Chapter 4 : FERMI SYSTEMS

10. THE HARTREE-FOCK APPROXIMATION

This method was first developed to describe many-electron atoms.

It is also applied in nuclear physics, for nuclear structure calculations.

A related topic : TDHF

nuclei. Hence a natural approach is to retain the single-particle picture and assume that *each particle moves in a single-particle potential that comes from its average interaction with all of the other particles.* The single-particle energy should then be the unperturbed energy plus the potential energy of interaction averaged over the states occupied by all of the other particles. This is the result

Consider N particles with the Hamiltonian

$$\hat{H}_0 = \int d^3x \; \hat{\psi}^\dagger_\alpha(\vec{x}) \underbrace{\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{x}) \right]}_{h_0} \hat{\psi}_\alpha(\vec{x})$$

$$\hat{H}_1 = \frac{1}{2}\int d^3x \, d^3x' \; \hat{\psi}^\dagger_\alpha(\vec{x})\, \hat{\psi}^\dagger_\beta(\vec{x}')\, V(\vec{x}-\vec{x}')\, \hat{\psi}_\beta(\vec{x}')\, \hat{\psi}_\alpha(\vec{x})$$

describes a spin independent 2 particle potential

$$V(\vec{x},\vec{x}')_{\lambda\lambda',\mu\mu'} = V(\vec{x}-\vec{x}')\,\delta_{\lambda\lambda'}\,\delta_{\mu\mu'}$$

Because of U(**x**) we do not have translation invariance. So, we cannot expand in momentum eigenfunctions $e^{i\mathbf{k}\cdot\mathbf{x}}$ (at least not easily). But we can expand in the eigenfunctions of h_0.

Assume these eigenfunctions are known:

$$h_0 \phi_j(\vec{x}) = \frac{-\hbar^2}{2m} \nabla^2 \phi_j + U(\vec{x}) \phi_j = \epsilon_j^0 \phi_j(\vec{x})$$

Examples

▲ For atoms, $U(\mathbf{x}) = -Ze^2 / |\mathbf{r}|$ *(fundamental)* + a mean field from the other electrons *(approximate).*
i.e., each electron is attracted to the nucleus and repelled by the mean field.

The position of the nucleus breaks the translation invariance.

$\varphi^0_j(\mathbf{x})$ are hydrogenic states.modified by the mean field.

Then $V(\mathbf{x}-\mathbf{x}')$ is the repulsion of two electrons *(fundamental)* minus the mean field.

▲ For nuclei, $U(\mathbf{x})$ = a *"mean field potential"*; each nucleon moves in an effective mean field due to the other nucleons.

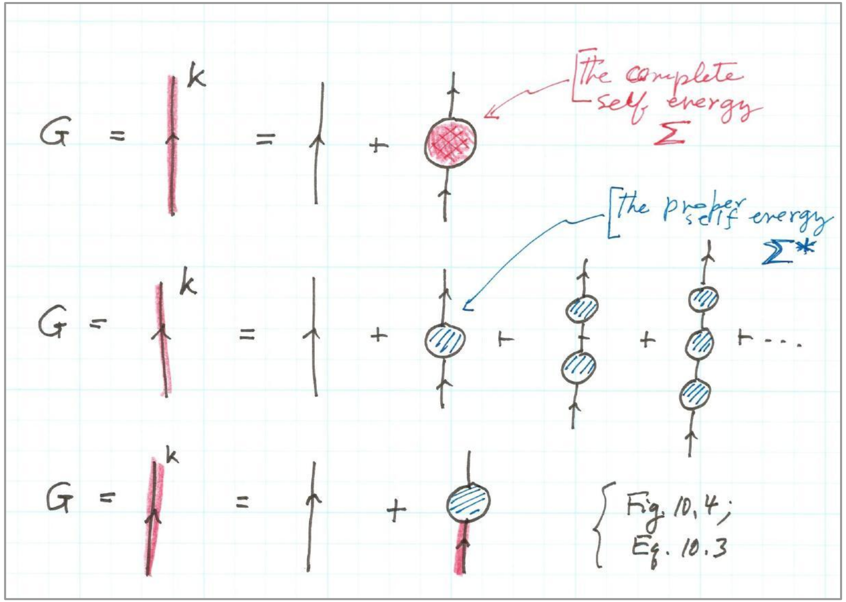
The center of mean field breaks the translation invariance.

