\dagger_{k\downarrow}|0\rangle + \frac{1}{2}\sum_{kk'} \frac{v_k v_{k'}}{u_k u_{k'}} a^\dagger_{k\uparrow} a^\dagger_{k\downarrow} a^\dagger_{k'\uparrow} a^\dagger_{k'\downarrow}|0\rangle + \cdots\right]}$$

which clearly reveals that the general BCS state has an indefinite number of particles.

- This means we'll want to minimize

$$\boxed{\langle BCS|\hat{K}|BCS\rangle} \quad \text{with} \quad \boxed{\hat{K} \equiv \hat{H} - \mu\hat{N}}$$

where the chemical potential μ acts as a Lagrange multiplier to enforce that $\langle BCS|\hat{N}|BCS\rangle = N$ (N particles on average).

- The 1/2 in front of the $(a^\dagger a^\dagger)^2$ term arises to account for the double counting of identical permutations (note that the $a^\dagger a^\dagger$ pairs always commute).
  - In general there will be $\frac{1}{n!}(a^\dagger a^\dagger)^n|0\rangle$

  $\Rightarrow |BCS\rangle$ is the expansion of an exponential.

- If we define $\boxed{A^\dagger = \sum_k \frac{v_k}{u_k} a^\dagger_{k\uparrow} a^\dagger_{k\downarrow}}$

then $\boxed{|BCS\rangle \propto e^{A^\dagger}|0\rangle = \sum_{\nu=0}^{\infty} \frac{1}{\nu!}(A^\dagger)^\nu|0\rangle}$

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- Does the $|BCS\rangle$ ansatz contain $|F\rangle$ as a special case?

Yes: Choose

$$\boxed{u_k = \begin{cases} 0 & |k|<k_f \\ 1 & |k|>k_f \end{cases} \quad \text{"particles"} \qquad v_k = \begin{cases} 1 & |k|<k_f \\ 0 & |k|>k_f \end{cases} \quad \text{"holes"}}$$

and then $\boxed{|BCS\rangle \longrightarrow \prod_k^{k_f} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} |0\rangle = |F\rangle}$

- So clearly $|BCS\rangle$ is a more general ground state, so it should be able to choose (variationally, that is) between a normal and superconducting ground state.

- We'll verify first that we get the correct result for $\langle F|\hat{K}|F\rangle$ as a special case of our general result.

- Claim:

$$\boxed{\langle BCS|\hat{K}|BCS\rangle = 2\sum_k (\epsilon_k^0 - \mu) v_k^2 - \frac{|\lambda|}{L}\sum_{kk'}(v_k^2 v_{k'}^2 + u_k v_k u_{k'} v_{k'})}$$

- We derive (or motivate) this later (or put it in a problem set!)

Check:

$$\begin{aligned}
\langle F|\hat{K}|K\rangle &= 2\sum_k^{k_f}(\epsilon_k^0 - \mu) - \frac{|\lambda|}{L}\sum_{kk'}\left[\theta(k_f-|k|)\theta(k_f-|k'|) + 0\right] \\
&= 2\frac{L}{2\pi}\int_{-k_f}^{k_f} dk\left(\frac{k^2}{2m} - \mu\right) - \frac{|\lambda|}{L}\left(\frac{L}{2\pi}\right)^2\left(\int_{-k_f}^{k_f} dk\right)^2 \\
&= \frac{L}{\pi}\left(2\frac{k_f^3}{6m} - 2\mu k_f\right) - \frac{|\lambda| L}{4\pi^2} 4k_f^2 \\
&= L\rho\left[\left(\frac{1}{3}\frac{k_f^2}{2m} - \mu\right) - \left(\frac{1}{4}|\lambda|\rho\right)\right] = E - \mu N
\end{aligned}$$

$$\Rightarrow \boxed{E/N = \frac{1}{3}\frac{k_f^2}{2m} - \frac{1}{4}|\lambda|\rho} \quad \checkmark$$

which agrees with our previous result. Note that μ just dropped out.

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Let's take $\langle BCS|\hat{K}|BCS\rangle$ as given and minimize it.

