4/16/03

Let's return to the quadratic term before doing the fermion integration

$$\int dx \begin{pmatrix} \psi_1^\dagger & \psi_2 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial \tau} - \frac{\nabla^2}{2m} - \mu & -\Delta_c \\ -\Delta_c^* & \frac{\partial}{\partial \tau} + \frac{\nabla^2}{2m} + \mu \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2^\dagger \end{pmatrix} + \frac{1}{|\lambda|}|\Delta_c|^2$$

and go to a uniform system $\Delta_c(x) \to \Delta_c$ and Fourier transform: (also take $1 \to \uparrow$ and $2 \to \downarrow$)

$$\sum_\omega \sum_k \begin{pmatrix} \psi_\uparrow^\dagger(k) & \psi_\downarrow(-k) \end{pmatrix} \begin{pmatrix} -i\omega + \xi_k & -\Delta_c \\ -\Delta_c^* & -i\omega - \xi_k \end{pmatrix} \begin{pmatrix} \psi_\uparrow(k) \\ \psi_\downarrow^\dagger(-k) \end{pmatrix} + LT\frac{|\Delta_c|^2}{|\lambda|}$$

Now think about diagonalizing the matrix $\Rightarrow$ introduce a rotated basis of Grassman fields:

$$\begin{pmatrix} \psi_\uparrow(k) \\ \psi_\downarrow^\dagger(-k) \end{pmatrix} = \begin{pmatrix} \cos\chi_k & +\sin\chi_k \\ -\sin\chi_k & \cos\chi_k \end{pmatrix} \begin{pmatrix} \alpha(k) \\ \beta^\dagger(-k) \end{pmatrix}$$

and choose χ_k so that we get a diagonal matrix.

This is accomplished (surprise, surprise!) by

$$\cos 2\chi_k = \frac{\xi_k}{\sqrt{\xi_k^2 + |\Delta_c|^2}} \qquad \sin 2\chi_k = \frac{|\Delta_c|}{\sqrt{\xi_k^2 + |\Delta_c|^2}}$$

(checked with Mathematica)

Inverting the transformation,

$$\begin{pmatrix} \alpha(k) \\ \beta^\dagger(-k) \end{pmatrix} = \begin{pmatrix} \cos\chi_k & -\sin\chi_k \\ +\sin\chi_k & \cos\chi_k \end{pmatrix} \begin{pmatrix} \psi_\uparrow(k) \\ \psi_\downarrow^\dagger(-k) \end{pmatrix}$$

4/16/03

which is precisely the Bogolyubov transformation from (270) when we make the same identifications of u_k and v_k:

$$\boxed{u_k = \cos\chi_k} \quad \text{and} \quad \boxed{v_k = \sin\chi_k}$$

Mathematica check:

```
In[1]:= r1 = {{Cos[χ], Sin[χ]}, {-Sin[χ], Cos[χ]}};

In[2]:= MatrixForm[r1]

Out[2]//MatrixForm=
        ( Cos[χ]   Sin[χ] )
        (-Sin[χ]   Cos[χ] )

In[3]:= r1t = Transpose[r1];

In[4]:= MatrixForm[r1t]

Out[4]//MatrixForm=
        ( Cos[χ]  -Sin[χ] )
        ( Sin[χ]   Cos[χ] )

In[5]:= mid = {{-I ω + ξ, -Δ}, {-Δ, -I ω - ξ}};

In[6]:= MatrixForm[mid]

Out[6]//MatrixForm=
        ( ξ - i ω     -Δ     )
        (   -Δ     -ξ - i ω  )

In[7]:= Ek = Sqrt[ξ^2 + Δ^2]

Out[7]= Sqrt[Δ^2 + ξ^2]

In[8]:= MatrixForm[Simplify[r1t.mid.r1] /. {Cos[2 χ] → ξ / Ek, Sin[2 χ] → Δ / Ek}]

Out[8]//MatrixForm=
        ( Δ^2/Sqrt[Δ^2+ξ^2] + ξ^2/Sqrt[Δ^2+ξ^2] - i ω          0          )
        (          0          -Δ^2/Sqrt[Δ^2+ξ^2] - ξ^2/Sqrt[Δ^2+ξ^2] - i ω )
```

