Quantum Theory of Many-Particle Systems, Phys. 540

- Anomalous propagators for fermions
- BCS
- Baym-Kadanoff strategy: propagator ↔ excited states

- Other questions about last class and assignments?
- Comments?

Finite temperature formalism

- Diagram technique can also be developed for systems at finite T
- In fact, same diagrams appear but there are some significant differences including e.g. Matsubara sums
- Focus on fermions

- Introduce finite T propagator (logical choice)
  \[ G_T(\alpha, \beta; t, t') = -\frac{i}{\hbar} \left\langle T [a_{\alpha\Omega}(t)a_{\beta\Omega}^\dagger(t')] \right\rangle = -\frac{i}{\hbar} \text{Tr} \left( \hat{\rho}_G T [a_{\alpha\Omega}(t)a_{\beta\Omega}^\dagger(t')] \right) \]
  
  - as before \( \hat{\rho}_G = \frac{e^{-\beta(H-\mu\hat{N})}}{Z_G} \)
  
  - Employ grand-canonical description so time evolution (as for bosons) governed by \( \hat{\Omega} = \hat{H} - \mu\hat{N} \)
  
  - Particle number conserved on average --> chemical potential
Modified Heisenberg picture

- Choice (other authors continue with standard version)
  
  \[ a_{\alpha\Omega}(t) = \exp\left\{ \frac{i}{\hbar} \hat{\Omega} t \right\} a_{\alpha} \exp\left\{ -\frac{i}{\hbar} \hat{\Omega} t \right\} \]

- Real-time propagator not ready for perturbation expansion
- Remember: used time-dependent Schrödinger equation before
- Here: other evolution equation for the operator \( \exp(-\hat{\Omega} \tau / \hbar) \)
- relating it to \( \exp(-\beta \hat{\Omega}) \)
- Introduce \( a_{\alpha\Omega}(\tau) = \exp\left\{ \frac{\hat{\Omega} \tau}{\hbar} \right\} a_{\alpha} \exp\left\{ -\frac{\hat{\Omega} \tau}{\hbar} \right\} \tau \) real
- and \( a_{\beta\Omega}^\dagger(\tau) = \exp\left\{ \frac{\hat{\Omega} \tau}{\hbar} \right\} a_{\beta}^\dagger \exp\left\{ -\frac{\hat{\Omega} \tau}{\hbar} \right\} \)

- Not adjoints!
- \( \tau \Rightarrow \tau \) requires imaginary time-ordering operation \( T_{\tau} \)
- smallest to the right etc. keeping fermion sign

Temperature/imaginary time sp propagator

- Define (dropping \( \text{i} \) as in the literature)

  \[
  G_T(\alpha, \beta; \tau - \tau') = -\frac{1}{\hbar} \left\langle T_{\tau} [a_{\alpha\Omega}(\tau) a_{\beta\Omega}^\dagger(\tau')] \right\rangle
  = -\frac{1}{\hbar} \text{Tr} \left( \hat{\rho}_G T_{\tau} [a_{\alpha\Omega}(\tau) a_{\beta\Omega}^\dagger(\tau')] \right)
  \]

- Notation: only \( \tau - \tau' \) dependence
- Quasiperiodic \( \tau - \tau' \) dependence
- Put \( \tau' = 0 \) and write

  \[
  G_T(\alpha, \beta; \tau) = -\frac{1}{\hbar Z_G} \left\{ \theta(\tau) \text{Tr} \left( e^{-(\beta - \tau / \hbar)} \hat{\Omega} a_{\alpha} e^{-\tau \hat{\Omega} / \hbar} a_{\beta}^\dagger \right) \\
  - \theta(-\tau) \text{Tr} \left( e^{-(\beta + \tau / \hbar)} \hat{\Omega} a_{\beta}^\dagger e^{\tau \hat{\Omega} / \hbar} a_{\alpha} \right) \right\}
  \]

- with \( Z_G = \text{Tr} \left( e^{-\beta (\hat{H} - \mu \hat{N})} \right) \)

  \[
  = \sum_N \sum_n \langle \Psi^N_n | e^{-\beta (\hat{H} - \mu \hat{N})} | \Psi^N_n \rangle = \sum_N \sum_n e^{-\beta (\mu_n - \mu) N} 
  \]

- and employing invariance of Trace \( \text{Tr} \left( \hat{A}\hat{B} \ldots \hat{X}\hat{Y} \right) = \text{Tr} \left( \hat{Y}\hat{A}\hat{B} \ldots \hat{X} \right) \)
Periodicity

- Weight factor in imaginary-time propagator in sum over states
  \[ e^{-(\beta \pm \tau / \hbar)\hat{\Omega}} \]
- Spectrum of grand potential not bounded from above
- \( \rightarrow \) Temperature propagator only defined for \( -\beta \hbar \leq \tau \leq \beta \hbar \) ensuring convergence
- Compare propagator for \( -\beta \hbar < \tau < 0 \) with the one at \( \tau + \beta \hbar \)
  \[
  G_T(\alpha, \beta; \tau) = \frac{1}{\hbar Z_G} \text{Tr} \left( e^{-(\beta + \tau / \hbar)\hat{\Omega}} a_\beta^\dagger e^{\tau \hat{\Omega}/\hbar} a_\alpha \right)
  \]
  \[
  G_T(\alpha, \beta; \tau + \beta \hbar) = -\frac{1}{\hbar Z_G} \text{Tr} \left( e^{\tau \hat{\Omega}/\hbar} a_\alpha e^{-(\beta + \tau / \hbar)\hat{\Omega}} a_\beta^\dagger \right)
  \]
- Cyclic property of trace then shows the antiperiodicity
  \[
  G_T(\alpha, \beta; \tau) = -G_T(\alpha, \beta; \tau + \beta \hbar)
  \]

Expansion in discrete frequencies

- Propagator continuous function over \([-\beta \hbar, \beta \hbar]\)
- Boundary condition implies that function can be repeated with period \(2\beta \hbar\)
- Allows expansion as a discrete Fourier series
  \[
  G_T(\alpha, \beta; \tau) = \frac{1}{\hbar \beta} \sum_{n=-\infty}^{+\infty} e^{-iE_n \tau / \hbar} G_T(\alpha, \beta; E_n)
  \]
  \[
  E_n = \frac{(2n + 1)\pi}{\beta}
  \]
- Coefficients contain equivalent information
  \[
  G_T(\alpha, \beta; E_n) = \frac{1}{2} \int_{-\beta \hbar}^{\beta \hbar} d\tau \ e^{iE_n \tau / \hbar} G_T(\alpha, \beta; \tau) = \int_{0}^{\beta \hbar} d\tau \ e^{iE_n \tau / \hbar} G_T(\alpha, \beta; \tau)
  \]
- \( \rightarrow \) temperature propagator in imaginary energy domain
Noninteracting temperature propagator

• Helpful to consider noninteracting Fermi system with
  \( \hat{\Omega}_0 = \hat{H}_0 - \mu \hat{N} \)

• Notation
  \( Z_F^0 = \text{Tr} \left( e^{-\beta \hat{\Omega}_0} \right) \quad \text{and} \quad \rho_G^0 = \frac{e^{-\beta \hat{\Omega}_0}}{Z_F^0} \)

• Then
  \[ G_T^{(0)}(\alpha, \beta; \tau - \tau') = -\frac{1}{\hbar} \langle T_{\tau}[a_{\alpha 0}(\tau) a_{\beta 0}^\dagger(\tau')] \rangle_0 \]
  \[ = -\frac{1}{\hbar} \text{Tr} \left( \rho_G^0 T_{\tau}[a_{\alpha 0}(\tau) a_{\beta 0}^\dagger(\tau')] \right) \]

