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Monday 8805 Class

- Finish from 10/29/14 notes
  - 7 correspondence of model and full field theory (see Appendix A)
  - 8 Green's function
  - 9 finite range potential

- Nonperturbative expansions
  - Recap 6 from 10/29/14
  - 2 - 4 (11/3/14)
  - brief: auxiliary fields 5
- Euclidean vs. Minkowski space 6, 7

- Self-consistent Hartree-Fock at T=0 with real time propagators.
  - 8 - 11
  - Details via Piazza

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· Nonperturbative approximations

- We have diagrammatic expansions to calculate the ground state energy or finite temperature thermodynamic functions in perturbation theory
- What if pert. theory is inadequate?

· Here: Nonperturbative "conserving approximation" that sum infinite classes of diagrams. [Also called "phi-derivable"]

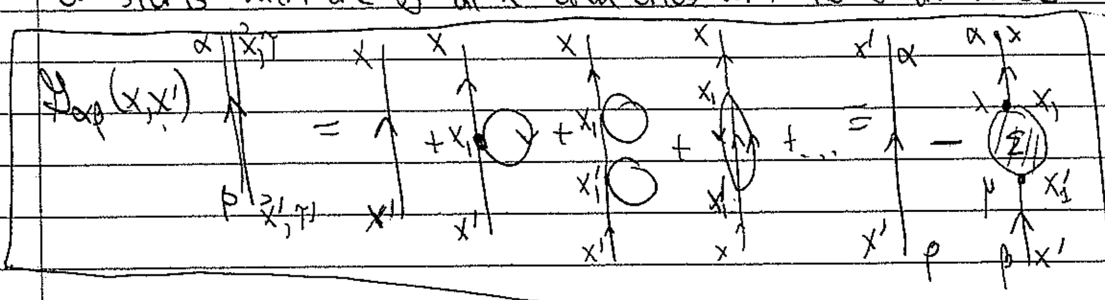
· First, go back to one body Green's function:

$$\mathcal{G}_{\alpha\beta}(\vec{x}\tau;\vec{x}'\tau') = \frac{\int \mathcal{D}(\bar{\psi}\psi)\,\psi_\alpha(\vec{x}\tau)\,\psi^\dagger_\beta(\vec{x}'\tau')\,e^{-S_E}}{\int \mathcal{D}(\bar{\psi}\psi)\,e^{-S_E}}$$

$$= \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\,T\left[\hat{\psi}_\alpha(\vec{x}\tau)\,\hat{\psi}^\dagger_\beta(\vec{x}'\tau')\right]\right] / \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]$$

- See Appendix A for more details on field operators.

· In the diagrammatic expansion, each term is either $\mathcal{G}^0_{\alpha\beta}(x,x')$ with $x=(\vec{x},\tau)$ or starts with one $\mathcal{G}^0$ at x' and ends with another at x. So



is the general structure, where the "improper self-energy" Σ stands for all possible (connected) diagram insertions.

In equation form, this is an integral equation (defining the self energy)

$$\boxed{\mathcal{G}_{\alpha\beta}(x,x') = \mathcal{G}^0_{\alpha\beta}(x,x') - \int d\tau_1 d^3x_1 \int d\tau_1' d^3x_1'\, \mathcal{G}^0_{\alpha\lambda}(x,x_1)\,\Sigma(x_1,x_1')_{\lambda\mu}\,\mathcal{G}^0_{\mu\beta}(x_1',x')}$$

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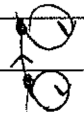
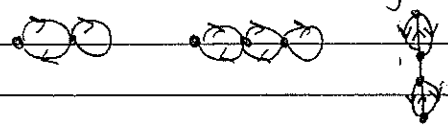
But we can go further. Compare two 2^{nd} order contributions to Σ:

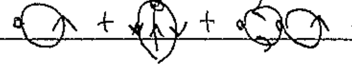
 and 

$\Rightarrow$ each part of the left diagram looks like a self-energy piece, because there is a single line joining them.

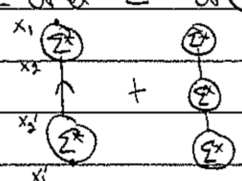
$\Rightarrow$ call it 1PR "one-particle reducible"

- The right diagram is 1PI "one-particle irreducible" because it does not fall into two pieces when a single line is cut (unlike the left diagram).
  - Check: are the following 1PR or 1PI?



