Essential introduction to NEGF methods for real-time simulations

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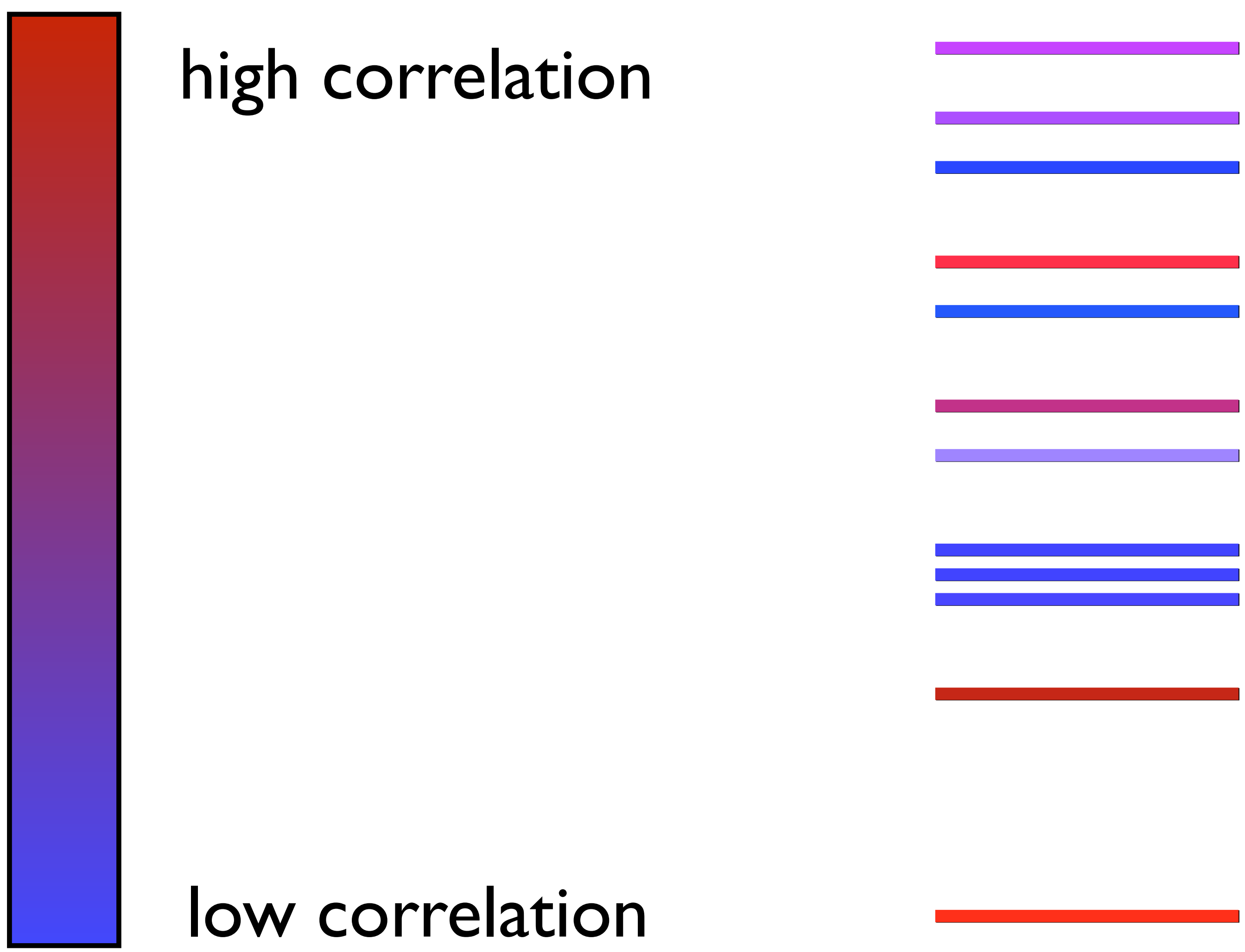
Strongly correlated systems ?

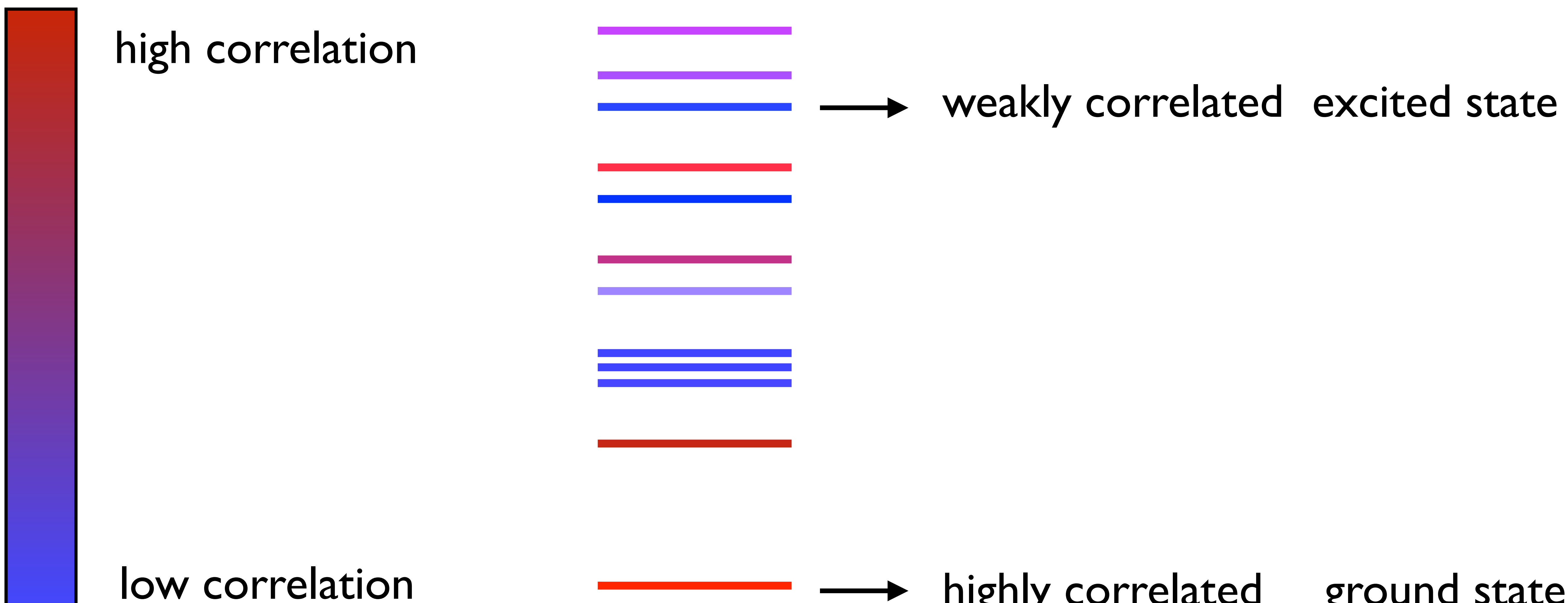
Spectrum



Not necessarily same type of correlations

Strongly correlated systems ?

Spectrum



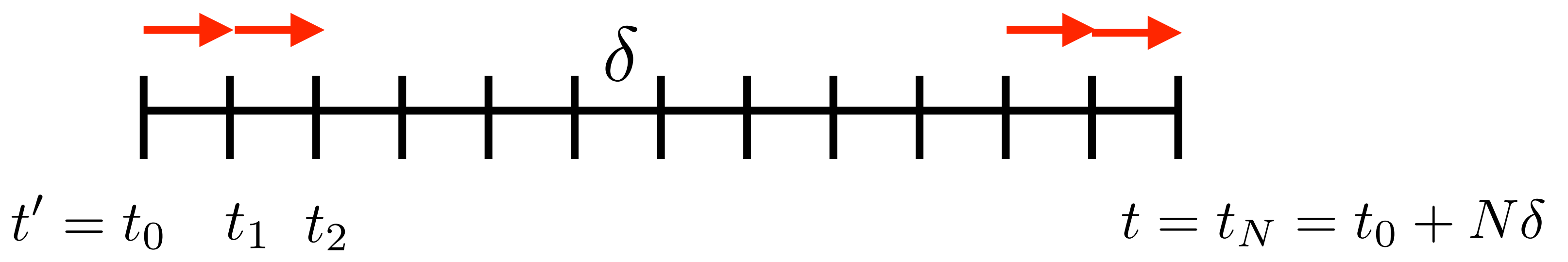
Extra difficulties in nonequilibrium

- More than just one state… how many? It depends on the time-dependent perturbation
- Different states may experience different correlation effects
- No equilibrium shortcuts: everything changes in time

Preparing the stage

$$\mathrm{i}\frac{d}{dt}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle \quad \Longrightarrow \quad |\Psi(t)\rangle = \hat{U}(t,0)|\Psi_g\rangle$$

Evolution operator for $t > t'$



$$\hat{U}(t,t') =$$

(forward evolution)

From the group property: $\hat{U}(t,t')\hat{U}(t',t) = \hat{1}$

$$\hat{U}(t',t) = \lim_{\delta\to 0} e^{\mathrm{i}\delta\hat{H}(t_0)}e^{\mathrm{i}\delta\hat{H}(t_1)}\dots e^{\mathrm{i}\delta\hat{H}(t_{N-1})}e^{\mathrm{i}\delta\hat{H}(t_N)} = \bar{\mathcal{T}}\left\{e^{-\mathrm{i}\int_t^{t'} d\bar{t}\,\hat{H}(\bar{t})}\right\}$$

(backward evolution)

Time-dependent averages

$$O(t) = \langle \Psi_g | \hat{U}(0,t) \hat{O} \hat{U}(t,0) | \Psi_g \rangle$$

correlation is everywhere

Adiabatic switching of the interaction: for $t < 0$

$$\hat{H}_\eta(t) = \hat{H}_0 + e^{-\eta|t|} \hat{H}_{\rm int} \quad \Rightarrow \quad |\Psi_g\rangle = \hat{U}(0,-\infty)|\Phi_g\rangle$$

noninteracting ground state

Let's try again

$$O(t) = \langle \Phi_g | \hat{U}(-\infty,t) \hat{O} \hat{U}(t,-\infty) | \Phi_g \rangle$$

$$= \langle \Phi_g | \bar{\mathcal{T}} \left\{ e^{-{\rm i}\int_t^{-\infty} d\bar{t}' \, \hat{H}(\bar{t}')} \right\} \hat{O} \, \mathcal{T} \left\{ e^{-{\rm i}\int_{-\infty}^{t} d\bar{t} \, \hat{H}(\bar{t})} \right\} |\Phi_g\rangle$$

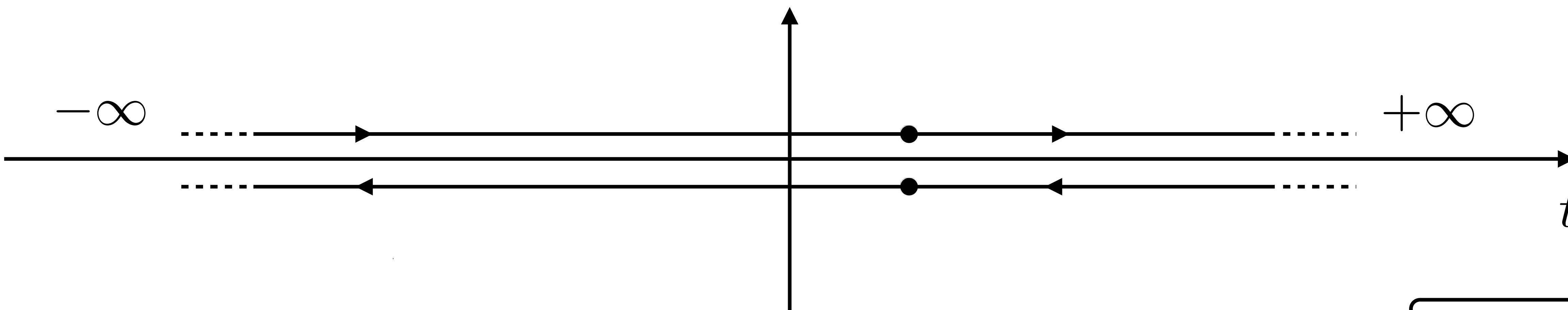
Time-dependent averages

Times on the contour: $z = t_-$ (forward branch) $z = t_+$ (backward branch)