We can simplify that last result a bit more to get

$$S = TL\frac{|\Delta_0|^2}{|\lambda|} + \sum_{w}\sum_{k}\begin{pmatrix}\alpha^\dagger(k) & \beta(-k)\end{pmatrix}\begin{pmatrix}-i\omega + \sqrt{\xi_k^2+|\Delta_0|^2} & 0 \\ 0 & -i\omega - \sqrt{\xi_k^2+|\Delta_0|^2}\end{pmatrix}\begin{pmatrix}\alpha(k) \\ \beta^\dagger(-k)\end{pmatrix}$$

$$= TL\frac{|\Delta_0|^2}{|\lambda|} + \sum_{w}\sum_{k}\left(-i\omega + \sqrt{\xi_k^2+\Delta_0^2}\right)\left(\alpha^\dagger(k)\alpha(k) + \beta^\dagger(k)\beta(k)\right)$$

4/16/03

Which is the action corresponding to the Hamiltonian from before:

$$\mathcal{H}_2 = \sum_k E_k \left(\alpha^\dagger(k)\alpha(k) + \beta^\dagger(k)\beta(k) \right)$$

What about the Hartree-Fock piece we had before?

- In our two effective action expansions, we made two different choices for getting rid of the $|\lambda|^2 \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1$ term

i) $\sigma \to \psi_1^\dagger \psi_1 + \psi_2^\dagger \psi_2$ $\left[\frac{1}{2}|\lambda|\left(\psi_\alpha^\dagger \psi_\alpha\right)^2 \right]$

ii) $\Delta \to |\lambda| \psi_2 \psi_1$

- The leading term in the σ-expansion included the Hartree-Fock contribution $E_{HF} = -\frac{N}{2}\rho^2$ or $E_{HF}/N = -\frac{N}{2}\rho$

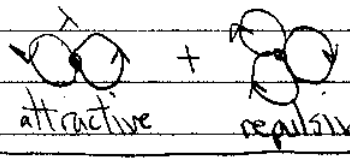
- If we solved either expansion exactly (ie, to all orders), we should get the same answer whether we choose i), ii) or $\frac{1}{2}[i) + ii)]$.
- However, if we truncate the expansion, we are incorporating two different types of physics. Nagaosa in his "QFT in Condensed Matter Physics" book says: "Here, a physical picture or intuition is necessary, because no general method exists."
  - We would like effective field theory (EFT) to provide such a method, but we haven't figured it out yet.

- Nagaosa argues that the most physically reasonable approximation is i) + ii) (rather than $\frac{1}{2}[i) + ii)]$) $\Rightarrow$ if restricted in momentum space, actually non-overlapping $\Rightarrow$ do both.
  - In practice this is what is done in nuclear models.

4/16/03

- So if we are going to put in both the particle-hole (ph) physics [type i)] and the particle-particle (pp) physics [type ii)], how do we do this in a finite nucleus?
  - For example, we want to know the ground state energy and density distribution for a wide range of nuclei, including the effects of pairing.
  - For all but the lightest nuclei, a "first-principles" calculation based on a nucleon-nucleon potential matched to scattering phase shifts is not possible.
  - Here we'll consider an alternative: energy functional methods (the most common are called Skyrme-Hartree-Fock and Relativistic Mean Field approaches).

- In PS#4, problem 1, we consider a simple energy function (not a functional, since the density ρ is for a uniform system $\Rightarrow$ independent of $\vec{r}$).
  - The form was motivated as

kinetic +  +

$$\Rightarrow \boxed{\mathcal{E}(\rho) = \frac{3}{5}\frac{\hbar_F^2}{2m}\rho + \frac{3}{8}t_0\rho^2 + \frac{1}{8}t_3\rho^3}$$

- Here $t_0 \propto \lambda$ and $t_3 \propto \beta$ is the conventional Skyrme notation.
- The energy per particle is

$$\boxed{\epsilon(\rho) \equiv E/N = \frac{\mathcal{E}(\rho)}{\rho} = \frac{3}{5}\frac{\hbar_F^2}{2m} + \frac{3}{8}t_0\rho + \frac{1}{8}t_3\rho^2}$$

- The full Skyrme functional has separate proton (ρ_p) and neutron (ρ_n) densities, as well as additional terms proportional to ρk_F^2, $(\nabla\rho)^2$ [which vanishes here], and some dependence on spin-orbit terms.

4/16/03

- You were given the conditions that nuclear matter (as extrapolated from the interior of heavy nuclei) is in equilibrium when

$$\boxed{\rho_0 \doteq 0.16\ \text{fm}^{-3}} \qquad \boxed{\mathcal{E}(\rho_0) \doteq -16.\ \text{MeV}}$$

Equilibrium implies $\boxed{\left.\frac{d\mathcal{E}}{d\rho}\right|_{\rho=\rho_0} = 0}$

$\Rightarrow$ in this case we have two equations that are linear in two unknowns ($\{t, \beta\}$ or $\{t_0, t_3\}$).