- The diagrams in Σ that are 1PI are called the "proper" self-energy and designated Σ^* =  + ...

- Diagrammatically, Σ and Σ^* are related by

Σ = Σ^* −  + ...

or, in equations (suppressing spin indices)

$$\boxed{\Sigma(x_1,x_1') = \Sigma^*(x_1,x_1') - \int d^4x_2\, d^4x_2'\, \Sigma^*(x_1,x_2)\, G^0(x_2,x_2')\, \Sigma^*(x_2',x_1') + \ldots}$$

where $\int d^4x_2$ means $\int d\tau_2\, d^3x_2$, etc.

- Now we can insert this equation back into our original equation for G to derive another integral equation:

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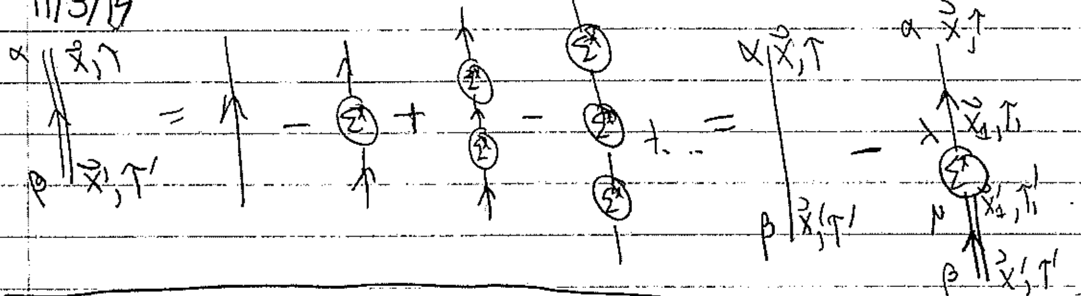

$$\boxed{\Rightarrow \mathcal{G}_{\alpha\beta}(x,x') = \mathcal{G}^0_{\alpha\beta}(x,x') - \int^\beta d\tau_1\, d\vec{x}_1 \int^\beta d\tau_1'\, d\vec{x}_1'\, \mathcal{G}^0_{\alpha\lambda}(x,x_1)\,\Sigma^*(x_1,x_1')_{\lambda\mu}\,\mathcal{G}_{\mu\beta}(x_1',x')}$$

- This is "Dyson's equation" for the propagator ("2-point function")
  - Note that it is like the previous equation for $\mathcal{G}$ except in the integral $\Sigma \to \Sigma^*$ and $\mathcal{G}^0 \to \mathcal{G}$.

- If we approximate Σ^* to some order in perturbation theory, we get an <u>all</u> orders approximation to $\mathcal{G}$!

- Think of the Dyson's equation as a matrix equation (in spin and space time indices)

$$\underline{\underline{\mathcal{G}}} = \underline{\underline{\mathcal{G}}}^0 + \underline{\underline{\mathcal{G}}}^0 \underline{\underline{\Sigma}}^* \underline{\underline{\mathcal{G}}} \Rightarrow \underline{\underline{\mathcal{G}}} - \underline{\underline{\mathcal{G}}}^0 \underline{\underline{\Sigma}}^* \underline{\underline{\mathcal{G}}} = \mathcal{G}^0$$

or $(\underline{\underline{1}} - \underline{\underline{\mathcal{G}}}^0 \underline{\underline{\Sigma}}^*)\underline{\underline{\mathcal{G}}} = \underline{\underline{\mathcal{G}}}^0 \Rightarrow \underline{\underline{\mathcal{G}}} = (\underline{\underline{1}} - \underline{\underline{\mathcal{G}}}^0 \underline{\underline{\Sigma}}^*)^{-1} \underline{\underline{\mathcal{G}}}^0 \Rightarrow \boxed{\underline{\underline{\mathcal{G}}}^{-1} = \underline{\underline{\mathcal{G}}}^{0-1}(\underline{\underline{1}} - \underline{\underline{\mathcal{G}}}^0 \underline{\underline{\Sigma}}^*) = \underline{\underline{\mathcal{G}}}^{0-1} - \underline{\underline{\Sigma}}^*}$

Recall that $\underline{\underline{\mathcal{G}}}^{0-1} = \frac{\partial}{\partial\tau} + \frac{\nabla^2}{2m}$, so Σ^* is like an external potential.