Operators on the contour: $\hat{O}(t_-) = \hat{O}(t_+) \equiv \hat{O}(t)$

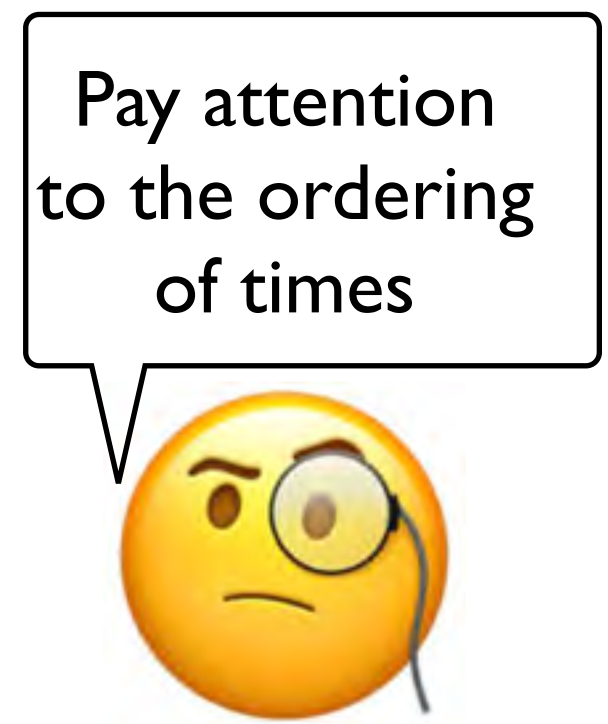
CONTOUR IDEA

$$O(t) = \langle \Phi_g | \mathcal{T}_\gamma \left\{ e^{-\mathrm{i} \int_\gamma d\bar{z}\, \hat{H}(\bar{z})} \hat{O}(z) \right\} | \Phi_g \rangle$$



$$O(t) = \langle \Phi_g | \hat{U}(-\infty, t) \hat{O} \hat{U}(t, -\infty) | \Phi_g \rangle$$

$$= \langle \Phi_g | \bar{\mathcal{T}} \left\{ e^{-\mathrm{i} \int_t^{-\infty} d\bar{t}'\, \hat{H}(\bar{t}')} \right\} \hat{O}\, \mathcal{T} \left\{ e^{-\mathrm{i} \int_{-\infty}^{t} d\bar{t}\, \hat{H}(\bar{t})} \right\} | \Phi_g \rangle$$



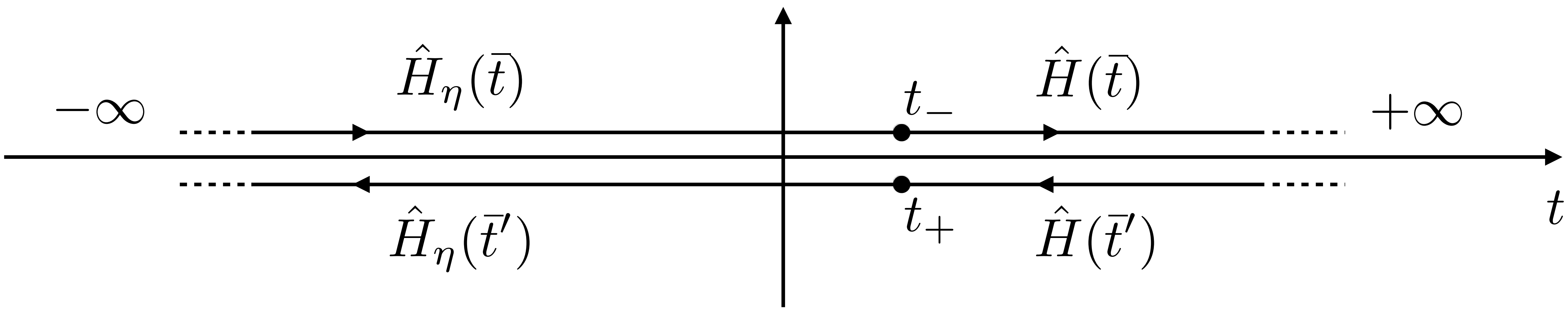
Time-dependent averages

Times on the contour: $z = t_-$ (forward branch) $z = t_+$ (backward branch)

Operators on the contour: $\hat{O}(t_-) = \hat{O}(t_+) \equiv \hat{O}(t)$

CONTOUR IDEA

$$O(t) = \langle \Phi_g | \mathcal{T}_\gamma \left\{ e^{-\mathrm{i} \int_\gamma d\bar{z}\, \hat{H}(\bar{z})} \hat{O}(z) \right\} |\Phi_g\rangle$$



Examples: $z = t_-$

$$O(t) = \langle \Phi_g | \underbrace{\bar{\mathcal{T}} \left\{ e^{-\mathrm{i} \int_\infty^{-\infty} d\bar{t}'\, \hat{H}(\bar{t}')} \right\}}_{\hat{U}(-\infty,\infty)} \underbrace{\mathcal{T} \left\{ e^{-\mathrm{i} \int_t^{\infty} d\bar{t}\, \hat{H}(\bar{t})} \right\}}_{\hat{U}(\infty,t)} \hat{O}\, \underbrace{\mathcal{T} \left\{ e^{-\mathrm{i} \int_{-\infty}^{t} d\bar{t}\, \hat{H}(\bar{t})} \right\}}_{\hat{U}(t,-\infty)} |\Phi_g\rangle$$

$$= \langle \Phi_g | \hat{U}(-\infty, t) \hat{O} \hat{U}(t, -\infty) | \Phi_g \rangle$$

NEGF

NEGF is a nonperturbative approach to calculate time-dependent averages

The fundamental bit is the contour Green's function

$$G_{ij}(z,z') \equiv \frac{1}{\mathrm{i}} \langle \Phi_g | \mathcal{T}_\gamma \left\{ e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})} \hat{d}_i(z) \hat{d}_j^\dagger(z') \right\} |\Phi_g\rangle$$

Probability amplitude that a hole created in i at time t is found in j at time t'

If z is earlier than z' (lesser Green's function)

$$G_{ij}(z,z') = -\frac{1}{\mathrm{i}} \langle \Phi_g | \hat{U}(-\infty,t')\, \hat{d}_j^\dagger\, \hat{U}(t',t)\, \hat{d}_i\, \hat{U}(t,-\infty) |\Phi_g\rangle \equiv G_{ij}^<(t,t')$$

Probability amplitude that an electron created in j at time t' is found in i at time t

If z is later than z' (greater Green's function)

$$G_{ij}(z,z') = \frac{1}{\mathrm{i}} \langle \Phi_g | \hat{U}(-\infty,t) \hat{d}_i \hat{U}(t,t') \hat{d}_j^\dagger \hat{U}(t',-\infty) |\Phi_g\rangle \equiv G_{ij}^>(t,t')$$

What can we get from G ?

Time-dependent average of one-body operators $\hat{O} = \sum_{ij} O_{ij} \hat{d}_i^\dagger \hat{d}_j$

$$O(t) = \sum_{ij} O_{ij} \langle \Phi_g | \hat{U}(-\infty, t) \hat{d}_i^\dagger \hat{d}_j \hat{U}(t, -\infty) | \Phi_g \rangle = -\mathrm{i} \sum_{ij} O_{ij} G_{ji}^<(t,t)$$

Time-dependent average of interaction energy (two-body operator)

$$E_{\mathrm{int}}(t) = \frac{1}{4\mathrm{i}} \sum_{ij} \left[\mathrm{i} \left(\frac{d}{dt} - \frac{d}{dt'} \right) \delta_{ij} - 2 h_{ij}(t) \right] G_{ji}^<(t,t') \Big|_{t=t'}$$

Momentum-resolved photoemission current

$$I_{\mathbf{k}}(t) = 2 \sum_{ij} \int d\bar{t}\, \mathrm{Re} \left[\Sigma_{ij,\mathbf{k}}(t,\bar{t}) G_{ji}^<(\bar{t},t) \right]$$

How do we get G ?

Starting point — Inside the contour ordering the operators commute, e.g.,

$$\mathcal{T}_\gamma \left\{ \hat{H}_0(z)\hat{H}_{\rm int}(z') \right\} = \mathcal{T}_\gamma \left\{ \hat{H}_{\rm int}(z')\hat{H}_0(z) \right\}$$

Back to the definition

$$\hat{H}(z) = \hat{H}_0(z) + \hat{H}_{\rm int}(z)$$

$$G_{ij}(z,z') \equiv \frac{1}{\rm i}\langle\Phi_g|\mathcal{T}_\gamma \left\{ e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\hat{d}_i(z)\hat{d}_j^\dagger(z') \right\}|\Phi_g\rangle$$

$$= \frac{1}{\rm i}\langle\Phi_g|\mathcal{T}_\gamma \left\{ e^{-{\rm i}\int_\gamma d\bar{z}\,\hat{H}_0(\bar{z})} e^{-{\rm i}\int_\gamma d\bar{z}\,\hat{H}_{\rm int}(\bar{z})}\hat{d}_i(z)\hat{d}_j^\dagger(z') \right\}|\Phi_g\rangle$$

$$= \frac{1}{\rm i}\sum_{n=0}^{\infty}\frac{(-{\rm i})^n}{n!}\int_\gamma dz_1\dots dz_n$$

$$\times\langle\Phi_g|\mathcal{T}_\gamma \left\{ e^{-{\rm i}\int_\gamma d\bar{z}\,\hat{H}_0(\bar{z})}\hat{H}_{\rm int}(z_1)\dots\hat{H}_{\rm int}(z_n)\hat{d}_i(z)\hat{d}_j^\dagger(z') \right\}|\Phi_g\rangle$$

How do we get G ?

Starting point — Inside the contour ordering the operators commute, e.g.,

$$\mathcal{T}_\gamma \left\{ \hat{H}_0(z) \hat{H}_{\text{int}}(z') \right\} = \mathcal{T}_\gamma \left\{ \hat{H}_{\text{int}}(z') \hat{H}_0(z) \right\}$$

Go back to the definition

$$\hat{H}(z) = \hat{H}_0(z) + \hat{H}_{\text{int}}(z)$$

$$G_{ij}(z, z') \equiv \frac{1}{\mathrm{i}} \langle \Phi_g | \mathcal{T}_\gamma \left\{ e^{-i \int_\gamma d\bar{z}\, \hat{H}(\bar{z})} \hat{d}_i(z) \hat{d}_j^\dagger(z') \right\} | \Phi_g \rangle$$

$$= \frac{1}{\mathrm{i}} \langle \Phi_g | \mathcal{T}_\gamma \left\{ e^{-\mathrm{i} \int_\gamma d\bar{z}\, \hat{H}_0(\bar{z})} e^{-\mathrm{i} \int_\gamma d\bar{z}\, \hat{H}_{\text{int}}(\bar{z})} \hat{d}_i(z) \hat{d}_j^\dagger(z') \right\} | \Phi_g \rangle$$

$$G_{ij}(z, z') = \frac{1}{\mathrm{i}} \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_\gamma dz_1 \ldots dz_n$$

$$\times \langle \Phi_g | \mathcal{T}_\gamma \left\{ e^{-\mathrm{i} \int_\gamma d\bar{z}\, \hat{H}_0(\bar{z})} \hat{H}_{\text{int}}(z_1) \ldots \hat{H}_{\text{int}}(z_n) \hat{d}_i(z) \hat{d}_j^\dagger(z') \right\} | \Phi_g \rangle$$

How do we get G ?

Same expansion as the standard time-ordered Green's function !!!