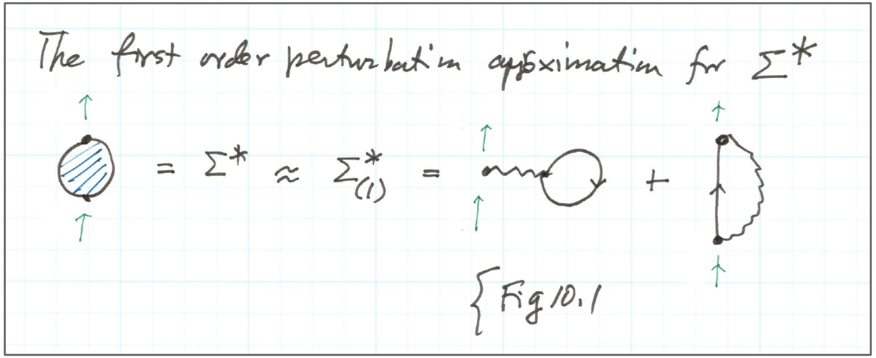
Then $V(\mathbf{x},\mathbf{x}') = V_{NN}(\mathbf{x}-\mathbf{x}') - U(\mathbf{x}) - U(\mathbf{x}')$

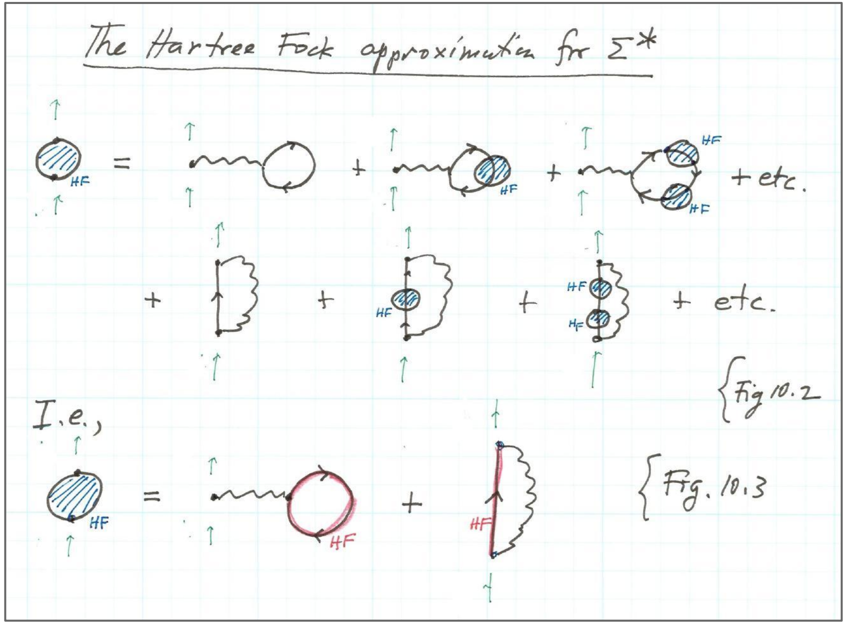
The idea is that the mean field describes the structure of nuclear states, in a first approximation; then treat
$V = V_{NN}$ – the mean field,
as a perturbation.