• Ensemble average over noninteracting systems

• Easy to show that
  \( \hbar \frac{\partial}{\partial \tau} a_{\alpha 0}(\tau) = [\hat{\Omega}_0, a_{\alpha 0}(\tau)] \)
  \[ = \exp \left\{ \hat{\Omega}_0 \tau / \hbar \right\} \left[ \hat{\Omega}_0, a_\alpha \right] \exp \left\{ -\hat{\Omega}_0 \tau / \hbar \right\} \]
  \[ = - (\varepsilon_\alpha - \mu) a_{\alpha 0}(\tau) = -\varepsilon_\alpha a_{\alpha 0}(\tau) \]

• assuming sp eigenstates of noninteracting Hamiltonian \((\varepsilon_{\alpha \mu} = \varepsilon_\alpha - \mu)\)

• Solution
  \( a_{\alpha \Omega_0}(\tau) = e^{-\varepsilon_\alpha \mu \tau / \hbar} a_\alpha \)
  similarly
  \( a_{\alpha \Omega_0}^\dagger(\tau) = e^{\varepsilon_\alpha \mu \tau / \hbar} a_\alpha^\dagger \)

Noninteracting temperature propagator

• So not related by Hermitian conjugation!

• Evaluate propagator
  \[ G_T^{(0)}(\alpha, \beta; \tau - \tau') = -\frac{1}{\hbar} \left\{ \theta(\tau - \tau') e^{-\varepsilon_\alpha \mu \tau / \hbar} e^{\varepsilon_\beta \mu \tau' / \hbar} \langle a_{\alpha} a_{\beta}^\dagger \rangle_0 \right. \]
  \[ - \left. \theta(\tau' - \tau) e^{-\varepsilon_\alpha \mu \tau' / \hbar} e^{\varepsilon_\beta \mu \tau / \hbar} \langle a_{\beta}^\dagger a_{\alpha} \rangle_0 \right\} \]
  \[ = -\frac{1}{\hbar} \delta_{\alpha \beta} e^{-\varepsilon_{\alpha \mu}(\tau - \tau') / \hbar} \left\{ \theta(\tau - \tau') (1 - n_{\alpha 0}^0) - \theta(\tau' - \tau) n_{\alpha 0}^0 \right\} \]

• Only diagonal terms and already evaluated
  \( \langle a_{\alpha} a_{\alpha}^\dagger \rangle_0 = 1 - \langle a_{\alpha}^\dagger a_{\alpha} \rangle_0 = 1 - n_{\alpha 0}^0 \)

• with
  \( \langle a_{\alpha}^\dagger a_{\alpha} \rangle_0 = n_{\alpha 0}^0 = \frac{1}{\exp \{ \beta \varepsilon_{\alpha \mu} \} + 1} \)

• Compare \( T=0 \) -> sharp distinction (blurred at finite \( T \))
  \[ G^{(0)}(\alpha, \beta; t - t') = G_{+}^{(0)}(\alpha, \beta; t - t') + G_{-}^{(0)}(\alpha, \beta; t - t') \]
  \[ = -\frac{i}{\hbar} \delta_{\alpha \beta} \left\{ \theta(t - t') \theta(\alpha - F) e^{-\frac{i}{\hbar} \varepsilon_{\alpha}(t-t')} - \theta(t' - t) \theta(F - \alpha) e^{\frac{i}{\hbar} \varepsilon_{\alpha}(t'-t)} \right\} \]
Energy formulation

• Check antiperiodicity: for \(-\hbar/\beta < \tau < 0\)

\[ G_T^{(0)}(\alpha, \beta; \tau) = \frac{1}{\hbar} \delta_{\alpha \beta} e^{-\varepsilon_{\alpha \mu} \tau/\hbar} n_0^\alpha \]

\[ G_T^{(0)}(\alpha, \beta; \tau + \hbar/\beta) = -\frac{1}{\hbar} \delta_{\alpha \beta} e^{-\varepsilon_{\alpha \mu} (\tau + \beta)/\hbar} (1 - n_0^\alpha) \]

• Note that \(-1 - n_0^\alpha = e^{\beta \varepsilon_{\alpha \mu} n_0^\alpha} \to OK\)

• Fourier coefficients

\[ G_T^{(0)}(\alpha, \beta; E_n) = \delta_{\alpha, \beta} \frac{1}{iE_n - \varepsilon_{\alpha \mu}} \]

• for sp basis of eigenstates of noninteracting Hamiltonian

• If not

\[ G_T^{(0)}(\alpha, \beta; E_n) = \sum_i \frac{z_{i\alpha} z_{i\beta}^*}{iE_n - \varepsilon_{i\mu}} \]

• with i labeling eigenstates of \(H_0\) and \(|i\rangle = \sum_{\alpha} z_{i\alpha} |\alpha\rangle\)

• HF at finite T later

Interaction-picture expansion at finite T

• Similar to T=0 development \(\to\) only sketch

• Start from \(\hat{\Omega} = \hat{\Omega}_0 + \hat{H}_1\) and equivalent of Schrödinger eq.

\[ \hbar \frac{\partial}{\partial \tau} \exp(-\hat{\Omega} \tau/\hbar) = -\hat{\Omega} \exp(-\hat{\Omega} \tau/\hbar) \]

• Heisenberg picture finite T

\[ \hat{O}_\Omega(\tau) = \exp\left\{ \hat{\Omega} \tau/\hbar \right\} \hat{O}_S \exp\left\{ -\hat{\Omega} \tau/\hbar \right\} \]

• Corresponding I picture

\[ \hat{O}(\tau) = \exp\left\{ \hat{O}_0 \tau/\hbar \right\} \hat{O}_S \exp\left\{ -\hat{O}_0 \tau/\hbar \right\} \]

• Relate:

\[ \hat{O}_\Omega(\tau) = \exp\left\{ \hat{\Omega} \tau/\hbar \right\} \exp\left\{ -\hat{\Omega}_0 \tau/\hbar \right\} \hat{O}(\tau) \exp\left\{ \hat{\Omega}_0 \tau/\hbar \right\} \exp\left\{ -\hat{\Omega} \tau/\hbar \right\} \]

\[ = \hat{U}(0, \tau) \hat{O}(\tau) \hat{U}(\tau, 0) \]

• Evolution operator not unitary (but group property OK)

\[ \hat{U}(\tau, \tau') = \exp\left\{ \hat{O}_0 \tau/\hbar \right\} \exp\left\{ -\hat{\Omega}(\tau - \tau')/\hbar \right\} \exp\left\{ -\hat{O}_0 \tau'/\hbar \right\} \]

• also \(\hat{U}(\tau, \tau) = 1\)
Evolution equation

From previous results

\[
\frac{\hbar}{\partial \tau} \hat{U}(\tau, \tau') = \exp \left\{ \hat{\Omega}_0 \tau / \hbar \right\} \left( \hat{\Omega}_0 - \hat{\Omega} \right) \exp \left\{ -\hat{\Omega}(\tau - \tau') / \hbar \right\} \exp \left\{ -\hat{\Omega}_0 \tau' / \hbar \right\} \\
= \exp \left\{ \hat{\Omega}_0 \tau / \hbar \right\} \left( \hat{\Omega}_0 - \hat{\Omega} \right) \exp \left\{ -\hat{\Omega}_0 \tau / \hbar \right\} \hat{U}(\tau, \tau') \\
= -\hat{H}_1(\tau) \hat{U}(\tau, \tau')
\]

with

\[
\hat{H}_1(\tau) = \exp \left\{ \hat{\Omega}_0 \tau / \hbar \right\} \hat{H}_1 \exp \left\{ -\hat{\Omega}_0 \tau / \hbar \right\}
\]

