Implementation of the propagator method

Path integral representation

For the full propagator

$$K(x, \mathbf{R}, t; x', \mathbf{R}', 0) = \int_{x'}^{x} \int_{\mathbf{R}'}^{\mathbf{R}} \mathcal{D}x(t')\, \mathcal{D}\mathbf{R}(t')\, \exp\left\{ \frac{i}{\hbar} S[x(t'), \mathbf{R}(t')] \right\}$$

$$S[x(t'), \mathbf{R}(t')] = \int_0^t L(x(t'), \mathbf{R}(t'), \dot{x}(t'), \dot{\mathbf{R}}(t'))\, dt'$$

Initial density operator $\hat{\rho}(x', \mathbf{R}', y', \mathbf{Q}', 0) = \hat{\rho}(x', y', 0)\, \hat{\rho}(\mathbf{R}', \mathbf{Q}', 0),$

Reduced density operator as a function of time

$$\tilde{\rho}(x, y, t) = \int \int dx' dy'\, \mathcal{J}(x, y, t; x', y', 0)\, \tilde{\rho}(x', y', 0)$$

Super-propagator

$$\mathcal{J}(x,y,t;x',y',0) = \int\int\int d\mathbf{R}' d\mathbf{Q}' d\mathbf{R} \left\{ K(x,\mathbf{R},t;x',\mathbf{R}',0) \times K^*(y,\mathbf{R},t;y',\mathbf{Q}',0)\, \tilde{\rho}_R(\mathbf{R}',\mathbf{Q}',0) \right\}.$$

And if $$S[x(t'),\mathbf{R}(t')] = \tilde{S}_0[x(t')] + S_I[x(t'),\mathbf{R}(t')] + S_R[\mathbf{R}(t')]$$

$$\mathcal{J}(x,y,t;x',y',0) = \int_{x'}^{x}\int_{y'}^{y} \mathcal{D}x(t')\,\mathcal{D}y(t')\ \exp\left\{\frac{i}{\hbar}\tilde{S}_0[x(t')]\right\}\ \exp\left\{-\frac{i}{\hbar}\tilde{S}_0[y(t')]\right\} \times \mathcal{F}[x(t'),y(t')]$$

System decoupled from the bath $$\mathcal{J}(x,y,t;x',y',0) = K_0(x,t;x',0)\, K_0^*(y,t;y',0)$$

Minimal model

$$\mathcal{F}[x(t'),y(t')] = \int\int\int d\mathbf{R}'\,d\mathbf{Q}'\,d\mathbf{R}\,\rho_R(\mathbf{R}',\mathbf{Q}',0)\int_{\mathbf{R}'}^{\mathbf{R}}\int_{\mathbf{Q}'}^{\mathbf{R}}\mathcal{D}\mathbf{R}(t')\,\mathcal{D}\mathbf{R}(t')\;\times$$

$$\times\;\exp\left\{\frac{i}{\hbar}\Big[S_I[x(t'),\mathbf{R}(t')] - S_I[y(t'),\mathbf{Q}(t')] + S_R[\mathbf{R}(t')] - S_R[\mathbf{Q}(t')]\Big]\right\},$$

Forced harmonic oscillator action

$$\begin{aligned} S_{cl}^{(k)} \;\; = \;\; & \frac{m_k\omega_k}{2\sin\omega_k t}\Bigg[\left(R_k^2 + {R'_k}^2\right)\cos\omega_k t - 2R_kR'_k \\ & + \frac{2C_kR_k}{m_k\omega_k}\int_0^t x(t')\sin\omega_k t' dt' + \frac{2C_kR'_k}{m_k\omega_k}\int_0^t x(t')\sin\omega_k(t-t')dt' \\ & - \frac{2C_k^2}{m_k^2\omega_k^2}\int_0^t dt'\int_0^{t'} dt''x(t')x(t'')\sin\omega_k(t-t')\sin\omega_k t''\Bigg]. \end{aligned}$$

averaged over

$$\rho_R(\mathbf{R}', \mathbf{Q}', 0) = \prod_k \rho_R^{(k)}(R'_k, Q'_k, 0) =$$

$$= \prod_k \frac{m_k\omega_k}{2\pi\hbar\sinh\left(\frac{\hbar\omega_k}{k_BT}\right)} \exp - \left\{ \frac{m_k\omega_k}{2\hbar\sinh\left(\frac{\hbar\omega_k}{k_BT}\right)} \left[\left({R'_k}^2 + {Q'_k}^2\right)\cosh\left(\frac{\hbar\omega_k}{k_BT}\right) - 2R'_kQ'_k \right] \right\}$$