- A comment about units and putting back the $\hbar$'s. The usual choice of units is

$\mathcal{E}(\rho) \rightarrow$ MeV
$\mathcal{E}(\rho) \rightarrow$ MeV-fm^{-3}
$m \rightarrow$ 939 MeV (averaged proton/neutron)
$k_F \rightarrow$ fm^{-1} (also MeV some times) 1.3–1.4 fm^{-1} at equilibrium
$\rho \rightarrow$ fm^{-3}

- If $\boxed{\rho = \frac{g k_F^3}{6\pi^2} \xrightarrow{g=4} \frac{2k_F^3}{3\pi^2}} \Rightarrow \boxed{k_F(\rho) = \left(\frac{3\pi^2\rho}{2}\right)^{1/3} \text{ in fm}}$

how do we get $\frac{k_F^2}{2m}$ in MeV from $\frac{\text{fm}^{-2}}{\text{MeV}}$?

$\Rightarrow$ the choice of units implies we have taken $\hbar = c = 1$ (or, more precisely, we are measuring angular momentum in units of $\hbar$ and speed in units of c).

To convert, use $\boxed{\hbar c = 197.33\ \text{MeV-fm}}$

- In detail: $\frac{k_F^2}{2m} \rightarrow \frac{\hbar^2 k_F^2}{2m} \rightarrow \frac{(\hbar c)^2 k_F^2}{2mc^2} = \frac{(\hbar c)^2}{2M}\left(\frac{3\pi^2\rho}{2}\right)^{2/3} = \frac{(197)^2}{2\cdot 939}\left(\frac{3\pi^2\rho}{2}\right)^{2/3}$

- In practice: just figure out how many powers of MeV-fm are needed and the details take care of themselves!

fm^{-2}/MeV $\rightarrow$ need to kill two fm^{-1} $\rightarrow$ (MeV-fm)^2 is the factor.

4/16/03

Exercises: Use $\hbar c = 200$ MeV-fm for the estimates.

a) What is k_{F_0} in MeV? Are nucleons in a nucleus nonrelativistic?

b) What is the approximate range in fm of a one-pion exchange potential ($m_\pi = 140$ MeV)? Rho meson exchange ($m_\rho = 770$ MeV).

What about t_0 and t_3 units?

- For Skyrme models, it is conventional to take the t_i in units of MeV-$(\text{fm})^n$, where n cancels the dimensions of ρ^2, ρ^3, etc.
  - Typically $t_0 \simeq -1000$ MeV-fm^3
    $t_3 \simeq 10000$ MeV-fm^6

- Question: Are these big or small numbers?
  - The energy function looks like it could be an expansion in density → can we justify omitting a ρ^3 term. What is the expected error if we do?
  - Units of MeV-$(\text{fm})^n$ don't tell us if we have an expansion parameter → we need to identify appropriate physics scales
  - Claim: low-energy effective field theories of QCD associate with $\pi\pi \to \rho$ a scale $1/(f_\pi^2 \Lambda_\chi)$ where $f_\pi \simeq 100$ MeV is the pion decay constant and $\Lambda_\chi \simeq 1$ GeV (closer to 600 MeV in practice) is the scale of the spontaneous breaking of chiral symmetry.

⇒ the expansion parameter is $\frac{\rho}{f_\pi^2 \Lambda_\chi}$.

Exercise: What is this roughly in the interior of a nucleus (take $\Lambda_\chi \simeq 600$ MeV)? Is it a good expansion?

- Note: The pion is the (approximate) Goldstone boson of spontaneously broken chiral symmetry ($m_\pi^2 \ll m_\rho^2$). Approximate since $m_u, m_d \neq 0$.

4/16/03

- The existence of expansion parameters motivates the use of energy functions where we guess (or, better, derive) the form of the terms, truncate, and fit the coefficients to finite density data rather than to scattering data.
  - We will justify this approach using density functional theory or DFT, which is widely used in quantum chemistry and condensed matter physics.