Only difference is: time t ⟶ contour time z

Dyson equation on the contour

$$G(z,z') = G_0(z,z') + \int_\gamma dz_1 dz_2\, G_0(z,z_1)\Sigma(z_1,z_2)G(z_2,z')$$

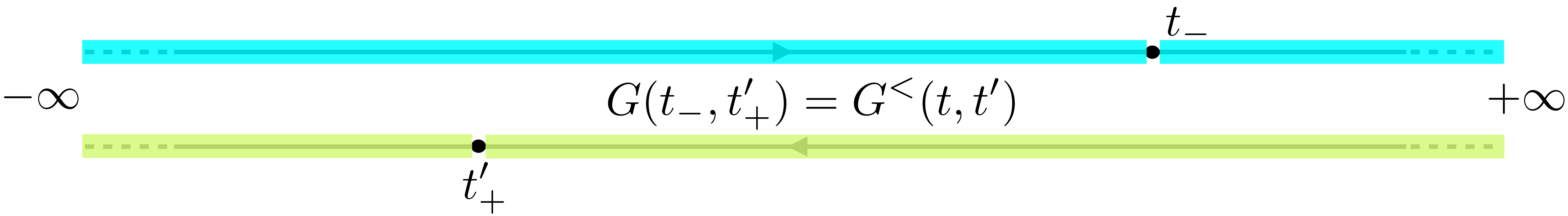
$$= G_0(z,z') + \int_\gamma dz_1 dz_2\, G(z,z_1)\Sigma(z_1,z_2)G_0(z_2,z')$$

$$G_{ij}(z,z') = \frac{1}{\mathrm{i}} \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_\gamma dz_1 \dots dz_n$$

$$\times \langle \Phi_g | \mathcal{T}_\gamma \left\{ e^{-\mathrm{i} \int_\gamma d\bar{z}\, \hat{H}_0(\bar{z})} \hat{H}_{\mathrm{int}}(z_1) \dots \hat{H}_{\mathrm{int}}(z_n) \hat{d}_i(z) \hat{d}_j^\dagger(z') \right\} |\Phi_g\rangle$$

The Kadanoff-Baym equations

We must convert the eom into equations for the real-time functions $G^<$ and $G^>$



$$\left[\mathrm{i}\frac{d}{dt} - h(t)\right] G^<(t,t') = \int_\gamma d\bar{z}\, \Sigma(t_-, \bar{z}) G(\bar{z}, t'_+)$$

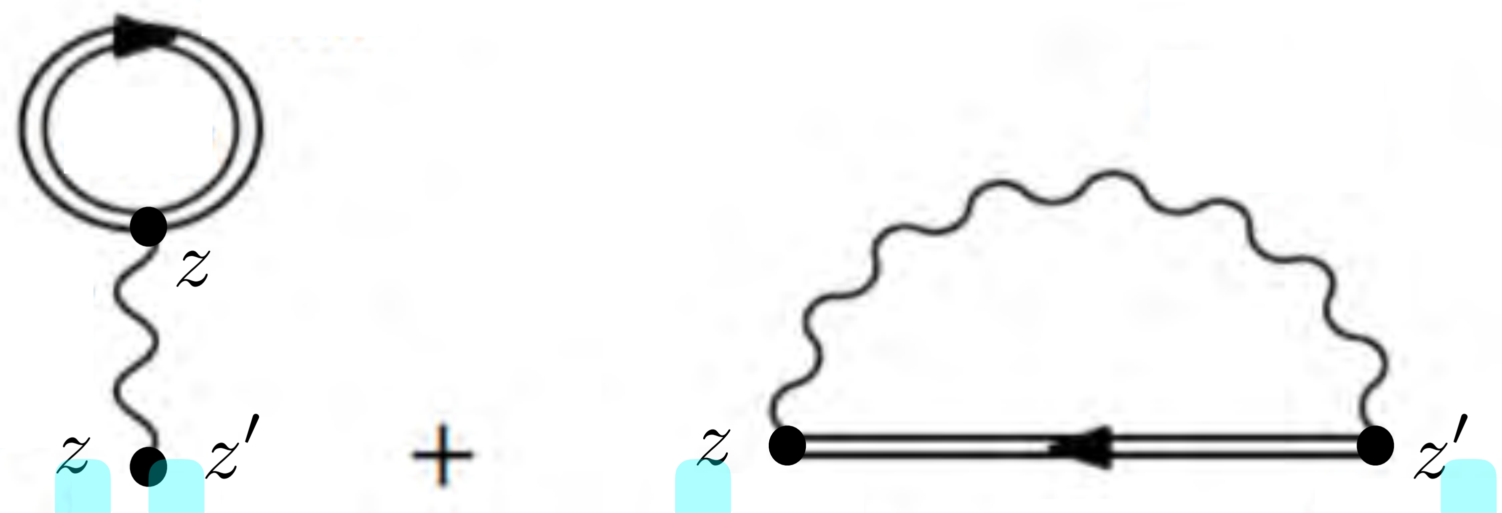
$$= \int_{-\infty}^{t} d\bar{t}\, \underbrace{\Sigma(t_-, \bar{t}_-) G(\bar{t}_-, t'_+)}_{\Sigma^>(t,\bar{t}) G^<(\bar{t},t')} + \int_{t}^{\infty} d\bar{t}\, \underbrace{\Sigma(t_-, \bar{t}_-) G(\bar{t}_-, t'_+)}_{\Sigma^<(t,\bar{t}) G^<(\bar{t},t')}$$

$$+ \int_{\infty}^{t'} d\bar{t}\, \underbrace{\Sigma(t_-, \bar{t}_+) G(\bar{t}_+, t'_+)}_{\Sigma^<(t,\bar{t}) G^<(\bar{t},t')} + \int_{t'}^{-\infty} d\bar{t}\, \underbrace{\Sigma(t_-, \bar{t}_+) G(\bar{t}_+, t'_+)}_{\Sigma^<(t,\bar{t}) G^>(\bar{t},t')}$$

$$= \int_{-\infty}^{t} d\bar{t} \left[\Sigma^>(t,\bar{t}) - \Sigma^<(t,\bar{t})\right] G^<(\bar{t}, t') - \int_{-\infty}^{t'} d\bar{t}\, \Sigma^<(t,\bar{t}) \left[G^>(\bar{t}, t') - G^<(\bar{t}, t')\right]$$

Intermezzo: the self-energy

$$\Sigma_{ij}(z, z') =$$

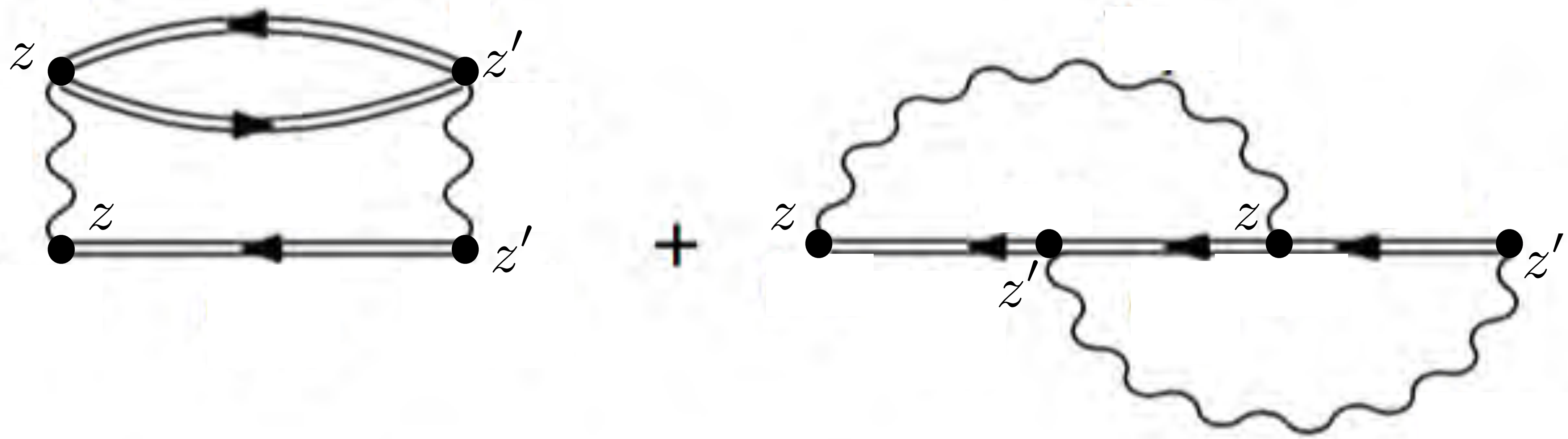


$$= \delta(z, z') \sum_{mn} \big(v_{imnj} - v_{imjn}\big) \rho_{nm}(t) = \delta(z, z') V_{\mathrm{HF},ij}(t)$$

$$\boxed{G(z, z^{+}) = G^{<}(t, t) = \mathrm{i}\rho(t)}$$

Intermezzo: the self-energy

$\Sigma_{ij}(z, z') =$



$$= \mathrm{i}^2 \sum_{rpn} \sum_{mqs} v_{irpn} v_{mqsj} \left[-G_{nm}(z, z') G_{sr}(z', z) G_{pq}(z, z') + G_{nq}(z, z') G_{sr}(z', z) G_{pm}(z, z') \right]$$

$$\Sigma(z, z') \to \Sigma^{\lessgtr}(t, t')$$

$$\Downarrow$$

$$G_{nm}(z, z') G_{sr}(z', z) G_{pq}(z, z') \to G^{\lessgtr}_{nm}(t, t') G^{\gtrless}_{sr}(t', t)^{\lessgtr} G^{\lessgtr}_{pq}(t, t')$$

Back to KBE

$$\mathrm{i}\frac{d}{dt}G^<(t,t') = h(t)G^<(t,t') + \int^{t} d\bar{t}\Big[\Sigma^>(t,\bar{t}) - \Sigma^<(t,\bar{t})\Big]G^<(\bar{t},t') - \int^{t'} d\bar{t}\,\Sigma^<(t,\bar{t})\Big[G^>(\bar{t},t') - G^<(\bar{t},t')\Big]$$

$$-\mathrm{i}\frac{d}{dt'}G^<(t,t') = G^<(t,t')h(t') + \int^{t} d\bar{t}\Big[G^>(t,\bar{t}) - G^<(t,\bar{t})\Big]\Sigma^<(\bar{t},t') - \int^{t'} d\bar{t}\,G^<(t,\bar{t})\Big[\Sigma^>(\bar{t},t') - \Sigma^<(\bar{t},t')\Big]$$

Time-stepping numerical solution scales like the number of time steps
N (for t) x N (for t') x N (for the integral) = N^3

Is there any chance to reduce the computational cost?

Back to KBE

$$\mathrm{i}\frac{d}{dt}G^<(t,t') = h(t)G^<(t,t') + \int^t d\bar{t}\Big[\Sigma^>(t,\bar{t}) - \cancel{\Sigma^<(t,\bar{t})}\Big]G^<(\bar{t},t') - \int^{t'} d\bar{t}\,\Sigma^<(t,\bar{t})\Big[G^>(\bar{t},t') - \cancel{G^<(\bar{t},t')}\Big]$$

$$-\mathrm{i}\frac{d}{dt'}G^<(t,t') = G^<(t,t')h(t') + \int^t d\bar{t}\Big[G^>(t,\bar{t}) - \cancel{G^<(t,\bar{t})}\Big]\Sigma^<(\bar{t},t') - \int^{t'} d\bar{t}\,G^<(t,\bar{t})\Big[\Sigma^>(\bar{t},t') - \cancel{\Sigma^<(\bar{t},t')}\Big]$$

