Time-dependent adiabatic *GW*

Jinyuan Wu

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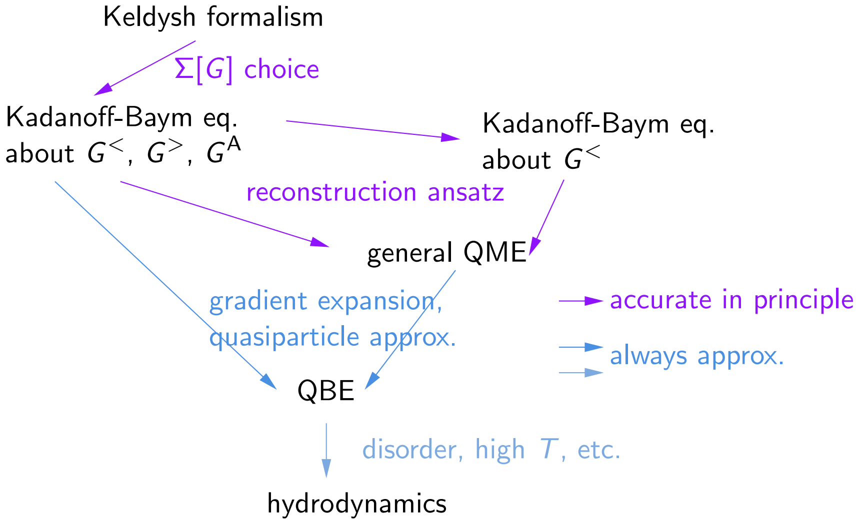
Relation between formalisms



Non-equilibrium Green function

Motivation

$$\langle A \rangle = \langle S^{-1} \mathcal{T}_t (S A_\mathrm{I}(t)) \rangle \,, \quad S = U(\infty, -\infty) \tag{1}$$

Non-equilibrium state: not pure; contains excited state components; $|\Psi_n\rangle$ is excited state $\Rightarrow S\,|\Psi_n\rangle \neq \mathrm{e}^{\mathrm{i}\,\alpha}\,|\Psi_n\rangle \Rightarrow$ we can't peel the S^{-1} off!!

Solution Four (instead of one) types of propagators: (note S^{-1} is *anti*-time ordered)

$\langle \psi^\dagger \psi \rangle$

contraction

$\langle \psi \psi^\dagger \rangle$

contraction

$\tilde{\mathcal{T}} \mathrm{e}^{\mathrm{i} \int \mathrm{d}t \; H_\mathrm{I}}$ $\quad \mathcal{T}$ observable $\quad \mathcal{T} \mathrm{e}^{-\mathrm{i} \int \mathrm{d}t \; H_\mathrm{I}}$

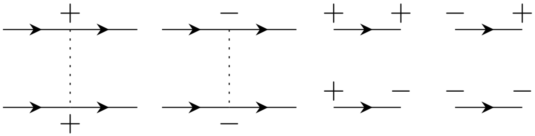
anti-time-ordered contraction $\qquad$ time-ordered contraction

Keldysh formalism

Four types of (fermionic) propagators

$$
\begin{aligned}
\mathrm{i}\,G^{--} &= \mathrm{i}\,G^{\mathrm{c}} = \langle \mathcal{T}\,\psi_1\psi_2^\dagger\rangle\,, \quad \mathrm{i}\,G^{++} = \mathrm{i}\,G^{\mathrm{a}} = \langle \tilde{\mathcal{T}}\psi_1\psi_2^\dagger\rangle\,, \\
\mathrm{i}\,G^{+-} &= \mathrm{i}\,G^{>} = \langle \psi_1\psi_2^\dagger\rangle\,, \quad \mathrm{i}\,G^{-+} = \mathrm{i}\,G^{<} = -\langle \psi_2^\dagger\psi_1\rangle\,.
\end{aligned}
\tag{2}
$$