- Solving for t_0, t_3 or λ, β using Mathematica:
  - To solve the simultaneous equations (the real ones have at least another term!)

$$a\rho_0 + b\rho_0^2 = e_0$$
$$a + 2b\rho_0 = 0$$

use:

NOTE!

```
Solve[ {a*rhoϕ + b*rhoϕ^2 == eϕ,        ← equations as a list
        a + 2*b*rhoϕ == 0},
       {a, b}]                          ← parameters to be solved for
```

The answer will be in the form:

```
{ {a -> 123}, {b -> 456} }
```

(or in terms of rhoϕ and eϕ if you didn't assign numbers)

- You can plug this in by hand, but its better to use the /. substitution command. Eg. (note there is no kinetic energy!!!)

```
EoverA[rho_] := a*rho + b*rho^2
rhoϕ = .16
eϕ = -16
DerivEoverA[rho_] = D[EoverA[rho], rho]
ans = Solve[ {EoverA[rhoϕ] == eϕ, DerivEoverA[rhoϕ] == 0},
             {a, b}]
```

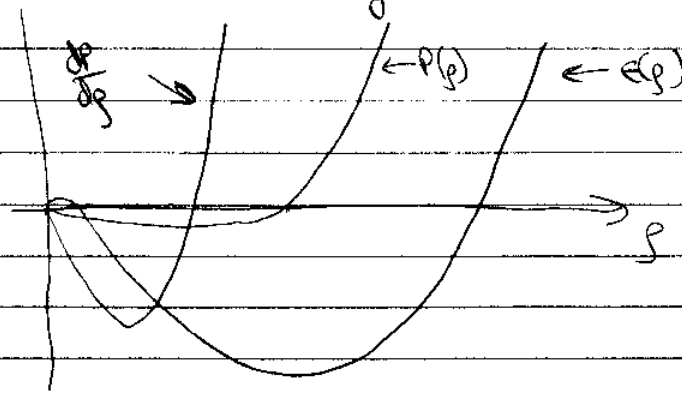
set the answer equal to a variable

```
Plot [{EoverA[rho] /. ans, Pressure[rho] /. ans, DerivPressure[rho] /. ans},
      {rho, 0, .4}, PlotRange -> {-30, 20}]
```

(where you need to define Pressure and DerivPressure).

4/16/03

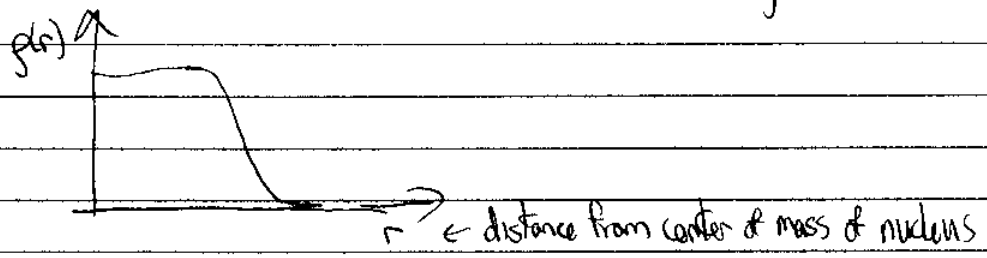
You should find something like



What do these curves tell us about nuclei?

- Are they consistent with the liquid drop picture?

Ok, we have an energy functional, how does this help us in a finite nucleus, where we expect the density not to be a constant but to look something like



Claim: There exists an energy functional $E[\rho(\vec{r})]$ that when the exact ground state density $\rho_{gs}(\vec{r})$ is inserted, gives the exact ground state energy E_{gs}:

$$\boxed{E_{gs} = E[\rho_{gs}(\vec{r})]}$$

and, this density minimizes the functional (variational principle).

$$\boxed{\left.\frac{\delta E[\rho]}{\delta \rho(\vec{r})}\right|_{\rho_{gs}(\vec{r})} = 0}$$

But how do we find (or guess) this $E[\rho]$?

4/16/03

Let's preview how this can work using our recent effective action results...

- Go back to (246) (without the chemical potential μ):

$$Z[J] = e^{iW[J]} = \int \mathcal{D}[\psi^\dagger,\psi]\,\mathcal{D}\sigma\; e^{i\left[\int d^4x\, \psi^\dagger_\alpha \underbrace{\left(i\frac{\partial}{\partial t} - \frac{\nabla^2}{2m} - C_0\sigma(x)\right)}_{G^{-1}}\psi_\alpha(x) + \frac{1}{2}C_0(\sigma(x))^2 + J(x)\sigma(x)\right]}$$

$$= \int \mathcal{D}\sigma\; e^{\frac{g}{2}\mathrm{Tr}\ln G^{-1}(x,y)}\, e^{\frac{1}{2}C_0\int d^4x(\sigma(x))^2}\, e^{i\int d^4x J(x)\sigma(x)}$$

Then the effective action (see (230) and thereabouts)

$$\Gamma[\sigma_c] \equiv W[J] - \int d^4x\, J(x)\sigma_c(x)$$

$$= \frac{g}{2i}\mathrm{Tr}\ln\left[G_H^{-1}(x,y)\right] + \frac{C_0}{2}\int d^4x(\sigma_c(x))^2 + (\text{higher orders})$$

which we'll label $\Gamma_{LO}[\sigma_c]$ as before.