Subtraction and evaluation in t=t'

$$\mathrm{i}\left(\frac{d}{dt} + \frac{d}{dt'}\right)G^<(t,t')\Big|_{t=t'} - \Big[h(t), G^<(t,t)\Big] = I(t) + I^\dagger(t)$$

$$-\frac{d}{dt}\rho(t) \qquad -\mathrm{i}\Big[h(t),\rho(t)\Big] \qquad = \int^t d\bar{t}\,\Big[\Sigma^>(t,\bar{t})G^<(\bar{t},t) - \Sigma^<(t,\bar{t})G^>(\bar{t},t)\Big]$$

$$+\mathrm{h.c.}$$

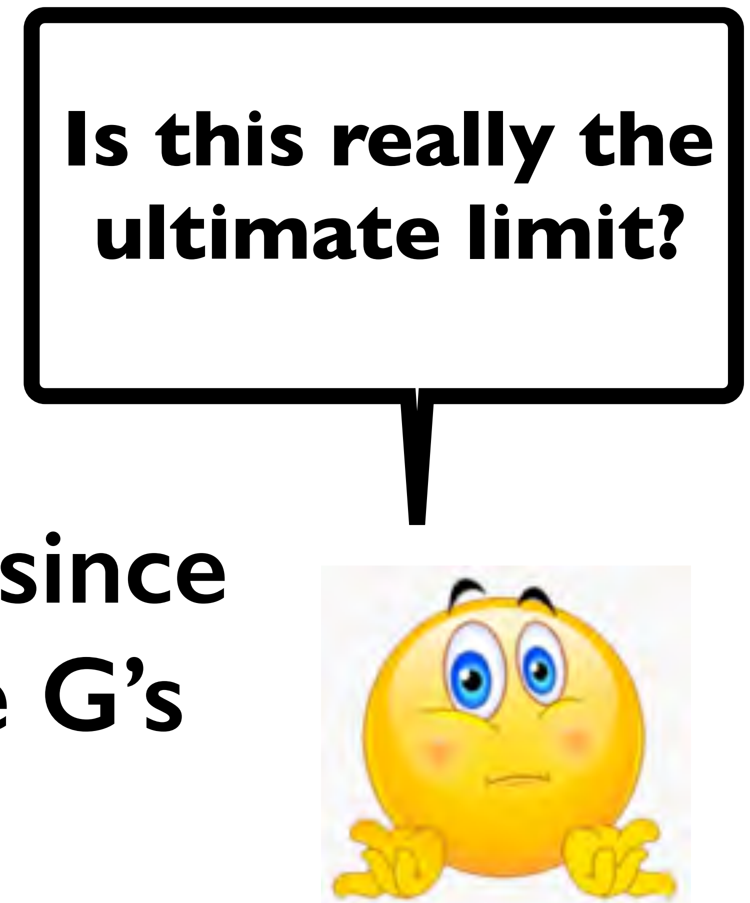
To summarize

- Through the GKBA we can generate an eom for the density matrix for *any* self-energy approximation

- Time-stepping algorithm to solve NEGF+GKBA eom scales like N^2

- GKBA is exact at the mean-field level

- GKBA partially neglects self-consistency since diagrams are calculate with mean-field-like G's



Back to the collision integral

$$I(t) = \int^{t} d\bar{t} \left[\Sigma^{>}(t,\bar{t}) G^{<}(\bar{t},t) - \Sigma^{<}(t,\bar{t}) G^{>}(\bar{t},t) \right]$$

Using the 2-nd order self-energy previoulsy derived $\quad \chi^{0,>}_{\substack{pq\\rs}}(t,t')\, w_{\substack{qj\\sm}}\, \chi^{0,<}_{\substack{jl\\mn}}(\bar{t},t)$

$$\left[\Sigma^{>}(t,\bar{t}) G^{<}(\bar{t},t) \right]_{il} = \mathrm{i}^2 \sum_{rpn} v_{irpn} \sum_{jmqs} \underline{(v_{qmsj} - v_{mqsj})} \underline{G^{>}_{nm}(t,\bar{t})} \underline{G^{<}_{sr}(\bar{t},t) G^{>}_{pq}(t,\bar{t})} \underline{G^{<}_{jl}(\bar{t},t)}$$

Highlight the mathematic structure:

$$w_{\substack{qj\\sm}} \equiv v_{mqsj} - v_{qmsj} = w^{*}_{\substack{jq\\ms}} \qquad \chi^{0,\gtrless}_{\substack{pq\\rs}}(t,t') \equiv -\mathrm{i} G^{\gtrless}_{pq}(t,t') G^{\lessgtr}_{sr}(t',t)$$

$$I_{il}(t) = -\mathrm{i} \sum_{rpn} v_{irpn}\, \mathcal{G}_{\substack{pl\\rn}}(t)$$

$$\boldsymbol{\mathcal{G}}(t) = -\mathrm{i} \int^{t} d\bar{t} \left[\boldsymbol{\chi}^{0,>}(t,\bar{t})\, \boldsymbol{w}\, \boldsymbol{\chi}^{0,<}(\bar{t},t) - \boldsymbol{\chi}^{0,<}(t,\bar{t})\, \boldsymbol{w}\, \boldsymbol{\chi}^{0,>}(\bar{t},t) \right]$$

The $\mathcal{G}$ in GKBA

$$\boldsymbol{\mathcal{G}}(t) = -\mathrm{i}\int^{t} d\bar{t}\left[\boldsymbol{\chi}^{0,>}(t,\bar{t})\,\boldsymbol{w}\,\boldsymbol{\chi}^{0,<}(\bar{t},t) - \boldsymbol{\chi}^{0,<}(t,\bar{t})\,\boldsymbol{w}\,\boldsymbol{\chi}^{0,>}(\bar{t},t)\right]$$

$t > t'$

$$\chi^{0,>}_{\substack{pq\\rs}}(t,t') = \mathrm{i}\underbrace{\sum_a G^{\mathrm{R}}_{pa}(t,t')(\rho_{aq}(t') - \delta_{aq})}_{-G^{>}_{pq}(t,t')}\underbrace{\sum_b \rho_{sb}(t')G^{\mathrm{A}}_{br}(t',t)}_{G^{<}_{sr}(t',t)}$$

$$P^{\mathrm{R}}_{\substack{pa\\rb}}(t,t') \equiv \mathrm{i}\,G^{\mathrm{R}}_{pa}(t,t')G^{\mathrm{A}}_{br}(t',t)$$

$$\rho^{(2)>}_{\substack{aq\\bs}}(t') \equiv (\rho_{aq}(t') - \delta_{aq})\rho_{sb}(t')$$

$t < t'$

$$\chi^{0,>}_{\substack{pq\\rs}}(t,t') = \mathrm{i}\underbrace{\sum_a(\rho_{pa}(t) - \delta_{pa})G^{\mathrm{A}}_{aq}(t,t')}_{G^{>}_{pq}(t,t')}\underbrace{\sum_b G^{\mathrm{R}}_{sb}(t',t)\rho_{br}(t)}_{-G^{<}_{sr}(t',t)}$$

The $\mathcal{G}$ in GKBA

$$\boldsymbol{\mathcal{G}}(t) = -\mathrm{i}\int^{t} d\bar{t}\left[\boldsymbol{\chi}^{0,>}(t,\bar{t})\,\boldsymbol{w}\,\boldsymbol{\chi}^{0,<}(\bar{t},t) - \boldsymbol{\chi}^{0,<}(t,\bar{t})\,\boldsymbol{w}\,\boldsymbol{\chi}^{0,>}(\bar{t},t)\right]$$

In short for all times

$$\boldsymbol{\chi}^{0,>}(t,t') = \boldsymbol{P}^{\mathrm{R}}(t,t')\boldsymbol{\rho}^{(2)>}(t') - \boldsymbol{\rho}^{(2)>}(t)\boldsymbol{P}^{\mathrm{A}}(t,t')$$

$$\rho^{(2)>}_{\substack{aq\\bs}}(t') \equiv (\rho_{aq}(t') - \delta_{aq})\rho_{sb}(t')$$

Mutatis mutandis

$$\boldsymbol{\chi}^{0,<}(t,t') = \boldsymbol{P}^{\mathrm{R}}(t,t')\boldsymbol{\rho}^{(2)<}(t') - \boldsymbol{\rho}^{(2)<}(t)\boldsymbol{P}^{\mathrm{A}}(t,t')$$

$$\rho^{(2)<}_{\substack{aq\\bs}}(t) \equiv \rho_{aq}(t)(\rho_{sb}(t) - \delta_{sb})$$

$$\boldsymbol{\mathcal{G}}(t) = \mathrm{i}\int^{t} d\bar{t}\,\boldsymbol{P}^{\mathrm{R}}(t,\bar{t})\boldsymbol{\Psi}(\bar{t})\boldsymbol{P}^{\mathrm{A}}(\bar{t},t)$$

$$\boldsymbol{\Psi}(t) = \boldsymbol{\rho}^{(2)>}(\bar{t})\boldsymbol{w}\boldsymbol{\rho}^{(2)<}(\bar{t}) - \boldsymbol{\rho}^{(2)<}(\bar{t})\boldsymbol{w}\boldsymbol{\rho}^{(2)>}(\bar{t})$$

Time-linear ODE scheme (Joost, Schlünzen, Bonitz PRL 2019)

$$\mathcal{G}(t) = \mathrm{i}\int^{t} d\bar{t}\, \boldsymbol{P}^{\mathrm{R}}(t,\bar{t})\boldsymbol{\Psi}(\bar{t})\boldsymbol{P}^{\mathrm{A}}(\bar{t},t)$$

$$\boldsymbol{\Psi}(t) = \boldsymbol{\rho}^{(2)>}(\bar{t})\boldsymbol{w}\boldsymbol{\rho}^{(2)<}(\bar{t}) - \boldsymbol{\rho}^{(2)<}(\bar{t})\boldsymbol{w}\boldsymbol{\rho}^{(2)>}(\bar{t})$$

$$\mathrm{i}\frac{d}{dt}\boldsymbol{P}^{\mathrm{R}}(t,\bar{t}) = \boldsymbol{h}^{(2)}(t)\boldsymbol{P}^{\mathrm{R}}(t,\bar{t})$$

$$\boldsymbol{P}^{\mathrm{R}}(t^{+},t) = \mathrm{i}\,\mathbf{1}$$

Using

$$\frac{d}{dt}\int^{t} d\bar{t}\, f(t,\bar{t}) = f(t^{+},t) + \int^{t} d\bar{t}\,\frac{d}{dt}f(t,\bar{t})$$

$$\mathrm{i}\frac{d}{dt}\mathcal{G}(t) = -\boldsymbol{\Psi}(t) + \boldsymbol{h}^{(2)}(t)\mathcal{G}(t) - \mathcal{G}(t)\boldsymbol{h}^{(2)}(t)$$

$$\mathrm{i}\frac{d}{dt}\rho(t) = h(t)\rho(t) - \rho(t)h(t) - \mathrm{i}\left(I(t) + I^{\dagger}(t)\right)$$

$$I_{il}(t) = -\mathrm{i}\sum_{rpn} v_{irpn}\,\mathcal{G}_{\substack{pl\\rn}}(t)$$

Linear scaling achieved

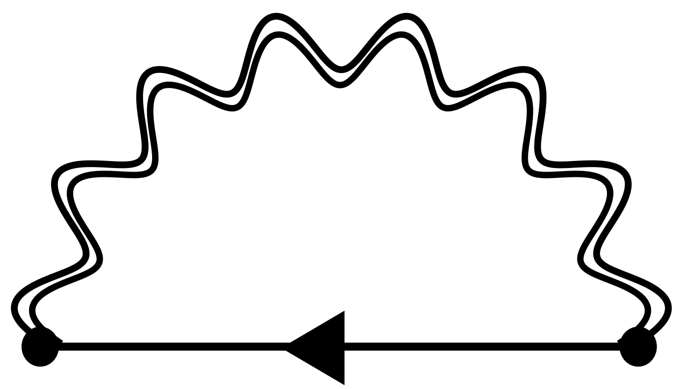
Beyond second-order self-energies

Don't get too excited, the trick works just for a second-order self-energy

Not really !!!

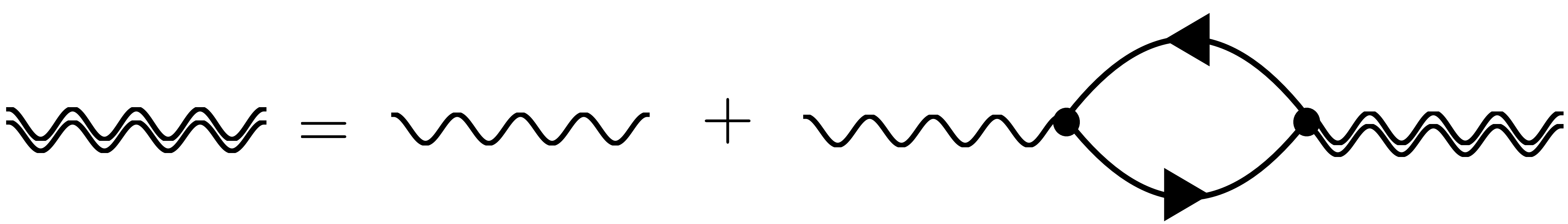
Joost, Schlünzen, Bonitz PRB 2020

$\Sigma =$



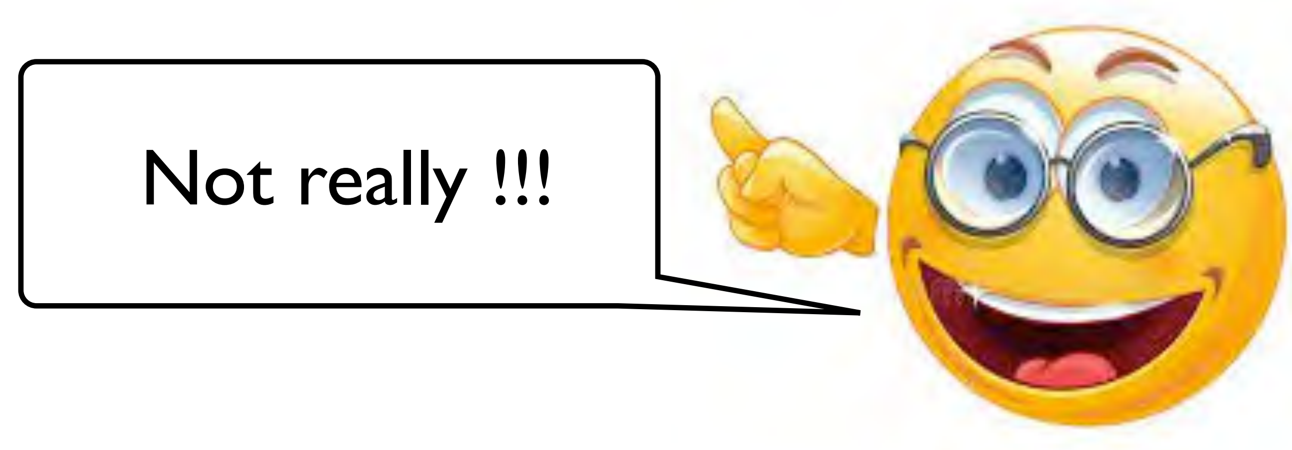
GW

$W =$



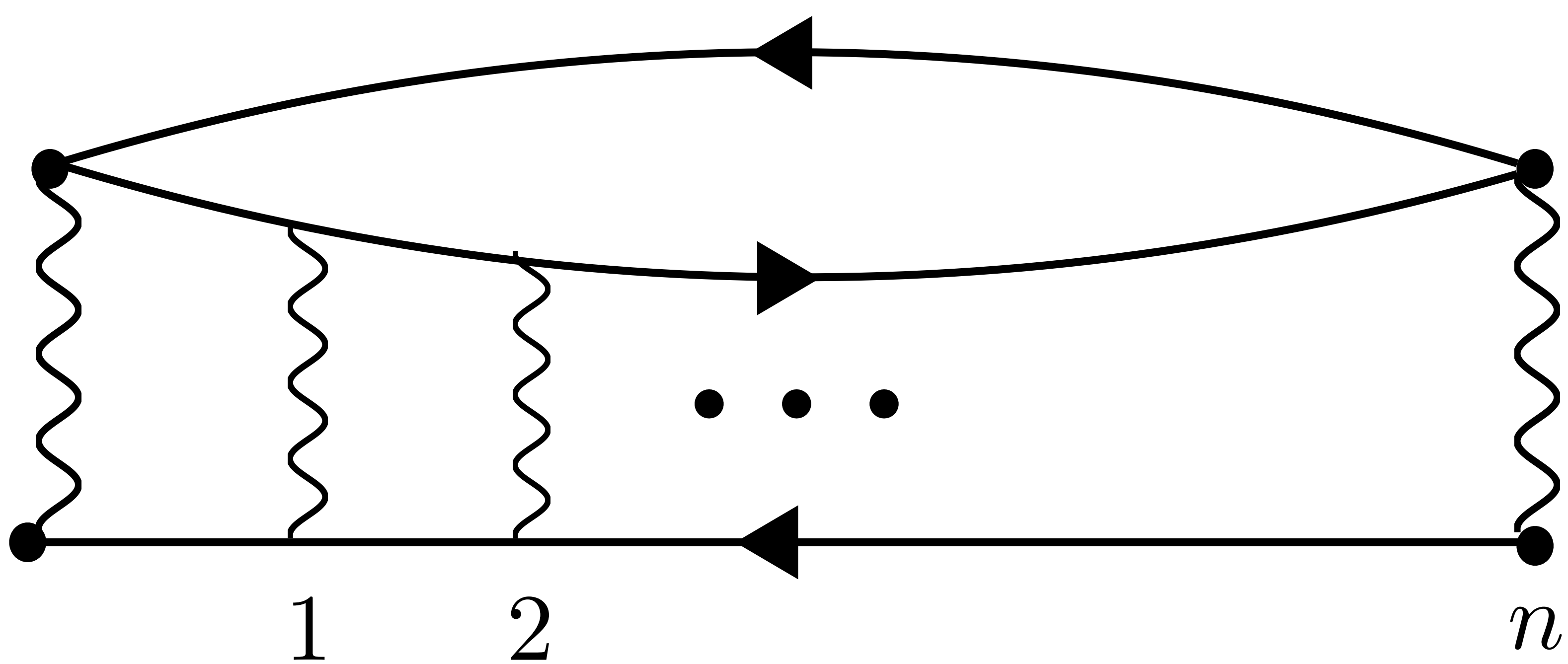
Beyond second-order self-energies

Joost, Schlünzen, Bonitz PRB 2020



T-matrix
ph

$$\Sigma = \sum_{n=1}^{\infty}$$



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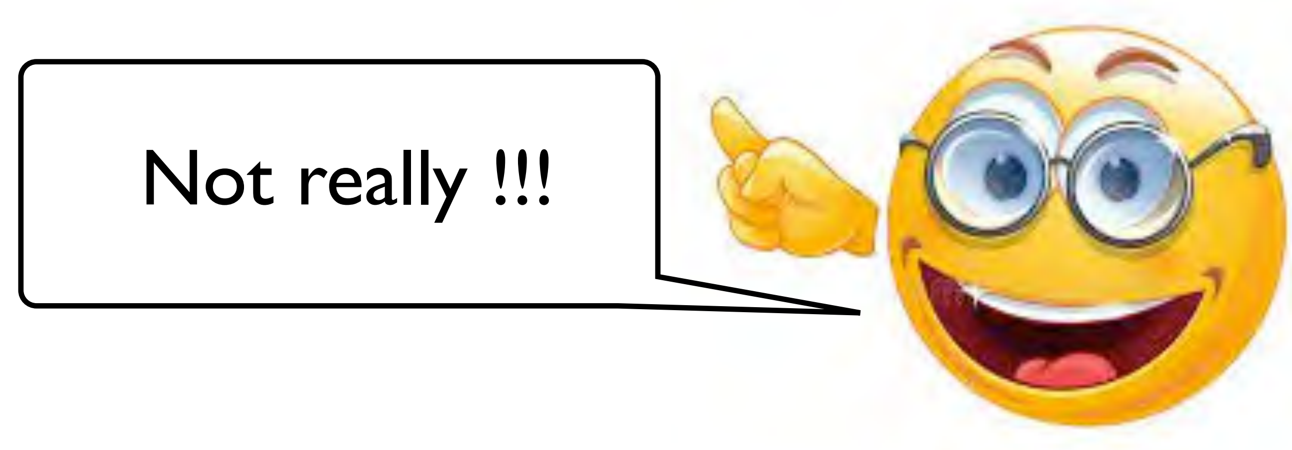
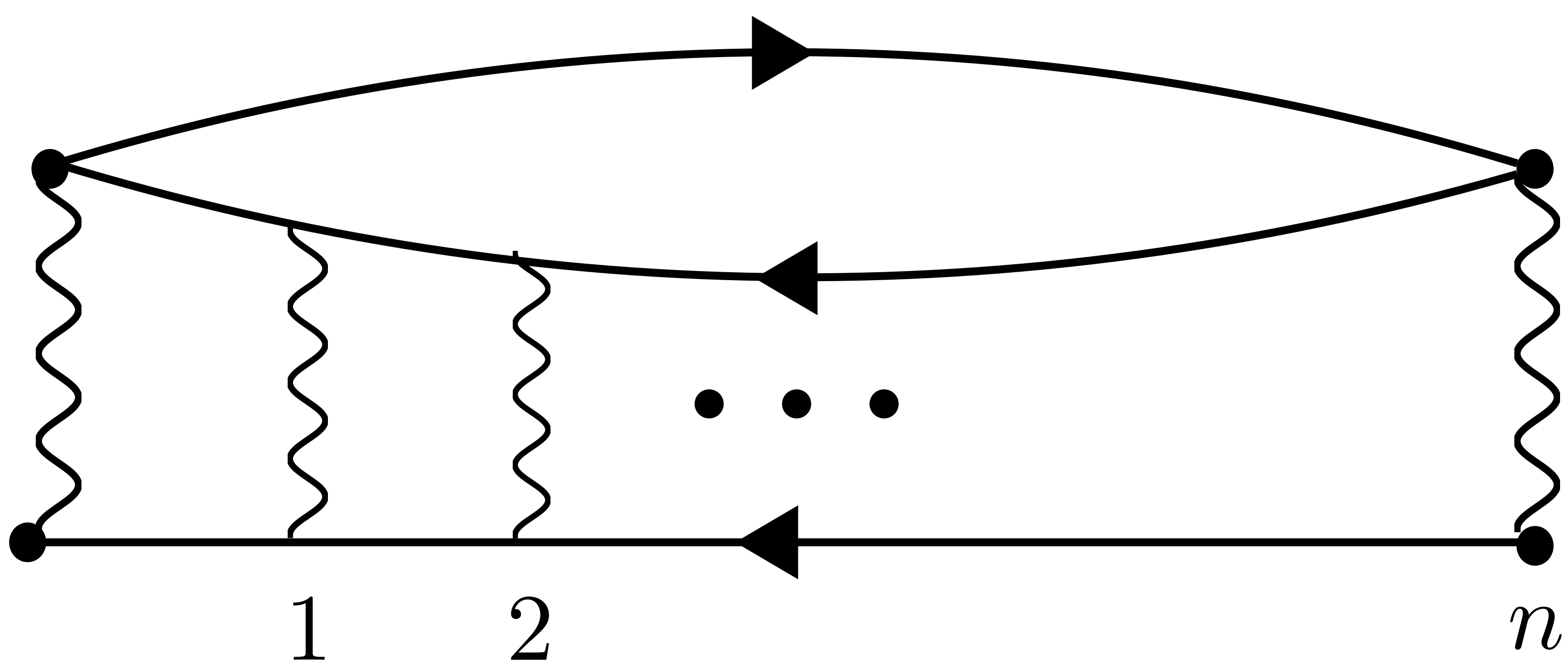


T-matrix
pp

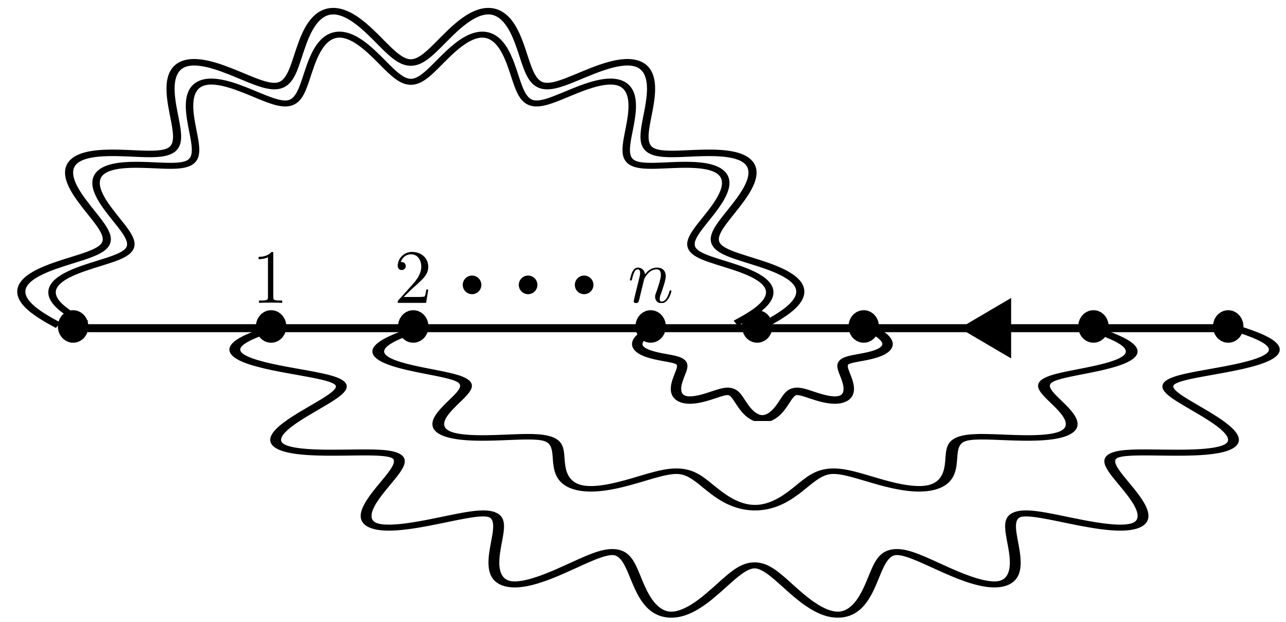
$$\Sigma = \sum_{n=1}^{\infty}$$

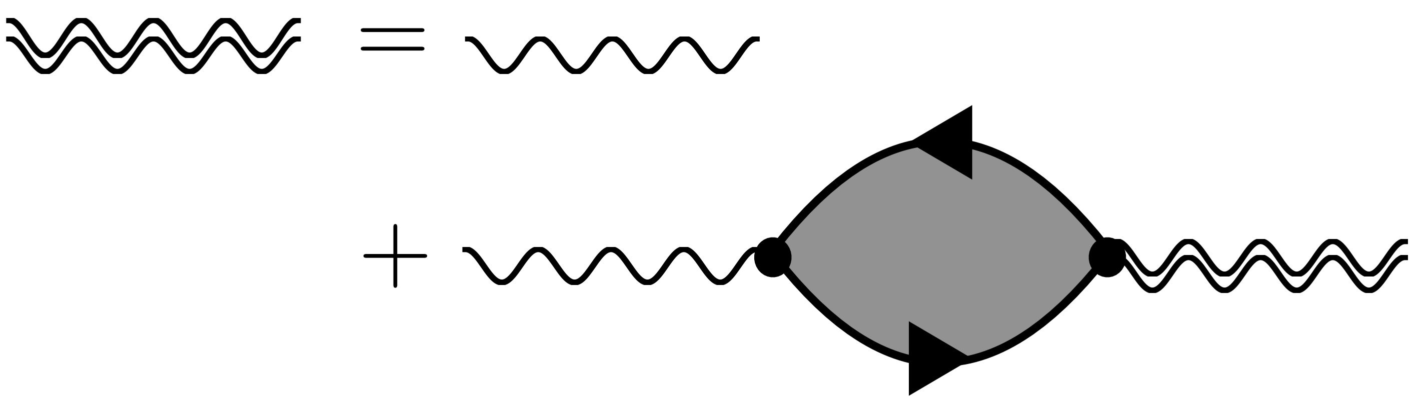


Beyond second-order self-energies

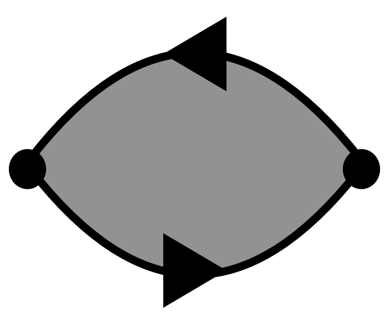
Pavlyukh, Perfetto, GS PRB 2021

$$\Sigma = \sum_{n=0}^{\infty}$$

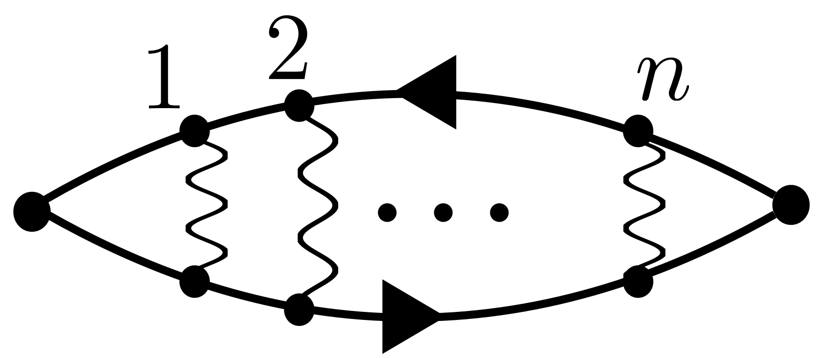




GW+X



$$= \sum_{n=0}^{\infty}$$



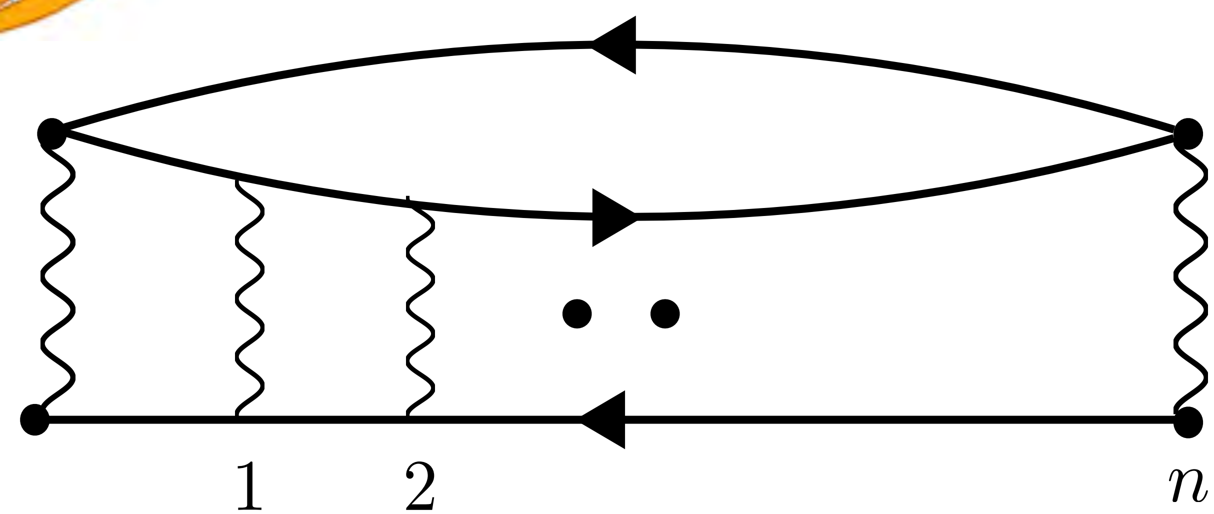
Beyond second-order self-energies

Pavlyukh, Perfetto, GS PRB 2021

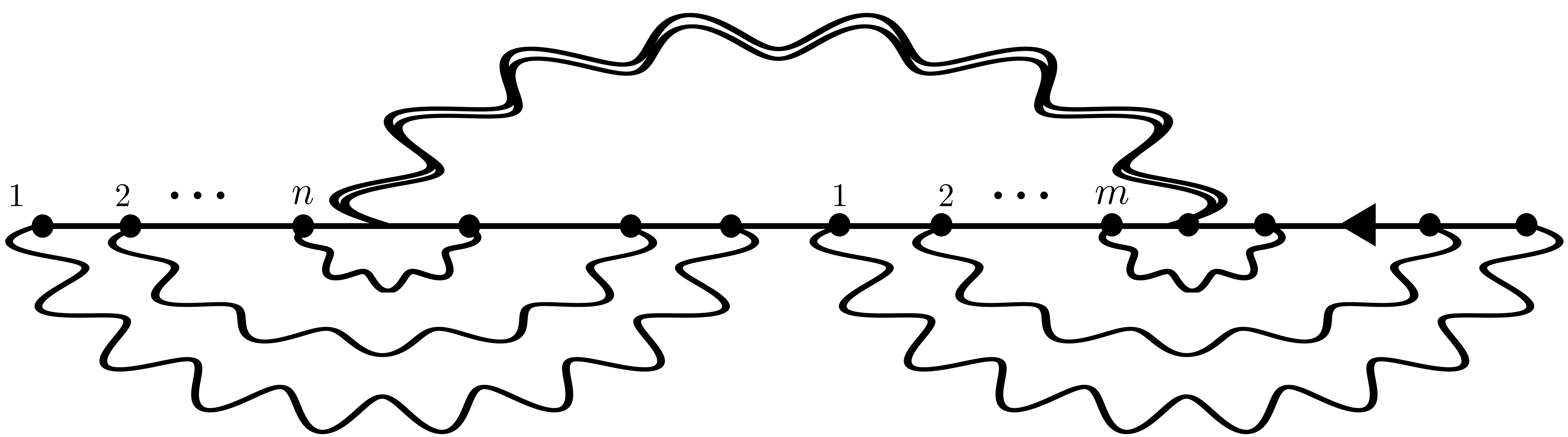
T-matrix

ph + X

$$\Sigma = \sum_{n=1}^{\infty}$$



$$+ \sum_{n=1}^{\infty} \sum_{m=0}^{\infty}$$



Beyond second-order self-energies

PHYSICAL REVIEW LETTERS **127**, 036402 (2021)

Fast Green's Function Method for Ultrafast Electron-Boson Dynamics

Daniel Karlsson,[1] Robert van Leeuwen,[1] Yaroslav Pavlyukh,[2,3] Enrico Perfetto,[3,4] and Gianluca Stefanucci[3,4]
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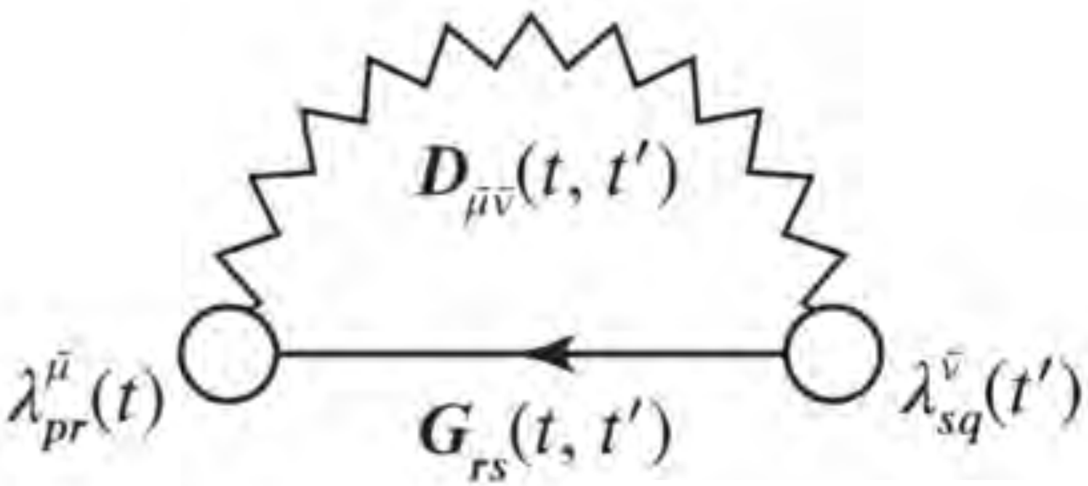
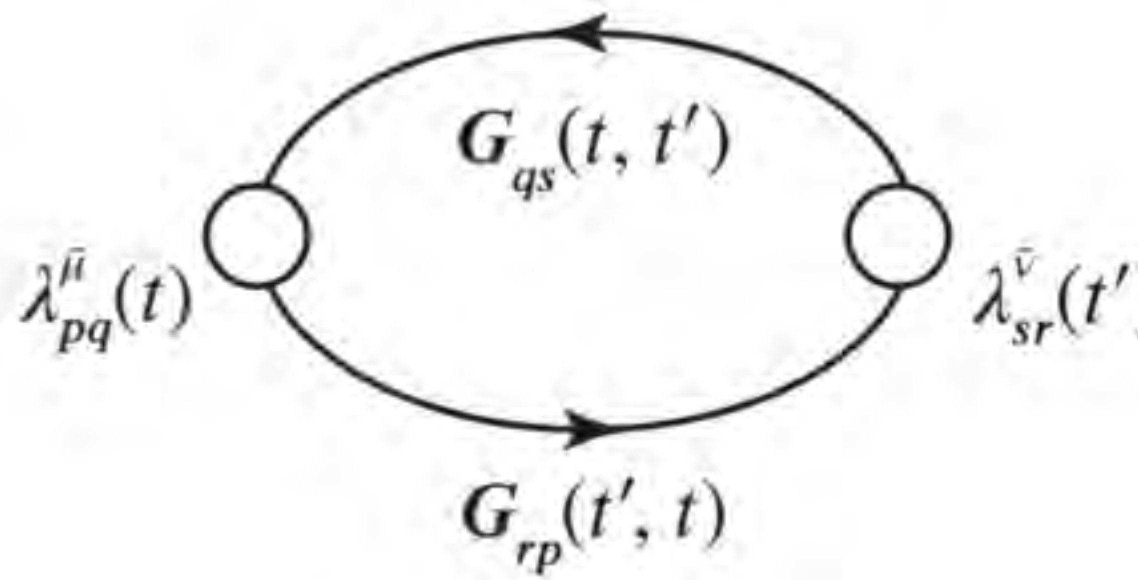
$\boldsymbol{\Sigma}_{pq}(t,t') \;=$



Electron self-energy due to phonons

Phonon self-energy due to electrons

$\boldsymbol{\Pi}_{\bar\mu\bar\nu}(t,t') \;=$



How do the eom change ???

$$\mathrm{i}\frac{d}{dt}\rho(t) = h(t)\rho(t) - \rho(t)h(t) - \mathrm{i}\Big(I(t) + I^{\dagger}(t)\Big)$$

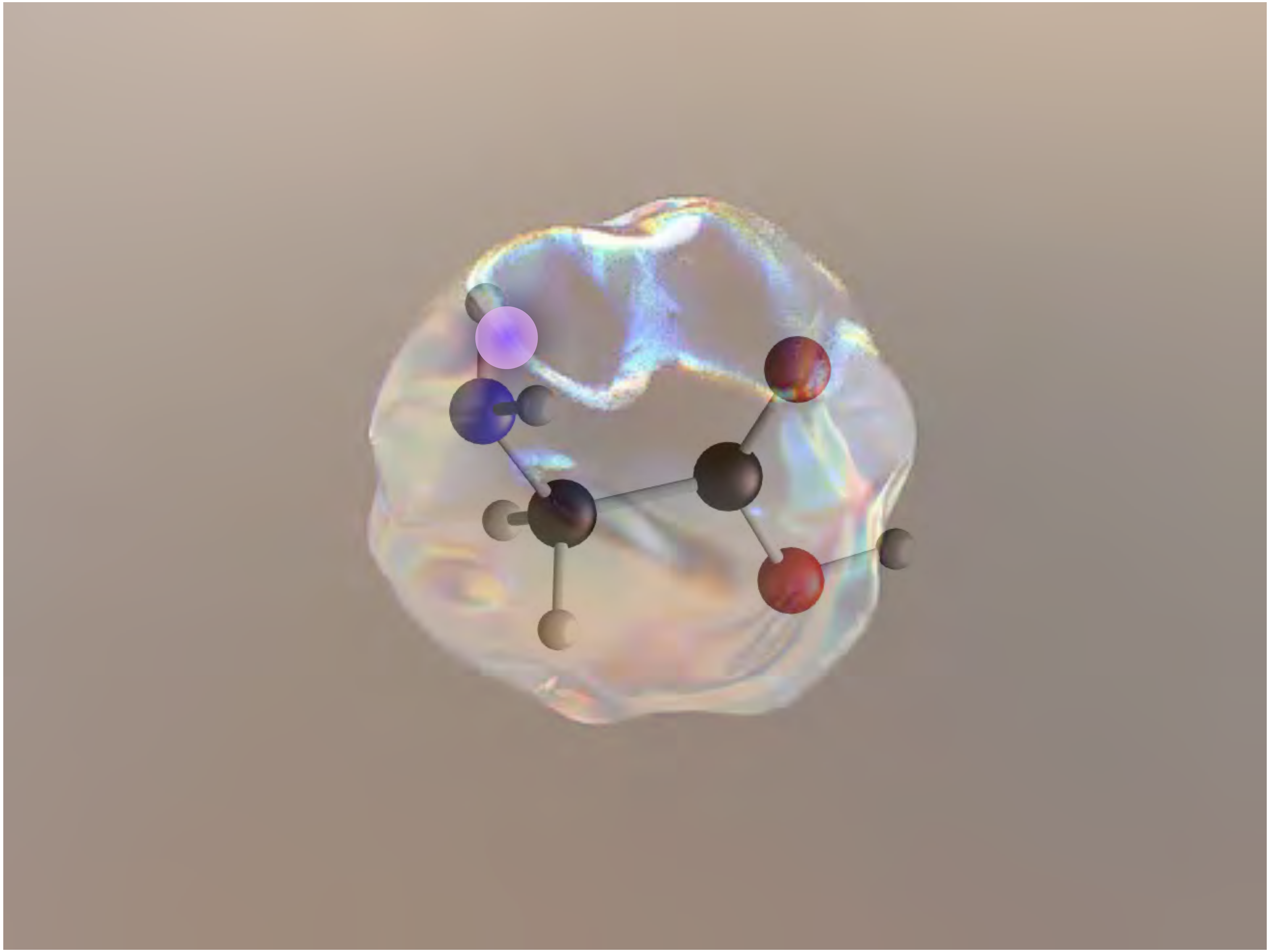
$$I_{il}(t) = -\mathrm{i}\sum_{rpn} v_{irpn}\, \mathcal{G}_{\substack{pl\\rn}}(t)$$

$$\mathrm{i}\frac{d}{dt}\boldsymbol{\mathcal{G}}(t) = -\boldsymbol{\Psi}(t) + \boldsymbol{h}^{(2)}(t)\boldsymbol{\mathcal{G}}(t) - \boldsymbol{\mathcal{G}}(t)\boldsymbol{h}^{(2)}(t)$$

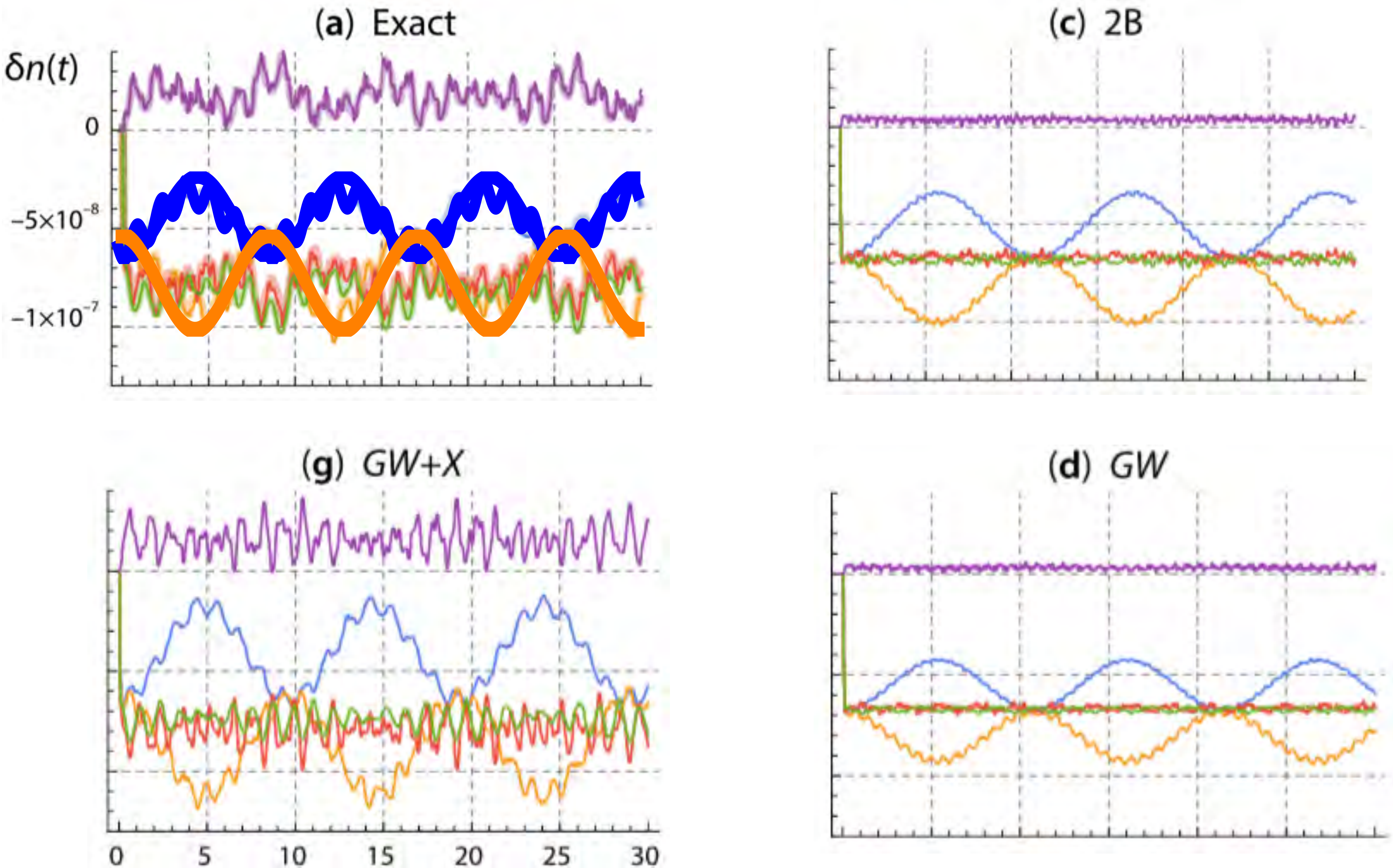
$\boldsymbol{h}^{(2)} \downarrow \boldsymbol{h}^{(2)}_{\text{eff}}$ $\qquad$ $\boldsymbol{h}^{(2)} \downarrow \boldsymbol{h}^{(2)\dagger}_{\text{eff}}$

$$\boldsymbol{h}^{(2)}_{\text{eff}}(t) \equiv \boldsymbol{h}^{(2)}(t) - \Big(\boldsymbol{\rho}^{(2),>}(t) - \boldsymbol{\rho}^{(2),<}(t)\Big)\,\boldsymbol{w}$$

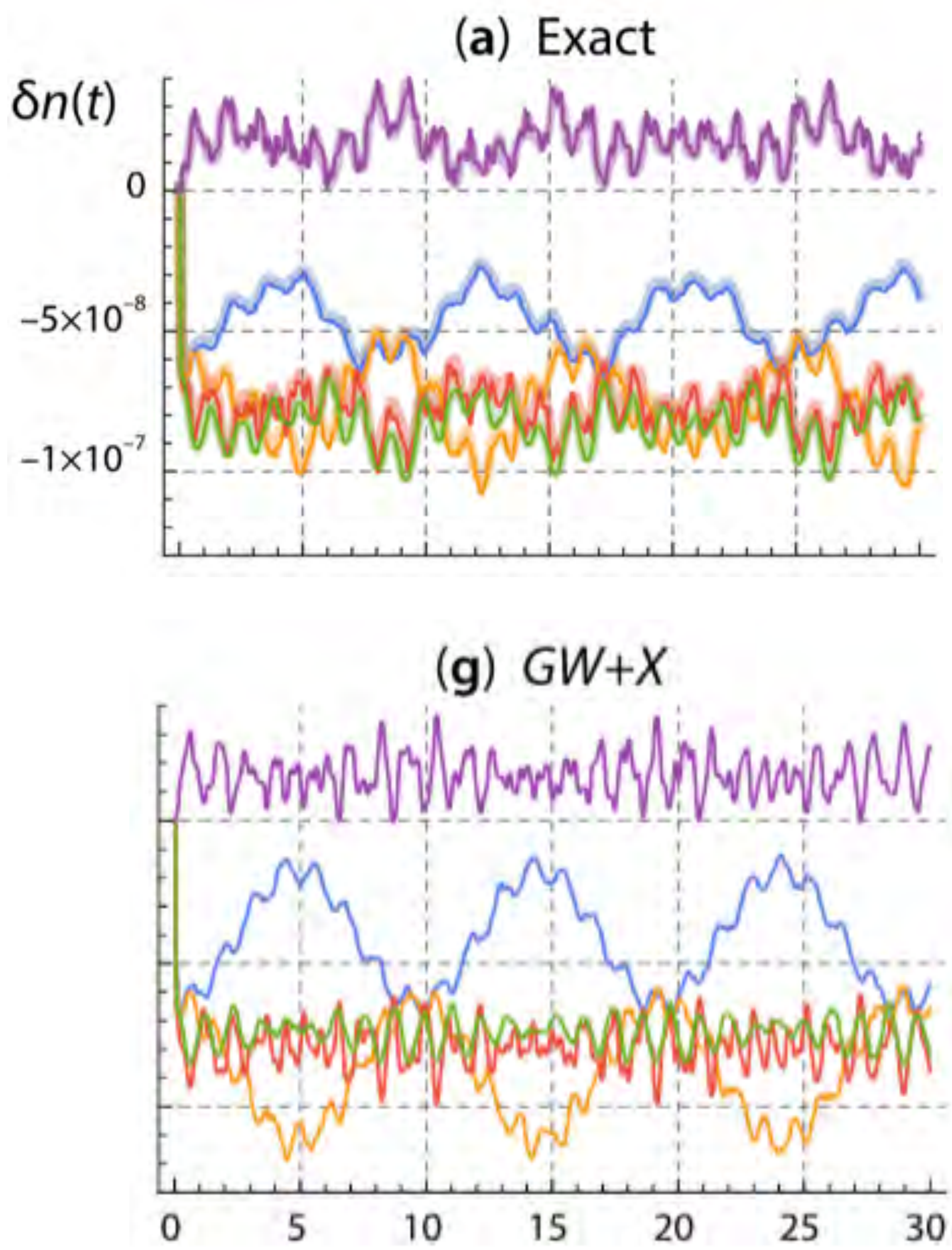
Photoinduced dynamics in organic molecule

