Supporting Information: Matsubara dynamics approximation to generalized multi-time correlation functions.

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CONTENTS

I. INTEGRATION OF NON-MATSUBARA MODES

Here we provide a step-by-step derivation of the Matsubara limit of the general ring-polymer correlation function

$$\begin{aligned}
&\left\langle O_n(t_n)\overleftrightarrow{J_n}\cdots\overleftrightarrow{J_2}O_1(t_1)\overleftrightarrow{J_1}O_0(t_0)\right\rangle_M = \\
&\frac{Z_N^{-1}N^N}{(2\pi\hbar)^N}\int d\mathbf{Q}\int d\mathbf{P}\ \left[e^{-\beta\hat{H}}\right]_{\overline{N}}(\mathbf{Q},\mathbf{P}) \\
&\times\left\{\left[\hat{O}_n(t_n)\right]_N\overleftrightarrow{J_n}\cdots\overleftrightarrow{J_2}\left[\hat{O}_1(t_1)\right]_N\overleftrightarrow{J_1}\left[\hat{O}_0(t_0)\right]_N\right\},
\end{aligned} \tag{1}$$

where

$$\overleftrightarrow{J} = \begin{cases}\lim_{\substack{N\to\infty\\ M<<N}}\overleftrightarrow{s} = \overleftrightarrow{\Lambda}_M \\ \lim_{\substack{N\to\infty\\ M<<N}}\overleftrightarrow{c} = \overleftrightarrow{1}\end{cases} \tag{2}$$

with

$$\overleftrightarrow{\Lambda}_M = \sum_{j=-\bar{M}}^{\bar{M}}\overleftarrow{\frac{\partial}{\partial P_j}}\overrightarrow{\frac{\partial}{\partial Q_j}} - \overleftarrow{\frac{\partial}{\partial Q_j}}\overrightarrow{\frac{\partial}{\partial P_j}}, \tag{3}$$

and where

$$\left[\hat{O}(t)\right]_N(\mathbf{Q},\mathbf{P}) \ = \ e^{\bar{\mathcal{L}}_M t}O(\mathbf{Q}), \tag{4}$$

with

$$\bar{\mathcal{L}}_M = \lim_{\substack{N\to\infty\\ M<<N}}\mathcal{L}_N^{\mathbf{Q},\mathbf{P}} = \sum_{j=-\bar{M}}^{\bar{M}}\left[\frac{P_j}{m}\overrightarrow{\frac{\partial}{\partial Q_j}} - \frac{\partial V(\mathbf{Q})}{\partial Q_j}\overrightarrow{\frac{\partial}{\partial P_j}}\right], \tag{5}$$

and

$$O(\mathbf{Q}) = \frac{1}{N}\sum_{j=1}^{N}O(\sum_{k=-\bar{N}}^{\bar{N}}\sqrt{N}T_{jk}Q_k). \tag{6}$$

Note that we have discarded the contribution of the non-Matsubara modes to the exact Janus operator and have taken the Matsubara limit ($N\to\infty, M << N$) to linearize the Sine/Cosine couplings [Eq. (2)] as well as the Liouvillian [Eq. (5)]. We remark that the Liouvillian $\bar{\mathcal{L}}_M$ still depends on non-Matsubara $\mathbf{Q}$ modes through the potential $V(\mathbf{Q})$.

We start by recognizing that in normal mode coordinates, the generalized Boltzmann factor $\left[e^{-\beta\hat{H}}\right]_{\overline{N}}$ is given by

$$\left[e^{-\beta\hat{H}}\right]_{\overline{N}}(\mathbf{Q},\mathbf{P}) \ = \ \left(\frac{mN}{2\pi\beta_N\hbar^2}\right)^{N/2}\int d\mathbf{D}\ \prod_{l=-\bar{N}}^{\bar{N}}\left(e^{\frac{i}{\hbar}NP_lD_l}\right)$$

$$\times \exp\left(-\frac{\beta_N}{2}\sum_{l=-\bar{N}}^{\bar{N}}\left[V(\eta_l^+(\mathbf{Q},\mathbf{D}))+V(\eta_l^-(\mathbf{Q},\mathbf{D}))\right]\right)$$
$$\times \exp\left(-\beta\sum_{l=-\bar{N}}^{\bar{N}}\left[\frac{m}{2}\omega_l^2 Q_l^2+\frac{m}{2}\Omega_l^2 D_l^2+m\omega_l\Omega_l D_l Q_{-l}\right]\right), \tag{7}$$

with

$$\eta_l^{\pm}(\mathbf{Q},\mathbf{D}) \;=\; \sum_{k=-\bar{N}}^{\bar{N}}\sqrt{N}T_{lk}Q_k \pm \sum_{k=-\bar{N}}^{\bar{N}}\sqrt{N}T_{lk}\frac{D_k}{2}, \tag{8}$$

and where $\omega_l = \frac{2}{\beta_N\hbar}\sin(\pi l/N)$ and $\Omega_l = \frac{1}{\beta_N\hbar}\cos(\pi l/N)$.

