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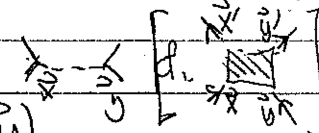
Friday 8805 Class

more general (non-local)

Recap the general Hartree-Fock (HF) discussion

- Restricted (for now) to local $\hat{V} \Rightarrow V(\vec{x},\vec{y})$



  - Translationally invariant means $V(\vec{x},\vec{y}) = V(\vec{x}-\vec{y})$
- Limited variational calculation $\Rightarrow$ trial wave function is the best Slater determinant from your choice of A single-particle wavefunctions $\{\phi_i(\vec{x})\}$, $i = 1,\ldots,A$ where i = complete set of quantum #'s
  - Piazza: Why do ϕ_i and ϕ_j have to be different for $i \neq j$? like $\{n l j m_j m_t\}$ or $\{\vec{k}, m_s, m_t\}$
  - Generally think of $\vec{x} \equiv \{\vec{r},\sigma,\tau\} \Rightarrow \int d\vec{x} \Rightarrow \sum_\alpha \sum_\beta \int d^3 r \rightarrow$ ← matrix indices

    as all the coordinates in a representation

    so we can have $V(\vec{x},\vec{y}) = \dfrac{g^2}{4\pi} \dfrac{e^{-m_\pi|\vec{r}_x-\vec{r}_y|}}{|\vec{r}_x-\vec{r}_y|}(\vec{\sigma}_1\cdot\vec{\sigma}_2)(\vec{\tau}_1\cdot\vec{\tau}_2)$ ← matrix indices for both

Non-local: $\vec{r}_x, \vec{r}_{x'}$ and $\vec{r}_y, \vec{r}_{y'}$

- So $|\Psi_{HF}\rangle = \det\{\phi_i(\vec{x}),\ i = 1\cdots A\}$ ⇐ antisymmetric product wave function
  - Question: What if we just used $\phi_1(\vec{x}_1)\cdot\phi_2(\vec{x}_2)\,\phi_3(\vec{x}_3)\cdots\phi_A(\vec{x}_A)$ without antisymmetrizing? Is this a variational calculation? (Note: we violate the principle of anti-symmetry, don't we? Does this make it unphysical?)

Historical: what do the terms first quantized and second quantized mean? Are they good names?

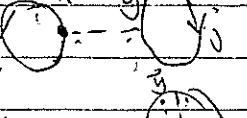
- Take $\hat{H} = \sum_{i=1}^{A} \hat{T}(\vec{x}_i) + \frac{1}{2}\sum_{i,j=1}^{A} \hat{V}(\vec{x}_i,\vec{x}_j)$ in 1st quantized form

Then (see section 8 notes)

$$\langle \Psi_{HF}|\hat{H}|\Psi_{HF}\rangle = \sum_{i=1}^{A} \frac{1}{2m}\int d\vec{x}\, \nabla\phi_i^* \cdot \nabla\phi_i$$

from Ring + Schuck notation

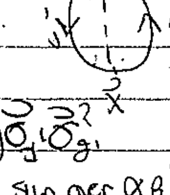
H: $\displaystyle + \frac{1}{2}\sum_{i,j=1}^{A} \int d\vec{x} \int d\vec{y}\ |\phi_i(\vec{x})|^2\, V(\vec{x},\vec{y})\, |\phi_j(\vec{y})|^2$



definite i,j from integral

(no contraction of indices)

F: $\displaystyle -\frac{1}{2}\int d^3x \int d^3y\ \underbrace{\sum_{i=1}^{A} \phi_i^*(\vec{x})\,\phi_i(\vec{y})}_{\rho(\vec{x},\vec{y})}\, V(\vec{x},\vec{y})\, \underbrace{\sum_{j=1}^{A} \phi_j^*(\vec{y})\,\phi_j(\vec{x})}_{\rho(\vec{y},\vec{x})}$



What would these look like in detail if $V(\vec{x},\vec{y}) \Rightarrow V(\vec{r}_x,\vec{r}_y)\vec{\sigma}_1\cdot\vec{\sigma}_2$?

