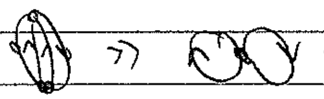
11/10/14

Monday 880S Class

linked on 880S page
2014_ect_3nf_carbone.pdf

- Finish up Hartree-Fock notes ⑧-⑪ from 11/3/14
  - pages ⑩ and ⑪ ⇒ ② and ③ here
  - then follow-up with Self Consistent Green's Function (SCGF) approach (slides + ③+)
- Does Hartree-Fock "work" (that is, is it a good initial approximation) for cold atoms in the unitary region?
  - For the uniform system $k_F a_s$ is the expansion parameter and corrections to HF go like powers of $k_F a_s$ ⇒ unitary region means $k_F a_s \gg 1$ ⇒ HF is poor approximation.

    Eg.  ← HF

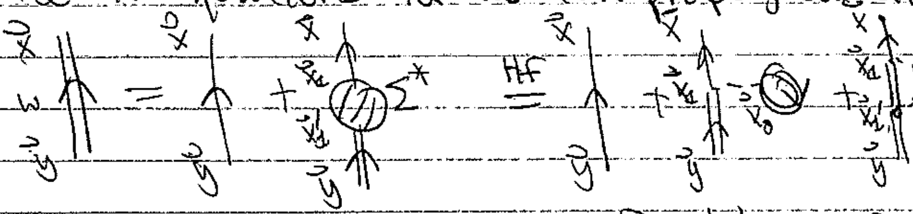
- For regular Coulomb atoms, HF is an excellent starting point, but not good enough for chemistry by itself.

- What about for nucleon-nucleon interactions?
  ⇒ it depends on the "resolution"
  - we'll do a survey of RG for NN interactions based on slides from the 2014 HUGS summer school, supplemented by notes. These slides are linked on the 880S home page.
    - look at lecture 4 for infinite matter
    - then lecture 1 for overview, lecture 2 for SRG details

11/10/14

Hartree-Fock recap . . .

The HF equations for the full propagator diagrammatically are:



or, in coordinate space as a function of frequency ω:

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

with
$$\boxed{\begin{aligned}\Sigma^*(\vec{x}_1,\vec{x}_1') = {} & -i\nu\,\delta^3(\vec{x}_1-\vec{x}_1')\int d^3x_2\, V(\vec{x}_1-\vec{x}_2)\int \frac{d\omega}{2\pi} e^{i\omega\eta}\, G(\vec{x}_2,\vec{x}_2,\omega) \\ & + iV(\vec{x}_1-\vec{x}_1')\int\frac{d\omega}{2\pi}e^{i\omega\eta}\, G(\vec{x}_1,\vec{x}_1',\omega)\end{aligned}}$$

Σ^* for HF is independent of frequency ω (because it has $\delta(t-t')$ time dependence) $\Rightarrow$ G will have the same structure as G^0 [why? Piazza]:

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

where we need to determine the single-particle wfs $\{\varphi_j(\vec{x})\}$ and energies ϵ_j.

- First: Σ^* looks like the HF potential

$$\boxed{\begin{aligned}\Sigma^*(\vec{x}_1,\vec{x}_1') &= \nu\,\delta^3(\vec{x}_1-\vec{x}_1')\int d^3x_2\, V(\vec{x}_1-\vec{x}_2)\sum_j|\varphi_j(\vec{x}_2)|^2\,\theta(\epsilon_F-\epsilon_j) \\ &\qquad - V(\vec{x}_1-\vec{x}_1')\sum_j\varphi_j(\vec{x}_1)\varphi_j^*(\vec{x}_1')\,\theta(\epsilon_F-\epsilon_j) \\ &= \delta^3(\vec{x}_1-\vec{x}_1')\int d^3x_2\, V(\vec{x}_1-\vec{x}_2)\,\rho(\vec{x}_2) - V(\vec{x}_1-\vec{x}_1')\sum_j\varphi_j(\vec{x}_1)\varphi_j^*(\vec{x}_1')\,\theta(\epsilon_F-\epsilon_j)\end{aligned}}$$

Now $G_0^{-1} = \omega - H_0 \Rightarrow \left(\omega + \frac{\nabla_1^2}{2m} - U(x_1)\right)\delta^3(\vec{x}_1-\vec{x}_1'')$

completeness

$$\int d^3x_1''\, G_0^{-1}(\vec{x}_1,\vec{x}_1'',\omega)\, G_0(\vec{x}_1'',\vec{x}_1',\omega) = \sum_j(\omega-\epsilon_j^0)\,\varphi_j^0(\vec{x}_1)\,\varphi_j^0(\vec{x}_1')^*\left[\frac{\theta(\epsilon_j^0-\epsilon_F^0)}{\omega-\epsilon_j^0+i\eta}+\frac{\theta(\epsilon_F^0-\epsilon_j^0)}{\omega-\epsilon_j^0-i\eta}\right] = \sum_j\varphi_j^0(\vec{x}_1)\,\varphi_j^0(\vec{x}_1')^* = \delta^3(\vec{x}_1-\vec{x}_1')$$