Diagrams

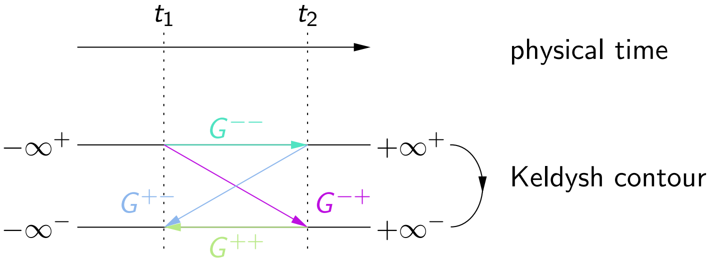


Self-energy

$$
G = \begin{pmatrix} G^{--} & G^{-+} \\ G^{+-} & G^{++} \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma^{--} & \Sigma^{-+} \\ \Sigma^{+-} & \Sigma^{++} \end{pmatrix}, \quad G = G_0 + G_0 \Sigma G\,. \tag{3}
$$

Alternative formulation: Keldysh contour

Keldysh contour The information in the G matrix can be alternatively stored in a time-ordered Green function on *Keldysh contour*



Green function EOM

From Keldysh contour to physical contour Lengreth theorem:

$$\begin{aligned} &(AB)^< = A^\mathrm{R} B^< + A^< B^\mathrm{A}, \quad (AB)^> = A^\mathrm{R} B^> + A^> B^\mathrm{A}, \\ &(AB)^\mathrm{R} = A^\mathrm{R} B^\mathrm{R}, \quad (AB)^\mathrm{A} = A^\mathrm{A} B^\mathrm{A}, \end{aligned} \tag{4}$$

where

$$\begin{aligned} &A^>(t_1, t_2) = A(t_1^+, t_2^-), \quad A^<(t_1, t_2) = A(t_1^-, t_2^+), \\ &A^\mathrm{R}(t_1, t_2) = \theta(t_1 - t_2)(A^> - A^<), \\ &A^\mathrm{A}(t_1, t_2) = -\theta(t_1 - t_2)(A^> - A^<). \end{aligned} \tag{5}$$

Mapping an equation on Keldysh contour to its counterpart on the physical time axis!

Derivation of EOM of $G^{<,>}$ and G^{A} I

Recommended references The following series:

- Václav Špička, Bedřich Velickỳ, and Anděla Kalvová. "Long and short time quantum dynamics: I. Between Green's functions and transport equations". In: *Physica E: Low-dimensional Systems and Nanostructures* 29.1-2 (2005), pp. 154–174
- Jørgen Rammer and H Smith. "Quantum field-theoretical methods in transport theory of metals". In: *Reviews of modern physics* 58.2 (1986), p. 323

Derivation of EOM of $G^{<,>}$ and G^{A} II

From self-energy correction to EOM From Lengreth theorem:

$$G = G_0 + G_0 \Sigma G \Rightarrow G^< = G_0^< + G_0^< \Sigma^{\mathrm{A}} G^{\mathrm{A}} + G_0^{\mathrm{R}} \Sigma^{\mathrm{R}} G^< + G_0^{\mathrm{R}} \Sigma^< G^{\mathrm{A}}, \quad (6)$$

$$G = G_0 + G \Sigma G_0 \Rightarrow G^< = G_0^< + G_0^{\mathrm{R}} \Sigma^{\mathrm{R}} G_0^< + G^{\mathrm{R}} \Sigma^< G_0^{\mathrm{A}} + G^< \Sigma^{\mathrm{A}} G^{\mathrm{A}}, \quad (7)$$

$$G^{\mathrm{A}} = G_0^{\mathrm{A}} + G_0^{\mathrm{A}} \Sigma^{\mathrm{A}} G^{\mathrm{A}}, \quad G^{\mathrm{R}} = G_0^{\mathrm{R}} + G_0^{\mathrm{R}} \Sigma^{\mathrm{R}} G^{\mathrm{R}}. \quad (8)$$

Getting rid of G_0 We define

$$G_0^{-1} := \mathrm{i}\, \partial_t - H_0, \quad (9)$$

and

$$G_0^{-1} G_0^{\mathrm{A,R}} = I, \quad G_0^{-1} G_0^{<,>} = 0. \quad (10)$$

Taking complex conjugate of the def. of $G_0^{<,>}$ we find (left arrow = apply ∂_t and H_0 to the second index of $G_0^{<,>}$)

$$G_0^{<,>} (-\mathrm{i}\, \overleftarrow{\partial}_{t_2} - H_0) = 0. \quad (11)$$