To perform the integration of the non-Matsubara modes in Eq. (1) we closely follow Ref. [1] and recognize that upon neglecting the non-Matsubara modes in the Janus operator, both the time-dependent observables $\left[\hat{O}(t)\right]_N$ [Eq. (4)] as well as the $\overleftrightarrow{J}$ couplings [Eq. (2)] are independent of the non-Matsubara momenta $\mathbf{P}$. The only dependence on the non-Matsubara momenta comes, therefore, from the Boltzmann factor $\left[e^{-\beta\hat{H}}\right]_{\overline{N}}$. Note that the integrals over non-Matsubara momenta modes are of the form

$$\int dP_l\; e^{\frac{i}{\hbar}NP_lD_l} \;=\; 2\pi\hbar\delta(ND_l) = \frac{2\pi\hbar}{N}\delta(D_l) \tag{9}$$

which allows us to also integrate the non-Matsubara 'stretch' variables D_l. As a result, the Boltzmann factor $\left[e^{-\beta\hat{H}}\right]_{\overline{N}}$ in Eq. (1) reduces to

$$\left[e^{-\beta\hat{H}}\right]_{\overline{N}}(\mathbf{Q},\mathbf{P}_M) \;=\; \left(\frac{mN}{2\pi\beta_N\hbar^2}\right)^{N/2}\left(\frac{2\pi\hbar}{N}\right)^{N-M}\int d\mathbf{D}_M\,\exp\left(\frac{i}{\hbar}N\sum_{l=-\bar{M}}^{\bar{M}}P_lD_l\right)$$
$$\times \exp\left(-\frac{\beta_N}{2}\sum_{l=1}^{N}\left[V(\eta_l^+(\mathbf{Q},\mathbf{D}_M))+V(\eta_l^-(\mathbf{Q},\mathbf{D}_M))\right]\right)$$
$$\times \exp\left(-\beta\sum_{l=-\bar{N}}^{\bar{N}}\frac{m}{2}\omega_l^2Q_l^2\right)$$
$$\times \exp\left(-\beta\sum_{l=-\bar{M}}^{\bar{M}}\left[\frac{m}{2}\Omega_l^2D_l^2+m\omega_l\Omega_lD_lQ_{-l}\right]\right) \tag{10}$$

where $\mathbf{P}_M$ and $\mathbf{D}_M$ include only Matsubara modes and

$$\eta_l^{\pm}(\mathbf{Q},\mathbf{D}_M) \;=\; \sum_{k=-\bar{N}}^{\bar{N}}\sqrt{N}T_{lk}Q_k \pm \sum_{k=-\bar{M}}^{\bar{M}}\sqrt{N}T_{lk}\frac{D_k}{2}. \tag{11}$$

In the $N \to \infty$ limit the Gaussian distributions over the Matsubara $\mathbf{D}_M$ modes in Eq. (10) become nascent Dirac delta functions. Indeed, note that the distribution over the D_l variable is of the Gaussian form

$$\begin{aligned} I_l &= \exp\left(\frac{i}{\hbar} N P_l D_l - \beta \frac{m}{2} \Omega_l^2 D_l^2 - \beta m \omega_l \Omega_l D_l Q_{-l}\right) \\ &= \exp\left(-\beta \frac{m}{2} \Omega_l^2 \left[D_l - i \frac{N}{\beta \hbar m \Omega_l^2} P_l + \frac{\omega_l}{\Omega_l} Q_{-l}\right]^2\right) \\ &\quad \times \exp\left(-\frac{N^2}{2\hbar^2 \beta m \Omega_l^2} P_l^2 + \frac{\beta m \omega_l^2}{2} Q_{-l}^2 - \frac{i}{\hbar} N \frac{\omega_l}{\Omega_l} P_l Q_{-l}\right). \end{aligned} \tag{12}$$

