Quantum Theory of Many-Particle Systems, Phys. 540

- $N \pm 2$ tp propagator with two times
- Scattering of two particles in free space
- Bound states of two particles
- Ladder diagrams and SRC in the medium
- Scattering of mean-field particles in the medium
- Cooper problem and pairing instabilities
- Bound pair states
- Other questions about last class and assignments?
- Comments?

Consequences for sp propagator in infinite systems

- Electron gas $\rightarrow$ plasmon $\rightarrow$ sp propagator
- Example of influence of collective state on sp properties
- Nuclear matter $\rightarrow$ SRC $\rightarrow$ sp propagator
- Example of influence of strong mutual repulsion on Fermi sea

- Diagrams with momentum conservation in infinite systems
- Volume terms from interactions cancel those arising from momentum integrations
- Propagator (sp) doesn't depend on spin/isospin quantum numbers for spin/isospin saturated system
- Label propagators with wave vectors (and energy) with beginning and end point labeled by discrete quantum numbers
Examples

- First-order term
  \[ G^{(1)}(k; E) = G^{(0)}(k; E) \]
  \[ \times \left\{ - \frac{i}{\nu} \sum_{m_\alpha m_\beta} \int \frac{d^3 k'}{(2\pi)^3} \langle km_\alpha k' m_\beta | V | km_\alpha k' m_\beta \rangle \right. \]
  \[ \times \left. \int_{C^\dagger} \frac{dE'}{2\pi} G^{(0)}(k'; E') \right\} G^{(0)}(k; E) \]

- includes extra summation over external quantum numbers to facilitate coupling to total spin etc.

- 2nd order (internal labeling as convenient)
  \[ \Sigma^{(2)}(k; E) = (-1)^2 \frac{1}{2} \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} \int \frac{d^3 q}{(2\pi)^3} \int \frac{d^3 k'}{(2\pi)^3} \frac{1}{\nu} \sum_{m_\alpha m_\beta m_\gamma m_\delta} \]
  \[ \times \langle km_\alpha k' - q/2m_\delta | V | k - q m_\gamma k' + q/2m_\delta \rangle \]
  \[ \times G^{(0)}(k' + q/2; E_1 + E_2) G^{(0)}(k' - q/2; E_2) G^{(0)}(k - q; E - E_1) \]
  \[ \times \langle k - q m_\gamma k' + q/2m_\delta | V | km_\alpha k' - q/2m_\delta \rangle \]

Self-energy in infinite system

- Exact self-energy similarly from
  \[ \Sigma^*(\gamma, \delta; E) = - \langle \gamma | U | \delta \rangle - i \int_{C^\dagger} \frac{dE'}{2\pi} \sum_{\nu, \nu'} \langle \gamma \mu | V | \delta \nu \rangle G(\nu, \mu; E') \]
  \[ + \frac{1}{2} \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} \sum_{e, \mu, \nu, \epsilon, \rho, \sigma} \langle \gamma \mu | V | e \nu \rangle G(e, \zeta; E_1) G(\nu, \rho; E_2) \]
  \[ \times G(\sigma, \mu; E_1 + E_2 - E) \langle \zeta \rho | \Gamma(E_1, E_2; E, E_1 + E_2 - E) | \delta \sigma \rangle \]

- to
  \[ \Sigma(k; E) = -U(k) \]
  \[ -i \frac{1}{\nu} \sum_{m_\alpha m_\beta} \int \frac{d^3 k'}{(2\pi)^3} \langle km_\alpha k' m_\beta | V | km_\alpha k' m_\beta \rangle \int_{C^\dagger} \frac{dE'}{2\pi} G(k'; E') \]
  \[ -i \frac{1}{2} \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} \int \frac{d^3 q}{(2\pi)^3} \int \frac{d^3 k'}{(2\pi)^3} \frac{1}{\nu} \sum_{m_\alpha m_\beta m_\gamma m_\delta} \]
  \[ \times \langle km_\alpha k' - q/2m_\delta | V | k - q m_\gamma k' + q/2m_\delta \rangle \]
  \[ \times G(k - q; E - E_1) G(k' + q/2; E_1 + E_2) G(k' - q/2; E_2) \]
  \[ \times \langle k - q m_\gamma k' + q/2m_\delta | \Gamma(E_1, E_2) | km_\alpha k' - q/2m_\delta \rangle \]
**Propagator**