Derivation of EOM of $G^{<,>}$ and G^{A} III

The Schrödinger-like Kadanoff-Baym eq. Applying G_0^{-1} to the left of (6) and to the right of (7):

$$(\mathrm{i}\,\partial_{t_1} - H_0)G^<(1,2) = \Sigma^{\mathrm{R}} G^< + \Sigma^< G^{\mathrm{A}}, \tag{12}$$

$$-\mathrm{i}\,\partial_{t_2} G^<(1,2) - G^< H_0 = G^{\mathrm{R}} \Sigma^< + G^< \Sigma^{\mathrm{A}}, \tag{13}$$

$$\Rightarrow \mathrm{i}(\partial_{t_1} + \partial_{t_2})G^< - [H_0, G^<] = \Sigma^{\mathrm{R}} G^< + \Sigma^< G^{\mathrm{A}} - G^{\mathrm{R}} \Sigma^< - G^< \Sigma^{\mathrm{A}}. \tag{14}$$

Mixed coordinates We define "average time" and "relative time":

$$T = \frac{t_1 + t_2}{2}, \quad t = t_1 - t_2, \tag{15}$$

$$\Rightarrow \frac{\partial}{\partial T} = \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2}. \tag{16}$$

We then do Fourier transform over t: similar to the equilibrium case. ($T \simeq$ driving, $t \simeq$ internal time evolution)

Towards a single-time formalism

Summary up to now

- *Accurate* EOMs about $G^{\mathrm{A,R}}$, and EOM of $G^<$:

$$\mathrm{i}\,\partial_T G^< - [H_0, G^<] = \Sigma^{\mathrm{R}} G^< + \Sigma^< G^{\mathrm{A}} - G^{\mathrm{R}} \Sigma^< - G^< \Sigma^{\mathrm{A}}. \tag{17}$$

  The RHS contains t (or ω) and $G^<$.
- Note: we can actually put the $t = 0$ part of Σ into H_0! $\Rightarrow$ Example: COHSEX TD-aGW

Goal Obtaining quantum kinetics:

- Quantum master equation (QME), i.e. EOM of $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2, t)$,
- and its downfolded version (in long wave length, well-defined quasiparticle limit), the quantum Boltzmann equation (QBE)

Problem Both LHS and RHS contain ω: problem too large.
What we want Obtaining a close form EOM about $G^<(T, t = 0)$

Quantum master equation

Reduced density matrix Single-electron density matrix:

$$\mathrm{i}\,\rho(T) = G^{<}(T, t=0) = \int \frac{\mathrm{d}\omega}{2\pi} G^{<}(T, \omega) \tag{18}$$

What we want Two types of reduction:

- Reducing Σ to an easy function of G, ideally $G^{<}$
- Reducing $G^{<}$ to $\rho(T)$

Reducing Σ

- Always possible: we can formally eliminate χ, ϵ, etc. from Hedin eq. and get a Σ about G i.e. about $G^{<}, G^{\mathrm{A,R}}$
- But then $G^{\mathrm{A,B}}$ can be eliminated with (8) as well
- In reality: a truncation is needed ...

Reconstruction of $G^<$ from ρ

Reconstruction theorem From ρ, $G^{\mathrm{A,R}}$ (which can be calculated using (8) from ρ), $G^<$ can be completely restored[1]

Constructive proof See (71) in the reference; note that

$$\begin{aligned}(G^{\mathrm{R}})^{-1}\theta(t_1-t_2)G^< &= (\partial_{t_1} - H_0 - \Sigma^{\mathrm{R}})\theta(t_1-t_2)G^< \\ &= \delta(t_1-t_2)G^< + \theta(t_1-t_2)(\partial_{t_1} - H_0 - \Sigma^{\mathrm{R}})G^< \\ &= \rho(t_1) + \cdots \end{aligned} \tag{19}$$

[1] Václav Špička, Bedřich Velický, and Anděla Kalvová. "Long and short time quantum dynamics: I. Between Green's functions and transport equations". In: *Physica E: Low-dimensional Systems and Nanostructures* 29.1-2 (2005), pp. 154–174.

