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

The action function 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 began 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 $C^{(2)}_{pp}(t_n)$ 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, N_ω points for the frequency integration, and (not exploiting symmetry) N_{orb}^2 for runs through p and q, leading to a total scaling of $O(N_O N_V^2 N_\omega N_{\text{orb}}^2)$. 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 $G_{pq}(\omega)$.