- **DE** \( G(k; E) = G^{(0)}(k; E) + G^{(0)}(k; E)\Sigma(k; E)G(k; E) \)
  \[ = \frac{E - \varepsilon(k) - \text{Re} \Sigma(k; E) + i\text{Im} \Sigma(k; E)}{(E - \varepsilon(k) - \text{Re} \Sigma(k; E))^2 + (\text{Im} \Sigma(k; E))^2} \]
- Only magnitude of wave vector needed
- Noninteracting propagator \( G^{(0)}(k; E) = \frac{\theta(k - k_F)}{E - \varepsilon(k) + i\eta} + \frac{\theta(k_F - k)}{E - \varepsilon(k) - i\eta} \)
- With \( \varepsilon(k) = \frac{\hbar^2 k^2}{2m} + U(k) \)
- Particle spectral function \( S_p(k; E) = \frac{-1}{\pi} \frac{\text{Im} \Sigma(k; E)}{(E - \varepsilon(k) - \text{Re} \Sigma(k; E))^2 + (\text{Im} \Sigma(k; E))^2} \)
- Hole spectral function \( S_h(k; E) = \frac{1}{\pi} \frac{\text{Im} \Sigma(k; E)}{(E - \varepsilon(k) - \text{Re} \Sigma(k; E))^2 + (\text{Im} \Sigma(k; E))^2} \)
- Dispersion relation (check)
  \[ G(k; E) = \int_{\varepsilon_F}^{\infty} \frac{dE'}{E - E'} \frac{S_p(k; E')}{E'} + \int_{-\infty}^{\varepsilon_F} \frac{dE'}{E - E'} \frac{S_h(k; E')}{E'} \]

**Other quantities**

- Energy per particle
  \[ \frac{E_0^N}{N} = \frac{\nu}{2\rho} \int \frac{d^3 k}{(2\pi)^3} \int_{\varepsilon_F}^{\infty} dE \left( \frac{\hbar^2 k^2}{2m} + E \right) S_h(k; E) \]
- Density \( \rho = \frac{\nu k_F^3}{6\pi^2} \) but also from
  \[ \rho = \frac{\nu}{2\pi^2} \int_0^{\infty} dk k^2 n(k) \]
- Integral over momentum distribution \( n(k) = \int_{-\infty}^{\varepsilon_F} dE S_h(k; E) \)
- Kinetic energy \( \frac{T}{N} = \frac{\nu}{2\pi^2 \rho} \int_0^{\infty} dk k^2 \frac{\hbar^2 k^2}{2m} n(k) \)
- Pressure at T=0 from density derivative of energy per particle
  \[ P = \rho^2 \frac{\partial (E/N)}{\partial \rho} = \rho [\varepsilon_F - (E/N)] \quad \text{using} \quad E/N = E/(\rho V) \]
- And \( \varepsilon_F = \partial E/\partial N \) so at saturation \( E/N = \varepsilon_F \) (H-vH theorem)
Self-energy in the electron gas

- Second-order is not appropriate for the electron gas
  \[
  \Sigma^{(2)}(k; E) = (-1)^2 \frac{1}{2} \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \sum \delta_{m_\alpha m_\beta m_\gamma m_\delta} V(k_m, k'_m | V | k - q/2m_\delta)
  \]
  \[
  \times G^{(0)}(k' + q/2; E_1 + E_2) G^{(0)}(k' - q/2; E_2) G^{(0)}(k - q; E - E_1)
  \times \langle k_m, k'_m + q/2m_\delta | V | k_m, k'_m - q/2m_\delta \rangle
  \]
- Consider direct matrix element in 2nd-order self-energy
  \[
  \langle k_m, k'_m - qm_\beta | V | k - qm_\gamma k'_m \delta \rangle \Rightarrow \delta_{m_\alpha m_\gamma} \delta_{m_\beta m_\delta} V(q)
  \]
  with \( V(q) = \frac{4\pi e^2}{q^2} \)
  
- Performing \( E_2 \) and \( k' \) integration and identifying noninteracting polarization propagator (including spin summations)
  \[
  \Sigma^{(2)}_D(k; E) = 2i \left( \frac{dE_1}{2\pi} \right) \left( \frac{d^3q}{(2\pi)^3} \right) V^2(q) G^{(0)}(k - q; E - E_1) \Pi^{(0)}(q; E_1)
  \]
  generates “infrared” divergence due to \( q^4 \) contribution so infinite! continues in higher order!

Higher-order terms

- Replace \( \Pi^{(0)} \) by \( \Pi^{(0)} 2V \Pi^{(0)} \) to generate 3rd order diagram and so on

- with worse divergences
- Remedy: sum all divergent terms replacing noninteracting polarization propagator by the RPA one (already encountered for discussion of plasmon)
- So evaluate
  \[
  \Sigma^{RPA}(k; E) = 2i \left( \frac{dE_1}{2\pi} \right) \left( \frac{d^3q}{(2\pi)^3} \right) V^2(q) G^{(0)}(k - q; E - E_1) \Pi^{RPA}(q; E_1)
  \]
Ring approximation