- How do we get the (free) energy? We might think $\int \mathcal{G}\Sigma \Rightarrow$ (Σ^* loop) because, if expanded, it has all the diagrams for $\ln Z/Z_0$.
  - But the factors are incorrect!

$\Rightarrow$ We'll come back and see how to do it correctly!

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Partition function for $V(\vec{x}-\vec{x}')$:

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$$

$$= \int \mathcal{D}[\psi^\dagger(x,\tau)\psi(\vec{x},\tau)]\; e^{-\int_0^\beta d\tau \int d^3x\, \psi^\dagger_\alpha(\vec{x}\tau)\left(\frac{\partial}{\partial\tau} - \frac{\nabla^2}{2m} - \mu\right)\psi_\alpha(\vec{x},\tau)}$$

$$\psi(\vec{x},\beta) = -\psi(\vec{x},0) \qquad \times e^{-\frac{1}{2}\int d\tau \int_0^\beta d^3x\, d^3x'\, \psi^\dagger_\beta(\vec{x}\tau)\psi^\dagger_\alpha(\vec{x}'\tau) V(\vec{x}-\vec{x}')\psi_\alpha(\vec{x}'\tau)\psi_\beta(\vec{x}\tau)}$$

$$\xrightarrow{V = -\lambda\delta^3(\vec{x}-\vec{x}')} \int \mathcal{D}[\psi^\dagger(x)\psi(x)]\; e^{-\int_0^\beta d\tau \int d^3x\, \psi^\dagger_\alpha(x)\left(\frac{\partial}{\partial\tau} - \frac{\nabla^2}{2m} - \mu\right)\psi_\alpha(x)}$$

$$\psi(\vec{x},\beta) = -\psi(\vec{x},0) \qquad \times e^{\frac{\lambda}{2}\int_0^\beta d\tau \int d^3x\, \psi^\dagger_\alpha(x)\psi^\dagger_\beta(x)\psi_\beta(x)\psi_\alpha(x)}$$

As we've seen, this is suitable for perturbation theory, but what about stochastic simulation?

- The fermion form with Grassman fields is not suitable

$\Rightarrow$ introduce an auxiliary field

analogy $1 = \dfrac{\int_{-\infty}^{\infty} d\sigma\, e^{-(\sigma-\sqrt{\lambda}\xi^2)^2}}{\int_{-\infty}^{\infty} d\sigma\, e^{-\sigma^2}}$ $\Rightarrow \int_{-\infty}^{\infty} d\xi\, e^{-a\xi^2 + \lambda\xi^4}$ (note sign) $= N\int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} d\xi\, e^{-a\xi^2 + \cancel{\lambda\xi^4}}\, e^{-\sigma^2 + 2\sigma\sqrt{\lambda}\xi^2}\, \cancel{e^{-\lambda\xi^4}}$

$\Rightarrow$ we can do the Gaussian ξ integral leaving one over σ.

In path integral Z with full $V(\vec{x}-\vec{x}')$:

$$Z = \int \mathcal{D}(\psi^\dagger\psi)\mathcal{D}(\sigma(x))\, e^{-\int d\tau\, d\tau' \int d\vec{x}\, d\vec{x}'\, \psi^\dagger(x\tau)\left[\frac{\partial}{\partial\tau} - \mu - \frac{\nabla^2}{2m} + \frac{1}{2}\int d\vec{y}\, V(\vec{x}-\vec{y})\sigma(\vec{y},\tau)\right]_{\vec{x}\tau,\vec{x}'\tau'}\psi(\vec{x}',\tau')}$$

$$\overset{\text{integrand } \psi^\dagger\psi}{=} \int \mathcal{D}\sigma(x) \left[\det M(\sigma)\right]^2 e^{\frac{1}{2}\int d\tau \int d\vec{x}\, d\vec{x}'\, \sigma(\vec{x},\tau)V(\vec{x}-\vec{x}')\sigma(\vec{x}',\tau)}$$

where $M_{\vec{x}\tau;\vec{x}'\tau'} = \left[\frac{\partial}{\partial\tau} - \mu - \frac{\nabla^2}{2m} + \frac{1}{2}\int d\vec{y}\, V(\vec{x}-\vec{y})\sigma(\vec{y},\tau)\right]_{\vec{x}\tau,\vec{x}'\tau'}$

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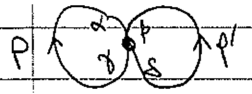
Previously we've evaluated the "bow tie" diagram using Feynman rules with real time (Minkowski) propagators.

