Lecture Wed.1

Many-body theory of electron-phonon interactions

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Lecture Summary

- Limitations of Rayleigh-Schrödinger perturbation theory
- Many-body Hamiltonian in quantum field theory
- Green’s function and the spectral function
- Electron-phonon self-energy
- Quasiparticle approximation
- Mass enhancement and electron lifetimes
Limitations of Rayleigh-Schrödinger perturbation theory

Kohn-Sham equations again

\[-\frac{\hbar^2}{2m_e} \nabla^2 \psi_n(r) + V_{\text{SCF}}(r; \tau_1, \tau_2, \cdots) \psi_n(r) = E_n \psi_n(r)\]
Limitations of Rayleigh-Schrödinger perturbation theory

Kohn-Sham equations again

\[-\frac{\hbar^2}{2m_e} \nabla^2 \psi_n(r) + V_{SCF}(r; \tau_1, \tau_2, \cdots) \psi_n(r) = E_n \psi_n(r)\]

- Adiabatic Born-Oppenheimer approximation
Limitations of Rayleigh-Schrödinger perturbation theory

Kohn-Sham equations again

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- Adiabatic Born-Oppenheimer approximation
- Nuclei described as classical particles
Limitations of Rayleigh-Schrödinger perturbation theory

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- Adiabatic Born-Oppenheimer approximation
- Nuclei described as classical particles
- Electron-phonon interactions depend on the XC functional
Kohn-Sham equations again

$$-\frac{\hbar^2}{2m_e} \nabla^2 \psi_n(r) + V_{\text{SCF}}(r; \tau_1, \tau_2, \cdots) \psi_n(r) = E_n \psi_n(r)$$

- Adiabatic Born-Oppenheimer approximation
- Nuclei described as classical particles
- Electron-phonon interactions depend on the XC functional
- Phonons are calculated from static displacements or DFPT
Breakdown of Rayleigh-Schrödinger perturbation theory

- Polaron liquid at the $\text{SrTiO}_3(001)$ surface

Figure from Wang et al, Nature Mater. 15, 835 (2016)
Breakdown of Rayleigh-Schrödinger perturbation theory

- Scanning tunneling spectra of 2H-NbS$_2$

• Raman $G$ peak of gated graphene

Left figure from Pisana et al, Nat. Mater. 6, 198 (2007)
Many-body Schrödinger’s equation

\[-\frac{\hbar^2}{2m_e} \sum_{i} \nabla_{i}^2 \Psi - \frac{\hbar^2}{2M_{\kappa}} \sum_{\kappa} \nabla_{\kappa}^2 \Psi - \sum_{i,\kappa} Z_{\kappa} v(r_{i}, \tau_{\kappa}) \Psi \]

\[+ \sum_{\kappa > \kappa'} Z_{\kappa} Z_{\kappa'} v(\tau_{\kappa}, \tau_{\kappa'}) \Psi + \sum_{i > j} v(r_{i}, r_{j}) \Psi = E_{\text{tot}} \Psi \]

\[v(r, r') = \frac{e^2}{4\pi \varepsilon_0 |r - r'|} \]
Many-body Schrödinger’s equation

\[-\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 \Psi - \frac{\hbar^2}{2M_\kappa} \sum_\kappa \nabla_\kappa^2 \Psi - \sum_{i,\kappa} Z_\kappa v(r_i, \tau_\kappa) \Psi \]

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\[v(r, r') = \frac{e^2}{4\pi\varepsilon_0 |r - r'|} \]

- We need to describe electrons and vibrations on the same footing
Many-body Schrödinger’s equation

\[ -\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 \Psi - \frac{\hbar^2}{2M_\kappa} \sum_\kappa \nabla_\kappa^2 \Psi - \sum_{i,\kappa} Z_\kappa v(r_i, \tau_\kappa) \Psi + \sum_{\kappa > \kappa'} Z_\kappa Z_{\kappa'} v(\tau_\kappa, \tau_{\kappa'}) \Psi + \sum_{i > j} v(r_i, r_j) \Psi = E_{\text{tot}} \Psi \]

\[ v(r, r') = \frac{e^2}{4\pi\epsilon_0 |r - r'|} \]

- We need to describe electrons and vibrations on the same footing
- The many-body Schrödinger equation is impractical for calculations
Field operators

\(N\)-electron wavefunction as a linear combination of Slater determinants

\[
\Psi(x_1, x_2, \cdots) = \sum_{mn} a_{mn} \hat{c}_m^\dagger \hat{c}_n |0_{KS}\rangle + \sum_{mnpq} b_{mnpq} \hat{c}_m^\dagger \hat{c}_n^\dagger \hat{c}_p \hat{c}_q |0_{KS}\rangle + \cdots
\]
Field operators

\[ N \)-electron wavefunction as a linear combination of Slater determinants

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Operators in second quantization

\[ V(x_1) + V(x_2) + \cdots \rightarrow \sum_{mn} V_{mn} \hat{c}_m \hat{c}_n \]
Field operators

$N$-electron wavefunction as a linear combination of Slater determinants

$$\Psi(x_1, x_2, \cdots) = \sum_{mn} a_{mn} \hat{c}_m \hat{c}_n |0_{KS}\rangle + \sum_{mnpq} b_{mnpq} \hat{c}_m \hat{c}_n \hat{c}_p \hat{c}_q |0_{KS}\rangle + \cdots$$

Operators in second quantization

$$V(x_1) + V(x_2) + \cdots \rightarrow \sum_{mn} V_{mn} \hat{c}_m \hat{c}_n$$

$$= \sum_m \sum_n \int dx \psi_m^*(x) V(x) \psi_n(x) \hat{c}_m \hat{c}_n$$
Field operators

\( N \)-electron wavefunction as a linear combination of Slater determinants

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\Psi(x_1, x_2, \cdots) = \sum_{mn} a_{mn} \hat{c}_m^\dagger \hat{c}_n |0_{KS}\rangle + \sum_{mnpq} b_{mnpq} \hat{c}_m^\dagger \hat{c}_n^\dagger \hat{c}_p \hat{c}_q |0_{KS}\rangle + \cdots
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Operators in second quantization