Existence of accurate quantum master equation In conclusion, in principle we can always write down something accurate like this:

$$\frac{\partial \rho}{\partial t} + \mathrm{i}\,[H_0, \rho] = \int_{-\infty}^{t} F[\rho(t')]\,\mathrm{d}t' \,, \tag{20}$$

where F is obtained from $\Sigma^{\mathrm{R}} G^{<} + \Sigma^{<} G^{\mathrm{A}} - G^{\mathrm{R}} \Sigma^{<} - G^{<} \Sigma^{\mathrm{A}}$, and $G^{\mathrm{R,A}}$ is reconstructed from ρ by doing a complete self-energy run, and $G^{<}$ is reconstructed from G^{A} and G^{R} and ρ.

. . . but of course simplification is needed

Gradient expansion: first step from QME to QBE

Mixed coordinates

$$\tilde{\rho}(\boldsymbol{p}, \boldsymbol{X}, t) = \int \mathrm{d}x \, \mathrm{e}^{-\mathrm{i}\, \boldsymbol{p} \cdot \boldsymbol{x}} \rho\left(\boldsymbol{X} + \frac{\boldsymbol{x}}{2}, \boldsymbol{X} - \frac{\boldsymbol{x}}{2}, t\right), \tag{21}$$

$$\frac{1}{\mathrm{i}} \widetilde{[H_0, \rho]} = \frac{\partial \epsilon}{\partial \boldsymbol{p}} \cdot \frac{\partial \tilde{\rho}}{\partial \boldsymbol{X}} - \frac{\partial \epsilon}{\partial \boldsymbol{X}} \cdot \frac{\partial \tilde{\rho}}{\partial \boldsymbol{p}} + \cdots \tag{22}$$

Gradient expansion Only take the first two terms: assuming no higher dependence

Issue: the definitions of G_0 and Σ

Ambiguity in the meaning of Σ

- In ordinary usage: G_0 directly from H_0
- But some prefer to move a part of Σ that looks like "effective potential" into H_0 ...
- G_0 contains "interactively corrected band structure"; Σ contains "scattering" – what is the distinction?

Comparison with similar issue in QBE

- When impurities are rare: they appear in collision integral
- When impurities are abundant: they lead to an impurity band ... and appear in the diffusion term?
- In QBE: it depends on the shape of the spectral function ...

Lacking proof of equivalence

- Do different division of labor between Σ and G_0 lead to consistent results?

A radical move towards quantum Boltzmann equation I

Approximations leading to QBE

- Smooth $U_{\text{ext}} \Rightarrow$ Gradient expansion:

$$[H_0, \rho] \longrightarrow \mathrm{i} \left(\frac{\partial \epsilon}{\partial \boldsymbol{p}} \cdot \frac{\partial \tilde{\rho}}{\partial \boldsymbol{X}} - \frac{\partial \epsilon}{\partial \boldsymbol{X}} \cdot \frac{\partial \tilde{\rho}}{\partial \boldsymbol{p}} + \cdots \right). \tag{23}$$

- Weakly correlated states $\Rightarrow$ Quasiparticle approx.:

$$G^{<}(\boldsymbol{X}, \boldsymbol{p}, T, \omega) = \mathrm{i} \underbrace{2\pi\delta(\omega - \xi_{\boldsymbol{p}} + \mu - U(\boldsymbol{X}, T))}_{A(\boldsymbol{X}, \boldsymbol{p}, T, \omega)} f(\boldsymbol{p}, \boldsymbol{X}, T), \tag{24}$$

$$G^{>}(\boldsymbol{X}, \boldsymbol{p}, T, \omega) = -\mathrm{i}\, A(\boldsymbol{X}, \boldsymbol{p}, T, \omega)(1 - f(\boldsymbol{p}, \boldsymbol{X}, T)). \tag{25}$$