- Those ones have Θ functions for momenta compared to the Fermi momentum with poles just below or above the real p_0 axis.
- The imaginary time ("Euclidean") propagators have poles for imaginary p_0 and include the chemical potential μ_0.

• Bowtie diagram in momentum space for energy density



- Same rules for spin and symmetry factor parts and vertex $\Rightarrow$ yield $\frac{1}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma})\delta_{\alpha\gamma}\delta_{\beta\delta}\cdot\lambda$
- The lines become momentum space Green's functions: $(T=0)$

$$\boxed{\mathcal{G}^0_{\alpha\beta}(p) = \frac{-\delta_{\alpha\beta}}{ip_0-(\epsilon^0_p-\mu_0)}} \quad \text{with} \quad \boxed{\epsilon^0_p = \frac{\hbar^2 p^2}{2m}}$$

(but not relativistic!)

instead of $\mathcal{G}^0_{\alpha\beta}(x,x')$ from before. Each line gets a four-momentum, which is conserved (no constraint here because p and p' both go in and out of the vertex).

- Integrate $\int\frac{d^4p}{(2\pi)^4}e^{ip_0\eta}$ over every four-momentum. $e^{ip_0\eta}$ is a convergence factor that tells us how to close contours. $\eta\to 0$ at end.
- ~~At $T\neq 0$, $p_0 \Rightarrow \omega_n$ a discrete frequency and we have "Matsubara sums".~~

$\Rightarrow$ 

$$= \frac{1}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma})\delta_{\alpha\gamma}\delta_{\beta\delta}\,\lambda\left[\int\frac{d^4p}{(2\pi)^4}\frac{-e^{ip_0\eta}}{ip_0-(\epsilon^0_p-\mu_0)}\right]\left[\int\frac{d^4p'}{(2\pi)^4}\frac{-e^{ip'_0\eta}}{ip'_0-(\epsilon^0_{p'}-\mu_0)}\right]$$

$$= \frac{\lambda}{2}\nu(\nu-1)\left[-\int\frac{d^3p}{(2\pi)^3}\Theta(\mu_0-\epsilon^0_p)\right]\left[-\int\frac{d^3p'}{(2\pi)^3}\Theta(\mu_0-\epsilon^0_{p'})\right]$$

$$= \frac{\lambda}{2}\left(1-\frac{1}{\nu}\right)\rho^2$$ which is what we got before for the energy density

- note that we close in the upper half plane so $e^{i(\mathrm{Re}\,p_0+i\,\mathrm{Im}\,p_0)\eta} \propto e^{-(\mathrm{Im}\,p_0)\eta}$ makes the integral converge. We pick up a pole if $\mu_0 > \epsilon^0_p$, otherwise 0.

Euclidean $\Longleftrightarrow$ Minkowski

$t \Longleftrightarrow -i\tau$ so $\mathcal{L}_E(x,\tau) = -\mathcal{L}(x,-i\tau)$ $\quad Z=\int e^{iS}$

or $\tau \Longleftrightarrow it$ or $\mathcal{L}(x,t) = -\mathcal{L}_E(x,it)$ $\quad Z=\int e^{-S_E}$

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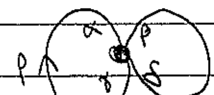
Check Minkowski vs. Euclidean versions.