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V(x_1) + V(x_2) + \cdots \rightarrow \sum_{mn} V_{mn} \hat{c}_m^\dagger \hat{c}_n
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\]

Field operators

\[
\hat{\psi}(x) = \sum_{n} \psi_n(x) \hat{c}_n
\]
Field operators

\(N\)-electron wavefunction as a linear combination of Slater determinants

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Operators in second quantization

\[
V(x_1) + V(x_2) + \cdots \quad \rightarrow \quad \sum_{mn} V_{mn} \hat{c}_m \hat{c}_n
\]

\[
= \sum_m \sum_n \int dx \psi_m^*(x) V(x) \psi_n(x) \hat{c}_m \hat{c}_n = \int dx \hat{\psi}^*(x) V(x) \hat{\psi}(x)
\]

Field operators

\[
\hat{\psi}(x) = \sum_n \psi_n(x) \hat{c}_n
\]
Many-body Hamiltonian in second quantization

Non-relativistic Hamiltonian of coupled electrons and nuclei

\[ \hat{H} = \hat{T}_e + \hat{T}_n + \hat{U}_{en} + \hat{U}_{ee} + \hat{U}_{nn} \]
Many-body Hamiltonian in second quantization

Non-relativistic Hamiltonian of coupled electrons and nuclei

\[ \hat{H} = \hat{T}_e + \hat{T}_n + \hat{U}_{en} + \hat{U}_{ee} + \hat{U}_{nn} \]

Electron kinetic energy

\[ \hat{T}_e = -\frac{\hbar^2}{2m_e} \int d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \nabla^2 \hat{\psi}(\mathbf{x}) \]
Many-body Hamiltonian in second quantization

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Electron-nucleus interaction

\[ \hat{U}_{en} = \int dr \int dr' \, \hat{n}_e(r) \hat{n}_n(r') v(r, r'), \quad \hat{n}_e(r) = \sum_{\sigma} \hat{\psi}^\dagger(x) \hat{\psi}(x) \]
Many-body Hamiltonian in second quantization

Non-relativistic Hamiltonian of coupled electrons and nuclei

\[ \hat{H} = \hat{T}_e + \hat{T}_n + \hat{U}_{en} + \hat{U}_{ee} + \hat{U}_{nn} \]

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Electron-nucleus interaction

\[ \hat{U}_{en} = \int d\mathbf{r} \int d\mathbf{r}' \, \hat{n}_e(\mathbf{r}) \hat{n}_n(\mathbf{r}') v(\mathbf{r}, \mathbf{r}'), \quad \hat{n}_e(\mathbf{r}) = \sum_\sigma \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \]

Electron-electron interaction

\[ \hat{U}_{ee} = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \, \hat{n}_e(\mathbf{r}) \left[ \hat{n}_e(\mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}') \right] v(\mathbf{r}, \mathbf{r}') \]
Time evolution of field operators

Ground state of $N$-electron system

\[ \hat{H} |N\rangle = E_N |N\rangle \]
Time evolution of field operators

Ground state of $N$-electron system

$s$-th excited state of $N+1$-electron system

$\hat{H}|N\rangle = E_N|N\rangle$

$\hat{H}|N + 1, s\rangle = E_{N+1,s}|N + 1, s\rangle$
### Time evolution of field operators

<table>
<thead>
<tr>
<th>State Description</th>
<th>Equation</th>
</tr>
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<tbody>
<tr>
<td>Ground state of $N$-electron system</td>
<td>$\hat{H}</td>
</tr>
<tr>
<td>$s$-th excited state of $N+1$-electron system</td>
<td>$\hat{H}</td>
</tr>
<tr>
<td>Excitation energy</td>
<td>$\varepsilon_s = E_{N+1,s} - E_N$</td>
</tr>
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Giustino, Lecture Wed.1
Time evolution of field operators

Ground state of $N$-electron system

$\hat{H}|N\rangle = E_N|N\rangle$

$s$-th excited state of $N+1$-electron system

$\hat{H}|N + 1, s\rangle = E_{N+1,s}|N + 1, s\rangle$

Excitation energy

$\varepsilon_s = E_{N+1,s} - E_N$

Heisenberg time evolution

$\hat{\psi}(x, t) = e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar}$

$i\hbar \frac{\partial}{\partial t} \hat{\psi}(x, t) = \left[ \hat{\psi}(x, t), \hat{H} \right]$
Time evolution of field operators

| Ground state of $N$-electron system | $\hat{H}|N\rangle = E_N|N\rangle$ |
|-------------------------------------|-----------------------------------|
| $s$-th excited state of $N+1$-electron system | $\hat{H}|N+1, s\rangle = E_{N+1,s}|N+1, s\rangle$ |
| Excitation energy | $\varepsilon_s = E_{N+1,s} - E_N$ |

Heisenberg time evolution

$$\hat{\psi}(x, t) = e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} \quad i\hbar\frac{\partial}{\partial t} \hat{\psi}(x, t) = \left[ \hat{\psi}(x, t), \hat{H} \right]$$

Exercise

$$\langle N|\psi(x, t)|N+1, s\rangle = \langle N|e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar}|N+1, s\rangle$$
Time evolution of field operators

Ground state of $N$-electron system

\[ \hat{H} |N\rangle = E_N |N\rangle \]

$s$-th excited state of $N+1$-electron system

\[ \hat{H} |N + 1, s\rangle = E_{N+1,s} |N + 1, s\rangle \]

Excitation energy

\[ \varepsilon_s = E_{N+1,s} - E_N \]

Heisenberg time evolution

\[ \hat{\psi}(x, t) = e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} \]

\[ i\hbar \frac{\partial}{\partial t} \hat{\psi}(x, t) = [\hat{\psi}(x, t), \hat{H}] \]

Exercise

\[ \langle N | \psi(x, t) | N + 1, s \rangle = \langle N | e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} | N + 1, s \rangle \]

\[ = \langle N | e^{iE_N t/\hbar} \hat{\psi}(x) e^{-iE_{N+1,s} t/\hbar} | N + 1, s \rangle \]
Time evolution of field operators

Ground state of $N$-electron system
\[ \hat{H}|N\rangle = E_N|N\rangle \]