Operator equation solved as before

\[
\hat{U}(\tau, \tau') = \sum_{n=0}^{\infty} \left( \frac{-1}{\hbar} \right)^n \frac{1}{n!} \int_{\tau}^{\tau'} d\tau_1 \cdots \int_{\tau}^{\tau_n} d\tau_n \text{Tr} \left[ \hat{H}_1(\tau_1) \cdots \hat{H}_1(\tau_n) \right]
\]

Rewrite earlier expression for evolution operator \star with \( \tau' = 0 \)

\[
\exp \left\{ -\hat{\Omega} \tau / \hbar \right\} = \exp \left\{ -\hat{\Omega}_0 \tau / \hbar \right\} \hat{U}(\tau, 0)
\]

With \( \tau = \beta \hbar \) --> expansion of grand partition function

\[
Z_G = \text{Tr} \left( e^{-\beta \hat{\Omega}} \right) = \text{Tr} \left( e^{-\beta \hat{\Omega}_0} \hat{U}(\hbar \beta, 0) \right) \\
= \sum_{n=0}^{\infty} \left( \frac{-1}{\hbar} \right)^n \frac{1}{n!} \int_0^{\hbar \beta} d\tau_1 \cdots \int_0^{\hbar \beta} d\tau_n \text{Tr} \left\{ e^{-\beta \hat{\Omega}_0} \text{Tr} \left[ \hat{H}_1(\tau_1) \cdots \hat{H}_1(\tau_n) \right] \right\}
\]

Development

\cdot \text{Basically copying Ch.8.2 from now on}

\cdot \text{Consider } \tau - \tau' > 0 \quad (\text{case of } \tau - \tau' < 0 \text{ analogous})

\[
G_{T+}(\alpha, \beta; \tau - \tau') = -\frac{1}{\hbar} \frac{\text{Tr} \left( e^{-\beta \hat{\Omega}_0} a_{\alpha \beta}(\tau) a_{\beta \alpha}^\dagger(\tau') \right)}{\text{Tr} \left( e^{-\beta \hat{\Omega}_0} \right)} \\
= -\frac{\text{Tr} \left( e^{-\beta \hat{\Omega}_0} \hat{U}(\hbar \beta, 0) \left[ \hat{U}(0, \tau) a_{\alpha \beta}(\tau) \hat{U}(\tau, 0) \right] \left[ \hat{U}(0, \tau') a_{\beta \alpha}^\dagger(\tau') \hat{U}(\tau', 0) \right] \right)}{\text{Tr} \left( e^{-\beta \hat{\Omega}_0} \hat{U}(\hbar \beta, 0) \right)},
\]

\[
= 1 \frac{\text{Tr} \left( e^{-\beta \hat{\Omega}_0} \hat{U}(\hbar \beta, 0) \right)}{\text{Tr} \left( e^{-\beta \hat{\Omega}_0} \hat{U}(\hbar \beta, 0) \right)}
\]

\cdot \text{Use expansion for evolution operators (interaction subscript)}

\[
e^{-\beta \hat{\Omega}_0} \sum_{n=0}^{\infty} \left( \frac{-1}{\hbar} \right)^n \frac{1}{n!} \sum_{k,l,m=0}^{\infty} \delta_{n,k+l+m} \frac{n!}{k!l!m!} \int_{\tau}^{\hbar \beta} dx_1 \cdots \int_{\tau}^{\hbar \beta} dx_k \\
\times \text{Tr} \left[ \hat{H}_1(x_1) \cdots \hat{H}_1(x_k) \right] a_{\alpha}(\tau) \int_{\tau'}^{\tau'} dy_1 \cdots \int_{\tau'}^{\tau'} dy_k \text{Tr} \left[ \hat{H}_1(y_1) \cdots \hat{H}_1(y_k) \right] a_{\beta}^\dagger(\tau') \\
\times \int_{\tau}^{\tau'} dz_1 \cdots \int_{\tau}^{\tau'} dz_m \text{Tr} \left[ \hat{H}_1(z_1) \cdots \hat{H}_1(z_m) \right] \\
= e^{-\beta \hat{\Omega}_0} \sum_{n=0}^{\infty} \left( \frac{-1}{\hbar} \right)^n \frac{1}{n!} \sum_{k,l,m=0}^{\infty} \delta_{n,k+l+m} \frac{n!}{k!l!m!} \int_{\tau}^{\hbar \beta} dx_1 \cdots \int_{\tau}^{\hbar \beta} dx_k \\
\times \text{Tr} \left[ \hat{H}_1(x_1) \cdots \hat{H}_1(x_k) \hat{H}_1(y_1) \cdots \hat{H}_1(y_k) \hat{H}_1(z_1) \cdots \hat{H}_1(z_m) a_{\alpha}(\tau) a_{\beta}^\dagger(\tau') \right]
\]
Development

- Combinatorial factor --> extend boundaries to \([0, \hbar/\beta]\)
- Final result
  \[
  G_T(\alpha, \beta; \tau - \tau') = -\frac{\hbar}{\hbar} \sum_{n=0}^{\infty} \left(\frac{-1}{\hbar}\right)^n \frac{1}{n!} \int_0^{\hbar/\beta} d\tau_1 \cdots \int_0^{\hbar/\beta} d\tau_n \left\langle \mathcal{T}_\tau \left[ \hat{H}_1(\tau_1) \cdots \hat{H}_1(\tau_n) a_\alpha(\tau) a_\beta(\tau') \right] \right\rangle_0
  \]
- Wick's theorem (no proof -> see Ch.24.2.1)
  \[
  \left\langle \mathcal{T}_\tau [\hat{x}_1 \hat{x}_2 \cdots \hat{x}_n] \right\rangle_0 = \text{sum of all fully contracted terms} = \left[ \hat{x}_1^\dagger \hat{x}_2^\dagger \hat{x}_3^\dagger \cdots \hat{x}_n^\dagger \right] + \left[ \hat{x}_1^\dagger \hat{x}_2^\dagger \hat{x}_3^\dagger \cdots \hat{x}_n^\dagger \right] + \ldots
  \]
- Contraction
  \[
  \hat{x}_i^\dagger \hat{x}_j^\dagger = \left\langle \mathcal{T}_\tau [\hat{x}_i \hat{x}_j] \right\rangle_0
  \]
- \(\times\) either addition or removal operator
- Only nonvanishing contraction
  \[
  a_\alpha^\dagger(\tau_i) a_\alpha(\tau_j) = -\hbar G_T^{(0)}(\alpha_i, \alpha_j; \tau_i - \tau_j) = -a_\alpha^\dagger(\tau_j) a_\alpha(\tau_i)
  \]

Diagrams at finite temperature

- Only connected diagrams
  \[
  G(\alpha, \beta; \tau - \tau') = -\frac{1}{\hbar} \sum_{n=0}^{\infty} \left(\frac{-1}{\hbar}\right)^n \frac{1}{n!} \int_0^{\hbar/\beta} d\tau_1 \cdots \int_0^{\hbar/\beta} d\tau_n \left\langle \mathcal{T}_\tau \left[ \hat{H}_1(\tau_1) \cdots \hat{H}_1(\tau_n) a_\alpha(\tau) a_\beta(\tau') \right] \right\rangle_0 \text{connected}
  \]
- No new diagrams but some changes in translation
- Rules for \(m\text{th}\) order \(G_T(\alpha, \beta, \tau - \tau')\)
  
  **Rule 1** Draw all topologically distinct and connected diagrams with \(m\) horizontal interaction lines for \(V\) (dashed) and \(2m + 1\) directed (using arrows) Green’s functions \(G_T^{(0)}\)
  