Resulting super-propagator

$$\mathcal{J}(x, y, t; x', y', 0) = \int_{x'}^{x}\int_{y'}^{y} \mathcal{D}x(t')\mathcal{D}y(t')\exp\frac{i}{\hbar}\Big\{\tilde{S}_0[x(t')] - \tilde{S}_0[y(t')] -$$

$$- \int_0^t\int_0^\tau d\tau d\sigma[x(\tau) - y(\tau)]\alpha_I(\tau - \sigma)[x(\sigma) + y(\sigma)]\Big\}\times$$

$$\times\exp - \frac{1}{\hbar}\int_0^t\int_0^\tau d\tau d\sigma[x(\tau) - y(\tau)]\alpha_R(\tau - \sigma)[x(\sigma) - y(\sigma)]\Big\}$$

Time kernels

$$\alpha_R(\tau-\sigma)=\sum_k \frac{C_k^2}{2m_k\omega_k}\ \coth\frac{\hbar\omega_k}{2k_BT}\ \cos\omega_k(\tau-\sigma)$$

$$\alpha_I(\tau-\sigma)=-\sum_k \frac{C_k^2}{2m_k\omega_k}\sin\omega_k(\tau-\sigma)$$

For ohmic dissipation

$$\eta(\tau-\sigma)=2M\gamma(\tau-\sigma)\equiv\sum_k \frac{C_k^2}{2m_k\omega_k^2}\cos\omega_k(\tau-\sigma) \qquad \alpha_I(\tau-\sigma)=\frac{d\eta(\tau-\sigma)}{d\tau}$$

$$\alpha_R(\tau-\sigma)=\frac{1}{\pi}\int_0^\Omega d\omega\ \eta\omega\ \coth\frac{\hbar\omega}{2k_BT}\ \cos\omega(\tau-\sigma)$$

$$\alpha_I(\tau-\sigma)=-\frac{1}{\pi}\int_0^\Omega d\omega\ \eta\omega\sin\omega(\tau-\sigma)=\frac{\eta}{\pi}\frac{d}{d(\tau-\sigma)}\int_0^\Omega d\omega\cos\omega(\tau-\sigma)$$

Double integral in the imaginary part of the super-propagator

$$\frac{\eta}{\pi}\int_0^t\int_0^\tau\int_0^\Omega [x(\tau)-y(\tau)]\,\frac{d}{d(\tau-\sigma)}\,\cos\omega(\tau-\sigma)\,[x(\sigma)+y(\sigma)]\,d\tau d\sigma d\omega$$

$$= -\frac{\eta\Omega}{\pi}\int_0^t [x^2(\tau)-y^2(\tau)]d\tau + \frac{\eta}{\pi}(x'+y')\int_0^t \frac{\sin\Omega\tau}{\tau}\,[x(\tau)-y(\tau)]\,d\tau$$

$$+\frac{\eta}{\pi}\int_0^t\int_0^\tau [x(\tau)-y(\tau)]\,\frac{\sin\Omega(\tau-\sigma)}{(\tau-\sigma)}\,[\dot{x}(\sigma)+\dot{y}(\sigma)]\,d\tau d\sigma$$

If $t >> \Omega^{-1}$ $\qquad \dfrac{1}{\pi}\dfrac{\sin\Omega(\tau-\sigma)}{\tau-\sigma} \approx \delta(\tau-\sigma)$ and then

$$\eta(x'+y')\int_0^t \frac{1}{\pi}\frac{\sin\Omega\tau}{\tau}\,[x(\tau)-y(\tau)]\,d\tau \rightarrow \eta(x'+y')\int_0^t \delta(\tau)\,[x(\tau)-y(\tau)]\,d\tau$$

$$\eta(x'+y')\int_{t'}^t \delta(\tau)\,[x(\tau)-y(\tau)]\,d\tau = \begin{cases} 0 & \forall \quad t'>0 \\ \eta(x'^2-y'^2)/2 & \text{if} \quad t'=0. \end{cases}$$

In contrast

$$\frac{\eta}{2}\int_0^t d\tau\,[x(\tau)-y(\tau)]\,\int_0^t \delta(\tau-\sigma)\,[\dot{x}(\sigma)+\dot{y}(\sigma)]\,d\sigma = \lim_{t'\rightarrow 0}\frac{\eta}{2}\int_{t'}^t d\tau\,[x(\tau)-y(\tau)]\,\int_{t'}^t \delta(\tau-\sigma)\,[\dot{x}(\sigma)+\dot{y}(\sigma)]\,d\sigma$$