$s$-th excited state of $N+1$-electron system
\[ \hat{H}|N+1, s\rangle = E_{N+1,s}|N+1, s\rangle \]

Excitation energy
\[ \varepsilon_s = E_{N+1,s} - E_N \]

Heisenberg time evolution
\[ \hat{\psi}(x, t) = e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} \]
\[ \imath\hbar \frac{\partial}{\partial t} \hat{\psi}(x, t) = \left[ \hat{\psi}(x, t), \hat{H} \right] \]

Exercise
\[ \langle N| \hat{\psi}(x, t)|N + 1, s\rangle = \langle N| e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} |N + 1, s\rangle \]
\[ = \langle N| e^{iE_N t/\hbar} \hat{\psi}(x) e^{-iE_{N+1,s} t/\hbar} |N + 1, s\rangle \]
\[ = \langle N| \hat{\psi}(x)|N + 1, s\rangle e^{-i\varepsilon_s t/\hbar} \]
Time evolution of field operators

Ground state of $N$-electron system

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$s$-th excited state of $N+1$-electron system

\[ \hat{H} |N+1, s\rangle = E_{N+1,s} |N+1, s\rangle \]

Excitation energy

\[ \varepsilon_s = E_{N+1,s} - E_N \]

Heisenberg time evolution

\[ \hat{\psi}(x, t) = e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} \quad \text{and} \quad i\hbar \frac{\partial}{\partial t} \hat{\psi}(x, t) = [\hat{\psi}(x, t), \hat{H}] \]

Exercise

\[
\begin{align*}
\langle N | \psi(x, t) | N + 1, s \rangle &= \langle N | e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} | N + 1, s \rangle \\
&= \langle N | e^{iE_N t/\hbar} \hat{\psi}(x) e^{-iE_{N+1,s} t/\hbar} | N + 1, s \rangle \\
&= \langle N | \hat{\psi}(x) | N + 1, s \rangle e^{-i\varepsilon_s t/\hbar} \\
&= f_s(x) \text{ Dyson orbital}
\end{align*}
\]
The Green’s function at zero temperature

\[ G(x_t, x'_t') = -\frac{i}{\hbar} \langle N | \hat{T} \hat{\psi}(x_t) \hat{\psi}^\dagger(x'_t') | N \rangle \]
The Green’s function at zero temperature

\[ G(x_t, x'_t') = -\frac{i}{\hbar} \langle N | \hat{T} \hat{\psi}(x_t) \hat{\psi}^\dagger(x'_t') | N \rangle \]

Time-ordered Green’s function

Wick’s time-ordering operator

electron in \( x' \) at time \( t' \)
The Green’s function at zero temperature

\[ G(x_t, x_{t'}) = -\frac{i}{\hbar} \langle N | \hat{T} \hat{\psi}(x_t) \hat{\psi}^\dagger(x'_{t'}) | N \rangle \]

\( \langle \text{electron in } x \text{ at time } t | \text{electron in } x' \text{ at time } t' \rangle \)
The Green’s function at zero temperature

\[ G(x_t, x_{t'}) = -\frac{i}{\hbar} \langle N| \hat{T} \hat{\psi}(x_t) \hat{\psi}^\dagger(x'_{t'}) | N \rangle \]

Time-ordered Green’s function

Wick’s time-ordering operator

\[ \langle \text{electron in } x \text{ at time } t \mid \text{electron in } x' \text{ at time } t' \rangle \]

\[ x_t \quad \bullet \quad \rightarrow \quad \bullet \quad x'_{t'} \]
The Green’s function at zero temperature

Consider $t > t'$ (electron injection)

$$G(x_t, x'_t) = -\frac{i}{\hbar} \langle N | \hat{\psi}(x_t) \hat{\psi}^\dagger(x'_t) | N \rangle$$
The Green’s function at zero temperature

Consider \( t > t' \) (electron injection)

\[
G(xt, x't') = -\frac{i}{\hbar} \langle N | \hat{\psi}(xt) \hat{\psi}^\dagger(x't') | N \rangle
\]

\[
= -\frac{i}{\hbar} \langle N | e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} e^{i\hat{H}t'/\hbar} \hat{\psi}^\dagger(x') e^{-i\hat{H}t'/\hbar} | N \rangle
\]
The Green’s function at zero temperature

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\]

\[
= -\frac{i}{\hbar} \langle N | \hat{\psi}(x) e^{-i(\hat{H} - E_N)(t-t')/\hbar} \hat{\psi}^\dagger(x') | N \rangle
\]
Consider $t > t'$ (electron injection)

\[
G(x_t, x_{t'}) = -\frac{i}{\hbar} \langle N | \hat{\psi}(x_t) \hat{\psi}^\dagger(x_{t'}) | N \rangle
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= -\frac{i}{\hbar} \langle N | e^{i\hat{H}t/\hbar} \hat{\psi}(x) e^{-i\hat{H}t/\hbar} e^{i\hat{H}t'/\hbar} \hat{\psi}^\dagger(x') e^{-i\hat{H}t'/\hbar} | N \rangle
\]

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= -\frac{i}{\hbar} \langle N | \hat{\psi}(x) e^{-i(\hat{H} - E_N)(t-t')/\hbar} \hat{\psi}^\dagger(x') | N \rangle
\]

\[
\sum_s |N + 1, s\rangle \langle N + 1, s|
\]
The Green’s function at zero temperature

Consider \( t > t' \) (electron injection)

\[
G(x_t, x_{t'}) = -\frac{i}{\hbar}\langle N | \hat{\psi}(x_t) \hat{\psi}^\dagger(x_{t'}) | N \rangle
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\]

\[
= -\sum_s \langle N + 1, s | N + 1, s \rangle
\]

\[
= -\frac{i}{\hbar} \sum_s f_s(x) f_s^*(x') e^{-i\varepsilon_s(t-t')/\hbar}
\]
The spectral function

After carrying out the same operation for $t < t'$ and Fourier transform

$$G(x, x', \omega) = \sum_s \frac{f_s(x)f_s^*(x')}{\hbar\omega - \varepsilon_s \mp i0^+} \mp \text{occ/unocc}$$
After carrying out the same operation for $t < t'$ and Fourier transform

$$G(x, x', \omega) = \sum_s \frac{f_s(x)f_s^*(x')}{\hbar\omega - \varepsilon_s \mp i0^+}$$

