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Density Functional Theory and Effective Field Theory

- The Skyrme approach to nuclei is very reminiscent of the Kohn-Sham DFT.
  - If we ignore the original derivation of the Skyrme energy functional in terms of the Skyrme "interaction", and concentrate instead on the functional itself, we can understand its success in describing nuclear ground states
  - Consider the functional as a local density plus gradient expansion of a DFT functional, just like those used in Coulomb problems.

- Unfortunately, we cannot at present validate the Skyrme functional by comparing it to an "ab initio" calculation of the energy per particle of nuclear matter.
  - "ab initio" in this case would mean in terms of two- and three-body (four-body?) potentials fit to NN and few-body scattering data.
  - We don't have the analog of a Coulomb potential, which can be derived (with well-defined corrections) from the underlying field theory QED. QCD is too hard (at present).
  - The difficulties in carrying out the ab initio program include technical difficulties in accurately solving the many-body problem and a limited knowledge of the many-body forces (three-body and higher).

- In the future, we might succeed in carrying out this program by using a chiral Lagrangian EFT to parametrize the low-energy NN and many-body forces.
  - There has been significant development along these lines in recent years.

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- To make the connection between EFT and DFT, we'll use the effective action formalism.
  - Argaman and Makov have established that DFT can be thought of in terms of Legendre transformations.
  - We have two things to figure out:
    - How to systematically carry out the Legendre transformation.
    - How to make the connection to Kohn-Sham orbitals.

- We can achieve both goal's for a short-ranged interaction following "Density Functional Theory for a Confined Fermi System with Short-Range Interaction," by Puglia, Bhattacharyya, and Furnstahl, nucl-th/0212071.
  - The system studied could be fermionic atoms in an optical trap $\Rightarrow$ harmonic confining potential.
  - The method is called the "inversion method."
  - See the paper for further references.

- We start with the short-range Lagrangian:

$$\boxed{\begin{aligned}\mathcal{L} = \psi^\dagger\left[i\frac{\partial}{\partial t} + \mu + \frac{\overrightarrow{\nabla}^2}{2m}\right]\psi - \frac{C_0}{2}(\psi^\dagger\psi)^2 + \frac{C_2}{16}\left[(\psi\psi)^\dagger(\psi\overleftrightarrow{\nabla}^2\psi) + h.c.\right] \\ + \frac{C_2'}{8}(\psi\overleftrightarrow{\nabla}\psi)^\dagger\cdot\psi\overleftrightarrow{\nabla}\psi + \ldots\end{aligned}}$$

with $\boxed{\overleftrightarrow{\nabla} = \overleftarrow{\nabla} - \overrightarrow{\nabla}}$

- Matching to the effective-range expansion determines C_0, C_2, C_2':

$$\boxed{C_0 = \frac{4\pi a_s}{m}} \quad \boxed{C_2 = C_0\frac{a_s r_s}{2}} \quad \boxed{C_2' = \frac{4\pi a_p^3}{m}}$$

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- We add an external potential: (note: it is time independent)

$$\boxed{\mathcal{L} \to \mathcal{L} - V(\vec{x})\psi^\dagger(x)\psi(x)}$$

which we will take for actual calculations to be an isotropic harmonic oscillator potential:

$$\boxed{V(\vec{x}) = \tfrac{1}{2} m\omega^2 |\vec{x}|^2}$$

- We write the generating functional with a source $J(x)$ coupled to the density operator $\psi^\dagger\psi$:

$$\boxed{Z[J] = e^{iW[J]} = \int \mathcal{D}\psi\,\mathcal{D}\psi^\dagger\; e^{i\int d^4x\,[\mathcal{L} + J(x)\psi^\dagger(x)\psi(x)]}}$$

Here x stands for $(\vec{x}, t)$, so the source is time-dependent in general.

- Note that we could absorb $V(\vec{x})$ into the definition of $J(x)$, since they both multiply $\psi^\dagger\psi$.
    - Since the original system we want corresponds to taking $J=0$, it is more convenient to leave them separate (otherwise we would be setting $J(x) = V(\vec{x})$ at the end).
    - $J(x)$ plays the role of an external magnetic field in our spin example. We want to find the ground state when it is set to zero.