Under the previous choice of the spectral function the final super-propagator is

$$J(x,x',t;y,y',0)=\int_{x'}^{x}\int_{y'}^{y}\mathcal{D}x(t')\mathcal{D}y(t')\times$$
$$\times\exp\frac{i}{\hbar}\left\{S_0[x(t')]-S_0[y(t')]-M\gamma\int_0^t(x\dot{x}-y\dot{y}+x\dot{y}-y\dot{x})dt'\right\}\times$$
$$\times\exp-\frac{2M\gamma}{\pi\hbar}\int_0^{\Omega}d\omega\,\omega\,\coth\frac{\hbar\omega}{2k_BT}\int_0^t\int_0^{\tau}d\tau d\sigma[x(\tau)-y(\tau)]\cos\omega(\tau-\sigma)[x(\sigma)-y(\sigma)]$$

In general

$$\mathcal{J}(x,x',t;y,y',0)=\int_{x'}^{x}\int_{y'}^{y}\mathcal{D}x(t')\mathcal{D}y(t')\exp\frac{i}{\hbar}\Bigg\{S_0[x(t')]-S_0[y(t')]-$$
$$-\int_0^t\int_0^{\tau}d\tau d\sigma[x(\tau)-y(\sigma)]M\gamma(\tau-\sigma)[\dot{x}(\tau)+\dot{y}(\sigma)]\Bigg\}\times$$
$$\times\exp-\frac{1}{\hbar}\int_0^t\int_0^{\tau}d\tau d\sigma[x(\tau)-y(\tau)]D(\tau-\sigma)[x(\sigma)-y(\sigma)]$$

With boundary condition $\mathcal{J}(x,y,0^+;x',y',0)=\delta(x-x')\delta(y-y')$

Quantum master equations

High temperature limit

$$\mathcal{J}(x,x',t;y,y',0)=\int_{x'}^{x}\int_{y'}^{y}\mathcal{D}x(t')\mathcal{D}y(t')$$

$$\times\exp\frac{i}{\hbar}\Big\{S_0[x(t')]-S_0[y(t')]-M\gamma\int_0^t(x\dot{x}-y\dot{y}+x\dot{y}-y\dot{x})dt'\Big\}$$

$$\times\exp-\frac{2M\gamma k_BT}{\hbar^2}\int_0^t d\tau[x(\tau)-y(\tau)]^2$$

We want to evaluate $\tilde{\rho}(x,y,t+\epsilon)=\int dx'\,dy'\,\mathcal{J}(x,y,t+\epsilon;x',y',t)\,\tilde{\rho}(x',y',t)$

where

$$\mathcal{J}(x,y,t+\epsilon;x',y',t)\approx\frac{1}{A^2}\exp\frac{i}{\hbar}f(x,y,x',y')$$

$$\times\exp\frac{i}{\hbar}\left\{\int_t^{t+\epsilon}\left(\frac{1}{2}M\dot{x}^2-V_0(x)\right)dt'+\int_t^{t+\epsilon}\left(\frac{1}{2}M\dot{y}^2-V_0(y)\right)dt'\right.$$

$$\left.-\int_t^{t+\epsilon}M\gamma\,(x\dot{y}-y\dot{x})\,dt'\right\}\exp-\frac{D(T)}{\hbar^2}\int_t^{t+\epsilon}(x-y)^2dt'$$

$$\frac{\partial\tilde{\rho}}{\partial t} = -\frac{\hbar}{2Mi}\frac{\partial^2\tilde{\rho}}{\partial x^2} + \frac{\hbar}{2Mi}\frac{\partial^2\tilde{\rho}}{\partial y^2} - \gamma(x-y)\frac{\partial\tilde{\rho}}{\partial x} + \gamma(x-y)\frac{\partial\tilde{\rho}}{\partial y}$$
$$+\frac{V(x)}{i\hbar}\tilde{\rho} - \frac{V(y)}{i\hbar}\tilde{\rho} - \frac{2M\gamma k_B T}{\hbar^2}(x-y)^2\tilde{\rho}$$

Which is the coordinate representation of

$$\frac{\partial\tilde{\rho}}{\partial t} = \frac{1}{i\hbar}[\mathcal{H}_0, \tilde{\rho}] + \frac{\gamma}{i\hbar}[q, \{p, \tilde{\rho}\}] - \frac{D}{\hbar^2}[x, [x, \tilde{\rho}]] \qquad D = D_{pp} = \eta k_B T$$