The poles of the Green’s function represent the electron addition/removal energies of the interacting many-body system.
The spectral function

After carrying out the same operation for $t < t'$ and Fourier transform

$$G(x, x', \omega) = \sum_s \frac{f_s(x)f^*_s(x')}{\hbar \omega - \varepsilon_s \mp i0^+} \mp \text{occ/unocc}$$

The poles of the Green’s function represent the electron addition/removal energies of the interacting many-body system

From the Green’s function we can obtain the spectral (density) function

$$A(x, \omega) = \frac{1}{\pi} |\text{Im } G(x, x, \omega)| = \sum_s |f_s(x)|^2 \delta(\hbar \omega - \varepsilon_s)$$
The spectral function

After carrying out the same operation for $t < t'$ and Fourier transform

$$G(x, x', \omega) = \sum_s \frac{f_s(x)f_s^*(x')}{\hbar\omega - \varepsilon_s \mp i0^+} \mp \text{occ/unocc}$$

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The spectra function is the many-body (local) density of states
The spectral function

After carrying out the same operation for $t < t'$ and Fourier transform

$$G(x, x', \omega) = \sum_s \frac{f_s(x)f^*_s(x')}{\hbar \omega - \varepsilon_s \mp i0^+} \mp \text{occ/unocc}$$

The poles of the Green's function represent the electron addition/removal energies of the interacting many-body system

From the Green's function we can obtain the spectral (density) function

$$A(x, \omega) = \frac{1}{\pi} |\text{Im } G(x, x, \omega)| = \sum_s |f_s(x)|^2 \delta(\hbar \omega - \varepsilon_s)$$

The spectra function is the many-body (local) density of states

- Usually it is presented as momentum-resolved $A(k, \omega)$
The spectral function

**Example:** a single complex pole

\[ \varepsilon_s = \varepsilon - i\Gamma \]
The spectral function

**Example: a single complex pole**

\[ \varepsilon_s = \varepsilon - i\Gamma \]

\[
G(x, x, t-t') = -\frac{i}{\hbar} |f_s(x)|^2 e^{-i\varepsilon(t-t')/\hbar} e^{-\Gamma(t-t')/\hbar}
\]
The spectral function

**Example: a single complex pole**

\[ \varepsilon_s = \varepsilon - i\Gamma \]

\[ G(x, x, t-t') = -\frac{i}{\hbar} |f_s(x)|^2 e^{-i\varepsilon(t-t')/\hbar} e^{-\Gamma(t-t')/\hbar} \]

\[ |G(x, x, t-t')| = \frac{1}{\hbar} |f_s(x)|^2 e^{-\Gamma(t-t')/\hbar} \]
The spectral function

Example: a single complex pole

\[ \varepsilon_s = \varepsilon - i\Gamma \]

\[ G(x, x, t-t') = -\frac{i}{\hbar} |f_s(x)|^2 e^{-i\varepsilon(t-t')/\hbar} e^{-\Gamma(t-t')/\hbar} \]

\[ |G(x, x, t-t')| = \frac{1}{\hbar} |f_s(x)|^2 e^{-\Gamma(t-t')/\hbar} \]

decay
The spectral function

**Example: a single complex pole**

\[ \varepsilon_s = \varepsilon - i\Gamma \]

\[
G(x, x, t-t') = -\frac{i}{\hbar} |f_s(x)|^2 e^{-i\varepsilon(t-t')/\hbar} e^{-\Gamma(t-t')/\hbar}
\]

\[
|G(x, x, t-t')| = \frac{1}{\hbar} |f_s(x)|^2 e^{-\Gamma(t-t')/\hbar} \quad \text{decay}
\]

\[
A(x, x, \omega) = \frac{1}{\pi} \frac{\Gamma}{(\hbar\omega - \varepsilon)^2 + \Gamma^2} |f_s(x)|^2
\]
The spectral function

**Example: a single complex pole**

$\varepsilon_s = \varepsilon - i\Gamma$

$$G(x, x, t-t') = -\frac{i}{\hbar} |f_s(x)|^2 e^{-i\varepsilon(t-t')/\hbar} e^{-\Gamma(t-t')/\hbar}$$

$$|G(x, x, t-t')| = \frac{1}{\hbar} |f_s(x)|^2 e^{-\Gamma(t-t')/\hbar}$$

$A(x, x, \omega) = \frac{1}{\pi} \frac{\Gamma}{(\hbar \omega - \varepsilon)^2 + \Gamma^2} |f_s(x)|^2$
The spectral function

\[ A(k, \omega) = \frac{1}{\pi} |\text{Im} \ G(k, \omega)| \]
The spectral function

\[ A(k, \omega) = \frac{1}{\pi} |\text{Im} \, G(k, \omega)| \]
The spectral function

$$A(k, \omega) = \frac{1}{\pi} |\text{Im } G(k, \omega)|$$

DFT density of states

many-body DOS

energy
The spectral function

\[ A(k, \omega) = \frac{1}{\pi} |\text{Im} \ G(k, \omega)| \]

DFT density of states

quasiparticle shift

many-body DOS

energy
The spectral function

\[ A(k, \omega) = \frac{1}{\pi} |\text{Im } G(k, \omega)| \]

- DFT density of states
- quasiparticle shift
- quasiparticle broadening

many-body DOS

energy
The spectral function

\[ A(k, \omega) = \frac{1}{\pi} |\text{Im } G(k, \omega)| \]

DFT density of states

\[ \text{many-body DOS} \]

boson energy

\[ \text{quasiparticle shift} \]

\[ \text{quasiparticle broadening} \]

energy
How to calculate the Green’s function

Equation of motion for field operators

\[
i \hbar \frac{\partial}{\partial t} \hat{\psi}(x,t) = \left[ \hat{\psi}(x,t), \hat{H} \right]
\]
How to calculate the Green’s function