The Hamiltonian

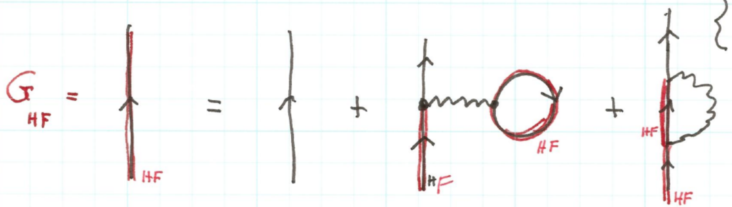
Diagrammatic analysis; Dyson's equation





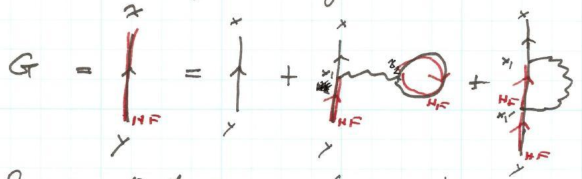


Dyson's equation for G in the H.F. approximation



{Fig. 10.5

So, we have, in diagrammatic form



In coordinate space (we can't use momentum space because the problem is not translation invariant)

$$G(xy) = G^0(xy) + \int d^4x_1\, d^4x_1'\, G^0(xx_1)\,\Sigma^*(x_1x_1')\,G(x_1'y)$$

where, calculated from Feynman rules, ← (HF approx, throughout)

$$\hbar\,\Sigma^*(x_1x_1') = -i\,\delta(t_1-t_1')$$

$$\Big\{ \delta^3(\vec{x}_1-\vec{x}_1')\cdot(2s+1)\cdot\int d^3x_2\, G(\vec{x}_2t_2;\vec{x}_2t_2^+)\,V(\vec{x}_1-\vec{x}_2)$$

$$- \quad V(\vec{x}_1-\vec{x}_1')\,G(\vec{x}_1t_1,\vec{x}_1'\,t_1^+)\Big\}$$

The Hamiltonian is independent of time --- that's translation invariance in time --- so we can Fourier expand in time and frequency.

Fourier transform in time and frequency

$$G(\vec{x}t;\vec{x}'t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \bar{G}(\vec{x}\vec{x}';\omega)$$

$$G^0(\vec{x}t;\vec{x}'t') = \int \frac{d\omega}{(2\pi)} e^{-i\omega(t-t')} \bar{G}^0(\vec{x}\vec{x}';\omega)$$

$$\Sigma^*(\vec{x}t,\vec{x}'t') = \Sigma^*(\vec{x},\vec{x}')\,\delta(t-t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \Sigma^*(\vec{x},\vec{x}')$$

$\Rightarrow$

$$\bar{G}(\vec{x}\vec{y};\omega) = \bar{G}^0(\vec{x}\vec{y};\omega) + \int d^3x_1\, d^3x_1'\, \bar{G}^0(\vec{x}\vec{x}_1;\omega)\,\bar{\Sigma}^*(\vec{x}_1,\vec{x}_1')\,\bar{G}(\vec{x}_1'y;\omega)$$

and

$$\hbar\bar{\Sigma}^*(\vec{x}_1\vec{x}_1') = -i(2s+1)\,\delta^3(\vec{x}_1-\vec{x}_1')\int d^3x_2\, V(\vec{x}_1-\vec{x}_2)\int d\omega\, e^{i\omega\eta}\,\bar{G}(\vec{x}_2,\vec{x}_2;\omega)$$
$$+\,iV(\vec{x}_1-\vec{x}_1')\int \frac{d\omega}{2\pi} e^{i\omega\eta}\,\bar{G}(\vec{x}_1\vec{x}_1';\omega) \qquad (\eta\to 0^+)$$

Also, we can expand in eigenfunctions of h_0.