In the limit $N \to \infty$, for l satisfying $l \leq |\bar{M}|$

$$\Omega_l = \frac{1}{\beta_N \hbar} \cos(\pi l / N) \xrightarrow{N \to \infty} \frac{1}{\beta_N \hbar}, \tag{13}$$

$$\omega_l = \frac{2}{\beta_N \hbar} \sin(\pi l / N) \xrightarrow{N \to \infty} \frac{2\pi l}{\beta \hbar}, \tag{14}$$

namely, $\Omega_l \sim O(N)$ and $\omega_l \sim O(1)$, and the Gaussian distributions become Dirac delta functions,

$$I_l \xrightarrow{N \to \infty} \left(\frac{2\pi \beta \hbar^2}{m N^2}\right)^{1/2} \delta(D_l)\; e^{-\frac{\beta}{2m} P_l^2 + \frac{\beta m \omega_l^2}{2} Q_{-l}^2 - i \beta \omega_l P_l Q_{-l}}. \tag{15}$$

Therefore, anticipating this limit, we replace the Gaussian integrals with delta functions in Eq. (10) and perform the integration over D_l to obtain

$$\begin{aligned} \left[e^{-\beta \hat{H}}\right]_{\overline{N}} (\mathbf{Q}, \mathbf{P}_M) &= \left(\frac{2\pi m}{\beta}\right)^{\frac{N-M}{2}} \exp\left(-\beta_N \sum_{l=1}^{N} V(q_l(\mathbf{Q}))\right) \\ &\quad \times \exp\left(-\frac{\beta}{2m} \sum_{l=-\bar{M}}^{\bar{M}} P_l^2 - i\beta \sum_{l=-\bar{M}}^{\bar{M}} \omega_l P_l Q_{-l}\right) \\ &\quad \times \exp\left(-\beta \frac{m}{2} \sum_{l=\bar{M}+1}^{\bar{N}} \omega_l^2 \left(Q_l^2 + Q_{-l}^2\right)\right) \end{aligned} \tag{16}$$

where

$$q_l(\mathbf{Q}) = \sum_{k=-\bar{N}}^{\bar{N}} \sqrt{N} T_{lk} Q_k. \tag{17}$$

We recognise that the non-Matsubara position modes $\mathbf{Q}$ in Eq. (16) are distributed according to Gaussian that in the $N \to \infty$ limit are nascent Dirac delta functions, namely

$$\exp\left(-\beta \frac{m}{2} \omega_l^2 Q_l^2\right) \xrightarrow{N \to \infty} \left(\frac{2\pi}{\beta m \omega_l^2}\right)^{1/2} \delta(Q_l). \tag{18}$$

Therefore, the non-Matsubara $\mathbf{Q}$ modes can be integrated out from Eq. (1), giving rise to the smooth distribution

$$q_l(\mathbf{Q}_M) \;=\; \sum_{k=-\bar{M}}^{\bar{M}} \sqrt{N} T_{lk} Q_k, \tag{19}$$

containing only Matsubara modes. Thus, upon integration of the the non-Matsubara $\mathbf{Q}$ modes, the Boltzmann factor becomes

$$\begin{aligned}\left[e^{-\beta\hat{H}}\right]_{\overline{N}}(\mathbf{Q},\mathbf{P}_M) \;=\; (2\pi\hbar)^{N-M}\,(2N)^{M-N}\,\mathcal{C}\,\exp\left(-\beta\frac{1}{N}\sum_{l=1}^{N} V(q_l(\mathbf{Q}_M))\right)\\ \times\exp\left(-\frac{\beta}{2m}\sum_{l=-\bar{M}}^{\bar{M}} P_l^2 - i\beta\sum_{l=-\bar{M}}^{\bar{M}}\omega_l P_l Q_{-l}\right),\end{aligned} \tag{20}$$

where

$$\begin{aligned}\mathcal{C} \;&=\; \left(\prod_{l=\bar{M}+1}^{\bar{N}} \frac{1}{\sin^2(\pi l/N)}\right)^{\frac{1}{2}} \left(\prod_{l=-\bar{N}}^{-\bar{M}-1} \frac{1}{\sin^2(\pi l/N)}\right)^{\frac{1}{2}}\\ &=\; \left(\prod_{l=\bar{M}+1}^{\bar{N}} \frac{1}{\sin(\pi l/N)}\right)^{2}.\end{aligned} \tag{21}$$