The RW quantum master equation: Lindblad form

$$\frac{\partial\tilde{\rho}}{\partial t} = \frac{1}{i\hbar}[\tilde{\mathcal{H}}, \tilde{\rho}] + \sum_n \left\{2A_n^\dagger\tilde{\rho}A_n - \tilde{\rho}A_nA_n^\dagger - A_nA_n^\dagger\tilde{\rho}\right\}$$

$$W(q,p,t) \equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \exp\left(\frac{ip\xi}{\hbar}\right) \tilde{\rho}\left(q - \frac{\xi}{2}, q + \frac{\xi}{2}, t\right) \, d\xi$$

$$\tilde{\rho}(x,y,t) = \int_{-\infty}^{+\infty} W\left(\frac{x+y}{2}, p, t\right) \exp\left(\frac{-ip(x-y)}{\hbar}\right) dp$$

$$\frac{\partial W}{\partial t} = -\frac{\partial}{\partial q}(pW) + \frac{\partial}{\partial p}\left[(2\gamma p + V'(q))\, W\right] + D\frac{\partial^2 W}{\partial p^2}$$

The equilibrium reduced density operator

Full operator $\langle x\mathbf{R}|e^{-\beta H}|y\mathbf{Q}\rangle = \rho(x,\mathbf{R};x,\mathbf{Q},\beta)$

Path integral representation

$$\rho(x,\mathbf{R};y,\mathbf{Q},\beta) = \int_y^x \int_{\mathbf{Q}}^{\mathbf{R}} \mathcal{D}q(\tau)\mathcal{D}\mathbf{R}(\tau)\exp -\frac{1}{\hbar}S_E[q(\tau),\mathbf{R}(\tau)]$$

Euclidean (imaginary time) action of the complete system

$$S_E[q(\tau),\mathbf{R}(\tau)] = \int_0^{\hbar\beta} d\tau \Big\{\frac{1}{2}M\dot{q}^2 + V(q) + \sum_k \Big(C_k q R_k + \frac{1}{2}m_k \dot{R}_k^2 + \frac{1}{2}m_k\omega_k^2 R_k^2\Big)\Big\}$$

Reduced density operator of the system

$$\begin{aligned}\tilde{\rho}(x,y,\beta) &\equiv \int d\mathbf{R}\ \rho(x,\mathbf{R};y,\mathbf{R},\beta) = \\ &= \int_y^x \mathcal{D}q(\tau)\int d\mathbf{R}\int_{\mathbf{R}}^{\mathbf{R}} \mathcal{D}\mathbf{R}(\tau)\exp -\frac{1}{\hbar}S_E[q(\tau),\mathbf{R}(\tau)]\end{aligned}$$

Final form

$$\tilde{\rho}(x,y,\beta) = \tilde{\rho}_0(\beta) \int_y^x \mathcal{D}q(\tau)\ \exp - \frac{1}{\hbar} S_{eff}[q(\tau)]$$

Prefactor

$$\tilde{\rho}_0(\beta) = \prod_k \frac{1}{2}\ \mathrm{cosech}\left(\frac{\hbar\beta\omega_k}{2}\right)$$

Effective euclidean action

$$S_{eff}[q(\tau)] = \int_0^{\hbar\beta} d\tau \left\{\frac{1}{2}M\dot{q}^2 + V(q)\right\} + \frac{1}{2}\int_{-\infty}^{+\infty} d\tau' \int_0^{\hbar\beta} d\tau \alpha(\tau-\tau')\{q(\tau)-q(\tau')\}^2$$

Imaginary time kernel

$$\alpha(\tau-\tau') \equiv \sum_k \frac{C_k^2}{4m_k\omega_k} \exp - \omega_k|\tau-\tau'| = \frac{1}{2\pi}\int_0^\infty d\omega\, J(\omega) \exp - \omega_k|\tau-\tau'|$$

Ohmic dissipation

$$\alpha(\tau-\tau') = \frac{1}{2\pi}\int_0^\infty d\omega\, \eta\omega \exp - \omega_k|\tau-\tau'| = \frac{\eta}{2\pi}\frac{1}{(\tau-\tau')^2}$$