This makes sense: we then have

$$A = \mathrm{i}(G^{\mathrm{R}} - G^{\mathrm{A}}) = \mathrm{i}(G^{>} - G^{<}). \tag{26}$$

- Gradient expansion in time domain $\Rightarrow$ Markovian collision integral

A radical move towards quantum Boltzmann equation II

Note

- The conditions are sufficient, but not necessary: in the formalism above, field renormalization (as in electron-phonon interaction) is not included, but by correcting the collision term (essentially, a mild breakdown of Fermi golden rule), a Boltzmann equation can still be established (with necessary corrections).
- The first condition and the rest two conditions are orthogonal: the first condition can also be used in QME: it gives the diffusion part of QBE
- The second and third conditions are used to simply the interactive RHS ($G^> \Sigma^< - G^< \Sigma^>$) into the collision integral.

A radical move towards quantum Boltzmann equation III

- $\Sigma^{<,>}$ are intuitively related to scattering but scattering $\neq$ non-pure state evolution ("incoherence"); Markovian also $\neq$ dissipation (counterexample: quantum optics beam splitter, which has a scattering matrix and splits beam immediately – but is totally pure-state i.e. coherent). Incoherence only appears due to ignoring other degrees of freedom (and not using an input-output formalism), which comes from higher-order correlation being ignored here.

A radical move towards quantum Boltzmann equation IV

Convolution in Green function EOM

$$AB := \int \mathrm{d}2\, A(1,2)B(2,3). \tag{27}$$

Gradient expansion, in $\boldsymbol{r}$ and t Taking Taylor expansion in $(\boldsymbol{r}, t)$

$$\begin{aligned} AB|_{\boldsymbol{X},\boldsymbol{p},T,\omega} &= A_{\boldsymbol{X},\boldsymbol{p},T,\omega} B_{\boldsymbol{X},\boldsymbol{p},T,\omega} \\ &\quad + \frac{\mathrm{i}}{2}\left(\frac{\partial A}{\partial \boldsymbol{X}} \cdot \frac{\partial B}{\partial \boldsymbol{p}} - \frac{\partial A}{\partial \boldsymbol{p}} \cdot \frac{\partial B}{\partial \boldsymbol{X}} - \frac{\partial A}{\partial T}\frac{\partial B}{\partial \omega} + \frac{\partial A}{\partial \omega}\frac{\partial B}{\partial T} \right) + \cdots \end{aligned} \tag{28}$$

We only keep the terms shown above.
$\Rightarrow [G^<, H_0]$ reduces to the diffusion term seen in QBE

Multi-band, spin index, etc. When we have discrete labels in $A, B, \ldots,$ quantities in (28) are matrices with these discrete indices

A radical move towards quantum Boltzmann equation V

Prototype of the collision integral Keeping only the first term in gradient expansion (28):

$$
\begin{aligned}
& \Sigma^{\mathrm{R}} G^{<} + \Sigma^{<} G^{\mathrm{A}} - G^{\mathrm{R}} \Sigma^{<} - G^{<} \Sigma^{\mathrm{A}} \\
\overset{\text{gradient exp.}}{\approx} \;& G^{<}(\Sigma^{\mathrm{R}} - \Sigma^{\mathrm{A}}) - (G^{\mathrm{R}} - G^{\mathrm{A}})\Sigma^{<} \\
=\;& G^{<}\Sigma^{>} - G^{>}\Sigma^{<} \\
\overset{\text{QP approx.}}{\approx} \;& \mathrm{i}\, A f(\boldsymbol{p}) \operatorname{Im} \Sigma - \text{incoming terms}
\end{aligned}
\tag{29}
$$

- Second line: the commutator terms assume the same form as that of (28), but are an order of magnitude smaller than it.
- Third line: from $A^{\mathrm{R}} - A^{\mathrm{A}} = A^{>} - A^{<}$
- The quasiparticle approximation (24) $\Rightarrow$ introduction of $f(\boldsymbol{p})$; the "out" part $\propto \operatorname{Im}\Sigma$ ($\operatorname{Im}\Sigma$ generally is even not well-defined)