Explicit evaluation of $\mathcal{C}$ can be performed using the identity

$$\prod_{n=1}^{N-1} \sin\left(\frac{n\pi}{N}\right) \;=\; \frac{N}{2^{N-1}}, \tag{22}$$

as follows:

$$\begin{aligned}\frac{N}{2^{N-1}} \;&=\; \prod_{n=1}^{N-1} \sin\left(\frac{n\pi}{N}\right)\\ &=\; \left[\prod_{n=1}^{\bar{N}} \sin\left(\frac{n\pi}{N}\right)\right]^2\\ &=\; \left[\prod_{n=1}^{\bar{M}} \sin\left(\frac{n\pi}{N}\right)\right]^2 \left[\prod_{n=\bar{M}+1}^{\bar{N}} \sin\left(\frac{n\pi}{N}\right)\right]^2\\ &=\; \left[\prod_{n=1}^{\bar{M}} \sin\left(\frac{n\pi}{N}\right)\right]^2 \mathcal{C}^{-1}\\ &=\; \left[\prod_{n=1}^{\bar{M}} \frac{n\pi}{N}\right]^2 \mathcal{C}^{-1}\end{aligned}$$

$$= \left(\frac{\pi}{N}\right)^{M-1} (\bar{M}!)^2 \mathcal{C}^{-1}, \tag{23}$$

giving

$$\mathcal{C} = \left(\frac{\pi}{N}\right)^{M-1} (\bar{M}!)^2 \frac{2^{N-1}}{N}. \tag{24}$$

Note that by virtue of the delta constraint that allows the integration of non-Matsubara $\mathbf{Q}$ [Eq. (18)], observables inside Eq. (1) effectively change as:

$$O(\mathbf{Q}) = \frac{1}{N} \sum_{j=1}^{N} V(q_j(\mathbf{Q})) \to O_M(\mathbf{Q}_M) = \frac{1}{N} \sum_{j=1}^{N} V(q_j(\mathbf{Q}_M)). \tag{25}$$

Therefore, time-evolved observables become

$$\left[\hat{O}(t)\right]_N = e^{\mathcal{L}_M t} O_M(\mathbf{Q}_M) \equiv O_M(t), \tag{26}$$

where now the Matsubara Liouvillian is given by

$$\mathcal{L}_M = \sum_{j=-\bar{M}}^{\bar{M}} \left[\frac{P_j}{m} \overrightarrow{\frac{\partial}{\partial Q_j}} - \frac{\partial V_M(\mathbf{Q})}{\partial Q_j} \overrightarrow{\frac{\partial}{\partial P_j}} \right] \tag{27}$$

depends only on Matsubara modes.

Introducing Eqs. (20) and (26) in Eq. (1), results in

$$\begin{aligned} &\left\langle O_n(t_n) \overleftrightarrow{J_n} \cdots \overleftrightarrow{J_2} O_1(t_1) \overleftrightarrow{J_1} O_0(t_0) \right\rangle_M = \\ &\frac{Z_N^{-1} \alpha_M}{(2\pi\hbar)^M} \int d\mathbf{Q} \int d\mathbf{P}\ e^{-\beta(H_M + i\theta_M)} \\ &\times \left\{ (O_n(t_n))_M \overleftrightarrow{J_n} \cdots \overleftrightarrow{J_2} (O_1(t_1))_M \overleftrightarrow{J_1} (O_0(t_0))_M \right\}, \end{aligned} \tag{28}$$

with

$$H_M(\mathbf{Q}, \mathbf{P}) = \sum_{l=-\bar{M}}^{\bar{M}} \frac{P_l^2}{2m} + V_M(\mathbf{Q}), \tag{29}$$

$$\theta_M(\mathbf{Q}, \mathbf{P}) = \sum_{l=-\bar{M}}^{\bar{M}} \omega_l P_l Q_{-l}, \tag{30}$$

and $\alpha_M = (2\pi)^{M-1} (\bar{M}!)^2$, and where we have dropped the M subscripts from the Matsubara positions and momenta since there is no longer a need to distinguish between the Matsubara and non-Matsubara modes.