  **Rule 2** Label the external points (\(\alpha\tau\) and \(\beta\tau'\)) using imaginary times. Label each interaction with an imaginary time \(\tau_i\) and sp quantum numbers
  \[
  \tau \Rightarrow \gamma_{\dot{\epsilon}} \cdots \delta_{\dot{\theta}} \Rightarrow (\gamma|\delta)_{V}[\epsilon|\theta]
  \]
  
  For each full line one writes
  \[
  \tau_i \Rightarrow \alpha \quad \Rightarrow G_T^{(0)}(\alpha, \beta; \tau_i - \tau_j)
  \]
  
  \[
  \tau_j \Rightarrow \beta
  \]
  
  **Rule 3** Sum (integrate) over all internal sp quantum numbers and integrate all \(m\) internal \(\tau_i\) over the interval \([0, \hbar/\beta]\)
  
  **Rule 4** Include a factor \((-\hbar)^m\) and \((-1)^F\) where \(F\) is the number of closed fermion loops
  
  **Rule 5** Interpret equal imaginary times in a propagator as
  \[
  G_T^{(0)}(\alpha, \beta; \tau - \tau')
  \]
Rules

- Rule 3: factor \((-\hbar)^m = \frac{-1}{\hbar} \left( \frac{-1}{\hbar} \right)^m \) \((-\hbar)^{2m+1}\)
- Rule 5: reflects original order of operators
- Extra rules for auxiliary potential (and similar for external potential except for sign)

**Rule 6** Label each \(U\) according to

\[
\Rightarrow \tau_i \quad \begin{array}{c} \alpha \\ \beta \end{array} \Rightarrow \langle \alpha | U | \beta \rangle
\]

**Rule 7** Include a factor \((-1)^k\) and \(k\) additional propagators \(G_T^{(0)}\)

**Example: first-order (antisymmetrized)**

\[
\begin{align*}
\tau & \Rightarrow \alpha \\
\tau_1 & \Rightarrow \begin{array}{c} \gamma \\ \delta \end{array} \\
\tau' & \Rightarrow \beta \\
\Rightarrow (1) \ (-\hbar) \int_0^{\beta \hbar} d\tau_1 \sum_{\gamma \delta} \langle \gamma \delta | V | \epsilon \theta \rangle G_T^{(0)}(\alpha, \gamma; \tau_1) \times G_T^{(0)}(\theta, \delta; \tau_1 - \tau') G_T^{(0)}(\epsilon, \beta; \tau_1 - \tau')
\end{align*}
\]

Energy rules

- Note: we now deal with discrete Fourier series
- Instead of integrations: sums over Matsubara frequencies
- \(m^{th}\) order \(G_T(\alpha, \beta, E_n)\)

**Rule 1** Draw all topologically distinct (direct) and connected diagrams with \(m\) horizontal interaction lines for \(V\) (dashed) and \(2m + 1\) directed (using arrows) Green’s functions \(G_T^{(0)}\)

**Rule 2** Label external points only with sp quantum numbers, e.g. \(\alpha\) and \(\beta\)
Label each interaction with sp quantum numbers

\[
\begin{array}{c} \alpha \\ \beta \end{array} \quad \Rightarrow \langle \alpha \beta | V | \gamma \delta \rangle = (\alpha \beta | V | \gamma \delta) - (\alpha \beta | V | \delta \gamma)
\]

For an arrow line one writes

\[
\begin{array}{c} \alpha \\ \beta \end{array} \quad \Rightarrow G_T^{(0)}(\alpha, \beta; E_k) = \delta_{\alpha, \beta} \frac{1}{E_k - E_k}
\]

but in such a way that energy is conserved for every \(V\)

**Rule 3** Sum (integrate) over all internal sp quantum numbers and sum over all \(m\) internal energies (which should be interpreted as Matsubara energies); a propagator starting and ending on the same interaction line should have a convergence factor \(e^{\frac{i}{\beta} E_k}\).

**Rule 4** Include a factor \((-1/\beta)^m\) and \((-1)^F\) where \(F\) is the number of closed fermion loops

**Rule 5** Include a factor of \(\frac{1}{2}\) for equivalent pairs of lines
**Rules**

- **Factor**: $(-1/\beta)^m$
  - discrete FT of an imaginary time term in this order yields $m+1$ $\tau$-integrations
  - $2m+1$ propagators from time to frequency: $1/(\hbar\beta)^{2m+1}$
  - time integrations: $m+1 \rightarrow$ Kronecker deltas $(m+1)$ each providing $\hbar\beta$
  - combine with original factor $-\hbar^m$

- Ordering for same interaction $\rightarrow \mathcal{G}_T(\alpha\beta; \tau = 0^− = -\eta)$

- So
  $$\mathcal{G}_T(\alpha, \beta; \tau = -\eta) = \frac{1}{\beta\hbar} \sum_{n=-\infty}^{+\infty} \mathcal{G}_T(\alpha, \beta; E_n) e^{i\eta E_n}$$

- **U rules**: Rule 6 Label each $U$ according to
  $$\begin{array}{ccc} 
  \bullet & \otimes & \bullet \\
  \alpha & \beta
  \end{array} \Rightarrow \langle \alpha | U | \beta \rangle$$

**Rule 7** Include a factor $(-1)^k$ and $k$ additional propagators $G^{(0)}$

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**Example**

- **First-order**
  $$\begin{array}{ccc}
  \bullet & \otimes & \bullet \\
  \alpha & \beta
  \end{array} \Rightarrow \sum_{\gamma\delta} G^{(0)}(\alpha, \gamma; E_n)$$

- Infinite sums over Matsubara energies $E_n = (2n + 1)\pi/\beta$ can be calculated by noting that the Fermi function $f(z) = 1/(1 + e^{\beta z})$ has its only singularities precisely at the imaginary Matsubara energies $iE_n$: all simple poles with residue $-1/\beta$

- Example: first-order self-energy
  $$\Sigma^{(1)}(\gamma, \delta; E_n) = \sum_{\theta} \langle \gamma\theta | V | \delta\theta \rangle S_{\theta}$$
First-order self-energy sum

- Energy sum
  \[ S_\theta = \frac{1}{\beta} \sum_{m=-\infty}^{+\infty} \frac{e^{i\eta E_m}}{iE_m - \varepsilon_\theta \mu} = \sum_m F(iE_m). \]

- where the analytic function \( F(z) = \frac{1}{\beta} \frac{e^{\eta z}}{z - \varepsilon_\theta \mu} \) has a pole on the real axis

- Consider contour counterclockwise along large circle (-\( \to \) infinity) centered at the origin for \( \int_C dz \ f(z) F(z) \) \( f(z) = \frac{1}{1 + e^{\beta z}} \)

- For \( |z| \to \infty \) integrand \( \to \frac{e^{z(\eta - \beta)}}{z} \) for \( \text{Re} \ z > 0 \) and \( \to \frac{e^{\eta z}}{z} \) for \( \text{Re} \ z < 0 \)

- Since \( 0 < \eta < \beta \) integral vanishes exponentially (infinite radius)

- Apply residue theorem -->

\[ S_\theta = \frac{1}{\beta} \sum_m \left( -\frac{1}{\beta} \right) F(iE_m) + \frac{1}{\beta} e^{\eta \varepsilon_\theta \mu} f(\varepsilon_\theta \mu) \]

- and therefore \( S_\theta = f(\varepsilon_\theta \mu) = n_\theta^0 \) yields thermal occupation