A radical move towards quantum Boltzmann equation VI

Obtaining the collision integral

$$\text{LHS} = \mathrm{i}\,\partial_T G^< - \mathrm{i}\left(\frac{\partial H_0}{\partial \boldsymbol{X}} \cdot \frac{\partial G^<}{\partial \boldsymbol{p}} - \frac{\partial H_0}{\partial \boldsymbol{p}} \cdot \frac{\partial G^<}{\partial \boldsymbol{X}}\right), \tag{30}$$

where the $-\frac{\partial H_0}{\partial T}\frac{\partial G^<}{\partial \omega} + \frac{\partial H}{\partial \omega}\frac{\partial G^<}{\partial T}$ terms vanish when H_0 contains no strong time dependence.

$$\text{RHS} = G^< \Sigma[\mathrm{i}\,G^>] - G^> \Sigma[\mathrm{i}\,G^<]. \tag{31}$$

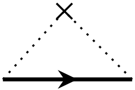
$G^<$ appears in the LHS once, so there is a $2\pi\,\mathrm{i}\,\delta(\omega - H)$ factor in the LHS; in the RHS suppose $\Sigma \sim G^n$, then the normalization factor coming with G is $(2\pi\,\mathrm{i}\,\delta(\omega - H))^{n+1}$; but since there are n propagators in Σ, we have $n-1$ frequency integrals connecting them to the "skeleton" of Σ, each with a factor of $1/2\pi$, so finally there is a $2\pi\delta(\omega - H)$ factor in the

A radical move towards quantum Boltzmann equation VII

RHS, which exactly is the factor seen in Fermi golden rule. The imaginary units always cancel each other finally.

Example: disorder self-energy The self-energy is

$$-\mathrm{i}\,\Sigma(\boldsymbol{p},\omega) =$$



$$= \sum_{\boldsymbol{q}} -\frac{1}{V} c |v(\boldsymbol{q}-\boldsymbol{p})|^2 \cdot \mathrm{i}\,G(\boldsymbol{q},\omega), \tag{32}$$

where each dotted line corresponds to $-\mathrm{i}\,gv(\boldsymbol{q}-\boldsymbol{p})/\sqrt{V}$, and c comes from averaging over the distribution of disorders.
The equation becomes

$$\begin{aligned} &\mathrm{i}\,\partial_T G^< - \mathrm{i}\left(\frac{\partial H_0}{\partial \boldsymbol{X}} \cdot \frac{\partial G^<}{\partial \boldsymbol{p}} - \frac{\partial H_0}{\partial \boldsymbol{p}} \cdot \frac{\partial G^<}{\partial \boldsymbol{X}}\right) \\ = &\frac{1}{V} \sum_{\boldsymbol{q}} c |v(\boldsymbol{p}-\boldsymbol{q})|^2 (G^<(\boldsymbol{p}) \cdot G^>(\boldsymbol{q}) - G^>(\boldsymbol{p}) \cdot G^<(\boldsymbol{q})), \end{aligned} \tag{33}$$

A radical move towards quantum Boltzmann equation VIII

and thus from quasiparticle approximation (f and A also depend on $\boldsymbol{X}$, T)

$$\frac{\mathrm{d}}{\mathrm{d}T}A(\boldsymbol{p})f(\boldsymbol{p}) = \int \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi)^d} c|v(\boldsymbol{p}-\boldsymbol{q})|^2 A(\boldsymbol{p})f(\boldsymbol{p})\cdot(-A(\boldsymbol{q}))(1-f(\boldsymbol{q}))+\boldsymbol{p}\leftrightarrow\boldsymbol{q}, \tag{34}$$

and integrating over ω we get

$$\frac{\mathrm{d}}{\mathrm{d}T}f(\boldsymbol{p}) = \int \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi)^d} c|v(\boldsymbol{p}-\boldsymbol{q})|^2(-2\pi)\delta(\epsilon_{\boldsymbol{p}}-\epsilon_{\boldsymbol{q}})f(\boldsymbol{p})(1-f(\boldsymbol{q}))+\boldsymbol{p}\leftrightarrow\boldsymbol{q}, \tag{35}$$

which is exactly what is obtained by intuitively inserting Fermi golden rule to the RHS of QBE.