Performing a similar integration of the non-Matsubara modes for the partition function Z_N results in

$$\begin{aligned} Z_N &= \frac{N^N}{(2\pi\hbar)^N}\int d\mathbf{Q}\int d\mathbf{P}\ \left[e^{-\beta\hat{H}}\right]_{\overline{N}}(\mathbf{Q},\mathbf{P}) \\ &= \frac{\alpha_M}{(2\pi\hbar)^M}\int d\mathbf{Q}\int d\mathbf{P}\ e^{-\beta(H_M+i\theta_M)} \\ &= \alpha_M Z_M, \end{aligned} \tag{31}$$

where in the last line we implicitly define Z_M. Introducing Eq. (31) into Eq. (28) gives the final result

$$\begin{aligned} &\left\langle O_n(t_n)\overleftrightarrow{J_n}\cdots\overleftrightarrow{J_2}O_1(t_1)\overleftrightarrow{J_1}O_0(t_0)\right\rangle_M = \\ &\frac{Z_M^{-1}}{(2\pi\hbar)^M}\int d\mathbf{Q}\int d\mathbf{P}\ e^{-\beta(H_M+i\theta_M)} \\ &\times\left\{\left(\hat{O}_n(t_n)\right)_M\overleftrightarrow{J_n}\cdots\overleftrightarrow{J_2}\left(\hat{O}_1(t_1)\right)_M\overleftrightarrow{J_1}\left(\hat{O}_0(t_0)\right)_M\right\}. \end{aligned} \tag{32}$$

II. PHASE-SPACE CONTINUITY IN MATSUBARA SUBSPACE

For convenience, we define the vector $\mathbf{X}_t = (\mathbf{Q}_t, \mathbf{P}_t)$ and $\nabla_t = (\partial/\partial\mathbf{Q}_t, \partial/\partial\mathbf{P}_t)$. [2, 3] Since in Matsubara dynamics the Matsubara modes follows classical evolution governed by the Hamiltonian H_M, it follows that

$$\begin{aligned} \nabla_t\cdot\dot{\mathbf{X}}_t &= \sum_j \frac{\partial\dot{Q}_{j,t}}{\partial Q_{j,t}} + \frac{\partial\dot{P}_{j,t}}{\partial P_{j,t}} \\ &= \sum_j \frac{\partial^2 H_M}{\partial Q_{j,t}\partial P_{j,t}} - \frac{\partial^2 H_M}{\partial P_{j,t}\partial Q_{j,t}} \\ &= 0, \end{aligned} \tag{33}$$

where we have used Hamilton's equations of motion in the second line. Eq. (33) states the incompressibility of the Matsubara phase-space. [2, 3]

On the other hand, the Jacobian matrix (cf. stability matrix) of the transformation generated by the dynamics is given by [2, 3]

$$\mathbf{J}(t) = \frac{\partial\mathbf{X}_t}{\partial\mathbf{X}_0}, \tag{34}$$

whose determinant governs the transformation of the volume element $d\mathbf{X}_0$ as

$$d\mathbf{X}_t = \det(\mathbf{J}(t))d\mathbf{X}_0. \tag{35}$$

The determinant of the matrix satisfies

$$\det(\mathbf{J}(t)) = e^{\mathrm{Tr}[\ln \mathbf{J}(t)]}, \tag{36}$$

and, therefore, its time derivative is given by

$$\frac{d}{dt}\det(\mathbf{J}(t)) = \det(\mathbf{J}(t))\mathrm{Tr}\left[\mathbf{J}(t)^{-1}\frac{d}{dt}\mathbf{J}(t)\right]. \tag{37}$$

From Eq. (34), the time derivative of the Jacobian matrix is given by

$$\frac{d}{dt}\mathbf{J}(t) = \frac{\partial \dot{\mathbf{X}}_t}{\partial \mathbf{X}_0}. \tag{38}$$

Therefore, it follows that the second term on the right hand side of Eq. (37) can be written using the chain rule as

$$\begin{aligned}
\mathrm{Tr}\left[\mathbf{J}(t)^{-1}\frac{d}{dt}\mathbf{J}(t)\right] &= \sum_{i,j}\frac{\partial X_{i,0}}{\partial X_{j,t}}\frac{\partial \dot{X}_{j,t}}{\partial X_{i,0}} \\
&= \sum_{i,j,k}\frac{\partial X_{i,0}}{\partial X_{j,t}}\frac{\partial \dot{X}_{j,t}}{\partial X_{k,t}}\frac{\partial X_{k,t}}{\partial X_{i,0}} \\
&= \sum_{j,k}\frac{\partial X_{k,t}}{\partial X_{j,t}}\frac{\partial \dot{X}_{j,t}}{\partial X_{k,t}} \\
&= \sum_{j}\frac{\partial \dot{X}_{j,t}}{\partial X_{j,t}} \\
&= \nabla_t \cdot \dot{\mathbf{X}}_t.
\end{aligned} \tag{39}$$