11/10/14

⇒ Hit the Dyson equation with G_0^{-1}. First schematically:

$$G_0^{-1}G = G_0^{-1}G_0 + G_0^{-1}G_0\Sigma^* G = 1 + \Sigma^* G$$

$$\Rightarrow \left[\omega - \left(\frac{-\nabla_1^2}{2m} + U(\vec{x}_1)\right)\right] G(\vec{x}_1, \vec{x}_1', \omega) = \delta^3(\vec{x}_1 - \vec{x}_1') + \int d^3x_2\, \Sigma^*(\vec{x}_1, \vec{x}_2) G(\vec{x}_2, \vec{x}_1', \omega)$$

Substitute the expansion for G and find (Piazza)

$$\boxed{\left[\frac{-\nabla_1^2}{2m} + U(\vec{x}_1)\right] \varphi_j(\vec{x}_1) + \int d^3x_2\, \Sigma^*(\vec{x}_1, \vec{x}_2)\varphi_j(\vec{x}_2) = \varepsilon_j \varphi_j(\vec{x}_1)}$$

which is the HF equation for φ_j.

[Check that if this works, then Dyson's equation is satisfied. If G has the correct BCs, what do we conclude?]

- So far we worked in coordinate space and derived an integro-differential equation that specified G^{HF}.
  - But more generally we will be in a single-particle basis, such as harmonic oscillators (or Hartree-Fock!)
  - We'll use $\alpha, \beta, \ldots$ to label the states (note that this includes any spin or isospin degrees of freedom as well — usually the spin will be coupled with orbital angular momentum).

The Hamiltonian is (following Carbone talk notation)

$$\hat{H} = \sum_\alpha \varepsilon_\alpha^0 a_\alpha^\dagger a_\alpha - \sum_{\alpha\beta} U_{\alpha\beta} a_\alpha^\dagger a_\beta + \frac{1}{4}\sum_{\substack{\alpha\gamma\\ \beta\delta}} V_{\alpha\gamma,\beta\delta}\, a_\alpha^\dagger a_\gamma^\dagger a_\delta a_\beta$$

← two body (antisymmetrized) potential

single particle energies; one-body potential

$$+ \frac{1}{36}\sum_{\substack{\alpha\gamma\epsilon\\ \beta\delta\eta}} W_{\alpha\gamma\epsilon,\beta\delta\eta}\, a_\alpha^\dagger a_\gamma^\dagger a_\epsilon^\dagger a_\eta a_\delta a_\beta$$

3-body (anti-symmetrized) potential

11/10/14

Now the (two-point) Green's function is [$G_{\alpha\beta} \equiv g_{\alpha\beta}$ in slides]

$$G_{\alpha\beta}(t,t') = \frac{1}{i}\langle \Psi_0^N | T[a_\alpha(t)\, a_\beta^\dagger(t')] | \Psi_0^N\rangle$$

where $|\Psi_0^N\rangle$ is the exact ground state with N particles (we'll use "N" instead of "A" here to match the slides)

$$T[a_\alpha(t)\, a_\beta^\dagger(t')] = \begin{cases} a_\alpha(t)\, a_\beta^\dagger(t') & t > t' \\ -a_\beta^\dagger(t')\, a_\alpha(t) & t < t' \end{cases}$$

and the Heisenberg operators are

$$\boxed{a_\alpha^\dagger(t) = e^{iHt} a_\alpha^\dagger e^{-iHt}} \quad \boxed{a_\alpha(t) = e^{iHt} c_\alpha e^{-iHt}}$$

so that

$$iG(\vec{x}t; \vec{x}'t') = \sum_{\alpha\beta} \varphi_\alpha(\vec{x})\, G_{\alpha\beta}(t,t')\, \varphi_\beta^*(\vec{x}')$$

(with implicit spin indices)

$\hat{H}|\Psi_n^{N'}\rangle = E_n^{N'}|\Psi_n^{N'}\rangle$ (also $\hat{N}|\Psi_n^{N'}\rangle = N'|\Psi_n^{N'}\rangle$)

Now insert complete sets of eigen-states $\sum_{n,N'} |\Psi_n^{N'}\rangle\langle\Psi_n^{N'}|$ in between the a_α and $a_\beta^\dagger$ operators.