Non-linear model

$$\mathcal{H}_{RI} = \mathcal{H}_R + \mathcal{H}_I(x(t')) \quad \Longrightarrow \quad \mathcal{F}\left[x(t'), y(t')\right] = \mathrm{Tr}_R\left(\rho_R U^\dagger_{RI}[y(t')]U_{RI}[x(t')]\right)$$

where $$i\hbar \frac{dU_{RI}(t)}{dt} = \mathcal{H}_{RI}(t)U_{RI}(t) \quad \Longrightarrow \quad U_{RI}(t) = \mathcal{T}\exp -\frac{i}{\hbar}\int_0^t dt'\mathcal{H}_{RI}(t')$$

In the interaction picture $$U_{RI}(t) = e^{-i\mathcal{H}_R t/\hbar}\,\mathcal{T}\exp -\frac{i}{\hbar}\int_0^t dt'\tilde{\mathcal{H}}_I[x(t')]$$

where $$\tilde{\mathcal{H}}_I[x(t')] \equiv e^{i\mathcal{H}_R t/\hbar}\mathcal{H}_I[x(t')]e^{-i\mathcal{H}_R t/\hbar}$$

$$\Downarrow$$

$$\mathcal{T}\exp -\frac{i}{\hbar}\int_0^t dt'\tilde{\mathcal{H}}_I[x(t')] \approx 1 - \frac{i}{\hbar}\int_0^t dt'\tilde{\mathcal{H}}_I[x(t')] - \frac{1}{\hbar^2}\int_0^t dt'\int_0^{t'} dt''\tilde{\mathcal{H}}_I[x(t')]\tilde{\mathcal{H}}_I[x(t'')]$$

and
$$\mathcal{F}\left[x(t'),y(t')\right] \approx 1-\frac{1}{\hbar^2}\int\limits_0^t dt'\int\limits_0^{t'} dt''\left(\left\langle \tilde{\mathcal{H}}_I[x(t')]\tilde{\mathcal{H}}_I[x(t'')]\right\rangle + \right.$$
$$\left. + \left\langle \tilde{\mathcal{H}}_I[y(t'')]\tilde{\mathcal{H}}_I[y(t')]\right\rangle - \left\langle \tilde{\mathcal{H}}_I[y(t')]\tilde{\mathcal{H}}_I[x(t'')]\right\rangle - \left\langle \tilde{\mathcal{H}}_I[y(t'')]\tilde{\mathcal{H}}_I[x(t')]\right\rangle\right)$$

Reexponentiating:
$$\mathcal{F}\left[x(t'),y(t')\right] = \exp -\frac{1}{\hbar^2}\int\limits_0^t dt'\int\limits_0^{t'} dt''\left(\left\langle \tilde{\mathcal{H}}_I[x(t')]\tilde{\mathcal{H}}_I[x(t'')]\right\rangle + \right.$$
$$\left. + \left\langle \tilde{\mathcal{H}}_I[y(t'')]\tilde{\mathcal{H}}_I[y(t')]\right\rangle - \left\langle \tilde{\mathcal{H}}_I[y(t')]\tilde{\mathcal{H}}_I[x(t'')]\right\rangle - \left\langle \tilde{\mathcal{H}}_I[y(t'')]\tilde{\mathcal{H}}_I[x(t')]\right\rangle\right)$$

where
$$\left\langle \tilde{\mathcal{H}}_I[x(t')]\tilde{\mathcal{H}}_I[x(t'')]\right\rangle = \frac{1}{2}\sum_k \left\{C_{-k}[x(t')]C_k[x(t'')] + \right.$$
$$\left. + C_k[x(t')]C_{-k}[x(t'')]\right\}\alpha_k(t'-t'')$$

Using that $\langle R_k(t')R_{k'}(t'')\rangle = 0$ except for $k' = -k$ when

$$\alpha_k(t'-t'') \equiv \langle R_k(t')R_{-k}(t'')\rangle$$

$$\alpha_k(t'-t'') = \frac{\hbar}{\pi}\int\limits_{-\infty}^{\infty} d\omega \mathrm{Im}\chi_k(\omega)\frac{e^{-i\omega(t'-t'')}}{1-e^{-\omega\hbar\beta}}$$

the influence functional reads $\mathcal{F}[x(t'),y(t')] = \exp -\frac{1}{\hbar^2}\int_0^t dt' \int_0^{t'} dt''$

$$\times\left\{\sum_k \kappa_k\kappa_{-k}\alpha_k(t'-t'')\left[\cos k(x(t')-x(t'')) - \cos k(y(t')-x(t''))\right] + \right.$$

$$\left. + \sum_k \kappa_k\kappa_{-k}\alpha_k^*(t'-t'')\left[\cos k(y(t')-y(t'')) - \cos k(y(t'')-x(t'))\right]\right\}$$