H: $\int d^3r_x \int d^3r_y\, [\phi_i^*(\vec{r}_x)]_\alpha (\sigma_1^a)_{\alpha\beta} [\phi_i(\vec{r}_x)]_\beta\, V(\vec{r}_x,\vec{r}_y)\, \phi_j^*(\vec{r}_y)_\gamma (\sigma_2^a)_{\gamma\delta}\, \phi_j(\vec{r}_y)_\delta$ with implied sum over $\alpha,\beta,\gamma,\delta$

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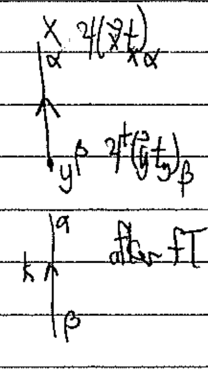
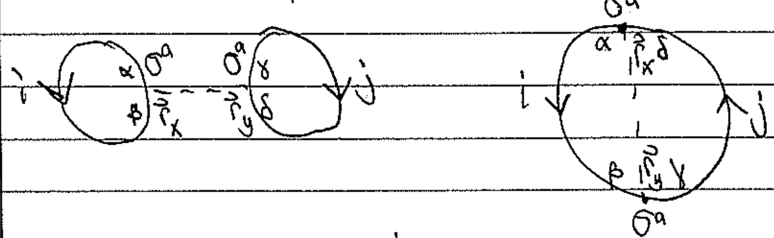
The Fock term is (note that the "1" and "2" go away) later: propagators or Green's functions

$$\int d^3r_x \int d^3r_y\, \phi^*_i(\vec r_x)_\alpha\, \sigma^a_{\alpha\delta}\, \phi_j(\vec r_x)_\delta\, V(\vec r_x, \vec r_y)\, \phi^*_j(\vec r_y)_\gamma\, \sigma^a_{\gamma\beta}\, \phi_j(\vec r_y)_\beta$$



Check the correspondence to the Feynman diagrams:



· The i and j label lines: ↑i

Piazza: · Is there an issue with anti commuting? ⇒ e.g., uncertain minus signs?

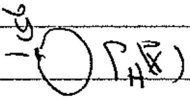
· The Lagrangian version would be $(\psi^\dagger\sigma^a\psi)(\psi^\dagger\sigma^a\psi)$, which is much closer to the diagram. (in Ring and Schuck's version, the contractions are in $\vec x, \vec y$)

- But check minus sign overall!

· Then $\dfrac{\delta}{\delta\phi^*_i(\vec x)}\left(\langle\Psi_{HF}|\hat H|\Psi_{HF}\rangle - \sum_{j=1}^{A}\varepsilon_j \int d\vec y\, |\phi_j(\vec y)|^2\right) = 0$

$$\Rightarrow \left[-\frac{\nabla^2}{2m} + \Gamma_H(\vec x)\right]\phi_i(\vec x) + \int d\vec y\, \Gamma_F(\vec x, \vec y)\, \phi_i(\vec y) = \varepsilon_i \phi_i(\vec x)$$

$$\Gamma_H(\vec x) = \int d\vec y\, V(\vec x, \vec y) \sum_{j=1}^{A} |\phi_j(\vec y)|^2$$



$$\Gamma_F(\vec x, \vec y) = -V(\vec x, \vec y) \sum_{j=1}^{A} \phi^*_j(\vec y)\, \phi_j(\vec x)$$

Some physics comments:

· In $|\Psi_{HF}\rangle$, each of the A particles occupies a definite single-particle state (up to antisymmetry from identical particles)

⇒ each particle moves in a single-particle potential that comes from its average interaction with all other particles, accounting for identical particles.

· Must be solved self-consistently

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'Self-consistency solution procedure':

1. Start the cycle. Suppose we have guesses for the A wf's $\phi_i(\vec{x})$ [e.g. harmonic oscillator lowest energies]. Alternative would be to guess Γ_H and Γ_F.

2. Calculate $\Gamma_H(\vec{x})$ and $\Gamma_F(\vec{x},\vec{y})$ by substitution.

3. Solve integro-diff. eq. for the lowest A $\phi_i(\vec{x})$'s and ε_i's.

4. Check how much the ε_i's have changed. If change is within a specified tolerance, go to 5. If not, go to 2.

Questions: (for Piazza)

- Does this always converge? How can we accelerate convergence?
- Step 3 and lowest sounds potentially problematic, (open shell?, changed occ.)
- What if the occupancy is not either 0 or 1 for each state i in a particular iteration?
- What if you did this at finite temperature with a chemical potential?