$\Leftarrow$ contribution to energy density E/V at $T \to 0$

symmetry factor is $\frac{1}{2}$

Minkowski	Euclidean
$\frac{i}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma})\delta_{\alpha\gamma}\delta_{\beta\delta}$	$\frac{1}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma})\delta_{\alpha\gamma}\delta_{\beta\delta}$
$\times(-iC_0)$	$\times(C_0)$
$\times\int\frac{d^4p}{(2\pi)^4}\, i\left[\frac{\theta(\lvert\vec{p}\rvert-k_F)}{p_0-\epsilon_p^0+i\epsilon}+\frac{\theta(k_F-\lvert\vec{p}\rvert)}{p_0-\epsilon_p^0-i\epsilon}\right]e^{ip_0\eta}$	$\times\int\frac{d^4p}{(2\pi)^4}\left[\frac{-1}{ip_0-(\epsilon_p^0-\mu_0)}e^{ip_0\eta}\right]$
$\times\int\frac{d^4p'}{(2\pi)^4}\, i\left[\frac{\theta(\lvert\vec{p}'\rvert-k_F)}{p_0'-\epsilon_{p'}^0+i\epsilon}+\frac{\theta(k_F-\lvert\vec{p}'\rvert)}{p_0'-\epsilon_{p'}^0-i\epsilon}\right]e^{ip_0'\eta}$	$\times\int\frac{d^4p'}{(2\pi)^4}\left[\frac{-1}{ip_0'-(\epsilon_{p'}^0-\mu_0)}e^{ip_0'\eta}\right]$

same spin factors

(vertex factor of i or $-i$) e^{iS} vs. e^{-S_E}

$$= \frac{C_0}{2}\nu(\nu-1)\left[\int\frac{d^3p}{(2\pi)^3}\theta(k_F-\lvert\vec{p}\rvert)\right]\left[\int\frac{d^3p'}{(2\pi)^3}\theta(\mu_0-\epsilon_{p'}^0)\right]$$

These are the same; use either!

$$= \frac{C_0}{2}\left(1-\frac{1}{\nu}\right)\rho^2 \quad \text{where} \quad \rho=\frac{\nu k_F^3}{6\pi^2},\ \mu_0=\frac{k_F^2}{2m}$$

- Note that we are just taking $p_0 \to ip_0$, as implied by the Wick rotation.

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Goal: Recover HF result from Feyman rules resummed

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

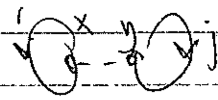
$$\left[-\frac{\nabla^2}{2m} + \Gamma_H(\vec{x})\right]\phi_i(\vec{x}) + \int d\vec{y}\, \Gamma_F(\vec{x},\vec{y})\,\phi_i(\vec{y}) = \varepsilon_i\,\phi_i(\vec{x})$$

$$\Gamma_H(\vec{x}) = \int d^3y\, V(\vec{x},\vec{y}) \sum_{j=1}^{A} |\phi_j(\vec{y})|^2 = \int d^3y\, V(\vec{x},\vec{y})\,\rho(\vec{y},\vec{y})$$

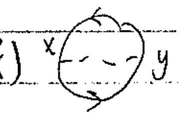
$$\Gamma_F(\vec{x},\vec{y}) = -V(\vec{x},\vec{y}) \sum_{j=1}^{A} \phi_j^\dagger(\vec{y})\,\phi_j(\vec{x}) = -V(\vec{x},\vec{y})\,\rho(\vec{y},\vec{x})$$

$$E_{HF} = \sum_{i=1}^{A} \frac{1}{2m}\int d\vec{x}\, \nabla\phi_i^\dagger \nabla\phi_i$$

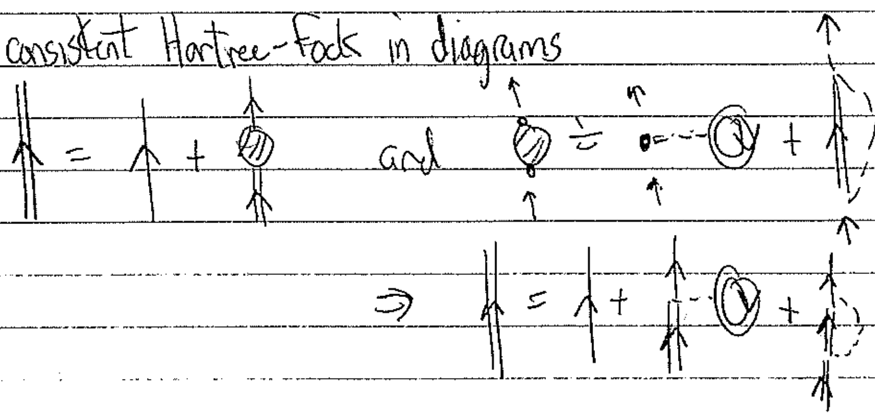
$$+ \frac{1}{2}\int d\vec{x}\int d\vec{y}\, \sum_i |\phi_i(\vec{x})|^2\, V(\vec{x},\vec{y}) \sum_j |\phi_j(\vec{y})|^2$$