Using that $\mathrm{Im}\chi_k(-\omega) = -\mathrm{Im}\chi_k(\omega)$ we can write

$$\alpha_k(t'-t'') = \alpha_k^{(R)}(t'-t'') + i\alpha_k^{(I)}(t'-t'')$$

where $\alpha_k^{(R)}(t'-t'') = \frac{\hbar}{\pi}\int_0^\infty d\omega \mathrm{Im}\chi_k(\omega)\cos\omega(t'-t'')\coth(\hbar\beta\omega/2)$

and $\alpha_k^{(I)}(t'-t'') = -\frac{\hbar}{\pi}\int_0^\infty d\omega \mathrm{Im}\chi_k(\omega)\sin\omega(t'-t'')$

If when $\omega\to 0$ we use $\mathrm{Im}\chi_k(\omega) \approx f(k)\omega\theta(\Omega-\omega)$

We get
$$\mathcal{F}[x(t'),y(t')] = \exp - \frac{1}{\hbar^2} \int_0^t dt' \int_0^{t'} dt'' \sum_k \kappa_k \kappa_{-k} \alpha_k^{(R)}(t'-t'') \times$$
$$[\cos k(x(t')-x(t'')) - \cos k(y(t')-x(t'')) + \cos k(y(t')-y(t'')) - \cos k(y(t'')-x(t'))]$$
$$\times \exp \frac{i}{2\hbar} \sum_k \kappa_k \kappa_{-k} f(k) k \int_0^t dt' \sin k(y(t')-x(t'))\,(\dot{x}(t')+\dot{y}(t'))$$

Linearizing this expression
$$\mathcal{F}[x(t'),y(t')] = \exp \left\{ \frac{i\eta}{2\hbar} \int_0^t dt' (y(t')-x(t'))\,(\dot{x}(t')+\dot{y}(t')) - \right.$$
$$- \frac{\eta}{\hbar\pi} \int_0^t dt' \int_0^{t'} dt'' (x(t')-y(t'))(x(t'')-y(t'')) \times$$
$$\left. \times \int_0^\infty d\omega\, \omega \coth\left(\frac{\hbar\beta\omega}{2}\right) \cos\omega(t'-t'') \right\}$$

$$\eta = \sum_k k^2 \kappa_k \kappa_{-k} f(k)$$

Collision model

Non-interacting particles in 1-D $$\mathcal{H} = \frac{p^2}{2M} + \sum_{i=1}^{N} U(q_i - q) + \sum_{i=1}^{N} \frac{p_i^2}{2m}$$

Reduced density operator $$\tilde{\rho}(x,y,t) = \int dq_1 dq_2 ... dq_N \langle x, q_1, ..., q_N | e^{-i\frac{\mathcal{H}t}{\hbar}} \rho(0) e^{i\frac{\mathcal{H}t}{\hbar}} | y, q_1, ..., q_N \rangle$$

Translation $$\mathcal{U} = \exp \frac{i}{\hbar} \sum_{j=1}^{N} p_j q$$

$$\tilde{\rho}(x,y,t) = \int dq_1 dq_2 ... dq_N \langle x, q_1, ..., q_N | \mathcal{U}^{-1} e^{-i\frac{\mathcal{H}'t}{\hbar}} \rho'(0) e^{i\frac{\mathcal{H}'t}{\hbar}} \mathcal{U} | y, q_1, ..., q_N \rangle =$$

$$= \int dq_1 dq_2 ... dq_N \langle x, q_1, ..., q_N | \mathcal{U}^{-1} \rho'(t) \mathcal{U} | y, q_1, ..., q_N \rangle$$

$$\mathcal{H}' = \mathcal{U}\mathcal{H}\mathcal{U}^{-1} = \frac{1}{2M}\left(p - \sum_{j=1}^{N} p_j\right)^2 + \sum_{j=1}^{N}\left(\frac{p_j^2}{2m} + U(q_j)\right) \qquad \rho'(0) = \mathcal{U}\rho(0)\mathcal{U}^{-1}$$

Inserting identities $$\tilde{\rho}(x,y,t) = \int ... \int dq_1 dq_2 ... dq_N dr_1 dr_2 ... dr_N$$
$$\times \langle r_1, ..., r_N | e^{-\frac{i}{\hbar} \sum_{j=1}^{N} p_j (x-y)} | q_1, ..., q_N \rangle \langle x, q_1, ..., q_N | \rho'(t) | y, r_1, ..., r_N \rangle$$