- Add Fock term: represented by $G^{(0)} W^{(0)}$
- Approximation known as $GW$
- Self-consistent formulation $GW$
- Note
  - medium modification important so should be included self-consistently
  - drawback: f-sum rule no longer conserved and no plasmon (see later)
- Evaluate self-energy using Lehmann representation
  \[
  \Pi(q, E) = -\frac{1}{\pi} \int_0^{\infty} dE' \frac{\text{Im} \, \Pi(q, E')}{E - E' + i\eta} + \frac{1}{\pi} \int_{-\infty}^0 dE' \frac{\text{Im} \, \Pi(q, E')}{E - E' - i\eta}
  \]
- RPA generates discrete poles (plasmons)
- Plasmon term above Fermi energy (im part)
  \[
  \text{Im} \, \Sigma^{RPA}_p(k; E) = \pi \frac{d^3q}{(2\pi)^3} \theta(|k - q| - k_F) \theta(q_c - q) \times \delta(E - E_p(q) - \epsilon(k - q)) \left( \frac{\partial \Pi^{(0)}(q, E)}{\partial E} \right)^{-1} \]

Development

- Algebra somewhat lengthy
- When $q=0$ point included, integrand requires expansion yielding a logarithmic singularity (Hedin 1967)
- From delta-function: occurs at $E = \pm E_p(0) + \epsilon(k)$ (+ for $k > k_F$)
- Results (only plasmon)
  \[ r_s = 2 \]
- Real part singular for $k = k_F$
Continuum contribution

- Employ corresponding dispersion relation
  \[ \Pi_c^{RPA}(q, E) = -\frac{1}{\pi} \int_{E_-}^{E_+} dE' \frac{\text{Im} \, \Pi_c^{RPA}(q, E')}{E - E' + i\eta} + \frac{1}{\pi} \int_{-E_+}^{-E_-} dE' \frac{\text{Im} \, \Pi_c^{RPA}(q, E')}{E - E' - i\eta} \]

- Insert in self-energy

- For energies above the Fermi energy
  \[ \text{Im} \, \Sigma_c^{RPA}(k; E) = \frac{2}{(2\pi)^3} V^2(q) \int_{E_-}^{E_+} dE' \text{Im} \, \Pi_c^{RPA}(q, E') \theta(|k - q| - k_F) \delta(E - E' - \varepsilon(k - q)) \]

  similarly for energies below

- Real part from
  \[ \text{Re} \, \Sigma^{RPA}(k; E) = \Sigma^{HF}(k) + \frac{\mathcal{P}}{\pi} \int_{-\infty}^{+\infty} dE' \left| \text{Im} \, \Sigma^{RPA}(k; E') \right| \frac{E - E'}{E - E'} \]

  Continuum only

  Much smaller than plasmon terms

Spectral functions

- From self-energy and Dyson equation -> spectral functions

- Wave vectors deep inside Fermi sea: two distinct features

- Because of the vanishing of the imaginary part in certain regions there may be multiple solutions to
  \[ E_Q(k) = \frac{\hbar^2 k^2}{2m} + \text{Re} \, \Sigma^{RPA}(k; E_Q(k)) \]

  outside these domains -> more than one delta-function solution possible with
  \[ Z_Q(k) = \left( 1 - \left. \frac{\partial \text{Re} \, \Sigma^{RPA}(k; E)}{\partial E} \right|_{E=E_Q(k)} \right)^{-1} \]

  Almost realized for \( k/k_F = 0.2 \) at \( r_s = 2 \)

  Peak is referred to as the “plasmaron”
• \( r_s = 2 \)
• Only plasmon

• Integrated strength:
• \( n(k) \) for \( r_s = 1 \) and \( 2 \)

\[
\Pi^f(k; q, E) = \int_\varepsilon_F^{\infty} d\tilde{E} \int_{-\infty}^{\varepsilon_F} d\tilde{E}' \frac{S_p(k + q/2; \tilde{E})S_h(k - q/2; \tilde{E}')}{E - (\tilde{E} - \tilde{E}')} + i\eta \\
- \int_{-\infty}^{\varepsilon_F} d\tilde{E} \int_{\varepsilon_F}^{\infty} d\tilde{E}' \frac{S_h(k + q/2; \tilde{E})S_p(k - q/2; \tilde{E}')}{E + (\tilde{E}' - \tilde{E}) - i\eta}
\]
Development

• For positive energies

\[
\text{Im } \Pi^f(k; q, E) = -\pi \int_{E_F}^{\infty} d\tilde{E} \int_{-\infty}^{E+\tilde{E}} d\tilde{E}' S_p(k+q/2; \tilde{E}) S_h(k-q/2; \tilde{E}') \delta(E-(\tilde{E}-\tilde{E}'))
\]

\[
= -\pi \int_{E_F}^{E+E_F} d\tilde{E} S_p(k+q/2; \tilde{E}) S_h(k-q/2; \tilde{E}-E)
\]