$\Rightarrow$ only $N' = N+1$ and $N' = N-1$ survive (fill in steps on Piazza)

$$\Rightarrow G_{\alpha\beta}(t,t') = \frac{1}{i}\theta(t-t')\sum_m \langle\Psi_0^N|a_\alpha|\Psi_m^{N+1}\rangle\langle\Psi_m^{N+1}|a_\beta^\dagger|\Psi_0^N\rangle e^{-i(E_m^{N+1}-E_0^N)(t-t')}$$

$$-\frac{1}{i}\theta(t'-t)\sum_n \langle\Psi_0^N|a_\beta^\dagger|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|a_\alpha|\Psi_0^N\rangle e^{i(E_n^{N-1}-E_0^N)(t-t')}$$

$$= G_{\alpha\beta}(t-t')$$

$\Rightarrow$ we can Fourier transform from $t-t'$ to frequency ω. $\Rightarrow$ for any time-independent Hamiltonian.

11/10/14

$$\Rightarrow G_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} d(t-t')\, e^{i\omega(t-t')}\, G_{\alpha\beta}(t-t')$$

We can do this directly, or use

$$\theta(\pm(t-t')) = \mp \frac{1}{2\pi i}\int_{-\infty}^{\infty} d\omega\, \frac{e^{-i\omega(t-t')}}{\omega \pm i\eta} \qquad \text{where } \eta \to 0^+$$

The result is the Lehmann (or "spectral) representation:

$$\boxed{\begin{aligned} G_{\alpha\beta}(\omega) = &\sum_m \frac{\langle \Psi_0^N | a_\alpha | \Psi_m^{N+1}\rangle \langle \Psi_m^{N+1} | a_\beta^\dagger | \Psi_0^N \rangle}{\omega - (E_n^{N+1} - E_0^N) + i\eta} \quad \leftarrow \text{(quasi) particles} \\ &- \sum_n \frac{\langle \Psi_0^N | a_\beta^\dagger | \Psi_n^{N-1}\rangle \langle \Psi_n^{N-1} | a_\alpha | \Psi_0^N \rangle}{\omega - (E_0^N - E_k^{N-1}) - i\eta} \quad \leftarrow \text{(quasi) holes} \end{aligned}}$$

$\Rightarrow$ see slides 3-4 of Carbone talk.

The spectral function is the imaginary part of $G_{\alpha\beta}(\omega)$.

- Easy to extract because only i is in denominators

$$\Rightarrow \text{use } \frac{1}{x \pm i\eta} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x)$$

$$\Rightarrow S_{\alpha\beta}(\omega) \equiv S^p_{\alpha\beta}(\omega) + S^h_{\alpha\beta}(\omega)$$

where
$$S^p_{\alpha\beta}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G^p_{\alpha\beta}(\omega) = \sum_m \langle \Psi_0^N | a_\alpha | \Psi_m^{N+1}\rangle \langle \Psi_m^{N+1} | a_\beta^\dagger | \Psi_0^N \rangle \times \delta(\omega - (E_m^{N+1} - E_0^N))$$

is the (quasi) particle spectral function and

$$S^h_{\alpha\beta}(\omega) = +\frac{1}{\pi}\,\mathrm{Im}\, G^h_{\alpha\beta}(\omega) = \sum_n \langle \Psi_0^N | a_\beta^\dagger | \Psi_n^{N-1}\rangle \langle \Psi_n^{N-1} | a_\alpha | \Psi_0^N \rangle \times \delta(\omega - (E_0^N - E_n^{N-1}))$$

$G_{\alpha\beta}(\omega)$ can be reconstructed completely:

$$G_{\alpha\beta}(\omega) = \int d\omega' \frac{S^p_{\alpha\beta}(\omega')}{\omega - \omega' + i\eta} + \int d\omega' \frac{S^h_{\alpha\beta}(\omega')}{\omega - \omega' - i\eta}$$

[advanced and retarded have only $+i\eta$ or $-i\eta$, respectively]

11/10/14

· Now we can write Dyson's equation for $G_{\alpha\beta}(\omega)$, with a more general diagrammatic approximation to $\Sigma^*(\omega)$ [beyond HF, Σ^* depends on ω].

· Following the Carbone talk, Σ^* is formed from an approximation to the "vertex", which is a 4-pt function (two lines in, two lines out).
  - The self-consistency procedure is outlined on slides 4 to 8 of the Carbone talk for two body interactions.
  - The extension to 3-body forces is discussed in the rest of the talk.

· The energy follows from the "Koltun sum rule" (see slides 27-30).

· Solve the Dyson's equation by iteration (or possibly a more sophisticated method?)