But, as $$\langle x^n(t) \rangle = \int dx x^n \tilde{\rho}(x,x,t)$$

We have $$\langle x^n(t) \rangle = \int ... \int dx dq_1 ... dq_N x^n \langle x, q_1, ..., q_N | \rho'(t) | x, q_1, ..., q_N \rangle$$

On the other hand $$\langle p(t) \rangle = \int \int dx\, dy\, \delta(x-y) \frac{\hbar}{2i} \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) \tilde{\rho}(x,y,t)$$

And then $$\langle p(t) \rangle = \frac{\hbar}{2i} \int \int dx\, dy\, \delta(x-y) \int ... \int dq_1 dq_2 ... dq_N dr_1 dr_2 ... dr_N$$
$$\times \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) \Bigg\{ \langle r_1, ..., r_N | e^{-\frac{i}{\hbar} \sum_{j=1}^{N} p_j (x-y)} | q_1, ..., q_N \rangle$$
$$\times \langle x, q_1, ..., q_N | \rho'(t) | y, r_1, ..., r_N \rangle \}$$

or $$\langle p(t)\rangle = \frac{\hbar}{2i}\int ... \int dx dq_1 dq_2 ... dq_N$$
$$\times \lim_{x\to y}\left\{\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)\langle x, q_1, ..., q_N|\rho'(t)|y, q_1, ..., q_N\rangle\right\}$$

Then, all we need is $\tilde{\rho}'(x,y,t) = \int ... \int dq_1 dq_2 ... dq_N \langle x, q_1, ..., q_N|\rho'(t)|y, q_1, ..., q_N\rangle$

with $\rho'(0) = \rho_s \rho'_{eq} = \rho_s e^{-\beta \mathcal{H}_R}$

$$\mathcal{H}_R = \sum_{j=1}^{N}\left(\frac{p_j^2}{2m} + U(q_j)\right) \rightarrow \mathcal{H}' = \frac{1}{2M}\left(p - \sum_{i,j}\hbar g_{ij} a_i^\dagger a_j\right)^2 + \sum_i (\hbar\Omega_i - \mu) a_i^\dagger a_i$$

where $g_{ij} = \frac{1}{\hbar}\langle i|p'|j\rangle$

$$\tilde{\rho}'(x,y,t) = \int dx' \int dy' \mathcal{J}(x,y,t;x',y',0)\rho_s(x',y',0)$$

$$\mathcal{J}(x,y,t;x',y',0) = \int ... \int dq_1 ... dq_N dr_1 ... dr_N ds_1 .. ds_N \langle x, q_1, ..., q_N| \exp -\frac{i}{\hbar}\mathcal{H}'t|x', r_1, ..., r_N\rangle$$
$$\times \langle r_1, ..., r_N| \exp -\beta\mathcal{H}_R|s_1, ..., s_N\rangle\langle y', s_1, ..., s_N| \exp \frac{i}{\hbar}\mathcal{H}'t|y, q_1, ..., q_N\rangle$$

Path integral or c-number representation

$$\mathcal{J}(x,y,t;x',y',0) = \int \dots \int d\mu(\boldsymbol{\alpha})\, d\mu(\boldsymbol{\alpha}')\, d\mu(\boldsymbol{\gamma}')\, \langle x, \boldsymbol{\alpha}| \exp -\frac{i}{\hbar}\mathcal{H}' t | x', \boldsymbol{\alpha}'\rangle$$

$$\times \langle \boldsymbol{\alpha}'| \exp -\beta \mathcal{H}_e |\boldsymbol{\gamma}'\rangle \langle y', \boldsymbol{\gamma}'| \exp \frac{i}{\hbar}\mathcal{H}' t | y, \boldsymbol{\alpha}\rangle$$

$$\mathcal{J}(x,y,t;x',y',0) = \int_{x'}^{x}\int_{y'}^{y} \mathcal{D}x(t')\,\mathcal{D}y(t')\,\mathcal{F}[x,y]\, \exp \frac{i}{\hbar}\left(S_0[x] - S_0[y]\right)$$