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Let's try the uniform system with local $V(\vec{x},\vec{y}) = C_0\,\delta^3(\vec{x}-\vec{y})$

For step 1, let's guess $\phi_i(\vec{x}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}_i\cdot\vec{x}}\,\eta_\alpha$ where $\vec{k}_i$ are the discrete momentum levels and α is the spin coordinate $\eta = \begin{pmatrix}1\\0\end{pmatrix}$ or $\begin{pmatrix}0\\1\end{pmatrix}$ so if $\alpha = 1,2$ then $\eta = \begin{pmatrix}1\\0\end{pmatrix}$ mean $\eta_{\alpha=1} = 1$, $\eta_{\alpha=2} = 0$

Take A lowest k_i^2's.

$$\Rightarrow \Gamma_H(\vec{x}) = \int d^3y\, C_0\,\delta^3(\vec{x}-\vec{y}) \sum_{j=1}^{A} |\phi_j(\vec{y})|^2$$

$$= \underbrace{C_0 \frac{1}{\Omega}\cdot \frac{\Omega}{(2\pi)^3}\int^{k_F} d^3k \cdot \nu}_{\rho \;\leftarrow\; \text{independent of } \vec{x}} \quad \leftarrow \text{from } \eta^\dagger_\alpha \eta_\alpha = \nu$$

What if $V(\vec{x}-\vec{y})$ unspecified? (but spin independent)

$$\Gamma_H(\vec{x}) = \int d^3y\, V(\vec{x}-\vec{y}) \sum_{j=1}^{A} |\phi_j(\vec{y})|^2 = \int d^3y\, V(\vec{x}-\vec{y})\cdot \rho \quad \leftarrow \text{still independent of } \vec{x}$$

What is $\int d^3y\, V(\vec{x}-\vec{y})$? Any volume integral can be thought of as a Fourier transform with $\vec{k}=0$.

- First switch to $\vec{y}' = \vec{y}-\vec{x}$ and use $V(-\vec{y}') = V(\vec{y}')$
  [or use $\vec{y}' = \vec{x}-\vec{y}$ and $\int d^3y = \int d^3y'$ after variable interchange

$$\Rightarrow \int d^3y\, V(\vec{x}-\vec{y}) = \int d^3y'\, V(\vec{y}') = \int d^3y'\, V(\vec{y}')\, e^{-i\vec{k}\cdot\vec{y}'}\Big|_{\vec{k}=0} = \tilde{V}(0)$$

$$\Rightarrow \Gamma_H(\vec{x})_{\alpha\beta} = \rho\,\tilde{V}(0)\,\delta_{\alpha\beta} \Rightarrow C_0\,\rho \text{ in our case of contact interaction}$$

$\Rightarrow$ spatial constant in S-eqn

$$\Gamma_F(\vec{x},\vec{y})_{\alpha\beta} = -V(\vec{x}-\vec{y})\,\delta_{\alpha\beta}\,\frac{1}{\Omega}\frac{\Omega}{(2\pi)^3}\int^{k_F} d^3k\, e^{i\vec{k}\cdot(\vec{x}-\vec{y})}$$

$$\Rightarrow \int d^3y\, \Gamma_F(\vec{x},\vec{y})_{\alpha\beta}\,\phi_i(\vec{y})_\alpha = -\int^{k_F} \frac{d^3k'}{(2\pi)^3} \int d^3y\, V(\vec{x}-\vec{y})\, e^{i\vec{k}'\cdot(\vec{x}-\vec{y})}\, \frac{1}{\sqrt{\Omega}} e^{i\vec{k}_i\cdot\vec{y}}\,\delta_{\alpha\beta}\,\eta_\alpha$$

$$\underset{\vec{y}'=\vec{x}-\vec{y}}{=} -\int^{k_F} \frac{d^3k'}{(2\pi)^3} \underbrace{\int d^3y'\, V(\vec{y}')\, e^{i\vec{k}'\cdot\vec{y}'}\, e^{-i\vec{k}_i\cdot\vec{y}'}}_{\tilde{V}(\vec{k}-\vec{k}')}\, \underbrace{\frac{1}{\sqrt{\Omega}} e^{i\vec{k}_i\cdot\vec{x}}\,\eta_\beta}_{\phi_i(\vec{x}) \text{ again}}$$