Equation of motion for field operators

\[ i\hbar \frac{\partial}{\partial t} \hat{\psi}(x,t) = \left[ \hat{\psi}(x,t), \hat{H} \right] = \left[ -\frac{\hbar^2}{2m_e} \nabla^2 + \int dr' v(r, r') \hat{n}(r't) \right] \hat{\psi}(x,t) \]

total charge, electrons & nuclei
How to calculate the Green’s function

Equation of motion for field operators

\[
i\hbar \frac{\partial}{\partial t} \hat{\psi}(x, t) = \left[ \hat{\psi}(x, t), \hat{H} \right] = \left[ -\frac{\hbar^2}{2m_e} \nabla^2 + \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \hat{n}(\mathbf{r}' t) \right] \hat{\psi}(x, t)
\]

total charge, electrons & nuclei

\[
i\hbar \frac{\partial}{\partial t_1} \hat{\psi}(1) = \left[ -\frac{\hbar^2}{2m_e} \nabla_1^2 + \int d2v(12) \hat{n}(2) \right] \hat{\psi}(1)
\]
How to calculate the Green’s function

Equation of motion for field operators

\[ i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{x}t) = \left[ \hat{\psi}(\mathbf{x}, t), \hat{H} \right] = \left[ -\frac{\hbar^2}{2m_e} \nabla^2 + \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \hat{n}(\mathbf{r}'t) \right] \hat{\psi}(\mathbf{x}t) \]

Equation of motion for Green’s function

\[ \left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_e} \nabla_1^2 \right] G(12) + \frac{i}{\hbar} \int d\mathbf{r} v(13) \langle \hat{T} \hat{n}(3) \hat{\psi}(1) \hat{\psi}^\dagger(2) \rangle = \delta(12) \]
How to calculate the Green’s function

Equation of motion for field operators

\[
i\hbar \frac{\partial}{\partial t} \hat{\psi}(x,t) = \left[ \hat{\psi}(x,t), \hat{H} \right] = \left[ -\frac{\hbar^2}{2m_e} \nabla^2 + \int d\mathbf{r'} v(\mathbf{r}, \mathbf{r'}) \hat{n}(\mathbf{r'} t) \right] \hat{\psi}(x,t)
\]

\[
i\hbar \frac{\partial}{\partial t_1} \hat{\psi}(1) = \left[ -\frac{\hbar^2}{2m_e} \nabla^2_1 + \int d2v(12) \hat{n}(2) \right] \hat{\psi}(1)
\]

Equation of motion for Green’s function

\[
\left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_e} \nabla^2_1 \right] G(12) + \frac{i}{\hbar} \int d3v(13) \langle \hat{T} \hat{n}(3) \psi(1) \psi^\dagger(2) \rangle = \delta(12)
\]

4 field operators → 2-particle Green’s function

\[
\langle \hat{T} \psi^\dagger(3) \psi(3) \psi(1) \psi^\dagger(2) \rangle = [\text{Hartree}] + [\text{Fock}] + G_2(31, 32)
\]
How to calculate the Green’s function

\[
\left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_e} \nabla_1^2 - V_{\text{tot}}(1) \right] G(12) - \int d^3 \Sigma(13) G(32) = \delta(12)
\]

\[V_{\text{tot}}(1) = \int d^2 v(12) \langle \hat{n}(2) \rangle\]

rewrite 2-particle Green’s function using self-energy \( \Sigma \)
How to calculate the Green’s function

\[
\left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_e} \nabla^2_1 - V_{\text{tot}}(1) \right] G(12) - \int d^3 \Sigma(13) G(32) = \delta(12)
\]

\[V_{\text{tot}}(1) = \int d^2 v(12) \langle \hat{n}(2) \rangle\]

rewrite 2-particle Green’s function using self-energy \(\Sigma\)

Express the Green’s function in terms of Dyson’s orbitals

\[
\left[ -\frac{\hbar^2}{2m_e} \nabla^2 + V_{\text{tot}}(r) \right] f_s(x) + \int dx' \Sigma(x, x', \varepsilon_s / \hbar) f_s(x') = \varepsilon_s f_s(x)
\]
How to calculate the Green’s function

\[
\left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_e} \nabla^2 - V_{\text{tot}}(1) \right] G(12) - \int d3 \Sigma(13) G(32) = \delta(12)
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\[V_{\text{tot}}(1) = \int d2 v(12) \langle \hat{n}(2) \rangle\]

rewrite 2-particle Green’s function using self-energy \( \Sigma \)

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Sources of electron-phonon interaction
How to calculate the Green’s function

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\left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_e} \nabla_1^2 - V_{\text{tot}}(1) \right] G(12) - \int d^3 \Sigma(13) G(32) = \delta(12)
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rewrite 2-particle Green’s function using self-energy \( \Sigma \)

Express the Green’s function in terms of Dyson’s orbitals

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\left[ -\frac{\hbar^2}{2m_e} \nabla^2 + V_{\text{tot}}(r) \right] f_s(x) + \int dx' \Sigma(x, x', \varepsilon_s / \hbar) f_s(x') = \varepsilon_s f_s(x)
\]

Sources of electron-phonon interaction
How to calculate the self-energy

Electron self-energy from Hedin-Baym’s equations

\[ \Sigma(12) = i\hbar \int d(34) \ G(13) \ \Gamma(324) W(41^+) \]
How to calculate the self-energy

Electron self-energy from Hedin-Baym’s equations

$$\Sigma(12) = i\hbar \int d(34) \ G(13) \ \Gamma(324)W(41^+)$$

Green’s function
How to calculate the self-energy

Electron self-energy from Hedin-Baym’s equations

$$\Sigma(12) = i\hbar \int d(34) \, G(13) \Gamma(324) W(41^+)$$

- Green’s function
- Vertex
How to calculate the self-energy

Electron self-energy from Hedin-Baym’s equations

\[ \Sigma(12) = i\hbar \int d(34) \, G(13) \, \Gamma(324) \, W(41^+) \]

- Green's function
- Vertex
- Screened Coulomb interaction
How to calculate the self-energy

Electron self-energy from Hedin-Baym’s equations

\[ \Sigma(12) = i\hbar \int d(34) \, G(13) \, \Gamma(324) W(41^+) \]