- Same technique for higher-order diagrams

- Second-order self-energy

\[ \Sigma^{(2)}(\gamma, \delta; E_n) = \frac{1}{2} \sum_{\lambda \epsilon \theta} \langle \gamma \lambda | V | \epsilon \theta \rangle \langle \epsilon \theta | V | \delta \lambda \rangle S_{\lambda \epsilon \theta} \]
more energy sums

\[ S_{\lambda \epsilon \theta} = -\frac{1}{\beta^2} \sum_{k,m=-\infty}^{+\infty} \frac{1}{(iE_k - \epsilon \epsilon_{\mu})} \frac{1}{(iE_m - \epsilon \theta_{\mu})} \frac{1}{(iE_k + E_m - E_n - \epsilon \lambda_{\mu})} \]

\[ = -\frac{1}{\beta^2} \sum_{k,m} \frac{1}{iE_k - \epsilon \epsilon_{\mu}} G(iE_m) \]

• Now relevant analytic function is

\[ G(z) = \frac{1}{(z - \epsilon \theta_{\mu})} \frac{1}{(z + i(E_k - E_n) - \epsilon \lambda_{\mu})} \]

• \( \rightarrow \) single pole real axis plus additional ones

• Imaginary part of the latter EVEN multiples of \( \pi/\beta \) and don’t coincide with the poles of the Fermi function

• Again large circle contour of \( \int_C dz \, f(z)G(z) \) vanishes so residue theorem yields

\[ 0 = \sum_m \left( -\frac{1}{\beta} \right) G(iE_m) + \frac{f(\epsilon \theta_{\mu}) - f(\epsilon \lambda_{\mu})}{\epsilon \theta_{\mu} - \epsilon \lambda_{\mu} + i(E_k - E_n)} \]

• Note: \( f(\epsilon \lambda_{\mu} + i(E_n - E_k)) = f(\epsilon \lambda_{\mu}) \) was used

Final summation

• Inserting this result yields

\[ S_{\lambda \epsilon \theta} = -\frac{1}{\beta} \sum_{k=-\infty}^{+\infty} \frac{f(\epsilon \theta_{\mu}) - f(\epsilon \lambda_{\mu})}{(iE_k - \epsilon \epsilon_{\mu})(iE_k - iE_n + \epsilon \theta_{\mu} - \epsilon \lambda_{\mu})} \]

• Use the same procedure to evaluate remaining Matsubara sum

\[ S_{\lambda \epsilon \theta} = \frac{f(\epsilon \theta_{\mu}) - f(\epsilon \lambda_{\mu})}{iE_n + \epsilon \lambda_{\mu} - \epsilon \theta_{\mu} - \epsilon \epsilon_{\mu}} (f(\epsilon \epsilon_{\mu}) - f(iE_n + \epsilon \lambda_{\mu} - \epsilon \theta_{\mu})) \]

\[ = \frac{n_0^0(1 - n_0^0)(1 - n_0^0) + (1 - n_0^0)n_0^0n_0^0}{iE_n + \epsilon \lambda_{\mu} - \epsilon \theta_{\mu} - \epsilon \epsilon_{\mu}} \]

• Compare with \( T=0 \) evaluation in second-order self-energy

\[ \frac{\theta(\epsilon - F)\theta(\nu - F)\theta(F - \lambda)}{E - (\epsilon + \epsilon + \epsilon - \lambda) + i\eta} \quad + \quad \frac{\theta(F - \epsilon)\theta(F - \nu)\theta(\lambda - F)}{E + (\epsilon - \lambda - \epsilon - \nu) - i\eta} \]

• and note similarities and differences
Quantum Theory of Many-Particle Systems, Phys. 540

- Imaginary time / temperature propagator
- Diagrammatic expansion
- Examples of first- and second-order self-energy calculations doing Matsubara sums
- Other questions about last class and assignments?
- Comments?

Spectral representation

- What information is contained in finite T propagator?
- Select removal part of propagator (time version $\rightarrow 0^-$)

\[ \hbar G_T(\alpha, \beta; 0^-) = \frac{1}{Z_G} \text{Tr} \left( e^{-\beta \hat{\Omega}} a_\beta^+ a_\alpha \right) = \langle a_\beta^+ a_\alpha \rangle \]

- So for a one-body operator: ensemble average

\[ \langle \hat{O} \rangle = \sum_{\alpha, \beta} \langle \alpha | O | \beta \rangle \hbar G_T(\beta, \alpha; 0^-) \]

- In imaginary-energy version

\[ \frac{1}{\beta} \sum_n e^{i\eta E_n} G_T(\alpha, \beta; E_n) = \langle a_\beta^+ a_\alpha \rangle \]

- Also at finite temperature it is possible to obtain the ensemble average of the two-body interaction from sp propagator (book)
Insert exact eigenstates

- Helps clarify content of sp propagator at finite T
- For \( \tau > 0 \)
  \[
  G_T(\alpha, \beta; \tau) = -\frac{1}{\hbar Z_G} \text{Tr} \left( e^{-\beta \hat{\Omega}} e^{\hat{\Omega} \tau / \hbar} a_\alpha e^{-\Omega \tau / \hbar} a_\beta^\dagger \right)
  = -\frac{1}{\hbar Z_G} \sum_{kl} e^{-\beta \Omega_k} z_{kl\alpha} z_{kl\beta}^* e^{-\tau (\Omega_l - \Omega_k) / \hbar}
  \]
- with \( z_{kl\alpha} = \langle \Psi_k | a_\alpha | \Psi_l \rangle \)
- Note double sum (unlike \( T=0 \)) so amplitudes more general
- Energy version
  \[
  G_T(\alpha, \beta; E_n) = -\frac{1}{\hbar Z_G} \sum_{kl} z_{kl\alpha} z_{kl\beta}^* e^{-\beta \Omega_k} \int_0^{\beta \hbar} d\tau \, e^{(\Omega_k - \Omega_l + i E_n) \tau / \hbar}
  = \frac{1}{Z_G} \sum_{kl} z_{kl\alpha} z_{kl\beta}^* \frac{e^{-\beta \Omega_l} + e^{-\beta \Omega_k}}{i E_n + \Omega_k - \Omega_l}
  \]

Connection

- Connection possible between
  \[
  G_T(\alpha, \beta; E_n) = -\frac{1}{\hbar Z_G} \sum_{kl} z_{kl\alpha} z_{kl\beta}^* e^{-\beta \Omega_k} \int_0^{\beta \hbar} d\tau \, e^{(\Omega_k - \Omega_l + i E_n) \tau / \hbar}
  = \frac{1}{Z_G} \sum_{kl} z_{kl\alpha} z_{kl\beta}^* \frac{e^{-\beta \Omega_l} + e^{-\beta \Omega_k}}{i E_n + \Omega_k - \Omega_l}
  \]
- and real-time propagator
  \[
  G_T(\alpha, \beta; t - t') = -\frac{i}{\hbar} \left\langle T [a_{\alpha \alpha}(t) a_{\beta \beta}(t')] \right\rangle = -\frac{i}{\hbar} \text{Tr} \left( \hat{T} [a_{\alpha \alpha}(t) a_{\beta \beta}(t')] \right)
  \]
- with FT
  \[
  G_T(\alpha, \beta; E) = \int_{-\infty}^{+\infty} dt(t - t') e^{i E(t-t')/\hbar} G_T(\alpha, \beta; t - t')
  \]
  \[
  G_T(\alpha, \beta; E) = \frac{1}{i \hbar Z_G} \sum_{kl} z_{kl\alpha} z_{kl\beta}^* e^{i (\Omega_k - \Omega_l)(t-t')/\hbar} \left\{ e^{-\beta \Omega_k} - \theta(t-t') e^{-\beta \Omega_l} \right\}
  \]
- then FT --> Lehmann
  \[
  G_T(\alpha, \beta; E) = \frac{1}{Z_G} \sum_{kl} z_{kl\alpha} z_{kl\beta}^* \left( \frac{e^{-\beta \Omega_k}}{E + \Omega_k - \Omega_l + i \eta} + \frac{e^{-\beta \Omega_l}}{E + \Omega_k - \Omega_l - i \eta} \right)
  \]
Spectral functions