$\Rightarrow$ Is a solution with $\epsilon_k = \frac{k^2}{2m} + \rho\,\tilde{V}(0) - \int^{k_F} \frac{d^3k'}{(2\pi)^3}\,\tilde{V}(\vec{k}-\vec{k}')$

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Check $\langle \Psi_{HF} | \hat{H} | \Psi_{HF} \rangle$ for uniform system with local $V(\vec{x},\vec{y}) = C_0 \delta^3(\vec{x}-\vec{y})$

$$\Rightarrow \phi_i(\vec{x}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}_i\cdot\vec{x}} \eta_\alpha$$

Kinetic: $\sum_{i=1}^{N} \frac{1}{2m} \int d^3x \, \nabla\phi_i^* \cdot \nabla\phi_i$

$$\Rightarrow E^{(0)} = \nu \sum_{\vec{k}}^{k_F} \frac{1}{2m} \int d^3x \frac{1}{\Omega} (-i\vec{k}\cdot i\vec{k}) e^{-i\vec{k}\cdot\vec{x}} e^{i\vec{k}\cdot\vec{x}} \cancel{\eta^\dagger\eta}$$

$$= \frac{\nu}{\Omega} \int^{k_F} \frac{d^3k}{(2\pi)^3} \frac{k^2}{2m} \int d^3x \cancel{\frac{1}{\Omega}} \cdot 1 = \frac{3}{5} \frac{k_F^2}{2m} \rho \quad \checkmark$$

direct $\frac{1}{2} \sum_{i,j=1}^{N} \int d^3x \int d^3y \, |\phi_i(\vec{x})|^2 \underbrace{V(\vec{x},\vec{y})}_{C_0\delta^3(\vec{x}-\vec{y})} |\phi_j(\vec{y})|^2$

$$\longrightarrow \frac{C_0}{2} \left(\nu \sum_{\vec{k}}^{k_F} 1\right)\left(\nu \sum_{\vec{k}} 1\right) \underbrace{\int d^3x \frac{1}{\Omega}\frac{1}{\Omega}}_{\frac{1}{\Omega}} = \frac{C_0}{2}\left(\frac{\nu}{\Omega}\sum_{\vec{k}}^{k_F}(1)\right)^2 = \frac{C_0}{2}\rho^2 \quad \checkmark$$

exchange $(-)\frac{1}{2} \sum_{i,j=1}^{N} \int d^3x \int d^3y \, \phi_i^*(\vec{x}) \phi_i(\vec{y}) \underbrace{V(\vec{x},\vec{y})}_{C_0\delta^3(\vec{x}-\vec{y})} \phi_j^*(\vec{y}) \phi_j(\vec{x})$

spin contractions are now different $\quad \delta_{\alpha\beta}\delta_{\beta\alpha} = \nu$

$$\longrightarrow -\frac{C_0}{2}\frac{1}{\nu}\left(\frac{\nu}{\Omega}\sum_{\vec{k}}^{k_F}(1)\right)^2 = -\frac{C_0}{2}\frac{1}{\nu}\rho^2 \quad \checkmark$$

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$\Rightarrow$ The plane wave guess is already the self-consistent result, with ϵ_k^0

For $V(\vec{x}-\vec{y}) = C_0\,\delta^3(\vec{x}-\vec{y})$, $\epsilon_k = \frac{k^2}{2m} + \rho\left(1-\frac{1}{\gamma}\right)C_0$

and $\langle \Psi_{HF}|\hat{H}|\Psi_{HF}\rangle = \frac{3}{5}\frac{k_F^2}{2m}\rho + \frac{C_0}{2}\left(1-\frac{1}{\gamma}\right)\rho^2$

$$\stackrel{?}{=} V\sum_k^{k_F} \epsilon_k \ ?$$

No, double counting of potential $\Rightarrow$ subtract $\frac{1}{2}\langle V\rangle$