$$-\frac{1}{2}\int d\vec{x}\int d\vec{y}\, \sum_{i,j} \phi_i^\dagger(\vec{x})\,\phi_i(\vec{x})\,V(\vec{x},\vec{y})\,\phi_j^\dagger(\vec{y})\,\phi_j(\vec{x})$$



Self-consistent Hartree-Fock in diagrams



• We'll follow Fetter and Walecka section 10, which uses a real-time $T=0$ formulation. A finite temperature, Euclidean version of the same discussion is in FTW section 27.

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Let's take $\hat{H} = \hat{H}_0 + \hat{H}_1$ where $\hat{H}_0$ includes a single-particle potential $U(\vec{x})$, which then defines a single-particle complete set of states: (here in first quantization)

$$H_0 \varphi_j^0(\vec{x}) = \left[-\frac{\nabla^2}{2m} + U(\vec{x})\right] \varphi_j^0(\vec{x}) = \varepsilon_j^0 \varphi_j^0(\vec{x})$$

- Even if $\hat{H} = \hat{T} + \hat{V}$, we can always write $\hat{H} = (\hat{T} + \hat{U}) + (\hat{V} - \hat{U}) \equiv \hat{H}_0 + \hat{H}_1$.

- In 2nd quantized form

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

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

where we can choose the φ_j^0 to be the basis for the field operators $\hat{\psi}_\alpha(\vec{x})$:

$$\hat{\psi}_\alpha(\vec{x}) = \sum_j \varphi_j^0(\vec{x})\, a_j \,; \quad \hat{\psi}_\alpha^\dagger(\vec{x}) = \sum_j \varphi_j^{0*}(\vec{x})\, a_j^\dagger$$

- Dyson's equation for Hartree-Fock is then (suppressing spin indices)

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

where the proper self-energy is

$$\Sigma^*(x_1,x_1') = -i\delta(t_1-t_1')\Big[\delta(\vec{x}_1-\vec{x}_1')\, \nu \int d^3x_2\, G(\vec{x}_2 t_2; \vec{x}_2 t_2^+) V(\vec{x}_1-\vec{x}_2) - V(\vec{x}_1-\vec{x}_1')\, G(\vec{x}_1 t_1; \vec{x}_1' t_1^+)\Big]$$

- $\hat{H}_0$ and $\hat{H}_1$ are both time independent, so switching to a Fourier representation in frequency makes sense.

$$G(\vec{x}t, \vec{x}'t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega(t-t')}\, G(\vec{x},\vec{x}';\omega) \quad \text{(similarly with } G^0\text{)}$$

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

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Let's first consider G^0 in terms of field operators:

$$\boxed{iG^0_{\alpha\beta}(\vec{x}t,\vec{x}'t') = \frac{\langle\Phi_0|T[\hat{\psi}_{H\alpha}(\vec{x}t)\hat{\psi}^\dagger_{H\beta}(\vec{x}'t')]|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle}}$$