Now expand in eigenfunctions of h_0

$$h_0\,\phi_j^0(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2\phi_j^0 + U(\vec{x})\phi_j^0 = \epsilon_j^0\,\phi_j^0(\vec{x})$$

$$\Rightarrow\quad G^0(\vec{x}t,\vec{x}'t') = \sum_j \phi_j^0(\vec{x})\,\phi_j^0(\vec{x}')^*\, e^{-i\epsilon_j^0(t-t')/\hbar}\left[\theta(t-t')\,\theta(\epsilon_j^0-\epsilon_F^0) - \theta(t'-t)\,\theta(\epsilon_F^0-\epsilon_j^0)\right]$$

where ϵ_F^0 = energy of the last filled state.

For the translation invariant case, $\phi_j^0(\vec{x}) = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{x}}$;
$\Rightarrow$ the momentum space G. F. $G^0(\vec{k},\omega)$ of chapter 3.

$$\bar{G}^0(\vec{x}\vec{x}';\omega) = \sum_j \phi_j^0(\vec{x})\,\phi_j^0(\vec{x}')^*\left[\frac{\theta(\epsilon_j^0-\epsilon_F^0)}{\omega-\epsilon_j^0/\hbar+i\eta} + \frac{\theta(\epsilon_F^0-\epsilon_j^0)}{\omega-\epsilon_j^0/\hbar-i\eta}\right]$$

Propagator and proper self energy

To Solve : $\bar{G} = \bar{G}^0 + \bar{G}^0 \bar{\Sigma}^* \bar{G}$

Let's try this form

(*)

$$\bar{G}(\vec{x}\vec{x}';\omega) = \sum_j \phi_j(\vec{x})\, \phi_j(\vec{x}')^* \left[\frac{\theta(\epsilon_j - \epsilon_F)}{\omega - \epsilon_j/\hbar + i\eta} + \frac{\theta(\epsilon_F - \epsilon_j)}{\omega - \epsilon_j/\hbar - i\eta} \right]$$

where $\{\phi_j(\vec{x})\}$ are a complete set of wave functions; with associated "energy" ϵ_j and $\epsilon_F =$ max occupied ϵ_j.

If it works then the equation for $\bar{G}$ will become an equation for ϕ_j and ϵ_j.

If it works then

$$\hbar\Sigma^*(\vec{x}_1,\vec{x}_1') = (2s+1)\,\delta^3(\vec{x}_1-\vec{x}_1')\int d^3x_2\, V(\vec{x}_1-\vec{x}_2) \sum_j |\phi_j(\vec{x}_2)|^2 \theta(\epsilon_F-\epsilon_j)$$
$$- V(\vec{x}_1-\vec{x}_1') \sum_j \phi_j(x_1)\, \phi_j(x_1')^* \theta(\epsilon_F-\epsilon_j)$$

$$= \delta^3(x_1-x_1')\int d^3x_2\, V(\vec{x}_1-\vec{x}_2)\, n(\vec{x}_2)$$
$$- V(\vec{x}_1-\vec{x}_1') \sum_j \phi_j(x_1)\, \phi_j(x_1')^* \theta(\epsilon_F-\epsilon_j)$$

NB $n(\vec{x}) = -i(2s+1)\int \frac{d\omega}{2\pi} e^{i\omega\eta} G(xx;\omega)$
$= (2s+1)\sum_j |\phi_j(x)|^2 \theta(\epsilon_F-\epsilon_j)$

Now we'll see that (*) works

$$G(xy;\omega) = G^0(xy;\omega) + G^0\Sigma^* G(xy;\omega)$$

Consider

$$(\hbar\omega - h_0)G^0(xy) = \sum_j (\hbar\omega - \hbar\omega_j^0)\, \phi_j(x)\phi_j^*(y) \left\{ \frac{\theta}{\omega-\omega_j^0} + \frac{\theta}{\omega-\omega_j^0} \right\}$$
$$= \hbar \sum_j \phi_j(x)\phi_j^*(y) = \hbar\,\delta^3(x-y)$$