Where $S_0[x] = \int_0^t dt' \frac{1}{2} M \dot{x}^2(t')$ and $\mathcal{F}[x,y] = \int \dots \int d\mu(\boldsymbol{\alpha})\, d\mu(\boldsymbol{\alpha}')\, d\mu(\boldsymbol{\gamma}')\, \rho_R(\boldsymbol{\alpha}'^*, \boldsymbol{\gamma}')$

$$\times \int_{\boldsymbol{\alpha}'}^{\boldsymbol{\alpha}^*} \mathcal{D}\mu(\boldsymbol{\alpha}) \int_{\boldsymbol{\gamma}'^*}^{\boldsymbol{\alpha}} \mathcal{D}\mu(\boldsymbol{\gamma}) \exp \frac{i}{\hbar}\left(S_{RI}[x,\boldsymbol{\alpha}] - S_{RI}^*[y,\boldsymbol{\gamma}^*]\right)$$

with

$$S_{RI}[x,\boldsymbol{\alpha}] = \int_0^t dt' \left(\frac{i\hbar}{2}\sum_n (\alpha_n^* \dot{\alpha}_n - \alpha_n \dot{\alpha}_n^*) + \dot{x}\sum_{m,n} \hbar g_{mn}\alpha_m^*\alpha_n - \sum_n (\hbar\Omega_n - \mu)\alpha_n^*\alpha_n \right)$$

And $\rho_R(\boldsymbol{\alpha}'^*, \boldsymbol{\gamma}') = \dfrac{\exp\left\{e^{-\beta(\hbar\Omega_n - \mu)}\alpha_n'^*\gamma_n'\right\}}{Z}$; $Z = \int d\mu(\boldsymbol{\alpha}) \exp\left\{e^{-\beta(\hbar\Omega_n-\mu)}|\alpha_n|^2\right\}$

This gives $\mathcal{F}[x,y] = [\det(1 \mp \bar{N}\Gamma[x,y])]^{\mp 1}$ with $\bar{N}_{ij} = \delta_{ij}\overline{n}_i$ and

$$\overline{n}_i = \frac{1}{e^{\beta(\Omega_i - \mu)} \mp 1}$$

Moreover $\Gamma_{nm}[x,y] = W_{nm}[x] + W^*_{nm}[y] + \sum_k W^*_{nk}[y] W_{km}[x]$

where $W_{nm}[x,\tau] = \int_0^\tau dt'\, W^{(0)}_{nm}(\dot{x},t') + \sum_k \int_0^\tau dt' \int_0^{t'} dt''\, W^{(0)}_{nk}(\dot{x},t') W_{km}(\dot{x},t'')$

with $W^{(0)}_{nm}(t') = i g_{nm} \dot{x}(t') e^{i(\Omega_n - \Omega_m)t'}(1 - \delta_{nm})$

Within Born approximation $\mathcal{F}[x,y] = \exp -\frac{i}{\hbar}\Phi_I[x,y] \exp -\frac{1}{\hbar}\Phi_R[x,y]$

$$\Phi_I = \int_0^t dt' \int_0^{t'} dt''(\dot{x}(t') - \dot{y}(t'))\hbar\Gamma_I(t'-t'')(\dot{x}(t'') + \dot{y}(t''))$$

$$\Phi_R = \int_0^t dt' \int_0^{t'} dt''(\dot{x}(t') - \dot{y}(t'))\hbar\Gamma_R(t'-t'')(\dot{x}(t'') - \dot{y}(t''))$$

where $$\Gamma_R(t) = \frac{1}{2}\sum_{i,j} |g_{ij}|^2(\overline{n}_i + \overline{n}_j \pm 2\overline{n}_i\overline{n}_j)\cos(\Omega_i - \Omega_j)t$$

and $$\Gamma_I(t) = \frac{1}{2}\sum_{i,j} |g_{ij}|^2(\overline{n}_i - \overline{n}_j)\sin(\Omega_i - \Omega_j)t$$

Defining the scattering function $$S(\omega,\omega') = \sum_{i,j} |g_{ij}|^2\delta(\omega - \Omega_i)\delta(\omega' - \Omega_j)$$

we have

$$\gamma(t) = -\frac{\hbar}{M}\frac{d\Gamma_I(t)}{dt} = -\frac{\hbar}{2M}\int d\omega\int d\omega' S(\omega,\omega')[\overline{n}(\omega) - \overline{n}(\omega')](\omega - \omega')\cos(\omega - \omega')t$$

$$D(t) = -\hbar\frac{d^2\Gamma_R}{dt^2} = \frac{\hbar^2}{2}\int d\omega\int d\omega' S(\omega,\omega')[\overline{n}(\omega) + \overline{n}(\omega') \pm 2\overline{n}(\omega)\overline{n}(\omega')](\omega - \omega')^2\cos(\omega - \omega')t$$