Dynamics of electron-phonon systems

Model electron-phonon Hamiltonian

$$H = \sum_{a=1}^{n} \epsilon_a |a\rangle\langle a| + \sum_{a=b=1}^{n} \sum_{i=1}^{N} \lambda_{abi} x_i |a\rangle\langle b| + \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N} \frac{m\omega_i^2 x_i^2}{2}$$

Expectation value of observable *M*

$$\mathrm{Tr}(M(0)\rho(t)) = \mathrm{Tr}(M(t)\rho(0))$$

$$\mathrm{Tr}(M(0)e^{-\frac{i}{\hbar}Ht}\rho(0)e^{\frac{i}{\hbar}Ht}) = \mathrm{Tr}(e^{\frac{i}{\hbar}Ht}M(0)e^{-\frac{i}{\hbar}Ht}\rho(0))$$

Liouville Equation for ρ

$$i\frac{\partial\rho}{\partial t} = \mathcal{L}\rho$$

$$i\frac{\partial\rho}{\partial t} = \frac{1}{\hbar}[H\rho - \rho H]$$

Heisenberg Equation for M

$$i\frac{dM}{dt} = -\mathcal{L}M$$

$$i\frac{dM}{dt} = \frac{1}{\hbar}(MH - HM)$$

Example of projection of ρ

$$\langle x|\rho|x'\rangle = \rho(x, x')$$

$$\int_{-\infty}^{\infty} dx' \delta(x - x')\rho(x, x') = \rho(x, x)$$

$$\int_{-\infty}^{\infty} dx' \delta(x - x')\rho(x, x) = \rho(x, x)$$

Derivation of Nakajima-Zwanzig master equation for $\mathcal{P}\rho(t)$

Projection operators $\mathcal{P}$ and $\mathcal{Q}$

$$\mathcal{P} + \mathcal{Q} = I \qquad \mathcal{P}^2 = \mathcal{P} \qquad \mathcal{Q}^2 = \mathcal{Q}$$

$$\mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0$$

$$\mathcal{P} i \frac{\partial \rho}{\partial t} = \mathcal{P} \mathcal{L} \rho$$

$$\mathcal{Q} i \frac{\partial \rho}{\partial t} = \mathcal{Q} \mathcal{L} \rho$$

$$i \frac{\partial \mathcal{P} \rho}{\partial t} = \mathcal{P} \mathcal{L} (\mathcal{P} + \mathcal{Q}) \rho$$

$$i \frac{\partial \mathcal{Q} \rho}{\partial t} = \mathcal{Q} \mathcal{L} (\mathcal{P} + \mathcal{Q}) \rho$$

$$\mathcal{Q} \rho(t) = e^{-i \mathcal{Q} \mathcal{L} t} \mathcal{Q} \rho(0) - i \int_0^t d\tau \, e^{-i \mathcal{Q} \mathcal{L} (t - \tau)} \mathcal{P} \rho(\tau)$$

Nakajima-Zwanzig master equation

$$i\frac{\partial \mathcal{P}\rho}{\partial t} = \mathcal{P}\mathcal{L}\mathcal{P}\rho(t) - i\int_0^t d\tau\, \mathcal{P}\mathcal{L}e^{-i\mathcal{Q}\mathcal{L}(t-\tau)}\mathcal{Q}\mathcal{L}\mathcal{P}\rho(\tau) + \mathcal{P}\mathcal{L}e^{-i\mathcal{Q}\mathcal{L}t}\mathcal{Q}\rho(0)$$

Special
case

$$\frac{\partial \mathcal{P}\rho}{\partial t} = -\int_0^t d\tau \mathcal{K}^{NZ}(t-\tau)\mathcal{P}\rho(\tau)$$

where

$$\mathcal{K}^{NZ}(t) = \int_0^t d\tau\, \mathcal{P}\mathcal{L}e^{-i\mathcal{Q}\mathcal{L}t}\mathcal{Q}\mathcal{L}\mathcal{P}$$

$$\frac{\partial \mathcal{P}\rho}{\partial t} = -\int_0^t d\tau \mathcal{K}^{NZ}(t-\tau)\mathcal{P}\rho(\tau)$$

$$s\mathcal{P}\rho(s) - \mathcal{P}\rho(0) = -K(s)\mathcal{P}\rho(s)$$

$$\mathcal{P}\rho(s) = \frac{1}{s+K(s)}\mathcal{P}\rho(0) \qquad \mathcal{P}\rho(t) = G(t)\mathcal{P}\rho(0)$$

$$G(t) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{st}\frac{1}{s+K(s)}$$

Time-convolutionless master equation

$$\mathcal{P}\rho(t) = G(t)\mathcal{P}\rho(0)$$

$$\frac{\partial \mathcal{P}\rho(t)}{\partial t} = F(t)\mathcal{P}\rho(t)$$

$$F(t) = \frac{\partial G(t)}{\partial t} G^{-1}(t)$$

$$\frac{\partial \mathcal{P}\rho}{\partial t} = -\int_0^t d\tau \mathcal{K}^{TCL}(\tau)\mathcal{P}\rho(t)$$

Projection of ρ

$$\mathcal{P}\rho = \sum_a |a\rangle\langle a|\rho_{eq}^{os}\,\mathrm{Tr}\left(|a\rangle\langle a|\rho\right)$$

$$= \sum_a |a\rangle P(a)\langle a|\rho_{eq}^{os}$$

Master equation P_a
for

$$\frac{dP_a}{dt} = \sum_b W_{ab}(t) P_b - \sum_b W_{ba}(t) P_a$$

$$W_{mn}(t) = 2\Re e \int_0^t d\tau \sum_{ij} \lambda_{nmi}\lambda_{mnj} \langle x_i x_j(\tau)\rangle e^{-i(\epsilon_n - \epsilon_m)\tau},$$

where

$$\langle x_i x_j(\tau)\rangle = \mathrm{Tr}\left(x_i x_j(\tau)\rho_{eq}^{os}\right)$$

Heisenberg equation approach

$$\frac{d(|a\rangle\langle a|)}{dt} = \frac{i}{\hbar}(H|a\rangle\langle a| - |a\rangle\langle a|H)$$

$$\frac{d(|a\rangle\langle a|)}{dt} = \frac{i}{\hbar}\sum_{bi}\lambda_{abi}(|b\rangle\langle a| - |a\rangle\langle b|)x_i$$

$$\frac{dx_i}{dt} = \frac{p_i}{m} \qquad \frac{dp_i}{dt} = -\frac{\omega_i^2 x_i}{m} - \sum_{ab}\lambda_{abi}|a\rangle\langle b|$$