• By integrating over wave vector \( k \) the dressed version of the Lindhard function is generated

\[
\Pi^f(q, E) = \int \frac{d^3k}{(2\pi)^3} \Pi^f(k; q, E)
\]

• Obey usual dispersion relation

\[
\Pi^f(q, E) = -\frac{1}{\pi} \int_0^\infty dE' \frac{\text{Im } \Pi^f(q, E')}{E-E'+i\eta} + \frac{1}{\pi} \int_0^0 dE' \frac{\text{Im } \Pi^f(q, E')}{E-E'-i\eta}
\]

• Plot for \( r_s = 2 \) (dashed)

• \( r_s = 4 \) (solid)

• noninteracting \( q/k_F = 0.25 \)

• Huge spreading for self-consistency

Polarization propagator

• As usual

\[
\Pi(q, E) = \frac{\Pi^f(q, E)}{1 - 2V(q)\Pi^f(q, E)}
\]

• and the screened Coulomb interaction becomes

\[
W(q, E) = V(q) + V(q)2\Pi^f(q, E)V(q)
\]

\[
+ V(q)2\Pi^f(q, E)V(q)2\Pi^f(q, E)V(q) + ...
\]

\[
= V(q) + 2V(q) \{ \Pi^f(q, E) + \Pi^f(q, E)2V(q)\Pi^f(q, E) + ... \} V(q)
\]

\[
= V(q) + 2V^2(q)\Pi(q, E)
\]

• Demonstrating that it has the same analytical properties as \( \Pi \)

\[
W(q, E) \equiv V(q) + \Delta W(q, E)
\]

\[
= V(q) - \frac{1}{\pi} \int_0^\infty dE' \text{Im } W(q, E') \frac{1}{E-E'+i\eta} + \frac{1}{\pi} \int_0^\infty dE' \text{Im } W(q, E') \frac{1}{E-E'-i\eta}
\]

\[
= V(q) - \frac{1}{\pi} \int_0^\infty dE' \text{Im } W(q, E') \frac{1}{E-E'+i\eta} + \frac{1}{\pi} \int_0^\infty dE' \text{Im } W(q, E') \frac{1}{E-E'+i\eta}
\]

\[
= \frac{1}{\pi} \int_0^\infty dE' \text{Im } W(q, E') \frac{1}{E-E'+i\eta} + \frac{1}{\pi} \int_0^\infty dE' \text{Im } W(q, E') \frac{1}{E-E'+i\eta}
\]
More development

• Imaginary part of screened Coulomb can be written as
  \[ \text{Im } W(q, E) = 2V^2(q) \text{Im } \Pi(q, E) \]
  \[ = 2V^2(q) \frac{\text{Im } \Pi^f(q, E)}{(1 - 2V(q) \text{ Re } \Pi^f(q, E))^2 + (2V(q) \text{ Im } \Pi^f(q, E))^2} \]

• Since \( \Delta W = 2V^2 \Pi \) the self-energy can be written as
  \[ \Sigma_{\Delta W}(k; E) = i \int \frac{dE_1}{2\pi} \int \frac{d^3q}{(2\pi)^3} G(k - q; E - E_1) \Delta W(q; E_1) \]

• Insert spectral representation and perform energy integration
  \[ \Sigma_{\Delta W}(k; E) = \frac{1}{\pi} \int \frac{d^3q}{(2\pi)^3} \int_{\varepsilon_F}^\infty d\tilde{E}' \int_{\varepsilon_F}^\infty d\tilde{E} S_p(k - q; \tilde{E}) \text{Im } W(q, \tilde{E}') \]
  \[ \quad \times \frac{E - \tilde{E}' - \tilde{E} + i\eta}{E - \tilde{E}' - \tilde{E} - i\eta} \]

• First term (particle domain)
  \[ \text{Im } \Sigma_{\Delta W}(k; E) = \int \frac{d^3q}{(2\pi)^3} \int_{\varepsilon_F}^0 d\tilde{E}' S_p(k - q; E - \tilde{E}') \text{Im } W(q, \tilde{E}') \]

• Hole domain
  \[ \text{Im } \Sigma_{\Delta W}(k; E) = -\int \frac{d^3q}{(2\pi)^3} \int_{E - \varepsilon_F}^{E - \varepsilon_F} d\tilde{E}' S_h(k - q; E - \tilde{E}') \text{Im } W(q, \tilde{E}') \]

Final steps

• Still need generalization of HF term
  \[ \Sigma_V(k) = -\int \frac{d^3k'}{(2\pi)^3} V(k - k') n(k') \]

• So GW self-energy becomes
  \[ \Sigma_{GW}(k; E) = \Sigma_V(k) - \frac{1}{\pi} \int_{\varepsilon_F}^{\infty} d\tilde{E}' \frac{\text{Im } \Sigma_{\Delta W}(k; E')}{E - \tilde{E}' + i\eta} + \frac{1}{\pi} \int_{-\infty}^{\varepsilon_F} d\tilde{E}' \frac{\text{Im } \Sigma_{\Delta W}(k; E')}{E - \tilde{E}' - i\eta} \]