- Green’s function
- Vertex
- Screened Coulomb interaction

\[ W = W_e + W_{ph} \]

\[ W_e(12) = \int d3 \, \epsilon_e^{-1}(13) v(32) \]
How to calculate the self-energy

Electron self-energy from Hedin-Baym’s equations

$$\Sigma(12) = i\hbar \int d(34) G(13) \Gamma(324) W(41^+)$$

Green’s function
Vertex
Screened Coulomb interaction

$$W = W_e + W_{ph}$$

$$W_e(12) = \int d3 \epsilon_e^{-1}(13)v(32)$$

Basically the standard GW method + screening from nuclei
How to calculate the self-energy

Screened Coulomb interaction from the nuclei

$$W_{ph}(12) = \sum_{\kappa \kappa'} \int d(34) \epsilon_e^{-1}(13) \frac{\partial V_\kappa(r_3)}{\partial \tau_\kappa} \cdot D_{\kappa \kappa'}(t_3 t_4) \cdot \epsilon_e^{-1}(24) \frac{\partial V_{\kappa'}(r_4)}{\partial \tau_{\kappa'}}$$
How to calculate the self-energy

Screened Coulomb interaction from the nuclei

\[ W_{ph}(12) = \sum_{\kappa \kappa'} \int d(34) \epsilon_e^{-1}(13) \frac{\partial V_{\kappa}(\mathbf{r}_3)}{\partial \tau_\kappa} \cdot D_{\kappa \kappa'}(t_3 t_4) \cdot \epsilon_e^{-1}(24) \frac{\partial V_{\kappa'}(\mathbf{r}_4)}{\partial \tau_{\kappa'}} \]
How to calculate the self-energy

Screened Coulomb interaction from the nuclei

\[ W_{\text{ph}}(12) = \sum_{\kappa\kappa'} \int d(34) \epsilon^{-1}(13) \frac{\partial V_\kappa(r_3)}{\partial \tau_\kappa} \cdot D_{\kappa\kappa'}(t_3 t_4) \cdot \epsilon^{-1}(24) \frac{\partial V_{\kappa'}(r_4)}{\partial \tau_{\kappa'}} \]

Displacement-displacement correlation function of the nuclei, a.k.a. the phonon Green’s function

\[ D_{\kappa\kappa'}(tt') = -\frac{i}{\hbar} \langle \hat{T} \Delta \hat{r}_\kappa(t) \Delta \hat{R}_{\kappa'}^T(t') \rangle \]
Diagrammatic representation of the self-energy

\[
\Sigma = W_e \quad G \quad \Gamma
\]

Standard GW self-energy (we will ignore this from now on)

Figure from Giustino,
Rev. Mod. Phys. 89,
015003 (2017)
Diagrammatic representation of the self-energy

Standard GW self-energy
(we will ignore this from now on)

Fan-Migdal self-energy
Diagrammatic representation of the self-energy

Standard GW self-energy (we will ignore this from now on)

Fan-Migdal self-energy

Debye-Waller self-energy

Improper self-energy: comes from

\[ V_{\text{tot}}(1) = \int d^2 v(12) \langle \hat{n}(2) \rangle \text{ term} \]
Diagrammatic representation of the self-energy

\[ \Sigma = W_e + G D + g^2_{DW} \]

Standard GW self-energy
(we will ignore this from now on)

Fan-Migdal self-energy

Debye-Waller self-energy
(Lecture Thu.2)

Improper self-energy: comes from
\[ V_{tot}(1) = \int d^2v(12)\langle \hat{n}(2) \rangle \text{ term} \]
Fan-Migdal self-energy

Fan-Migdal self-energy using Kohn-Sham states and DFPT phonons

\[
\Sigma_{nk}^{FM}(\omega) = \frac{1}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{BZ}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2
\]

\[
\times \left[ \frac{1 - f_{mk+q}}{\omega - \epsilon_{mk+q}/\hbar - \omega_{q\nu} + i\eta} + \frac{f_{mk+q}}{\omega - \epsilon_{mk+q}/\hbar + \omega_{q\nu} + i\eta} \right]
\]
Fan-Migdal self-energy

Fan-Migdal self-energy using Kohn-Sham states and DFPT phonons

\[
\Sigma_{nk}^{FM}(\omega) = \frac{1}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \times \left[ \frac{1 - f_{m\mathbf{k+q}}}{\omega - \varepsilon_{m\mathbf{k+q}}/\hbar - \omega_{\nu \mathbf{q}} + i\eta} + \frac{f_{m\mathbf{k+q}}}{\omega - \varepsilon_{m\mathbf{k+q}}/\hbar + \omega_{\nu \mathbf{q}} + i\eta} \right]
\]

Dynamical structure on the scale of the phonon energy
Fan-Migdal self-energy

Fan-Migdal self-energy using Kohn-Sham states and DFPT phonons

\[ \Sigma_{nk}(\omega) = \frac{1}{\hbar} \sum_{mn\nu} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \times \left[ \frac{1 - f_{m\mathbf{k}+\mathbf{q}}}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar - \omega_{\mathbf{q}\nu} + i\eta} + \frac{f_{m\mathbf{k}+\mathbf{q}}}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar + \omega_{\mathbf{q}\nu} + i\eta} \right] \]

Dynamical structure on the scale of the phonon energy
Fan-Migdal self-energy

Fan-Migdal self-energy using Kohn-Sham states and DFPT phonons

\[
\Sigma_{n\mathbf{k}}^{FM}(\omega) = \frac{1}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{BZ}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \times \left[ \frac{1 - f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu}}{\omega - \epsilon_{m\mathbf{k}+\mathbf{q}}/\hbar - \omega_{\mathbf{q}\nu} + i\eta} + \frac{f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu}}{\omega - \epsilon_{m\mathbf{k}+\mathbf{q}}/\hbar + \omega_{\mathbf{q}\nu} + i\eta} \right]
\]

Dynamical structure on the scale of the phonon energy
Fan-Migdal self-energy

Example: A single dispersionless phonon (Holstein model)
Fan-Migdal self-energy

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Fan-Migdal self-energy

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Fan-Migdal self-energy

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Example: A single dispersionless phonon (Holstein model)
Fan-Migdal self-energy

Example: A single dispersionless phonon (Holstein model)

change of velocity/mass

phonon energy

broadening

Giustino, Lecture Wed.1 24/35
Examples from experiments

- Velocity renormalization in MgB$_2$

Examples from experiments

- Velocity renormalization in Ca-decorated graphene on Au

\[ v = v_0 / 1.25 \]

Right figure adapted from Fedorov et al, Nat. Commun. 5, 3257 (2014)
Examples from calculations

- Velocity renormalization in $C_6CaC_6$ (EPW)

Figure adapted from Margine et al, Sci Rep. 6, 21414 (2016)
Examples from calculations

- Velocity renormalization and broadening in MgB$_2$

Figure from Figueren et al, Phys. Rev. B 79. 245103 (2009)
Quasiparticle shift and broadening

Spectral function from the self-energy

\[ A(k, \omega) = -\frac{1}{\pi} \text{Im} \sum_n \frac{1}{\hbar \omega - \epsilon_n k - \Sigma_n k(\omega)} \]
Quasiparticle shift and broadening

Spectral function from the self-energy

\[ A(k, \omega) = -\frac{1}{\pi} \text{Im} \sum_n \frac{1}{\hbar \omega - \varepsilon_{nk} - \Sigma_{nk}(\omega)} \]

Quasiparticle approximation:

*assume* Lorentzian peaks centered near \( \hbar \omega = E_{nk} \)

\[ \Sigma_{nk}(\omega) = \Sigma_{nk}(E_{nk}) + \frac{1}{\hbar} \left. \frac{\partial \text{Re}\Sigma_{nk}}{\partial \omega} \right|_{\omega = E_{nk}/\hbar} (\hbar \omega - E_{nk}) + \cdots \]
Quasiparticle shift and broadening

Spectral function from the self-energy

\[ A(k, \omega) = -\frac{1}{\pi} \text{Im} \sum_n \frac{1}{\hbar \omega - \varepsilon_{nk} - \Sigma_{nk}(\omega)} \]

Quasiparticle approximation:

*assume* Lorentzian peaks centered near \( \hbar \omega = E_{nk} \)

\[ \Sigma_{nk}(\omega) = \Sigma_{nk}(E_{nk}) + \frac{1}{\hbar} \left. \frac{\partial \text{Re}\Sigma_{nk}}{\partial \omega} \right|_{\omega = E_{nk}/\hbar} (\hbar \omega - E_{nk}) + \cdots \]

Define the *quasiparticle strength*

\[ Z_{nk} = \left[ 1 - \frac{1}{\hbar} \left. \frac{\partial \text{Re}\Sigma_{nk}(\omega)}{\partial \omega} \right|_{\omega = E_{nk}/\hbar} \right]^{-1} \]
Quasiparticle shift and broadening

Replace the Taylor expansion inside the spectral function

$$A(k, \omega) = -\frac{1}{\pi} \sum_n \frac{1}{\hbar \omega - \epsilon_n - \Sigma_n(E_{nk}) - (1 - 1/Z_n)(\hbar \omega - E_{nk})}$$
Quasiparticle shift and broadening

Replace the Taylor expansion inside the spectral function

\[
A(k, \omega) = -\frac{1}{\pi} \sum_n \frac{1}{\hbar \omega - \varepsilon_{nk} - \Sigma_{nk}(E_{nk}) - (1 - 1/Z_{nk})(\hbar \omega - E_{nk})}
\]

After rearranging\(^{(*)}\):

\[
A(k, \omega) = -\frac{1}{\pi} \sum_n \frac{Z_{nk}}{\hbar \omega - (E_{nk} + i\Gamma_{nk})}
\]

\(^{(*)}\)Requires the additional approximation \(|\partial \text{Im} \Sigma_{nk}/\partial \omega| \ll |\partial \text{Re} \Sigma_{nk}/\partial \omega|\)
Quasiparticle shift and broadening

Replace the Taylor expansion inside the spectral function

\[ A(k, \omega) = -\frac{1}{\pi} \sum_n \frac{1}{\hbar \omega - \varepsilon_{nk} - \Sigma_{nk}(E_{nk}) - (1 - 1/Z_{nk})(\hbar \omega - E_{nk})} \]

After rearranging\(^(*)\):

\[ A(k, \omega) = -\frac{1}{\pi} \sum_n \frac{Z_{nk}}{\hbar \omega - (E_{nk} + i\Gamma_{nk})} \]

\[ E_{nk} = \varepsilon_{nk} + \text{Re} \Sigma_{nk}(E_{nk}/\hbar) \quad \text{quasiparticle energy} \]

\(^(*)\)Requires the additional approximation \(|\partial \text{Im} \Sigma_{nk}/\partial \omega| \ll |\partial \text{Re} \Sigma_{nk}/\partial \omega|\)
Quasiparticle shift and broadening

Replace the Taylor expansion inside the spectral function

\[ A(k, \omega) = -\frac{1}{\pi} \sum_n \frac{1}{\hbar \omega - \varepsilon_{nk} - \Sigma_{nk}(E_{nk}) - (1 - 1/Z_{nk})(\hbar \omega - E_{nk})} \]

After rearranging\(^{(*)}\):

\[ A(k, \omega) = -\frac{1}{\pi} \sum_n \frac{Z_{nk}}{\hbar \omega - (E_{nk} + i\Gamma_{nk})} \]

\[ E_{nk} = \varepsilon_{nk} + \text{Re} \Sigma_{nk}(E_{nk}/\hbar) \quad \text{quasiparticle energy} \]

\[ \Gamma_{nk} = Z_{nk} \text{Im} \Sigma_{nk}(E_{nk}/\hbar) \quad \text{quasiparticle broadening} \]

\(^{(*)}\) Requires the additional approximation \(|\partial \text{Im} \Sigma_{nk}/\partial \omega| \ll |\partial \text{Re} \Sigma_{nk}/\partial \omega|\)
The mass enhancement parameter