- Introduce hermitian and antihermitian components of real-time propagator

\[ \mathcal{H} G_T(\alpha, \beta; E) = \frac{1}{2} \left( G_T(\alpha, \beta; E) + G^*_T(\beta, \alpha; E) \right) \]

\[ \mathcal{A} G_T(\alpha, \beta; E) = \frac{1}{2i} \left( G_T(\alpha, \beta; E) - G^*_T(\beta, \alpha; E) \right) \]

- Use Lehmann representation and the usual \( \frac{1}{x \pm i \eta} = \mathcal{P} \frac{1}{x \mp i \pi \delta(x)} \) \( \rightarrow \)

\[ \mathcal{H} G_T(\alpha, \beta; E) = \frac{1}{Z_G} \sum_{kl} z_{k\alpha} z_{k\beta}^* e^{-\beta \Omega_k} \mathcal{P} \frac{1 + e^{\beta(\Omega_k - \Omega_l)}}{E + \Omega_k - \Omega_l} \]

\[ \mathcal{A} G_T(\alpha, \beta; E) = \frac{\pi}{Z_G} \sum_{kl} z_{k\alpha} z_{k\beta}^* e^{-\beta \Omega_k} \delta(E + \Omega_k - \Omega_l)(e^{\beta(\Omega_k - \Omega_l)} - 1) \]

\[ = - \frac{\pi}{Z_G} \sum_{kl} z_{k\alpha} z_{k\beta}^* e^{-\beta \Omega_k} \delta(E + \Omega_k - \Omega_l)(1 + e^{\beta(\Omega_k - \Omega_l)}) \tanh\left( \frac{\beta E}{2} \right) \]

Dispersion relation

- Linked by dispersion relation

\[ \mathcal{H} G_T(\alpha, \beta; E) = -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{dE'}{E - E'} \mathcal{A} G_T(\alpha, \beta; E') \coth\left( \frac{\beta E'}{2} \right) \]

- Introduce spectral function matrix as basic quantity

\[ S(\alpha, \beta; E) = \frac{1}{Z_G} \sum_{kl} z_{k\alpha} z_{k\beta}^* e^{-\beta \Omega_k} \delta(E + \Omega_k - \Omega_l)(1 + e^{-\beta E}) \]

- since \( \mathcal{H} G_T(\alpha, \beta; E) = \mathcal{P} \int_{-\infty}^{+\infty} \frac{dE'}{E - E'} S(\alpha, \beta; E') \)

- and \( \mathcal{A} G_T(\alpha, \beta; E) = -\pi \tanh\left( \frac{\beta E}{2} \right) S(\alpha, \beta; E) \)
More spectral function matrix

• Rewrite spectral matrix

\[ S(\alpha, \beta; E) = \frac{1}{Z_G} \sum_{kl} z_{kl\alpha} z_{kl\beta}^* \delta(E + \Omega_k - \Omega_l)(e^{-\beta \Omega_k} + e^{-\beta \Omega_l}) \]

• Limit \( T \to 0 \) last factor filters only ground-state contribution from each summation

• Sum rule

\[ \int_{-\infty}^{+\infty} dE \ S(\alpha, \beta; E) = \frac{1}{Z_G} \sum_{kl} z_{kl\alpha} z_{kl\beta}^* (e^{-\beta \Omega_k} + e^{-\beta \Omega_l}) = \langle \hat{\rho} G a_\alpha a_\beta + \hat{\rho} G a_\beta a_\alpha \rangle = \delta_{\alpha\beta} \]

• Important: same spectral function matrix determines imaginary-energy propagator!!

\[ G_T(\alpha, \beta; E_n) = \int_{-\infty}^{+\infty} \frac{dE'}{iE_n - E'} S(\alpha, \beta; E') \]

Connection

• Appears convenient way to calculate one from the other propagator (the latter \( \to \) diagrams)

• Requires analytic continuation (OK)

• Real-time propagator obtained from

\[ S(\alpha, \beta; E) = \frac{1}{2\pi i} [G_T(\alpha, \beta; -iE - \eta) - G_T(\alpha, \beta; -iE + \eta)] = \frac{1}{\pi} AG_T(\alpha, \beta; -iE - \eta) \]

• and earlier results

• Example of noninteracting system in the book
Dyson equation

- Analysis identical to T=0
- So immediately (introducing irreducible self-energy at finite T)
  \[ G_T(\alpha, \beta; E_n) = G_T^{(0)}(\alpha, \beta; E_n) + \sum_{\gamma\delta} G_T^{(0)}(\alpha, \gamma; E_n) \Sigma(\gamma, \delta; E_n) G_T(\delta, \beta; E_n) \]
- Homogeneous systems (suppressing discrete quantum numbers)
  \[ G_T(p_\alpha, p_\beta; E_n) = \delta_{p_\alpha, p_\beta} G_T(p_\alpha; E_n) \]
- Inverse of noninteracting propagator
  \[ \frac{1}{G_T^{(0)}(p; E_n)} = iE_n - \varepsilon(p) + \mu \]
- So solution
  \[ G_T(p_\alpha; E_n) = \frac{1}{iE_n - \varepsilon(p) + \mu - \Sigma(p; E_n)} \]
- Spectral function (see previous slide)
  \[ S(p; E) = \frac{1}{\pi} \text{Im} \frac{1}{E - \varepsilon(p) + \mu - \Sigma(p; -iE - \eta)} \]

Observations

- Quasiparticle excitations --> energy
  \[ E_Q(p) = \varepsilon(p) - \mu + \text{Re} \Sigma(p; -iE_Q(p) - \eta) \]
- where spectral function peaks
- Width
  \[ W(p; E) = \frac{1}{\pi} \text{Im} \Sigma(p; -iE - \eta) \]
- Small near chemical potential at low temperature
- At finite temperature width remains finite
- Spectral functions illustrated later
Hartree-Fock at finite T

• Use self-consistent lowest-order self-energy
  \[ \Sigma^{HF}(\gamma, \delta; E_n) = \frac{1}{\beta} \sum_{\epsilon \theta} \langle \gamma \epsilon | V | \delta \theta \rangle \sum_k G_T(\theta, \epsilon; E_k)e^{i\eta E_k} \]

• Use result from Matsubara sum
  \[ \Sigma^{HF}(\gamma, \delta) = \sum_{\epsilon \theta} \langle \gamma \epsilon | V | \delta \theta \rangle \langle a^\dagger_\epsilon a_\theta \rangle \]

• average of tp interaction over ensemble average of one-body density matrix at finite T -- still static as for T=0

• Again HF solution has noninteracting form
  \[ G_T^{HF}(\alpha, \beta; E_n) = \sum_i \frac{z^{HF}_i z^{HF*}_i}{iE_n - \epsilon_{i\mu}} \]

• with
  \[ \sum_\delta \{ \langle \gamma | T | \delta \rangle + \Sigma^{HF}(\gamma, \delta) \} z^{HF*}_\delta = \epsilon^{HF}_i z^{HF}_\gamma \]

• self-consistency from
  \[ \Sigma^{HF}(\gamma, \delta) = \sum_{\epsilon \theta} \langle \gamma \epsilon | V | \delta \theta \rangle \left( \sum_i z^{HF}_i z^{HF*}_i f(\epsilon_i - \mu) \right) \]

more HF

• HF potential depends on HF orbitals but ALSO on HF spectrum through thermal occupation factors \( f(\epsilon_{i\mu}) \)

• Consequence for homogeneous system!