- We need to keep $u_k^2+v_k^2=1 \Rightarrow 2u_k\,du_k+2v_k\,dv_k=0$

  $\Rightarrow$ vary v_k and use this constraint on u_k.

$$\boxed{\begin{aligned}\Rightarrow \left(\frac{\partial}{\partial v_k}+\frac{\partial u_k}{\partial v_k}\frac{\partial}{\partial u_k}\right)\langle BCS|\hat{K}|BCS\rangle &= 0\\ = 4(\epsilon_k^0-\mu)v_k-\frac{|\lambda|}{L}\Big[4v_k\sum_{k'}v_{k'}^2+2u_k\sum_{k'}u_{k'}v_{k'}\\ +\left(-\frac{v_k}{u_k}\right)2v_k\sum_{k'}u_{k'}v_{k'}\Big] &= 0\end{aligned}}$$

So solve this along with $\boxed{u_k^2+v_k^2=1}$

- Group together the v_k terms with the definitions:

$$\boxed{\epsilon_k^{HF}\equiv\epsilon_k^0-\frac{|\lambda|}{L}\sum_{k'}v_{k'}^2=\epsilon_k^0-\frac{|\lambda|}{L}\frac{N}{2}=\epsilon_k^0-\frac{|\lambda|}{2}\rho}$$

and $\boxed{\xi_k\equiv\epsilon_k^{HF}-\mu}$ and $\boxed{\Delta\equiv\frac{|\lambda|}{L}\sum_{k'}u_{k'}v_{k'}}$

where we've used (again, derivation to follow!)

$$\boxed{\begin{aligned}\langle BCS|\hat{N}|BCS\rangle &= \sum_{k\alpha}\langle BCS|a_{k\alpha}^\dagger a_{k\alpha}|BCS\rangle\\ &= 2\sum_k v_k^2\end{aligned}}$$

- Note that ϵ_k^{HF} is the Hartree-Fock single-particle energy.

Our equation is now

$$\boxed{2\xi_k v_k u_k-[u_k^2-v_k^2]\Delta=0} \quad\text{or}\quad \boxed{2\xi_k u_k v_k=[u_k^2-v_k^2]\Delta}$$

let $\boxed{u_k\equiv\cos\chi_k}$ and $\boxed{v_k\equiv\sin\chi_k}$

$$\Rightarrow \boxed{2\xi_k\cos\chi_k\sin\chi_k=(\cos^2\chi_k-\sin^2\chi_k)\Delta} \Rightarrow \boxed{\xi_k\sin 2\chi_k=\Delta\cos 2\chi_k}$$

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From $\boxed{\tan 2\chi_k = \Delta/\xi_k}$ we find

$$\boxed{\sin 2\chi_k = \frac{\pm\Delta}{\sqrt{\Delta^2+\xi_k^2}}} \quad \text{and} \quad \boxed{\cos 2\chi_k = \frac{\pm\xi_k}{\sqrt{\Delta^2+\xi_k^2}}}$$

• If we consider the full $\hat{H}$, we'll see that the + signs are needed for the energy to be bounded from below. [Later!]

$$\Rightarrow \boxed{u_k v_k = \tfrac{1}{2}\sin 2\chi_k = \frac{\Delta}{2\sqrt{\Delta^2+\xi_k^2}}}$$

and

$$\boxed{\begin{aligned} u_k^2 = \cos^2\chi_k &= \tfrac{1}{2}(\cos^2\chi_k + 1 - \sin^2\chi_k) = \tfrac{1}{2}(1+\cos 2\chi_k) \\ &= \tfrac{1}{2}\left(1+\frac{\xi_k}{\sqrt{\Delta^2+\xi_k^2}}\right) \end{aligned}}$$

and $\boxed{v_k^2 = 1-u_k^2 = \tfrac{1}{2}\left(1-\xi_k/\sqrt{\Delta^2+\xi_k^2}\right)}$

Using the definition of Δ, we get the "gap equation"

$$\boxed{\Delta = \frac{|\lambda|}{L}\sum_k u_k v_k = \frac{|\lambda|}{2L}\sum_k \frac{\Delta}{\sqrt{\Delta^2+\xi_k^2}}}$$

so either

$\boxed{\text{i)}\ \Delta = 0}$

or

$$\boxed{\text{ii)}\quad 1 = \frac{|\lambda|}{2L}\sum_k \frac{1}{\sqrt{\Delta^2+\xi_k^2}}}$$

Next time: check the energy!