Comments on derivation of QBE

The role of the assumptions

- Gradient expansion does most of the heavy lifting job
- Quasiparticle approximation is used to write down an explicit collision integral
- The locality of the collision integral comes from gradient expansion on the temporal domain as well

Phenomenon covered

- Exciton is multi-band phenomenon, but multi-band QBE can be established; see Lifshitz's Statistical Physics: Theory of the Condensed State, §5 for a magnetic field-induced exciton
- Plasmon comes from long-range divergence of Hartree term (in BerkeleyGW the $\boldsymbol{q} = 0, \boldsymbol{G} = 0$ part is omitted)

A little beyond the quasiparticle approximation

ω dependence in Σ, no damping $\Rightarrow$ QBE with field renormalization.[2]

Example: electron-phonon interaction Renormalized QBE:

$$
\begin{aligned}
&(\partial_T + \nabla_{\boldsymbol{p}} E_{\boldsymbol{p}} \cdot \nabla_{\boldsymbol{R}} - \nabla_{\boldsymbol{R}}(E_{\boldsymbol{p}} + e\varphi) \cdot \nabla_{\boldsymbol{p}}) n_{\boldsymbol{p}} \\
&= -2\pi \int \frac{\mathrm{d}^3 \boldsymbol{p}'}{(2\pi)^3} Z_{\boldsymbol{p}} Z_{\boldsymbol{p}'} |g_{\boldsymbol{p}-\boldsymbol{p}'}|^2 \\
&\quad \times (n_{\boldsymbol{p}}(1 - n_{\boldsymbol{p}'})(1 + N(E_{\boldsymbol{p}} - E_{\boldsymbol{p}'})) - n_{\boldsymbol{p}'}(1 - n_{\boldsymbol{p}}) N(E_{\boldsymbol{p}} - E_{\boldsymbol{p}'})) \\
&\quad \times (\delta(E_{\boldsymbol{p}} - E_{\boldsymbol{p}'} - \omega_{\boldsymbol{p}-\boldsymbol{p}'}) - \delta(E_{\boldsymbol{p}} - E_{\boldsymbol{p}'} + \omega_{\boldsymbol{p}-\boldsymbol{p}'}))
\end{aligned}
\tag{36}
$$

$\Rightarrow$ Fermi golden rule is not accurate when field renormalization is strong

Another example: DMFT QBE[3]

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[2] Jørgen Rammer and H Smith. "Quantum field-theoretical methods in transport theory of metals". In: *Reviews of modern physics* 58.2 (1986), p. 323.

[3] Michael Wais et al. "Quantum Boltzmann equation for strongly correlated systems: Comparison to dynamical mean field theory". In: *Physical Review B* 98.13 (2018), p. 134312.

QBE in crystal

In crystal:

- If we work in $\boldsymbol{r}$ representation, $u_{n\boldsymbol{k}}$ means the relation between $\boldsymbol{r}$ and $\boldsymbol{k}$ is not simply Fourier transform; we can't define $f(\boldsymbol{X}, \boldsymbol{p})$ directly from Wigner transform.
- If we work in $\boldsymbol{k}$ representation, no well-defined $\boldsymbol{r}$ is initially given.

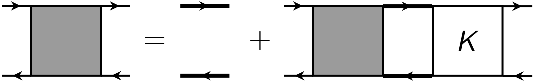
Solution

- Working in $\boldsymbol{k}$ representation; expanding $\varepsilon_{n\boldsymbol{k}} + e\boldsymbol{r} \cdot \boldsymbol{E}$ in this basis;
- TODO: prove that $\mathrm{i}\,\partial_{\boldsymbol{k}}$ is indeed the $\boldsymbol{r}$ appearing in electric field; after Wigner transform in $\boldsymbol{k}$ space, recover $\epsilon_{n\boldsymbol{k}} + e(\boldsymbol{r} + \boldsymbol{A}) \cdot \boldsymbol{E}$
- From semi-conservation law of $\boldsymbol{k}$ we get localized collision integral in RHS; the matrix elements of the screened Coulomb interaction are evaluated in $\psi_{n\boldsymbol{k}}$ basis as well.