• with DE self-consistency loop complete

• Holm and von Barth (1998) calculation employed sum of Gaussians
  \[ S(k; E) = \sum_n \frac{W_n(k)}{\sqrt{2\pi}\Gamma_n(k)} \exp \left\{ -\frac{(E - E_n(k))^2}{2\Gamma_n^2(k)} \right\} \]

• with GW\(^{(0)}\) to initiate parameters

• GW\(^{(0)}\) keeps screened Coulomb fixed but determines G self-consistently

• Both schemes require several iteration steps for the parameters
Results for GW

• No more plasmon! (no more $f$-sum rule too)
• Im part of noninteracting dressed polarization propagator has substantial imaginary part in large domain where plasmon used to reside $\rightarrow$ spreads plasmon strength
• Meaning?
• Self-energy $r_s = 4$ for $k=0$ and $k=k_F$
• GW solid
• $GW^{(0)}$ dashed
• Similar to $G^{(0)}W^{(0)}$

Spectral functions

• Still satellites in $GW^{(0)}$ dashed
• $r_s = 4$
• No satellites in GW (observed in Na)
• GW less correlated
• Illustrated by quasiparticle strength
• And momentum distribution
## Difficulties

- Bandwidth: difference between quasiparticle energies $k_F$ and 0
- Increases with self-consistency

- Problems?!?!
- Self-consistency physical
- Self-energy and plasmon worse
- Vertex corrections (exchange)?

- but correlation energy...

- Possible solution: Faddeev approach

## Energy per particle electron gas

- Fundamental issue related to DFT applications
- Quantum Monte Carlo available

- $-XC$ in table ($XC =$ exchange correlation energy per particle)

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- ⭐ famous paper: cited 6065 times (07/30/2009) and counting
- Green’s function results: $GW$ very close to QMC
- Particle number violations possible unless fully self-consistent
Assignment

- Choose a topic for your presentation!

Suggestions
- Dispersive optical model
- Spectral function of dilute Fermi gases
- Quasiparticle DFT
- Faddeev summation for self-energy
- Neutron matter equation of state

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- Self-energy in infinite systems
- Diagram rules
- Electron gas various forms of GW approximation
- Other questions about last class and assignments?
- Comments?
Nucleons in nuclear matter

- NN interaction requires summation of ladder diagrams
- Study influence of SRC on sp propagator
- Formulate in self-consistent form

\[ \langle km_\alpha m_{\alpha'} | \Gamma_{pphh}(K, E) | k'm_\beta m_{\beta'} \rangle \]

\[ = \langle km_\alpha m_{\alpha'} | V | k'm_\beta m_{\beta'} \rangle + \langle km_\alpha m_{\alpha'} | \Delta \Gamma_{pphh}(K, E) | k'm_\beta m_{\beta'} \rangle \]

\[ = \langle km_\alpha m_{\alpha'} | V | k'm_\beta m_{\beta'} \rangle + \frac{1}{2} \sum_{m_\gamma m_{\gamma'}} \int \frac{d^3 q}{(2\pi)^3} \langle km_\alpha m_{\alpha'} | V | q m_\gamma m_{\gamma'} \rangle \]

\[ \times G_{pphh}^f (K, q; E) \langle q m_\gamma m_{\gamma'} | \Gamma_{pphh}(K, E) | k'm_\beta m_{\beta'} \rangle \]

- employs noninteracting but dressed convolution of sp propagators

\[ G_{pphh}^f (K, q; E) = \int_{E_F}^{\infty} dE' \int_{E_F}^{\infty} dE'' \frac{S_p (q + K/2; E') S_p (K/2 - q; E'')}{E - E' - E'' + i\eta} \]

\[ - \int_{-\infty}^{E_F} dE' \int_{-\infty}^{E_F} dE'' \frac{S_h (q + K/2; E') S_h (K/2 - q; E'')}{E - E' - E'' - i\eta} \]

Lehmann representation

- Dispersion relation (arrows for location of poles in energy plane)

\[ \langle km_\alpha m_{\alpha'} | \Delta \Gamma_{pphh}(K, E) | k'm_\beta m_{\beta'} \rangle \]

\[ = -\frac{1}{\pi} \int_{2E_F}^{\infty} dE' \text{Im} \langle km_\alpha m_{\alpha'} | \Delta \Gamma_{pphh}(K, E') | k'm_\beta m_{\beta'} \rangle \]

\[ + \frac{1}{\pi} \int_{-\infty}^{2E_F} dE' \text{Im} \langle km_\alpha m_{\alpha'} | \Delta \Gamma_{pphh}(K, E') | k'm_\beta m_{\beta'} \rangle \]

\[ \equiv \langle km_\alpha m_{\alpha'} | \Delta \Gamma_1 (K, E) | k'm_\beta m_{\beta'} \rangle + \langle km_\alpha m_{\alpha'} | \Delta \Gamma_1 (K, E) | k'm_\beta m_{\beta'} \rangle \]

- Corresponding self-energy

\[ \Sigma_{\Delta \Gamma}(k; E) = -\frac{1}{\nu} \sum \int \frac{d^3 k'}{(2\pi)^3} \int \frac{dE'}{2\pi} G(k'; E') \]

\[ \times \langle \frac{1}{2} (k - k') m_\alpha m_{\alpha'} | \Delta \Gamma_{pphh}(K, E + E') | \frac{1}{2} (k - k') m_\alpha m_{\alpha'} \rangle \]

- Energy integral can be performed (note arrows)

\[ \Sigma_{\Delta \Gamma}(k; E) = \frac{1}{\nu} \sum \int \frac{d^3 k'}{(2\pi)^3} \int_{E_F}^{\infty} dE' \langle \frac{1}{2} (k - k') m_\alpha m_{\alpha'} | \Delta \Gamma_1 (E + E') | \frac{1}{2} (k - k') m_\alpha m_{\alpha'} \rangle S_h (k', E') \]

\[ - \frac{1}{\nu} \sum \int \frac{d^3 k'}{(2\pi)^3} \int_{-E_F}^{\infty} dE' \langle \frac{1}{2} (k - k') m_\alpha m_{\alpha'} | \Delta \Gamma_1 (E + E') | \frac{1}{2} (k - k') m_\alpha m_{\alpha'} \rangle S_p (k', E') \]

\[ \equiv \Delta \Sigma_1 (k; E) + \Delta \Sigma_1 (k; E) \]

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Final steps and implementation

- Total self-energy
  \[ \Sigma(k; E) = \Sigma_V(k) - \frac{1}{\pi} \int_{E_F}^{\infty} dE' \frac{\text{Im} \Sigma(k; E')}{E - E' + i\eta} + \frac{1}{\pi} \int_{-\infty}^{E_F} dE' \frac{\text{Im} \Sigma(k; E')}{E - E' - i\eta} \]
  \[ = \Sigma_V(k) + \Delta \Sigma_\downarrow(k; E) + \Delta \Sigma_\uparrow(k; E) \]
- Includes HF-like term
  \[ \Sigma_V(k) = \int \frac{d^3k'}{(2\pi)^3} \frac{1}{\nu} \sum_{m_\alpha m_{\alpha'}} \langle \frac{1}{2}(k - k') m_\alpha m_{\alpha'} | V | \frac{1}{2}(k - k') m_\alpha m_{\alpha'} \rangle n(k') \]
- Practical calculations first done with mean-field sp propagators in scattering equation
  \[ \Sigma_{\Delta}^{(0)}(k; E) = \frac{1}{\nu} \sum_{m_\alpha m_{\alpha'}} \int \frac{d^3k'}{(2\pi)^3} \langle \frac{1}{2}(k - k') m_\alpha m_{\alpha'} | \Delta \Gamma_{\downarrow}^{(0)}(E + \epsilon(k')) | \frac{1}{2}(k - k') m_\alpha m_{\alpha'} \rangle \theta(k_F - k') \]
  \[ - \frac{1}{\nu} \sum_{m_\alpha m_{\alpha'}} \int \frac{d^3k'}{(2\pi)^3} \langle \frac{1}{2}(k - k') m_\alpha m_{\alpha'} | \Delta \Gamma_{\uparrow}^{(0)}(E + \epsilon(k')) | \frac{1}{2}(k - k') m_\alpha m_{\alpha'} \rangle \theta(k' - k_F) \]

Results for mean-field input

- Realistic interactions generate pairing instabilities
- Avoid with “gap” is sp spectrum according to
  \[ \epsilon(k) = \begin{cases} \int dE \frac{E S_h(k, E)}{S_h(k, E)} & \text{for } k < k_F \\ \int dE \frac{E S_Q(k, E)}{S_Q(k, E)} = E_Q(k) & \text{for } k > k_F \end{cases} \]
- Hole strength spread so “sp energy” below QP energy --> gap
- Requires full knowledge of self-energy
- Self-consistent determination of sp spectrum
- Subsequent determination of self-energy constrained by sp spectrum --> imaginary part exhibits momentum dependent domains
Self-energy below Fermi energy

- Wave vectors 0.1 (solid), 0.51 (dotted), and 2.1 fm\(^{-1}\) (dashed)
- \(k_F = 1.36\) fm\(^{-1}\)
- Im part

Spectral functions with peaks at \(E_Q(k) = \frac{\hbar^2 k^2}{2m} + \text{Re} \Sigma(k; E_Q(k))\)

QP spectral function

\[ S_Q(k, E) = \frac{1}{\pi} \frac{Z_Q^2(k) | W(k) |}{(E - E_Q(k))^2 + (Z_Q(k) W(k))^2} \]

with \(W(k) = \text{Im} \Sigma(k; E_Q(k))\) and

\[ Z_Q(k) = \left\{ 1 - \left( \frac{\partial \text{Re} \Sigma(k; E)}{\partial E} \right)_{E=E_Q(k)} \right\}^{-1} \]

Spectral functions

- Near \(k_F\) about 70% of sp strength is contained in QP peak
- additional \(~13\%) distributed below the Fermi energy
- remaining strength (~17\%) above the Fermi energy
- Note “gap”
- Distribution narrows
- towards \(k_F\)
Spectral functions above the Fermi energy

- Wave vectors 0.79 (dotted), 1.74 (solid), and 3.51 fm\(^{-1}\) (dashed)
- Common distribution -> SRC
- For 0.79 -> 17%
- \(\varepsilon_F + 100\) MeV -> 13%
- above 500 MeV -> 7%
- Without tensor force:
  - strength only 10.5%
  - Momentum distribution
- \(n(0)\) same for different methods
- and interactions (not at \(k_F\))
- Solid: self-consistent

Self-consistent results

- Wave vectors 0.0 (solid), 1.36 (dotted), and 2.1 fm\(^{-1}\) (dashed)
- Limited set of Gaussians --&gt; self-consistent
- Spectral functions
- Main difference:
  - common strength
- Slightly less correlated
- \(Z_F\) from 0.72 to 0.75
**SRC and saturation**

- Energy sum rule
  \[
  \frac{E_0^N}{N} = \frac{\nu}{2\rho} \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\epsilon_F} dE \left( \frac{\hbar^2 k^2}{2m} + E \right) S_h(k;E)
  \]

- Contribution from high momenta after energy integral for different densities for Reid potential

**Saturation properties of nuclear matter**

- Colorful and continuing story

- Initiated by Brueckner: proper treatment of SRC in medium -> ladder diagrams but only include pp propagation

\[
\langle km_\alpha m_{\alpha'} | G(K,E) | k'm_\beta m_{\beta'} \rangle = \langle km_\alpha m_{\alpha'} | V | k'm_\beta m_{\beta'} \rangle + \frac{1}{2} \sum_{m,\gamma} \int \frac{d^3q}{(2\pi)^3} \langle km_\alpha m_{\alpha'} | V | q m_\gamma m_{\gamma'} \rangle \theta(|q+K/2| - k_F) \theta(|K/2 - q| - k_F) \frac{\theta(|q+K/2| - |K/2 - q|)}{E - \epsilon(q + K/2) - \epsilon(K/2 - q) + i\eta} \langle q m_\gamma m_{\gamma'} | G(K,E) | k'm_\beta m_{\beta'} \rangle
\]

- Brueckner G-matrix but Bethe-Goldstone equation...

- Dispersion relation

\[
\langle km_\alpha m_{\alpha'} | G(K,E) | k'm_\beta m_{\beta'} \rangle = \langle km_\alpha m_{\alpha'} | V | k'm_\beta m_{\beta'} \rangle - \frac{1}{\pi} \int_{2\epsilon_F}^{\infty} \frac{dE'}{E'} \Im \langle km_\alpha m_{\alpha'} | \Delta G(K,E') | k'm_\beta m_{\beta'} \rangle \frac{1}{E - E' + i\eta}
\]

\[
\equiv \langle km_\alpha m_{\alpha'} | V | k'm_\beta m_{\beta'} \rangle + \langle km_\alpha m_{\alpha'} | \Delta G(K,E') | k'm_\beta m_{\beta'} \rangle
\]

- Include HF term in “BHF” self-energy

\[
\Sigma_{BHF}(k;E) = \int \frac{d^3k'}{(2\pi)^3} \frac{1}{\rho} \sum_{m_\alpha m_{\alpha'}} \theta(k_F - k') \langle \frac{1}{2} (k - k') m_\alpha m_{\alpha'} | G(k + k'; E + \epsilon(k')) | \frac{1}{2} (k - k') m_\alpha m_{\alpha'} \rangle
\]

- Below Fermi energy: no imaginary part
• DE for $k < k_F$ yields solutions at
  $$\varepsilon_{BHF}(k) = \frac{\hbar^2 k^2}{2m} + \Sigma_{BHF}(k; \varepsilon_{BHF}(k))$$
  with strength $< 1$

• Since there is no imaginary part below the Fermi energy, no momenta above $k_F$ can admix -> problem with particle number

• Only sp energy is determined self-consistently

• Choice of auxiliary potential
  - Standard $U_s(k) = \Sigma_{BHF}(k; \varepsilon_{BHF}(k))$ only for $k < k_F$ (0 above)
  - Continuous $U_c(k) = \Sigma_{BHF}(k; \varepsilon_{BHF}(k))$ all $k$

• Only one calculation of $G$-matrix for standard choice

• Iterations for continuous choice

---

• Propagator
  $$G^{BHF}(k; E) = \frac{\theta(k - k_F)}{E - \varepsilon_{BHF}(k) + i\eta} + \frac{\theta(k_F - k)}{E - \varepsilon_{BHF}(k) - i\eta}$$

• Energy
  $$\frac{E_0^A}{A} = \frac{\nu}{2\rho} \int \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} + \frac{1}{2\rho} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \sum_{m_\alpha m_{\alpha'}} \theta(k_F - k)\theta(k_F - k') \langle \frac{1}{2}(k - k') m_\alpha m_{\alpha'} | G(k + k'; \varepsilon_{BHF}(k) + \varepsilon_{BHF}(k')) | \frac{1}{2}(k - k') m_\alpha m_{\alpha'} \rangle$$

• Rewrite using on-shell self-energy

• First term: kinetic energy free Fermi gas

• Compare
  $$E^{HF} = \frac{1}{2} \sum_p \theta(p_F - p) \left[ \frac{p^2}{2m} + \varepsilon^{HF}(p) \right] = T_{FG} + \frac{1}{2} \sum_{pp'} \theta(p_F - p)\theta(p_F - p') \langle pp' | V | pp' \rangle$$

• so BHF obtained by replacing $V$ by $G$
- Binding energy usually within 10 MeV from empirical volume term in the mass formula even for very strong repulsive cores
- Repulsion always completely cancelled by higher-order terms
- Minimum in density never coincides with empirical value when binding OK -> Coester band

**Historical perspective**

- First attempt using scattering in the medium  
  Brueckner 1954
- Formal development (linked cluster expansion)  
  Goldstone 1956
- Reorganized perturbation expansion (60s)  
  Bethe & students  
  BBG-expansion
- Variational Theory vs. Lowest Order BBG (70s) Clark (also crisis paper)  
  Pandharipande
- Variational results & next hole-line terms (80s) Day, Wiringa
- New insights from experiment & theory  
  NIKHEF Amsterdam about what nucleons are up to in the nucleus (90s)
- 3-hole line terms with continuous choice (90s) Baldo et al.
- Ongoing...
Some remarks

• Variational results gave more binding than G-matrix calculations
• Interest in convergence of Brueckner approach
• Bethe et al.: hole-line expansion
• G-matrix: sums all energy terms with 2 independent hole lines (noninteracting ...)
• Dominant for low-density
• Phase space arguments suggests to group all terms with 3 independent hole lines as the next contribution
• Requires technique from 3-body problem first solved by Faddeev -> Bethe-Faddeev summation
• Including these terms generates minima indicated by * in figure
• Better but not yet good enough

More

• Variational results and 3-hole-line results more or less in agreement
• Baldo et al. also calculated 3-hole-line terms with continuous choice for auxiliary potential and found that results do not depend on choice of auxiliary potential, furthermore 2-hole-line with continuous choice is already sufficient!
• Conclusion: convergence OK for a given realistic two-body interaction for the energy per particle
• Very recently: Monte Carlo calculations may modify this assessment
• Also: for other observables no such statements can be made
• Still nuclear matter saturation problem!
**Possible solutions**

- Include three-body interactions: inevitable on account of isobar
  - Simplest diagram: space of nucleons -> 3-body force
  - Inclusion in nuclear matter still requires phenomenology to get saturation right
  - Also needed for few-body nuclei; there is some incompatibility
- Include aspects of relativity
  - Dirac-BHF approach: ad hoc adaptation of BHF to nucleon spinors
  - Physical effect: coupling to scalar-isoscalar meson reduced with density
  - Antiparticles? Dirac sea? Three-body correlations?
  - Spin-orbit splitting in nuclei OK
  - Nucleons less correlated with higher density? (compare liquid $^3$He)

**Personal perspective**

- Based on results from (e,e'p) reactions as discussed here
  - Nucleons are dressed (substantially) and this should be included in the description of nuclear matter (depletion, high-momentum components in the ground state, propagation w.r.t. correlated ground state --> BHF?)
  - SRC dominate actual value of saturation density
    - From $^{208}$Pb charge density: 0.16 nucleons/fm$^3$
    - Determined from s-shell proton occupancy at small radius
    - Occupancy determined mostly by SRC (see next chapter)
- Result for SCGF of ladders
  - Ghent discrete approach
  - St. Louis gaussians (Libby Roth)
  - ccBHF --> SCGF closer to box
  - Do not include LRC