Here

$$G_H^{-1}(x,y) = \left[i\frac{\partial}{\partial t} + \frac{\nabla^2}{2m} - C_0\sigma_c(x)\right]\delta^4(x-y)$$

and the energy is $F_{LO} = -\Gamma_{LO}[\sigma_c^0]/T$ where $\left.\frac{\delta\Gamma_{LO}[\sigma_c]}{\delta\sigma_c}\right|_{\sigma_{c_0}} = 0$

- In a uniform system, we took $\sigma_c(x) \to \sigma_c = \text{constant}$ and found $\mathrm{Tr}\ln G_H^{-1}$ by diagonalizing it by going to momentum and frequency space:

$$g\,\mathrm{Tr}\ln G_H^{-1} = g\sum_{\vec{p}}\sum_{p_0}\ln\left(p_0 - e_{\vec{p}} + i\eta\,\mathrm{sgn}(|\vec{p}| - k_F)\right)$$

(boundary condition for N particles)

where $\sum_{p_0} \to T\int\frac{dp_0}{2\pi}$ and $e_{\vec{p}} \equiv \frac{p^2}{2m} + C_0\sigma_c$

The $\mathrm{Tr}\ln$ gave a sum of eigenvalues $e_{\vec{p}}$ up to ϵ_F and then we had a $\frac{1}{2}C_0\sigma_c^2$ term. $\left.\frac{\delta\Gamma_{LO}}{\delta\sigma_c}\right|_{\sigma_{c_0}} = 0 \Rightarrow \sigma_c^0 = \rho$ and $\Omega_{LO} = -\Gamma_{LO}[\sigma_c^0]/VT = \rho\left(\frac{3}{5}\frac{k_F^2}{2m} + \frac{C_0}{2}\rho\right)$

4/16/03

Now we find ϵ_α instead of e_β with $\sigma_c \to \sigma_c(\vec{x})$ time independent in the ground state (which means $\frac{\partial}{\partial t}$ is still diagonalized by going to p_0).

$\Rightarrow$ solve $\boxed{\left(-\frac{\nabla^2}{2m} + C_0\sigma(\vec{x})\right)\varphi_\alpha(\vec{x}) = \epsilon_\alpha \varphi_\alpha(\vec{x})}$

for all $\epsilon_\alpha < \epsilon_F$ (just count them until N states!)

Then $\boxed{-\frac{\Gamma_{Lo}[\sigma_c]}{T} = \sum_\alpha^{\epsilon_F} \epsilon_\alpha - \frac{1}{2}C_0 \int d^3x (\sigma_c(\vec{x}))^2}$

We need $\frac{\delta \epsilon_\alpha}{\delta \sigma_c(\vec{x})} = \frac{\delta}{\delta \sigma_c(\vec{x})} \int d^3y\, \varphi_\alpha^\dagger(\vec{y})\left(-\frac{\nabla^2}{2m} + C_0\sigma(y)\right)\varphi_\alpha(\vec{y})$

$= C_0 \varphi_\alpha^\dagger(\vec{x})\varphi_\alpha(\vec{x})$ [Why not $\frac{\delta \varphi_\alpha(\vec{y})}{\delta \sigma_c(\vec{x})}$ terms?]

$\Rightarrow \frac{-\delta \Gamma_{Lo}[\sigma_c]/T}{\delta \sigma_c(\vec{x})} = 0 = C_0 \sum_\alpha^{\epsilon_F} \varphi_\alpha^\dagger(\vec{x})\varphi_\alpha(\vec{x}) - C_0\sigma_c(\vec{x})$

or $\boxed{\sigma_c(\vec{x}) = \sum_\alpha^{\epsilon_F} \varphi_\alpha^\dagger(\vec{x})\varphi_\alpha(\vec{x}) = \rho(\vec{x})}$

Iteration plan:

1. guess $\sigma_c(\vec{x}) = \rho_{old}(\vec{x})$
2. plug into S-eqn and solve for $\{\epsilon_\alpha, \varphi_\alpha(\vec{x})\}$
3. Find $\rho_{new}(\vec{x}) = \sum_\alpha^{\epsilon_F} \varphi_\alpha^\dagger(\vec{x})\varphi_\alpha(\vec{x})$
4. repeat 2, 3 until $\rho(\vec{x})$ stops changing
5. evaluate E

Claim: We can make this procedure general with DFT!