BSE and single-electron kinetic theory

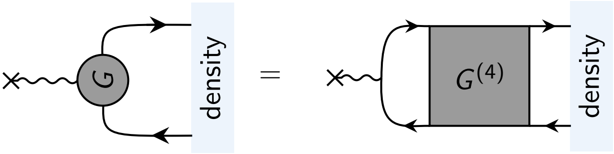
BSE for second-order correlation

Bethe–Salpeter equation (BSE)



(37)

What we need Linear response of single-electron under external field = BSE (simplest single-electron theory: QBE)



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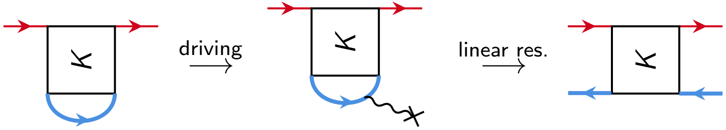
Next step: relation between K and Σ

Linear response of a single self-energy diagram

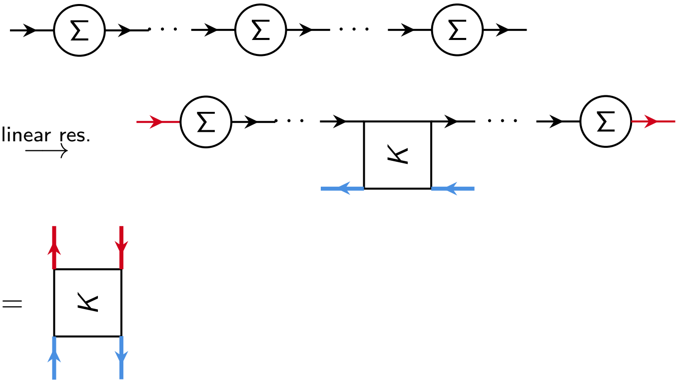
$\Sigma =$



(39)

Linking Σ with K

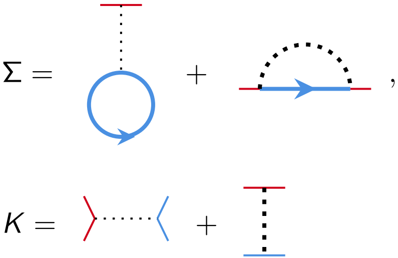
Whole picture



(40)

Linking Σ with K

Example: linear response from time-dependent GW = BSE



(41)

- First term = Electron Hartree term = Electron direct term = Exciton exchange term; $+1$ prefactor;
- Second term = Electron Fock term = Electron exchange term = Exciton direct term; (-1) prefactor.

Summary of formalisms

- Keldysh formalism (TODO: subtleties in initial correlation)
  - In principle we can get a closed equation system (with retardation) about G and hence $G^<$;
  - in practice $\Sigma[G]$ has to be truncated; n corrected propagator in $\Sigma =$ n-order non-trivial correlation
- $\Rightarrow$ ... and hence a (highly complicated) accurate quantum master equation
  - G needs to be reconstructed from ρ: reconstruction formalism
  - Issue: how to decide the division of labor between H_0 and Σ, when no physical pictures like "distinction between diffusion and collision" are available?
- Boltzmann formalism
  - Approximation 1: gradient expansion
  - Approximation 2: well-defined quasiparticle
  - Slight violation of approx. 2 (e.g. Z renormalization factor): Fermi golden rule no longer 100 % correct
- QBE $\Rightarrow$ hydrodynamics with random fluctuation

Overview

- ("Adiabatic") approximation for Σ: static limit of GW (i.e. $t = 0$) $=:$ static COHSEX
- In linear limit: W doesn't change $\Rightarrow$ only high-order correlation taken into account is the ladder approximation using static screening $=$ static screening BSE
- Σ has no $t \neq t'$ components $\Rightarrow$ Σ can be placed into H_0 $\Rightarrow$ TD-aGW usually carried out in QME framework

Introduction to COHSEX

Example: