Slides for Patryk's Notes

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Outline

1. Dunn

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Setup

We will work with an electron-boson Hamiltonian of the form

$$H = \sum_k \epsilon_k a_k^\dagger a_k + \frac{1}{2}\sum_q (P_q^\dagger P_q + \omega_q^2 Q_q^\dagger Q_q) + \sum_q \gamma_q Q_q \rho_q^\dagger \tag{1}$$

with HO position $Q_q = \sqrt{\frac{1}{2\Omega_q}}\left(b_q + b_{-q}^\dagger\right)$, momentum $P_q = i\sqrt{\frac{\Omega_q}{2}}\left(b_{-q}^\dagger - b_q\right)$, and density $\rho_q = \sum_k a_{k+q}^\dagger a_k \langle k+q|e^{iq\cdot r}|k\rangle$. In the presence of this interaction, the EOM for the electron annihilation operator is given by

$$\frac{da_k(t)}{dt} = -i\epsilon_k a_k(t) - i\sum_q g_{qk} Q_q(t) a_{k+q}(t) \tag{2}$$

$$\implies a_k(t) = e^{-i\epsilon_k t} T \exp\left[-i\int_0^t d\tau \sum_q Q_q(\tau)\Gamma_{qk}(\tau)\right] a_k \tag{3}$$

Proof

Start by introducing a rotated operator.

$$\tilde{a}_k(t) = e^{i\epsilon_k t} a_k(t) \tag{4}$$

$$\implies \frac{d\tilde{a}_k(t)}{dt} = i\epsilon_k e^{i\epsilon_k t} a_k(t) + e^{i\epsilon_k t} \frac{da_k(t)}{dt} \tag{5}$$

$$= -i \sum_q g_{qk} e^{i\epsilon_k t} Q_q(t) a_{k+q}(t) \tag{6}$$

$$= -i \sum_q g_{qk} Q_q(t) e^{i\left(\epsilon_k - \epsilon_{k+q}\right)t} \tilde{a}_{k+q}(t) \tag{7}$$

$$= -i \sum_q Q_q(t) \Gamma_{qk}(t) \tilde{a}_k(t) \tag{8}$$

$$\implies a_k(t) = e^{-i\epsilon_k t} T \exp\left[-i \int_0^t d\tau \sum_q Q_q(\tau) \Gamma_{qk}(\tau)\right] a_k \tag{9}$$

with $\Gamma_{qk}(t) = g_{qk} e^{i\epsilon_k t} e^{q \cdot \frac{d}{dk}} e^{-i\epsilon_k t} = g_{qk} e^{i\left(\epsilon_k - \epsilon_{k+q}\right)t} e^{q \cdot \frac{d}{dk}}$, where $e^{q \cdot \frac{d}{dk}}$ can be understood as a translation operator in k-space.

Retarded Green's function for an insulator

$$G_k(t) = i\Theta(t)e^{-i\epsilon_k t}\,\mathrm{Tr}\left[\rho T\left(\exp\left(-i\sum_q \int_0^t d\tau \frac{b_q(\tau)+b^\dagger_{-q}(\tau)}{\sqrt{2\Omega_q}}\Gamma_{qk}(\tau)\right)\right)\right] \tag{10}$$

$$= i\Theta(t)e^{-i\epsilon_k t}\left\langle 1 + TAB + \ldots\right\rangle_\rho \quad \text{(disconnected terms vanish)} \tag{11}$$

$$= i\Theta(t)e^{-i\epsilon_k t}\,T\exp\left[\underbrace{i\sum_q \int_0^t d\tau \int_0^\tau d\tau' D_q(\tau-\tau')\Gamma_{qk}(\tau)\Gamma_{-qk}(\tau')}\right] \tag{12}$$

with $D_q(\tau-\tau') = \frac{i}{2\Omega_q}\left((1+N(\Omega_q))e^{-i\Omega_q|\tau-\tau'|} + N(\Omega_q)e^{+i\Omega_q|\tau-\tau'|}\right)$ and the phonon occupation number $N(\Omega_q) = \frac{1}{e^{\frac{\Omega_q}{kT}}-1}$.

Approximation procedure

So with the underbraced differential operator as S

$$G_k(t) = i\Theta(t)\exp\left(-i\epsilon_k t - i\sum_{n=1}^{\infty}\frac{1}{n!}T\left[S^n\right]_c\right) \tag{13}$$

$$= i\Theta(t)\exp\left(iA_k(t)\right) \tag{14}$$

with $T\left[S^n\right]_c = T\left[S^n\right] - \sum_{m=1}^{n-1}\frac{(n-1)!}{m!(n-m-1)!}T\left[S^m\right]T\left[S^{n-m}\right]_c$, where $T[S]_c = T[S]$. To Nth order, we can write

$$G_k(t) = i\Theta(t)e^{-i\epsilon_k t}\prod_{n=1}^{N}e^{T[S^n]_c} \tag{15}$$

but thinking about it in this way does not lead to self-consistency.

Notions of self-consistency

Action function is introduced, which can be written as

$$A_k(t) = \phi_k(t) - i\sum_{n=1}^{\infty}\frac{1}{n!}T\left[\bar{S}^n\right]_c \tag{16}$$

where $\phi_k(t)$ can be chosen so as to improve the approximation with

$$\bar{S} = -i\int_0^t d\tau\left(\epsilon_k + \frac{d}{d\tau}\phi_k(\tau)\right) - i\sum_q\int_0^t d\tau\int_0^\tau d\tau' D_q\left(\tau-\tau'\right)\bar{\Gamma}_{-qk}(\tau)\bar{\Gamma}_{qk} \tag{17}$$

using the transformed vertex operators

$$\bar{\Gamma}_{qk}(\tau) \equiv \hat{U}(\tau)\Gamma_{qk}(\tau)\hat{U}^{-1}(\tau) = g_{qk}e^{-i\phi_k(\tau)}e^{q\cdot\frac{d}{dk}}e^{+i\phi_k(\tau)} \tag{18}$$

Dunn's choice

Dunn chooses $\phi_k(t) = -\epsilon_k t$, giving (to first order)

$$A_k(t) \equiv \phi_k(t) - iT[\bar{S}]_c \tag{19}$$

$$= -\epsilon_k t + i \sum_q |g_{qk}|^2 \left[(1 + N_q) \frac{e^{itb_-} - 1 - itb_-}{b_-^2} + N_q \frac{e^{itb_+} - 1 - itb_+}{b_+^2} \right. \tag{20}$$

where $b_\mp = \epsilon_k - \epsilon_{k-q} \mp \Omega_q$. Clearly, this resembles the Landau form of the cumulant, which is $C(t) = \int d\omega \frac{\beta(\omega)}{\omega^2} \left[e^{-i\omega t} + i\omega t - 1 \right]$. Then,

$$\epsilon_k \equiv -\lim_{t\to\infty} \frac{d}{dt} \mathrm{Re}\left(A_k(t)\right) \tag{21}$$

$$= \epsilon_k^{(0)} - \mathcal{P} \sum_q |g_{qk}|^2 \left[\frac{1 + N_q}{\epsilon_k - \epsilon_{k+q} - \Omega_q} + \frac{N_q}{\epsilon_k - \epsilon_{k+q} + \Omega_q} \right] \tag{22}$$

which gives an energy self-consistency condition.

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PJ's choice

He had $G_k(t) = i\Theta(t)e^{C_k(t)}$ and chose $\phi_k(t) = C_k(t)$, which gave

$$\frac{d\mathcal{G}_k(t)}{dt} = \frac{d}{dt}\left[-i\Theta(t)e^{C_k(t)}\right] \tag{23}$$

$$= \dot{C}_k(t)\mathcal{G}_k(t) \tag{24}$$

so

$$\mathcal{G}_k^{(n+1)}(t) = \mathcal{G}_k^{(0)}(t)\exp\left[i\sum_q \int_0^t d\sigma \int_0^\sigma d\tau\ |g_{qk}|^2\, D_q^{(0)}(\sigma-\tau)\frac{\mathcal{G}_{k-q}^{(n)}(\sigma)}{\mathcal{G}_{k-q}^{(n)}(\tau)}\frac{\mathcal{G}_k^{(n)}(\tau)}{\mathcal{G}_k^{(n)}(\sigma)}\right. \tag{25}$$

which for iterations $n \geq 2$, we use

$$\mathcal{G}_{\mathbf{k}}^{(n+1)}(t) = \mathcal{G}_{\mathbf{k}}^{(0)}(t)\exp\left(-i\sum_{\mathbf{q}}\int_0^t d\sigma \int_0^\sigma d\tau\, |g_{qk}|^2 \right. \tag{26}$$

$$\left. \times D_{\mathbf{q}}^0(\sigma-\tau)\mathcal{G}_{\mathbf{k}}^{(0)}(\tau-\sigma)\mathcal{G}_{\mathbf{k}-\mathbf{q}}^{(0)}(\sigma-\tau)e^{F^{(n)}(\mathbf{k},\mathbf{q},\sigma,\tau)}\right)$$

PJ's Solution

We introduce the notation

$$F^{(n)}(\mathbf{k},\mathbf{q},\sigma,\tau) = F_2^{(n)}(\mathbf{k},\mathbf{q},\sigma,\tau) + F_4^{(n)}(\mathbf{k},\mathbf{q},\sigma,\tau) + \cdots \tag{27}$$

where

$$F_i^{(n)}(\mathbf{k},\mathbf{q},\sigma,\tau) = C_i^{(n)}(\mathbf{k}-\mathbf{q},\sigma) - C_i^{(n)}(\mathbf{k}-\mathbf{q},\tau) - C_i^{(n)}(\mathbf{k},\sigma) + C_i^{(n)}(\mathbf{k},\tau) \tag{28}$$

So his self-consistency for the Greens function is recursive, involving higher order cumulants at each successive iteration. Past the second order cumulants, you begin double counting diagrams, which explains the negative spectral weight. Now, if we define $y_k(t) = e^{C_k(t)}$, the EOM is

$$\frac{dy_k(t)}{dt} = -i\sum_q \int_0^t d\tau\, |g_{qk}|^2\, D_q^{(0)}(t-\tau) e^{i(\epsilon_k-\epsilon_{k-q})(t-\tau)} \frac{y_k(\tau)y_{k-q}(t)}{y_{k-q}(\tau)} \tag{29}$$

which is a VIDE, and they solved it numerically using the appropriate methods.

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Littlewood

PJ showed that this method reduces to self-consistent Migdal, analogous to scGW, in the TDL, so this method does not seem useful for our purposes.

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Determining Fock matrix

$\boldsymbol{F}_{pq}$ is determined by D_{pq}. Then,

$$D_{pq} = \int_{-\infty}^{\infty} f(\omega - \mu) A_{pq}(\omega) d\omega \tag{30}$$

with the Fermi-Dirac distribution $f(\omega - \mu) = \frac{1}{e^{\beta(\omega-\mu)}+1}$, and the spectral function $A_{pq}(\omega) = -\frac{1}{\pi} \operatorname{Im} G^R_{pq}(\omega)$. So we need to get $G^R_{pq}(\omega)$. This can be achieved by accumulating data for $G^R_{pq}(t)$ at different time steps, and then performing a numerical Fourier transform.

$$G^R_{pq}(t) = -i\Theta(t) e^{-i\epsilon_p t} e^{C^{(2)}_{pq}(t)} \tag{31}$$

So we need to evaluate $C^{(2)}_{pq}(t_n)$ at each time step t_n. Note that after we determine $\boldsymbol{F}_{pq}$ for a given iteration, we can update the single particle energies ϵ_p in $G^0_{pp}(\omega)$ for the next iteration.

Evaluating the cumulant

$$C^{(2)}_{pq}(t) \equiv i \int \frac{d\omega}{2\pi} \frac{\tilde{\Sigma}^{(2)}_{pq}(\omega + \epsilon_p)}{(\omega + i\eta)^2} e^{-i\omega t} \tag{32}$$

$$\implies C^{(2)}_{pq}(t) = \frac{1}{2} \sum_{iab} \langle pi \,||\, ab \rangle \langle ab \,||\, qi \rangle \int \frac{d\omega}{2\pi} \frac{i e^{-i\omega t}}{\omega^2 \left(\omega - \epsilon^{ab}_{pi}\right)} \tag{33}$$

$$+ \frac{1}{2} \sum_{ija} \langle pa \,||\, ij \rangle \langle ij \,||\, qa \rangle \int \frac{d\omega}{2\pi} \frac{i e^{-i\omega t}}{\omega^2 \left(\omega - \epsilon^{ij}_{pa}\right)} \tag{34}$$

where $\epsilon^{ab}_{pi} = \epsilon_a + \epsilon_b - \epsilon_p - \epsilon_i$ and $\epsilon^{ij}_{pa} = \epsilon_i + \epsilon_j - \epsilon_p - \epsilon_a$. This is exact up to second order in the bare Coulomb interaction because the improper $\tilde{\Sigma}$ and proper Σ second-order self-energy are equivalent in MP partitioning, so the former has the form

$$\tilde{\Sigma}^{(2)}_{pq}(\omega) = \frac{1}{2} \sum_{iab} \frac{\langle pi||ab\rangle\langle ab||qi\rangle}{\omega + \epsilon_i - \epsilon_a - \epsilon_b} + \frac{1}{2} \sum_{ija} \frac{\langle pa||ij\rangle\langle ij||qa\rangle}{\omega + \epsilon_a - \epsilon_i - \epsilon_j} \tag{35}$$

Scaling analysis

In order to evaluate 34 with Fock self-consistency in mind, this would require the maximum scaling of $N_O N_V^2$ for the summations and (not exploiting symmetry) N_{orb}^2 for runs through p and q, leading to a total scaling of $O(N_O N_V^2 N_{\text{orb}}^2)$. Additionally, we need N_ω points for the frequency integration. For a given iteration, we accumulate data for the value of the interacting Green's function for all N_T time steps, with the intention of performing a numerical Fourier transform to obtain $G_{pq}(\omega)$. So we incur the prefactor of $N_T N_\omega$. Thus, the total scaling is $O(N_O N_V^2 N_{\text{orb}}^2 N_T N_\omega)$.