Therefore

$$(\hbar\omega - h_0)\,G(xy) = \hbar\,\delta^3(x-y) + \hbar\Sigma^* G\,(xy)$$

- Now project onto $\phi_\ell(y)$; $\int \phi_\ell(y)\, d^3y$

Note $\int G(x,y)\,\phi_\ell(y)\,d^3y = \phi_\ell(x)\left\{ \frac{\theta(\hbar\omega_\ell - \epsilon_F)}{\omega-\omega_\ell + i\eta} + \frac{\theta(\epsilon_F - \hbar\omega_\ell)}{\omega-\omega_\ell - i\eta} \right\}$

Thus

$$(\hbar\omega - h_0)\,\phi_\ell(x)\left\{ \frac{\theta}{\omega-\omega_\ell} + \frac{\theta}{\omega-\omega_\ell} \right\} = \hbar\phi_\ell(x) + \hbar\Sigma^*\phi_\ell(x)\left\{ \frac{\theta}{\omega-\omega_\ell} + \frac{\theta}{\omega-\omega_\ell} \right\}$$

- Now multiply by $\omega - \omega_\ell$

$$(\hbar\omega - h_0)\,\phi_\ell(x) = \hbar(\omega-\omega_\ell)\,\phi_\ell + \hbar\Sigma^*\phi_\ell(x)$$

$$h_0\phi_\ell + \hbar\Sigma^*\phi_\ell = \hbar\omega_\ell\,\phi_\ell = \epsilon_\ell\,\phi_\ell \qquad \text{Q.E.D.}$$

The Hartree-Fock equation

$$\epsilon_\ell \phi_\ell(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2\phi_\ell + U(\vec{x})\phi_\ell + \underbrace{\int d^3y\; \hbar\Sigma^*(\vec{x},\vec{y})\,\phi_\ell(\vec{y})}_{\text{a "non local" interaction potential.}}$$

$$\hbar\Sigma^*(\vec{x},\vec{y}) = \delta^3(\vec{x}-\vec{y})\int d^3x_2\, V(\vec{x}_1-\vec{x}_2)\, n(\vec{x}_2) - V(\vec{x}-\vec{y})\sum_j \phi_j(\vec{x})\,\phi_j(\vec{y})^*\,\Theta(\epsilon_F-\epsilon_j)$$

$$\epsilon_\ell \phi_\ell(\vec{x}) = -\frac{\hbar^2}{2m}\nabla^2\phi_\ell + U(\vec{x})\phi_\ell(\vec{x}) + V_{direct}(\vec{x})\,\phi_\ell(\vec{x}) + \int V_{exchange}(\vec{x},\vec{y})\,\phi_\ell(\vec{y})\,d^3y$$

where

$$V_{direct}(\vec{x}) = \int d^3x_2\, V(\vec{x}-\vec{x}_2)\, n(\vec{x}_2) \qquad \text{local, non linear}$$

$$V_{exchange}(\vec{x},\vec{y}) = -V(\vec{x}-\vec{y})\sum_j \phi_j(\vec{x})\,\phi_j^*(\vec{y})\,\Theta(\epsilon_F-\epsilon_j)$$

non local, non linear.

The relation to the *translation invariant* many-particle problem

Exercise: If $U(\vec{x})=0$ then $\phi_j^0(\vec{x}) = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{x}}$.

Also, $\phi_j(\vec{x}) = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{x}}$ and

$$\epsilon_j = \frac{\hbar^2k^2}{2m} + \hbar\Sigma^*(\vec{k}) \quad \text{where}$$

$$\hbar\Sigma^*(\vec{k}) = n\hat{V}_0(\vec{q}=0) - \int\frac{d^3k'}{(2\pi)^3}\,\hat{V}_0(\vec{k}-\vec{k}')\,\Theta(k_F-|\vec{k}'|)$$

“The self-consistent expressions for a uniform medium are identical to the expressions evaluated in 1st order perturbation theory; eqs. (9.35) and (9.36).“ The reason is because the unperturbed (plane-wave) eigenfunctions are also the self-consistent ones, for a translation invariant system.