Ground-state of H_0

- The time-ordered product means $\psi\psi^\dagger$ if $t>t'$ and $-\psi^\dagger\psi$ if $t<t'$.
- The Heisenberg field operators for $\hat{H}_0$ (or interaction picture) are $\boxed{\hat{\psi}_{H\alpha}(\vec{x}t) = e^{i\hat{H}_0 t}\hat{\psi}_\alpha(\vec{x})e^{-i\hat{H}_0 t}}$

$$\Rightarrow \boxed{\begin{aligned} iG^0_{\alpha\beta}(\vec{x}t,\vec{x}'t') &= \sum_j \varphi^0_j(\vec{x})\varphi^0_j(\vec{x}')\, e^{-i\epsilon^0_j(t-t')} \times\left[\theta(t-t')\langle\Phi_0|a_j a_j^\dagger|\Phi_0\rangle - \theta(t'-t)\langle\Phi_0|a_j^\dagger a_j|\Phi_0\rangle\right] \\ &= \sum_j \varphi^0_j(\vec{x})\varphi^0_j(\vec{x}')\, e^{-i\epsilon^0_j(t-t')} \times\left[\theta(t-t')\theta(\epsilon^0_j-\epsilon^0_F) - \theta(t'-t)\theta(\epsilon^0_F-\epsilon^0_j)\right]\end{aligned}}$$

where ϵ^0_F is the energy of the last filled state.

- Check that $\left[i\frac{\partial}{\partial t_x} + \frac{\nabla_x^2}{2m} - U(\vec{x})\right]G^0_{\alpha\beta}(\vec{x}t_x,\vec{x}'t_{x'}) = \delta^3(\vec{x}-\vec{x}')\,\delta(t_x-t'_x)\,\delta_{\alpha\beta}$

- If we calculate the Fourier transform: (Piazza!)

$$\boxed{\begin{aligned} G^0(\vec{x},\vec{x}',\omega) &= \int_{-\infty}^{\infty} d(t-t')\, e^{i\omega(t-t')}\, G^0(\vec{x}t,\vec{x}'t') \\ &= \sum_j \varphi^0_j(\vec{x})\varphi^0_j(\vec{x}')^*\left[\frac{\theta(\epsilon^0_j-\epsilon^0_F)}{\omega-\epsilon^0_j+i\eta} + \frac{\theta(\epsilon^0_F-\epsilon^0_j)}{\omega-\epsilon^0_j-i\eta}\right]\end{aligned}}$$

- If we took $U(\vec{x})\equiv 0$, then the $\varphi_j(\vec{x}) \to \frac{1}{\sqrt{\Omega}}e^{i\vec{k}_j\cdot\vec{x}}$ and $\epsilon^0_j \to k_j^2/2m$, recovering the result for G^0 from the non-interacting case.
- The analytic structure is simple poles at the non-interacting energies with residues given by the single-particle wave functions.
- This is an example of a <u>spectral representation</u>

- Defining the differential operator $L_1 = \omega - H_0 = \omega + \frac{\nabla_1^2}{2m} - U(\vec{x}_1)$

as expected from a Green's function

$$\Rightarrow L_1 G^0(\vec{x}_1,\vec{x}_1';\omega) = \sum_j(\omega-\epsilon^0_j)\varphi^0_j(\vec{x}_1)\varphi^0_j(\vec{x}_1')^*\left[\frac{\theta(\epsilon^0_j-\epsilon^0_F)}{\omega-\epsilon^0_j+i\eta} + \frac{\theta(\epsilon^0_F-\epsilon^0_j)}{\omega-\epsilon^0_j-i\eta}\right]$$

$$= \sum_j \varphi^0_j(\vec{x}_1)\varphi^0_j(\vec{x}_1')^* = \delta^3(\vec{x}_1-\vec{x}_1') \quad \text{by completeness.}$$

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- For Hartree-Fock, the full propagator G will also depend only on $t-t'$ and with Σ^* having a $\delta(t-t')$ dependence, the frequency Fourier transformation of the Dyson's equation is

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

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

- To solve this, we realize that because Σ^* (for HF) is independent of frequency, G will have the same structure as G^0:

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

where the single-particle wave functions $\{\varphi_j(\vec{x})\}$ have energy ϵ_j. How do we determine them?

- First we note that evaluating Σ^* looks like the HF potential from before:

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

- Now apply $L_1 = G_0^{-1}$ to the Dyson equation for G:

$$L_1 G(\vec{x}_1,\vec{x}_1',\omega) = \delta^3(\vec{x}_1-\vec{x}_1') + \int d^3x_2\, \Sigma^*(\vec{x}_1,\vec{x}_2)\,G(\vec{x}_2,\vec{x}_1',\omega)$$

We'll leave it as a Piazza exercise to show that this implies the HF equations:

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