• At finite T
  \[ \epsilon^{HF}(p) = \frac{p^2}{2m} + \sum_{p'} \langle pp' | V | pp' \rangle f(\epsilon^{HF}(p') - \mu) \]

• represents a self-consistency problem (see later for an example of momentum distribution in HF)

• Skip formalism for treatment of SRC at finite T

• Show some results
Applications

• Arnau Rios thesis results (University of Barcelona 2007)
• Realistic CDBonn interaction (moderately soft)
• Spectral functions for three typical momenta $\rightarrow 0, k_F, 2k_F$
• $T = 10$ MeV
• Dotted: Fermi function
• 5 densities
• Extra width $\leftrightarrow T$

Temperature dependence

• Same momenta
• Density $\rho = 0.16$ fm$^{-3}$
• Width computationally helpful compared to sharp features at $T=0$
• Zero at Fermi energy for $T=0$ disappears $\rightarrow$ at most a dip
• Tails hardly $T$-dependent
Momentum distribution

- Interplay between thermal and short-range correlations
- $T = 5 \text{ MeV}$
  - $\rho = 0.32 \text{ fm}^{-3}$
- Scales

Pairing at finite $T$

- Similar development as for $T=0$
- Direct transcription possible from $T=0$
- Gorkov equations
  \[
  G_{11T}(pm; E_n) = G_{11T}^{(0)}(pm; E_n) + G_{11T}^{(0)}(pm; E_n)\Sigma_{11}(pm; E_n)G_{11T}(pm; E_n) \\
  + G_{11T}^{(0)}(pm; E_n)\Sigma_{12}(pm; E_n)G_{21T}(pm; E_n)
  \]
  \[
  G_{21T}(pm; E_n) = G_{22T}^{(0)}(pm; E_n)\Sigma_{21}(pm; E_n)G_{11T}(pm; E_n) \\
  + G_{22T}^{(0)}(pm; E_n)\Sigma_{22}(pm; E_n)G_{21T}(pm; E_n)
  \]
- Noninteracting propagators
  \[
  G_{11T}^{(0)}(pm; E_n) = \frac{1}{iE_n - \varepsilon_{p\mu}}
  \]
  \[
  G_{22T}^{(0)}(pm; E_n) = \frac{1}{iE_n + \varepsilon_{p\mu}}
  \]
- Solution similar structure as for $T=0$
\[ G_{11}^{(0)}(p; E_n) = G_{11}^{N}(p; E_n) + G_{11}^{N}(p; E_n) \Sigma_{12}(p; E_n) G_{21}(p; E_n) \]
\[ G_{21}(p; E_n) = G_{22}^{N}(p; E_n) \Sigma_{21}(p; E_n) G_{11}^{N}(p; E_n) \]

* Check equivalence

* Useful for strong normal self-energy

\[ G_{21}(p; E_n) = G_{N22}^{(0)}(p; E_n) + \Sigma_{21}(p; E_n) G_{11}^{N}(p; E_n) \]

\[ G_{22}(p; E_n) = G_{N22}^{(0)}(p; E_n) + \Sigma_{21}(p; E_n) G_{11}^{N}(p; E_n) \]

\[ \Sigma_{21}(p; E_n) = \left(-1\right) \left(-\frac{1}{\beta}\right) \sum_{p'} \frac{W(p - p')}{V} \sum_{n} e^{iE_n} G_{21}(p' m; E_n) \]
\[ = \frac{1}{\beta} \sum_{p'} \frac{W(p - p')}{V} \sum_{n} e^{iE_n} G_{22}^{N}(p' m; E_n) \Sigma_{21}(p' m) G_{11}^{N}(p' m; E_n) \]

* Last equality from second Gorkov equation

* For now only include normal HF self-energy

\[ G_{22}^{N}(p; E_n) \rightarrow G_{22}^{HF}(p; E_n) = \frac{1}{iE_n + \chi_p} \]

* with \( \chi_p = \epsilon_{p\mu} + V_p \)

* Anticipate \( G_{11}^{N}(p; E_n) \rightarrow \frac{u_p^2}{iE_n - E_p} + \frac{v_p^2}{iE_n + E_p} \)

* with \( E_p = \sqrt{\chi_p^2 + \Delta_p^2} \)
Development

• As in Ch.22 we write \( \Sigma_{21}(pm) = \Delta_p s_m \)

• Combine, use same expressions for residues of superfluid propagators as in Ch.22, and evaluate Matsubara sum (decompose in partial fractions) \( \rightarrow \) gap equation at finite \( T \)

\[
\Delta_p = -\frac{1}{2} \sum_{p'} \frac{W(p-p') \Delta_{p'}}{E_{p'}} \text{tanh} \left( \frac{\beta E_{p'}}{2} \right)
\]

• Reduces to gap equation for \( T \rightarrow 0 \)

• Study for simplified case simulating normal superconductors when \( c \) is identified with Debye energy

• Same steps: \( 1 = \frac{\lambda}{2} \int_{-c}^{+c} d\chi \frac{D(\chi)}{\sqrt{\chi^2 + \Delta^2}} \text{tanh} \left( \frac{\beta}{2} \sqrt{\chi^2 + \Delta^2} \right) \)

• Study for \( T \rightarrow T_c \) where gap vanishes

Further development

• As in Ch.18 we extract density of states at the Fermi energy

• Using symmetry of the integrand and putting \( z = \beta \chi / 2 \)

\[
\frac{1}{\lambda D(0)} = \int_0^{\beta c/2} \frac{dz}{z} \text{tanh} z
\]

• Integrating by parts

\[
\frac{1}{\lambda D(0)} = [\ln z \text{tanh} z]_0^{\beta c/2} - \int_0^{\beta c/2} \frac{dz}{z} \ln z \text{sech}^2 z
\]

• Practical cases upper limit large \( \rightarrow \) infinity \( \rightarrow \) look up integral and rewrite \( k_B T_c = \frac{2 e^\gamma}{\pi} c e^{-1/\lambda D(0)} \approx 1.13 c e^{-1/\lambda D(0)} \)

• \( \gamma \approx 0.5772 \) Euler’s constant

• Compare with \( T=0 \) gap \( \rightarrow \) ratio \( \frac{\Delta_{T=0}}{k_B T_c} = \pi e^{-\gamma} \approx 1.76 \)

• In good agreement with data and independent of material

• Other results see book and FW
Gorkov equations with dressed propagators

• Infinite nuclear systems display pairing instabilities when ladder diagrams are summed

• BCS treatment of $^3S_1-^3D_1$ interaction generates large gaps inconsistent with empirical information

• But: SRC change sp propagators substantially → may have a large effect on pairing properties

• Study pairing with normal self-energy terms due to SRC included

• Normal propagator

\[
G_{22T}^N(pm; E_n) = \int_{-\infty}^{\infty} dE \frac{S(p; E)}{iE_n + E}
\]

• Superfluid propagator

\[
G_{11T}^N(pm; E_n) = \int_{-\infty}^{\infty} dE' \frac{S_s(p; E')}{iE_n - E'}
\]

Energy sum in gap equation

• Defines generalized denominator in gap equation

\[
- \frac{1}{2E_p'} \equiv \frac{1}{\beta} \sum_n e^{i\eta E_n} \int_{-\infty}^{\infty} dE \frac{S(p; E)}{iE_n + E} \int_{-\infty}^{\infty} dE' \frac{S_s(p; E')}{iE_n - E'}
\]

\[
= \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE' S(p; E)S_s(p; E') \frac{1 - f(E) - f(E')}{-E - E'}
\]

• In spite of denominator, integrand well-behaved (see earlier)

• Nuclear applications require gap equation in partial-wave basis to treat strong state dependence of NN interaction