Taking the $k$-derivatives of the quasiparticle energy $E_{nk}$ we find the velocity and mass renormalization

$$V_{nk} = \frac{v_{nk}}{1 + \lambda_{nk}}$$

$$M_{nk}^* = (1 + \lambda_{nk}) m_{nk}^*$$

(valid only for simple metals)
The mass enhancement parameter

Taking the $k$-derivatives of the quasiparticle energy $E_{nk}$ we find the velocity and mass renormalization

$$V_{nk} = \frac{v_{nk}}{1 + \lambda_{nk}}$$

$$M^*_{nk} = (1 + \lambda_{nk}) m^*_{nk}$$

(valid only for simple metals)

$\lambda_{nk}$ is the mass enhancement parameter

$$\lambda_{nk} = \frac{1}{Z_{nk}} - 1$$
The mass enhancement parameter

Taking the $k$-derivatives of the quasiparticle energy $E_{nk}$ we find the velocity and mass renormalization

$$V_{nk} = \frac{v_{nk}}{1 + \lambda_{nk}}$$

$$M_{nk}^* = (1 + \lambda_{nk}) m_{nk}^*$$

(valid only for simple metals)

$\lambda_{nk}$ is the mass enhancement parameter

$$\lambda_{nk} = \frac{1}{Z_{nk}} - 1 = -\frac{1}{\hbar} \left. \frac{\partial \Re \Sigma_{nk}(\omega)}{\partial \omega} \right|_{\omega=E_{nk}/\hbar}$$
The mass enhancement parameter

Taking the $k$-derivatives of the quasiparticle energy $E_{nk}$ we find the **velocity** and **mass** renormalization

$$V_{nk} = \frac{v_{nk}}{1 + \lambda_{nk}}$$

$$M_{nk}^* = (1 + \lambda_{nk}) m_{nk}^*$$

(valid only for simple metals)

$\lambda_{nk}$ is the **mass enhancement parameter**

$$\lambda_{nk} = \frac{1}{Z_{nk}} - 1 = -\frac{1}{\hbar} \left. \frac{\partial \text{Re} \Sigma_{nk}(\omega)}{\partial \omega} \right|_{\omega=E_{nk}/\hbar} = -\frac{1}{\hbar} \left. \frac{\partial \text{Im} \Sigma_{nk}(\omega)}{\partial \eta} \right|_{\omega=E_{nk}/\hbar}$$

(Cauchy-Riemann condition)
Electron lifetimes

\[ \tau_{nk} = \frac{\hbar}{2\Gamma_{nk}} = \frac{\hbar}{2|Z_{nk} \text{Im} \Sigma_{nk}(E_{nk}/\hbar)|} \]
Electron lifetimes

\[ \tau_{nk} = \frac{\hbar}{2\Gamma_{nk}} = \frac{\hbar}{2|Z_{nk} \text{Im} \Sigma_{nk}(E_{nk}/\hbar)|} \]

Common approximation: replace \( E_{nk} \) by \( \varepsilon_{nk} \) and set \( Z_{nk} = 1 \)
Electron lifetimes

\[ \tau_{nk} = \frac{\hbar}{2\Gamma_{nk}} = \frac{\hbar}{2|Z_{nk}\text{Im} \Sigma_{nk}(E_{nk}/\hbar)|} \]

Common approximation: replace \( E_{nk} \) by \( \varepsilon_{nk} \) and set \( Z_{nk} = 1 \)

\[ \frac{1}{\tau_{nk}} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{dq}{\Omega_{BZ}} |g_{nm\nu}(k, q)|^2 \]
\[ \times [(1 - f_{mk+q} + n_{q\nu})\delta(\varepsilon_{nk} - \hbar\omega_{q\nu} - \varepsilon_{mk+q})] \]
\[ + (f_{mk+q} + n_{q\nu})\delta(\varepsilon_{nk} + \hbar\omega_{q\nu} - \varepsilon_{mk+q})] \]
Electron lifetimes

\[
\tau_{nk} = \frac{\hbar}{2\Gamma_{nk}} = \frac{\hbar}{2|Z_{nk}\text{Im} \Sigma_{nk}(E_{nk}/\hbar)|}
\]

Common approximation: replace \(E_{nk}\) by \(\varepsilon_{nk}\) and set \(Z_{nk} = 1\)

\[
\frac{1}{\tau_{nk}} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{dq}{\Omega_{\text{BZ}}} |g_{nm\nu}(k, q)|^2 \times \left[ (1 - f_{mk+q} + n_{q\nu})\delta(\varepsilon_{nk} - \hbar\omega_{q\nu} - \varepsilon_{mk+q}) \right.
\]

photon emission

\[
+ (f_{mk+q} + n_{q\nu})\delta(\varepsilon_{nk} + \hbar\omega_{q\nu} - \varepsilon_{mk+q}) \]

photon absorption
Electron lifetimes

\[ \tau_{n\mathbf{k}} = \frac{\hbar}{2\Gamma_{n\mathbf{k}}} = \frac{\hbar}{2|Z_{n\mathbf{k}}\text{Im} \Sigma_{n\mathbf{k}}(E_{n\mathbf{k}}/\hbar)|} \]

Common approximation: replace \( E_{n\mathbf{k}} \) by \( \varepsilon_{n\mathbf{k}} \) and set \( Z_{n\mathbf{k}} = 1 \)

\[ \frac{1}{\tau_{n\mathbf{k}}} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{nm\nu}(\mathbf{k}, \mathbf{q})|^2 \times \left[(1 - f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}}) \text{ phonon emission} \right] \]
\[ + (f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}}) \text{ phonon absorption} \]

Standard Fermi Golden rule expression for lifetimes
Example from calculations

- Electron lifetimes in anatase TiO$_2$ (EPW)

Figure adapted from Verdi et al, Phys. Rev. Lett. 115, 176401 (2015)
Take-home messages

- Quantum field theory is extremely useful in the study of electron-phonon physics
- The electron-phonon self-energy works as in the GW method, but on much smaller energy scales
- We can calculate the change of the effective mass and band velocity induced by EPIs
- We can calculate electron lifetimes arising from EPIs
• F. Giustino, Rev. Mod. Phys. 89, 015003 (2017) [link]

• A. Marini, S. Poncé, and X. Gonze, Phys. Rev. B 91, 224310 (2015) [Link]


• Abrikosov et al, Methods of quantum field theory in statistical physics, 1964


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• G. D. Mahan, Many-Particle Physics (Plenum, 1993)