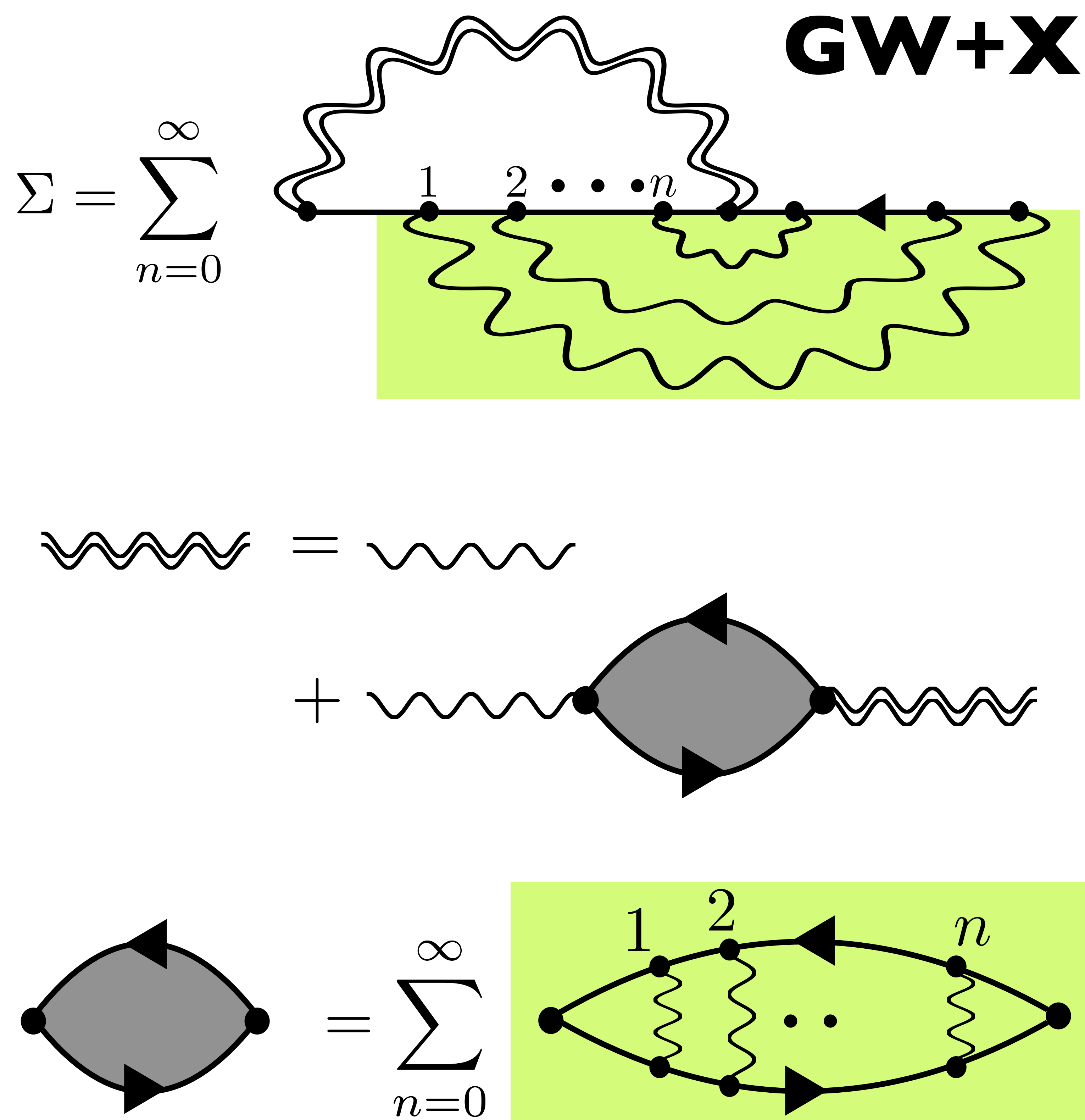


Photoinduced dynamics in organic molecule

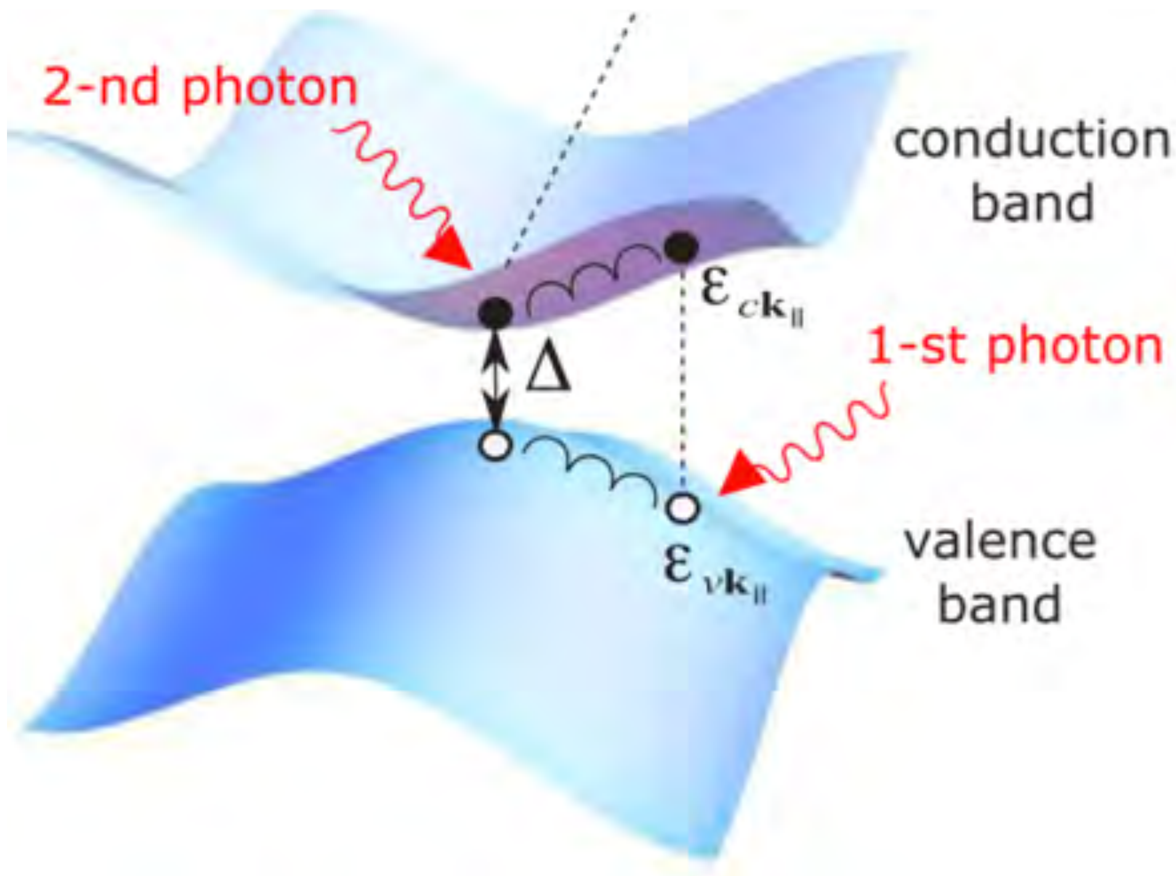


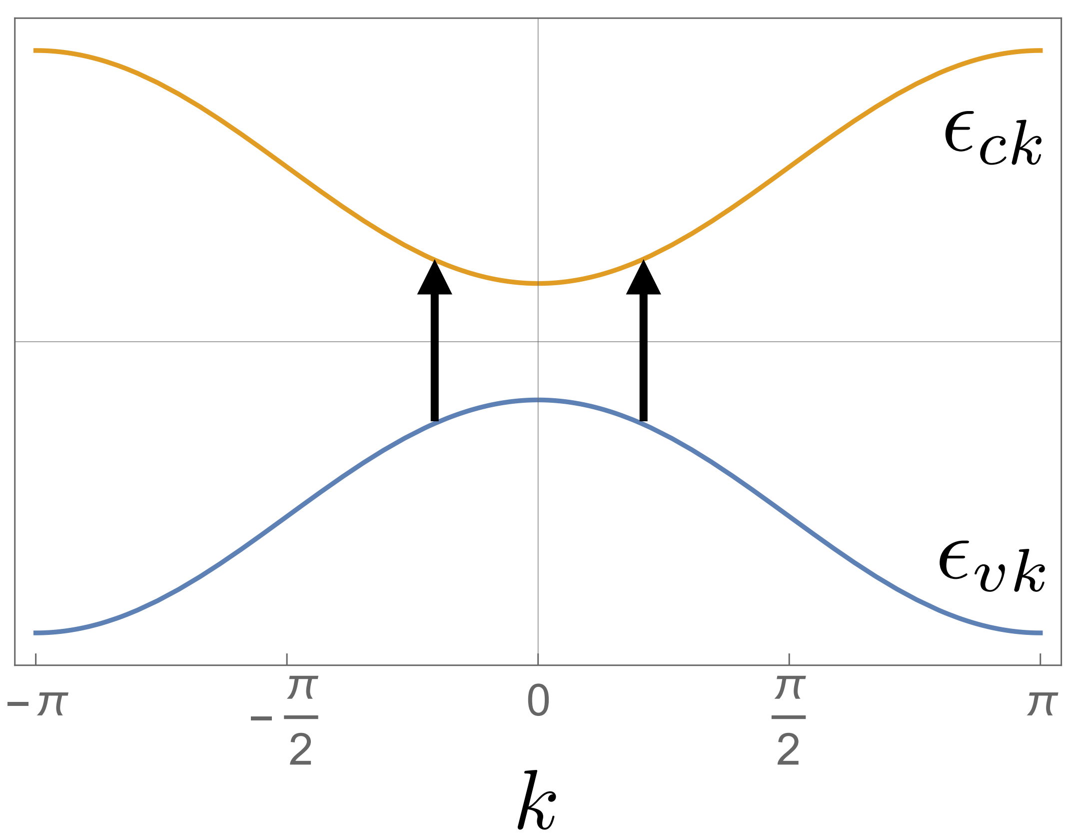
Photoinduced dynamics in organic molecule





Carrier and phonon relaxation





Conclusions

- Exceptional reduction in computational scaling of NEGF simulations

- Several nonperturbative approximations available

- Unifying method for electron-electron and electron-boson interations

- Possibility of merging NEGF with DFT for first-principles simulations

- Plenty of room for studying new nonequilibrium correlated phenomena

Advert

PostDoctoral Fellowship in Condensed Matter Theory

Ultrafast electron dynamics with NEGF

If you are interested just drop me an email: gianluca.stefanucci@roma2.infn.it

DEADLINE: October 30-th