• Also need pairing with S=1 quantum numbers for example

• Generalize gap equation to allow more general spin structure

\[
\Delta_{pmm'} = -\frac{1}{2} \sum_{p'\tilde{m}\tilde{m}'} (pm - pm'|V|p'\tilde{m} - p'\tilde{m}') \frac{\Delta p'\tilde{m}\tilde{m}'}{E_{p'}} \tanh \left( \frac{\beta E_{p'}}{2} \right)
\]
Generalized gap equation

- Total spin --> orbital angular momentum --> possible coupled channel --> total angular momentum

\[ \Delta_{pmm'} = \sum_{\ell m_{\ell}} \left( \frac{1}{2} m \frac{1}{2} m' |S \ m + m' \right) \]

\[ (S \ m + m' \ \ell \ m_{\ell} |J \ m + m' + m_{\ell}) Y_{\ell m_{\ell}}(\hat{p}) \Delta^{JST}_{\ell}(p) \]

- If energy denominator is angle-averaged (assumed in energy sum), gap function does not depend on projection of total angular momentum --> gap equation

\[ \Delta^{JST}_{\ell}(p) = -\frac{1}{2} \sum_{\ell'} \int_{0}^{\infty} dp' p'^2 \langle \ell' | V^{JST} | \ell' \rangle \Delta^{JST}_{\ell'}(p') \]

- Extra factor \( \frac{1}{2} \) --> antisymmetrized matrix elements

Link with BCS

- Energy sum

\[ -\frac{1}{2E_p} = \frac{1}{\beta} \sum_{n} e^{i\eta E_n} \int_{-\infty}^{\infty} dE \frac{S(p; E)}{iE_n + E} \int_{-\infty}^{\infty} dE' \frac{S_s(p; E')}{iE_n - E'} \]

\[ = \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE' S(p; E)S_s(p; E') \left( 1 - f(E) - f(E') \right) \frac{1}{-E - E'} \]

- Insert in energy sum

\[ S_s(p'; E') = \delta(E - \chi_{p'}) \]

\[ S_s(p'; E') = \left( \frac{E_{p'}}{2E_{p'}} \delta(E' - E_{p'}) + \frac{E_{p'} - \chi_{p'}}{2E_{p'}} \delta(E' + E_{p'}) \right) \]

- yields standard BCS equation

- Ignoring difference between \( S \) and \( S_s \), gap equation corresponds to homogeneous scattering equation at \( E_{tot} = 0 \) and total momentum zero --> ladder equation must generate a pole at that energy --> bound two-particle state --> pairing if fullfilled
Normal self-energy properties

- Temperature dependence of self-consistently calculated imaginary part of self-energy
- \( k = 225 \text{ MeV/c} \)
- \( T = 4, 7, \text{ and } 10 \text{ MeV above critical temperature for pairing} \)
- Empirical density
- CDBonn interaction
- \( T=0 \) extrapolated with the constraint that it vanishes at the Fermi energy

Normal self-energy for nuclear and neutron matter

- Both real and imaginary parts for Argonne V18 and CDBonn interactions
- \( k = 225 \text{ MeV/c} \)
- Nuclear matter normal density
- Neutron matter
  \( \rho = 0.08 \text{ fm}^{-3} \)
- \( T = 5 \text{ MeV} \)
- Different interactions!
- Depletion at \( k = 0 \) 11\% for CDBonn and 13\% for Argonne V18
**Numerical solution of the gap equation**

\[ \Delta(k) = \sum \langle k, \bar{k} | V | k', \bar{k}' \rangle \frac{\Delta(k')}{\omega - 2E(k')} \text{ with } E(k) = \sqrt{(\epsilon_k - \mu)^2 + \Delta(k)^2} \text{ and } \omega = 0 \]

Define:

\[ \delta(k) = \frac{\Delta(k)}{\omega - 2E(k)} \]

\[
\begin{bmatrix}
2E(k_1) + \langle k_1 | V | k_1 \rangle & \cdots & \langle k_1 | V | k_N \rangle \\
\vdots & \ddots & \vdots \\
\langle k_N | V | k_1 \rangle & \cdots & 2E(k_N) + \langle k_N | V | k_N \rangle
\end{bmatrix}
\begin{bmatrix}
\delta(k_1) \\
\vdots \\
\delta(k_N)
\end{bmatrix} = \omega
\begin{bmatrix}
\delta(k_1) \\
\vdots \\
\delta(k_N)
\end{bmatrix}
\]

**Eigenvalue problem for a pair of nucleons at \( \omega = 0 \)**

**Steps of the calculation:**

- Assume \( \Delta(k) \) and determine \( E(k) \)
- Solve eigenvalue equation and evaluate new \( \Delta(k) \)
  - If lowest eigenvalue \( \omega < 0 \) enhance \( \Delta(k) \) (resp. \( \delta(k) \))
  - If lowest eigenvalue \( \omega > 0 \) reduce \( \Delta(k) \)
- Repeat until convergence

**Pairing of strongly correlated nucleons**

**Standard BCS results**

- Gap functions for symmetric and neutron matter at corresponding densities
- Spectrum
  \[ \varepsilon(p) = \chi_p + \mu \]
- from
  \[ \varepsilon(p) = \frac{p^2}{2m} + \text{Re} \sum(p, \varepsilon(p) - \mu) \]
- extrapolated to \( T = 0 \)
  (necessary because of pairing instabilities)
- Nuclear matter gap too large but similar for both interactions

**Nuclear matter**

\[ ^3S_1-^3D_1 \quad \Delta = \sqrt{\Delta_0^2 + \Delta_2^2} \]

**Neutron matter**

\[ ^1S_0 \]

**Argonne V18 dashed**

QMPT 540
Pairing with dressed nucleons

- Clarify role of SRC and temperature
- Evaluate (note both correspond to normal spectral functions)
  \[
  \frac{1}{-2\tilde{\chi}_p} \equiv \int_{-\infty}^{+\infty} dE \int_{-\infty}^{+\infty} dE' S(p; E)S(p; E') \frac{1 - f(E) - f(E')}{-E - E'}
  \]
  - defining average energy denominator
- Mean-field limit uses \( S(p; E) = \delta(E - \chi_p) \) at \( T=0 \)
- Prescription generates
  \[
  \frac{1}{-2\tilde{\chi}_p} \xrightarrow{mf, T=0} \frac{1}{-2|\chi_p|}
  \]
  - \( \tilde{\chi}_p \) clarifies role of \( T \) and SRC
- \( T=0 \) qp; \( T=5 \) qp; \( T=5 \) with SRC

Gap in nuclear matter \( ^3S_1-^3D_1 \)

- Gap at the Fermi momentum
- CDBonn
  - Densities
    - 0.04 fm\(^{-3}\) dashed
    - 0.08 fm\(^{-3}\) dot-dashed
    - 0.16 fm\(^{-3}\) dotted
  - Thin lines: dressed
- Normal density no longer superfluid!!!!!!
- No longer inconsistent with empirical information from nuclei
- \( T \)-dependence \( \neq \) BCS
Superfluid spectral function

- Solid with
- Dashed without pairing
- $p = 193$ MeV/c
- $T = 0.5$ MeV
- Nuclear matter
  - $\rho = 0.08$ fm$^{-3}$
- Pairing effect \sim as BCS

\[ 2\pi S(p;E) \text{[MeV]}^{-1} \]
\[ E \text{[MeV]} \]

Gap in neutron matter

- $^1S_0$ gap in neutron matter as function of $T$ for CDBonn
- Densities
  - $0.02$ fm$^{-3}$ dashed
  - $0.04$ fm$^{-3}$ solid
  - $0.08$ fm$^{-3}$ dotted
  - thin with SRC
- No pairing at 0.08!
Comparison for neutron matter
with CBF & Monte Carlo PRL95,192501(2005)

End of lectures

• Hope you found the course useful
• Thanks for participating!
• Don’t forget to do course evals