- The density of the system while $J(x)$ is still on is

$$\boxed{\begin{aligned}\rho(x) \equiv \langle \psi^\dagger(x)\psi(x)\rangle_J &= \frac{\int \mathcal{D}\psi\,\mathcal{D}\psi^\dagger\,\psi^\dagger(x)\psi(x)\, e^{i\int d^4x'\,[\mathcal{L} + J(x')\psi^\dagger(x')\psi(x')]}}{Z[J]} \\ &= \frac{1}{iZ}\frac{\delta Z[J]}{\delta J(x)} = \frac{1}{i}\frac{\delta \ln Z[J]}{\delta J(x)} = \frac{\delta W[J]}{\delta J(x)}\end{aligned}}$$

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So now we do the Legendre transformation from $W[J]$ to $\Gamma[\rho]$:

$$\boxed{\Gamma[\rho] = W[J] - \int d^4x\, J(x)\, \rho(x)}$$

which ensures that $\Gamma[\rho]$ does not depend on $J(x)$. (I.e., $\delta\Gamma/\delta J(x) = 0$).

The idea in applying this equation is that we solve

$$\boxed{\frac{\delta W[J]}{\delta J(x)} = \rho(x)}$$

for $J(x)$ as a functional of $\rho(x)$, and substitute it above to construct $\Gamma[\rho]$. The possibility of inverting this relation uniquely is guaranteed by the same kind of physics that ensures us that we can solve for a chemical potential in terms of the number of particles. In particular, $W[J]$ is strictly concave.

- We can either use a chemical potential to enforce that

$$\boxed{\int \rho(x)\, d^3x = A}$$

is fixed, or else by hand make sure that this always holds. We'll do the latter by building $\rho(x)$ from A normalized wavefunctions - squared $\Rightarrow \rho(\vec{x}) = \sum_{i=1}^{A} |\varphi_i(\vec{x})|^2$ (see below).

- We will use time-independent sources from now on, which are appropriate for a ground states. It's possible we could miss the true ground state by neglecting these variations, but we'll check for them separately.

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- When we work with time-independent sources, every contribution to the effective action picks up an overall factor of the time interval over which the source acts, which we'll call T.
  - Just think of any diagram , which can only depend on time differences of the vertices, but we integrate over time everywhere. For N vertices, we can shift N-1 integrations to the time differences, leaving one free integration. For example:

$$\boxed{\begin{aligned}\int dt_1 \int dt_2\, f(t_1-t_2) &= \int dt_2 \int du_1\, f(u_1) \\ &= T \int du_1\, f(u_1)\end{aligned}} \quad \text{with } \boxed{u_1 = t_1 - t_2}$$

  and so on.
  - We'll divide out the T and identify the resulting energy functional:

$$\boxed{E[\rho] = -\Gamma[\rho]/T}$$

  (in the paper we also use $\Gamma[\rho] = -E[\rho]$). Note that we don't divide by the volume V here, as we have in the past, since we want the (finite) energy of a finite system, not the energy density of a uniform system.

- This energy functional is the ground-state energy when evaluated with the ground state density
  $\Rightarrow$ it is the Hohenberg-Kohn functional we are looking for.

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Let's check how this works out. Going back to

$$\boxed{\Gamma[\rho] = W[J] - \int d^4x\, J(x)\,\rho(x)},$$

we restrict ourselves to time independent sources and divide out T, defining $\boxed{\tilde{W}[J] \equiv W[J]/T}$

$$\Rightarrow \quad \boxed{E[\rho(\vec{x})] = -\tilde{W}[J(\vec{x})] + \int d^3y\, J(\vec{y})\,\rho(\vec{y})}$$

and $\boxed{\rho(\vec{x}) = \dfrac{\delta \tilde{W}[J]}{\delta J(\vec{x})}}$

Take $\dfrac{\delta}{\delta J(\vec{x})}$ of $E[\rho(\vec{x})]$:

$$\frac{\delta E[\rho(\vec{x})]}{\delta J(\vec{x})} = \int \left[\frac{\delta E[\rho]}{\delta \rho(\vec{y})}\frac{\delta \rho(\vec{y})}{\delta J(\vec{x})}\right] d^3y = \cancel{-\rho(\vec{x})} + \cancel{\rho(\vec{x})} + \int d^3y \left(\frac{\delta \rho(\vec{y})}{\delta J(\vec{x})}\right) J(\vec{y})$$

$$\Rightarrow \quad \boxed{\int d^3y \left(\frac{\delta E[\rho]}{\delta \rho(\vec{y})} - J(\vec{y})\right)\frac{\delta \rho(\vec{y})}{\delta J(\vec{x})} = 0}$$

But if $\delta\rho(\vec{y})/\delta J(\vec{x}) = 0$, that would mean we couldn't invert to find $J[\rho]$, so we must have instead that

$$\boxed{\frac{\delta E[\rho]}{\delta \rho(\vec{x})} = J(\vec{x})}$$

and since $J(\vec{x}) = 0$ is our original system, $E[\rho]$ is extremized for this ρ.

$\Rightarrow$ we have the second HK theorem.

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Now it is not immediately obvious that we can separate $E[\rho]$ into a piece independent of $v(\vec{x})$ and a universal piece, which is another claim of DFT.

- However, we can show the decomposition with a prudent change of variables.

Designate a $v(\vec{x}) \equiv 0$ version of $\tilde{W}[J]$ as $\tilde{W}_{v=0}$. Then since v and J appear in the combination $J-v$,

$$\boxed{\tilde{W}[J+v] = \tilde{W}_{v=0}[J]}$$

(that is, the $v(\vec{x})$ dependence is precisely cancelled) for any $J(\vec{x})$.

Call $J_\rho(\vec{x})$ the inversion of $\delta\tilde{W}/\delta J = \rho$ and $J^0_\rho(\vec{x})$ the inversion $\delta\tilde{W}_{v=0}/\delta J = \rho$ for the same density ρ. Then

$$\boxed{\frac{\delta\tilde{W}[J_\rho]}{\delta J(\vec{x})} = \rho(\vec{x}) = \frac{\delta\tilde{W}_{v=0}[J^0_\rho]}{\delta J(\vec{x})} = \frac{\delta\tilde{W}[J^0_\rho + v]}{\delta J(\vec{x})}}$$

or

$$\boxed{J_\rho(\vec{x}) = J^0_\rho(\vec{x}) + v(\vec{x})}$$

Thus we have

$$\boxed{\begin{aligned} E[\rho] &= -\tilde{W}[J_\rho] + \int d^3x\, J_\rho(\vec{x})\rho(\vec{x}) \\ &= \left[-\tilde{W}_{v=0}[J^0_\rho] + \int d^3x\, J^0_\rho(\vec{x})\rho(\vec{x})\right] + \int d^3x\, v(\vec{x})\rho(\vec{x}) \\ &= E_{v=0}[\rho] + \int d^3x\, v(\vec{x})\rho(\vec{x}) \end{aligned}}$$

which is the promised result!

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- Ok, so now we've got an expression, we still don't know how to use it. In particular, we don't know how to carry out the Legendre transformation and the inversion in particular.

- We're going to apply what is called the "inversion method" to an EFT expansion of our effective action.
  - We will call the expansion parameter λ generically. It could be $1/g$ in our "large N" expansion or $k_F a_s$ in our dilute expansion (λ actually just keeps track of the order — it is not really equal to $k_F a_s$, since k_F only appears at the end when we've evaluated the energy).

- So we write $\boxed{E = F[\rho, \lambda]}$

- This is important: The density $\rho(\vec{x})$ is an independent variable from λ; we can stick in any $\rho(\vec{x})$ we want.
- The special value of $\rho(\vec{x})$ in the exact ground state, which we'll call $\rho_g(\vec{x})$ will depend on λ through the extremization condition:

$$\boxed{\left.\frac{\delta E[\rho,\lambda]}{\delta\rho(\vec{x})}\right|_{\rho=\rho_g} = 0}$$

I.e., if λ is changed, a different $\rho_g(\vec{x})$ is needed to solve this equation.

- We define $E[\rho,\lambda]$ as before:

$$\boxed{E[\rho,\lambda] = -W[J,\lambda] + \int d^3x\, J(\vec{x})\rho(\vec{x})}$$

where $J(\vec{x})$ here is a functional of $\rho(\vec{x})$ and a function of λ,

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as dictated by

$$\boxed{\frac{\delta \tilde{W}[J,\lambda]}{\delta J(\vec{x})} = \rho(\vec{x})}$$

So as λ is changed, $J(\vec{x})$ must be adjusted so that the same $\rho(\vec{x})$ is obtained $\Rightarrow$ J depends on λ, in a nontrivial way.

- The basic idea of the inversion method is to expand everything in the $E[\rho,\lambda]$ equation in powers of λ, and then match equal powers.
  - The tricky part is that $J(\vec{x})$ [but NOT $\rho(\vec{x})$] depends on λ, so when we expand J, $\tilde{W}[J,\lambda]$ gets pretty complicated.

- We'll write

$$\boxed{\tilde{W}[J,\lambda] = \tilde{W}_0[J] + \tilde{W}_1[J] + \tilde{W}_2[J] + \ldots}$$

where the subscript indicates the (implicit) power of λ and $J(\vec{x})$ is any $J(\vec{x})$ as this stage.

- Similarly,

$$\boxed{E[\rho,\lambda] = E_0[\rho] + E_1[\rho] + E_2[\rho] + \ldots}$$

and

$$\boxed{J[\rho,\lambda] = J_0[\rho] + J_1[\rho] + \ldots}$$

Now we substitute and equate powers of λ. Remember that we are equating functionals of ρ.

- The zeroth order equation is

$$\boxed{E_0[\rho] = -\widetilde{W}_0[J_0] + \int d^3x\, J_0(\vec{x})\rho(\vec{x})}$$

The same sort of argument as before reveals

$$\boxed{\underbrace{\frac{\delta E_0[\rho]}{\delta\rho(\vec{x})} = \cancel{J_0(\vec{x})}}_{\text{From } \frac{\delta E[\rho]}{\delta\rho} = J(\vec{x}) \text{ to zeroth order}} = \int -\frac{\delta \widetilde{W}_0[J_0]}{\delta J_0(\vec{y})}\frac{\delta J_0(\vec{y})}{\delta\rho(\vec{x})}\, d^3y + \cancel{J_0(\vec{x})} + \int \rho(\vec{y})\frac{\delta J_0(\vec{y})}{\delta\rho(\vec{x})}\, d^3y}$$

or

$$\boxed{\int\left(\frac{\delta\widetilde{W}[J_0]}{\delta J_0(\vec{y})} - \rho(\vec{y})\right)\frac{\delta J_0(\vec{y})}{\delta\rho(\vec{x})}\, d^3y = 0}$$

which implies

$$\boxed{\rho(\vec{x}) = \frac{\delta \widetilde{W}_0[J_0]}{\delta J_0(\vec{x})}}$$

since $\delta J_0/\delta\rho \neq 0$ (convexity of $E_0[\rho]$).

Let's understand this equation: $\widetilde{W}_0$ describes the system with an external potential $v(\vec{x})$ and the source or potential $J_0(\vec{x})$, but is otherwise non-interacting (that is, only the kinetic energy in addition).

- Since $\widetilde{Z}_0$ is purely gaussian, the path integral can be done, yield a Tr Log for $\widetilde{W}_0$.
- When we plug in a $J(\vec{x})$ into $\widetilde{W}_0[J]$, that generates a $\rho(\vec{x})$ from $\delta\widetilde{W}_0[J]/\delta J(\vec{x})$.
- $J_0(\vec{x})$ is the particular function that generates $\rho(\vec{x})$.
- That such a function exists is the foundation of the Kohn-Sham approach to DFT.

In particular,

$$\boxed{\widetilde{W}[J_0] \propto \mathrm{Tr}\ln[(G^0_{ks})^{-1}]}$$

where $\boxed{G^0_{ks}(x,y) \equiv \left(i\frac{\partial}{\partial t} + \frac{\nabla^2}{2m} - V(\vec{x}) + J_0(\vec{x})\right)\delta^4(\vec{x}-\vec{y})}$

so that

$$\boxed{\left[i\partial/\partial t + \frac{\nabla^2}{2m} - V(\vec{x}) + J_0(\vec{x})\right] G^0_{ks}(\vec{x}t;\vec{x}'t') = \delta^3(\vec{x}-\vec{x}')\delta(t-t')}$$

We solve this the same way we did for the leading-order (LO) case of the large-N expansion with the auxiliary σ field:

- diagonalize $\partial/\partial t$ by going to frequency space.
- diagonalize the spatial part by introducing normalized single-particle orbitals satisfying

$$\boxed{\left(-\frac{\nabla^2}{2m} + V(\vec{x}) - J_0(\vec{x})\right)\varphi_i(\vec{x}) = \varepsilon_i\varphi_i(\vec{x})}$$

where i summarizes all the relevant quantum numbers and $\boxed{\int|\varphi_i(\vec{x})|^2 d\vec{x} = 1}$

- The subsequent discussion follows just as in the large-N LO discussion:

$$\boxed{\widetilde{W}_0[J_0] = -g\sum_{\varepsilon_i<\varepsilon_F}\varepsilon_i}$$

where ε_F is found by counting orbitals until the lowest A are filled (accounting for the spin degeneracy g.)

As before, $\boxed{\rho(\vec{x}) = \frac{\delta\widetilde{W}_0[J_0]}{\delta J_0(\vec{x})} = -g\sum_i^{\text{occ.}}\frac{\delta\varepsilon_i}{\delta J_0(\vec{x})} = g\sum_i^{\text{occ.}}\varphi_i^*(\vec{x})\varphi_i(\vec{x})}$

where the sum is over occupied ("occ.") states.

Thus the exact ground state density (when extremized) is given in terms of the

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orbitals of the Kohn-Sham non-interacting system.

- Substituting into the $E_0[\rho]$ expression, we find

$$\boxed{E_0[\rho] = g\sum_i \varepsilon_i + \int d^3x\, J_0(\vec{x})\,\rho(\vec{x})}$$

- If we introduce the kinetic energy functional $T_s[\rho]$ for the non interacting KS system,

$$\boxed{\begin{aligned} T_s[\rho] &= g\sum_i^{occ} \int d^3x\, \varphi_i^*(\vec{x})\left(\frac{-\nabla^2}{2m}\right)\varphi_i(\vec{x}) \\ &= g\sum_i^{occ} \varepsilon_i + \int \left(J_0(\vec{x}) - v(\vec{x})\right)\rho(\vec{x})\, d^3x \end{aligned}}$$

which gives an alternative expression for E_0:

$$\boxed{E_0[\rho] = T_s[\rho] + \int d^3x\, v(\vec{x})\,\rho(\vec{x})}$$

- Now if $E_0[\rho]$ were given as an explicit functional of ρ, then $J_0[\rho]$ would follow from a functional derivative wrt ρ. But that just takes us in circles with the current equations.
  - So at this point we have equations that looks like Kohn-Sham, but still no procedure to find $J_0(\vec{x})$.

- But we have all of the higher-order equations involving the $\{E_i[\rho], \tilde{W}_i[J], J_i[\rho]\}$ for $i \geq 1$.

- We know the diagrammatic expansion for $\tilde{W}_1[J]$, $\tilde{W}_2[J]$, and so on:

$\tilde{W}_1[J] \Rightarrow$  $\qquad \tilde{W}_2[J] \rightarrow$  $+$ 

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But the lines in this case are Green's functions in the presence of $V(\vec{x})$ and whatever $J(\vec{x})$ the $\tilde{W}_i$ are evaluated at. Let's check the leading order: (can you see where it comes from?)

$$\boxed{E_1[\rho] = -\tilde{W}_1[J_0] + \int J_1(\vec{x})\rho(\vec{x})\, d^3x - \int \frac{\delta \tilde{W}_0[J]}{\delta J(\vec{x})}\bigg|_{J=J_0(\vec{x})} J_1(\vec{x})\, d^3x}$$

which seems to require knowing $J_1(\vec{x})$ to find $E_1[\rho]$.

- But from before,

$$\boxed{\rho(\vec{x}) = \frac{\delta \tilde{W}_0[J]}{\delta J(\vec{x})}\bigg|_{J=J_0(\vec{x})}}$$

so the last two terms cancel, leaving

$$\boxed{E_1[\rho] = -\tilde{W}_1[J_0]}$$

Given $E_1[\rho]$, we can find $J_1(\vec{x})$ from

$$\boxed{\frac{\delta E[\rho]}{\delta \rho(\vec{x})} = J(\vec{x}) \xRightarrow{\text{each } i} \frac{\delta E_i[\rho]}{\delta \rho(\vec{x})} = J_i(\vec{x})}$$

since we simply match expansions of $E[\rho]$ and J.

So given $J_0(\vec{x})$, we can compute $\tilde{W}_0[J_0]$ and $\tilde{W}_1[J_0]$ using the Kohn-Sham Green's function for the lines:

$$\boxed{iG^0_{KS}(\vec{x}t, \vec{x}'t') = \sum_i \varphi_i(\vec{x})\varphi_i^*(\vec{x}')\, e^{-i\epsilon_i(t-t')}\left[\theta(t-t')\theta(\epsilon_i-\epsilon_F) - \theta(t'-t)\theta(\epsilon_F-\epsilon_i)\right]}$$

which yields 

$$\boxed{\tilde{W}_1[J_0] = \frac{1}{2} g(g-1) C_0 \int d^3x\, G^0_{KS}(x,x^+) G^0_{KS}(x,x^+) = -\frac{1}{2}\frac{(g-1)}{g} C_0 \int d^3x\, |\rho(\vec{x})|^2}$$

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or $$\boxed{E_1[\rho] = \frac{1}{2}\frac{g(g-1)}{g} C_0 \int d^3x\, |\rho(\vec{x})|^2}$$

- In this case, we can find $J_1(\vec{x})$ directly with a functional derivative w.r.t. $\rho(\vec{x})$.

- When we go to the next order, we find

$$\tilde{E}_2[\rho] = -\tilde{W}_2[J_0] + \int d^3x\, \cancel{J_2(\vec{x})}\rho(\vec{x}) - \int d^3x \frac{\delta \tilde{W}_0[J_0]}{\delta J_0(\vec{x})} \cancel{J_2(\vec{x})}$$
$$- \int d^3x \frac{\delta \tilde{W}_1[J_0]}{\delta J_0(\vec{x})} J_1(\vec{x}) - \frac{1}{2}\int d^3x\, d^3y \frac{\delta^2 \tilde{W}_0[J_0]}{\delta J_0(\vec{x})\,\delta J_0(\vec{y})} J_1(\vec{x}) J_1(\vec{y})$$

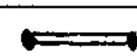
- The cancellation of the 2nd and 3rd terms continues to all orders, and ensures that we never need J_i to calculate E_i for any i. (We just need J_k for $k<i$.)

- We can replace $J_1(\vec{x})$ with

$$\boxed{J_1(\vec{x}) = \frac{\delta E_1[\rho]}{\delta \rho(\vec{x})} = \int d^3y \frac{\delta E_1}{\delta J_0(\vec{y})} \frac{\delta J_0(\vec{y})}{\delta \rho(\vec{x})} = -\int d^3y\, D^{-1}(\vec{x},\vec{y}) \frac{\delta \tilde{W}_1[J_0]}{\delta J_0(\vec{y})}}$$

where the "density-density" inverse correlator is

$$\boxed{D^{-1}(\vec{x},\vec{y}) \equiv \frac{\delta J_0(\vec{y})}{\delta \rho(\vec{x})} = -\left(\frac{\delta^2 \tilde{W}_0[J_0]}{\delta J_0(\vec{x})\,\delta J_0(\vec{y})}\right)}$$


D^{-1}

which means E_2 simplifies to

$$\boxed{\tilde{E}_2[\rho] = -\tilde{W}_2[J_0] - \frac{1}{2}\int d^3x\, d^3y \frac{\delta \tilde{W}_1[J_0]}{\delta J_0(\vec{x})} D^{-1}(\vec{x},\vec{y}) \frac{\delta \tilde{W}_1[J_0]}{\delta J_0(\vec{y})}}$$

$\Rightarrow$ $\tilde{E}_2[\rho] =$  $+$  $+$ 

$=$ 

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- We find a cancellation between the anomalous and extra diagrams. This continues for two more orders.
  - We can devise a set of Feynman rules involving the new piece , but this is just a detail.

- The appearance of D^{-1} is consistent with the general formalism of effective actions for local fields and non-local composite fields.
  - For local fields, the Legendre transformation removes one-particle intermediate states, leaving one-particle-irreducible diagrams.
  - For non-local composite fields [Cornwall-Jackiw-Tomboulis], the Legendre transformation removes two-particle intermediate states
  - So here the role of D^{-1} is to remove intermediate states propagating between (ψ^4)'s.

- Finally, we can find $J_0(\vec{x})$ by returning to:

$$\boxed{\begin{aligned} \left.\frac{\delta E[\rho,J]}{\delta\rho(\vec{x})}\right|_{\rho=\rho_g(\vec{x})} &= 0 \\ &= \left.\frac{\delta\left(E_0[\rho]+E_1[\rho]+E_2[\rho]+\dots\right)}{\delta\rho(\vec{x})}\right|_{\rho=\rho_g} \\ &= J_0(\vec{x}) + \left.\frac{\delta E_{int}[\rho]}{\delta\rho(\vec{x})}\right|_{\rho=\rho_g} \end{aligned}}$$

where the interaction energy is

$$\boxed{E_{int}[\rho] \equiv \sum_{i=1}^{\infty} E_i[\rho]}$$

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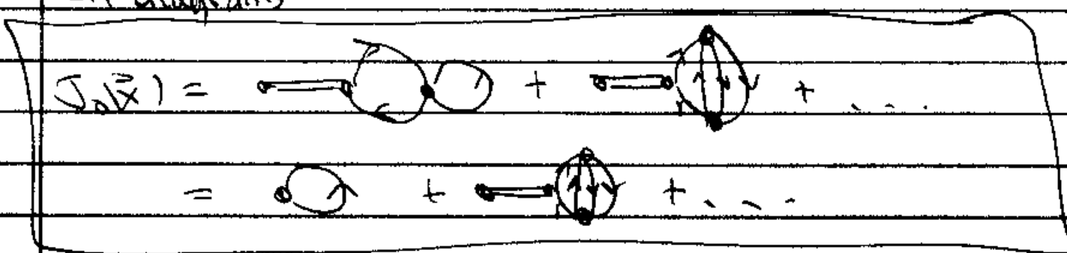
Thus, $$\boxed{J_0(\vec{x})\Big|_{\rho=\rho_g} = -\frac{\delta E_{int}[\rho]}{\delta\rho(\vec{x})}\Big|_{\rho=\rho_g} = \int D^{-1}(\vec{x},\vec{x}')\,\frac{\delta E_{int}[\rho]}{\delta J_0(\vec{x}')}\Big|_{\rho=\rho_g}}$$

In diagrams:



Here's the plan:

1. choose an approximation to $E_{int}[\rho]$ by truncating at some order in λ.
2. Make a guess for the Kohn-Sham potential $J_0(\vec{x})$
3. Calculate $E_{int}[\rho]$ starting from J_0. (find φ_i and ϵ_i)
4. Use the above equation to find a new $J_0(\vec{x})$
5. Repeat 3 and 4 until self-consistent.

- This procedure simplifies tremendously in the local density approximation, where

$$\boxed{E_{int}^{LDA}[\rho] = E_H[\rho(\vec{x})] + E_{xc}^{LDA}[\rho(\vec{x})]}$$

with

$$\boxed{E_{xc}^{LDA}[\rho(\vec{x})] \equiv \int d^3x\ \mathcal{E}_{2+}(\rho_0)\Big|_{\rho_0\to\rho(\vec{x})}}$$

Here $\mathcal{E}_{2+}$ is the energy density from the beach ball and higher diagrams, calculated at constant "local" density.

- See the paper for explicit expressions.

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The Kohn-Sham procedure is applied in the paper to fermionic atoms in a harmonic trap.

- We assume closed shells, which implies the densities and potentials will be purely radial.
- The iteration procedure is:

1. guess an initial density profile $\rho(r)$. Here the noninteracting density for A particles is fine.
2. Evaluate the local single-particle potential

$$\boxed{V_s[\rho(r)] \equiv V_s(r) \equiv V(r) - J_0(r)}$$

where $V(r)$ is the harmonic oscillator potential and to NNLO,

$$\boxed{\begin{aligned} J_0(\vec{x}) &= \frac{\delta}{\delta\rho(\vec{x})}\left[E_1[\rho] + E_{xc}^{LDA}[\rho]\right] \\ &= -\frac{(g-1)}{g}\frac{4\pi a_s}{m}\rho(\vec{x}) - \frac{7}{3}b_1\frac{a_s^2}{2m}(\rho(\vec{x}))^{4/3} - \frac{8}{3}(b_2 a_s^2 r_s + b_3 a_p^3 + b_4 a_s^3) \\ &\quad \times \frac{1}{2m}[\rho(\vec{x})]^{5/3} \end{aligned}}$$

(see the paper for b_1, b_2, b_3, b_4).

3. Solve the S-equation for the lowest A states:

$$\boxed{\left(-\frac{\nabla^2}{2m} + V_s(r)\right)\varphi_\alpha(\vec{x}) = \epsilon_\alpha \varphi_\alpha(\vec{x})}$$

4. Compute a new density: $\rho(r) = \sum_{\alpha=1}^{A} |\varphi_\alpha(\vec{x})|^2$
5. Repeat 2-4 until things (energy, ρ at selected points) stop changing (or changes are less than a tolerance) $\Rightarrow$ "self-consistency".

- See the figures in the paper for results!