Noticing that

$$\mathbf{J}(0) = \mathbf{1}, \tag{40}$$

it then follows from Eqs. (37) and (39) that

$$\begin{aligned}
\det(\mathbf{J}(t)) &= \exp\left(\int_0^t dt' \nabla_{t'} \cdot \dot{\mathbf{X}}_{t'}\right) \\
&= 1,
\end{aligned} \tag{41}$$

where we have used Eq. (33) in the last equality. It follows that

$$d\mathbf{X}_t = d\mathbf{X}_0, \tag{42}$$

which states the conservation of the Matsubara phase-space volume element along the dynamics.

Additional, defining the matrix [2, 3]

$$\mathbf{M} = \begin{pmatrix} \mathbf{0} & -\mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \tag{43}$$

where $\mathbf{0}$ and $\mathbf{1}$ are $M \times M$ zero and identity matrices, the Matsubara Poisson Bracket can be written as

$$\begin{aligned} \overleftrightarrow{\Lambda}_M &= \sum_j \overleftarrow{\frac{\partial}{\partial P_j}} \overrightarrow{\frac{\partial}{\partial Q_j}} - \overleftarrow{\frac{\partial}{\partial Q_j}} \overrightarrow{\frac{\partial}{\partial P_j}} \\ &= \overleftarrow{\nabla}_0 \mathbf{M} \overrightarrow{\nabla}_0^\dagger. \end{aligned} \tag{44}$$

Noting that

$$\overrightarrow{\nabla}_0^\dagger = \mathbf{J}(t)^\dagger \overrightarrow{\nabla}_t^\dagger, \tag{45a}$$

$$\overleftarrow{\nabla}_0 = \overleftarrow{\nabla}_t \mathbf{J}(t), \tag{45b}$$

and that

$$\begin{aligned} \mathbf{J}(t)\mathbf{M}\mathbf{J}(t)^\dagger &= \begin{pmatrix} \mathbf{0} & -\det(\mathbf{J}(t)) \\ \det(\mathbf{J}(t)) & \mathbf{0} \end{pmatrix} \\ &= \mathbf{M}, \end{aligned} \tag{46}$$

it follows that

$$\begin{aligned} \overleftrightarrow{\Lambda}_M &= \overleftarrow{\nabla}_0 \mathbf{M} \overrightarrow{\nabla}_0^\dagger \\ &= \overleftarrow{\nabla}_t \mathbf{J}(t)\mathbf{M}\mathbf{J}(t)^\dagger \overrightarrow{\nabla}_t^\dagger \\ &= \overleftarrow{\nabla}_t \mathbf{M} \overrightarrow{\nabla}_t^\dagger \\ &= \sum_j \overleftarrow{\frac{\partial}{\partial P_j(t)}} \overrightarrow{\frac{\partial}{\partial Q_j(t)}} - \overleftarrow{\frac{\partial}{\partial Q_j(t)}} \overrightarrow{\frac{\partial}{\partial P_j(t)}}, \end{aligned} \tag{47}$$

which proves that the Matsubara Poisson Bracket remains unchanged upon the change of variables $(\mathbf{Q}, \mathbf{P}) \to (\mathbf{Q}_t, \mathbf{P}_t)$.

III. MATSUBARA TCFS FOR HARMONIC OSCILLATOR

For a harmonic potential with natural frequency Ω of the form $V(\hat{q}) = \frac{1}{2} m\Omega^2 \hat{q}^2$, the Matsubara potential is given by

$$V_M(\mathbf{Q}) = \frac{1}{2} m\Omega^2 \sum_{k=-\bar{M}}^{\bar{M}} Q_k^2. \tag{48}$$

Moreover, since the dynamical evolution of the modes is decoupled from each other and classical, the dynamics is given by

$$
\begin{aligned}
Q_k(t) &= Q_k \cos(\Omega t) + \frac{P_k}{m\Omega} \sin(\Omega t), &\quad (49a)\\
P_k(t) &= P_k \cos(\Omega t) - m\Omega Q_k \sin(\Omega t). &\quad (49b)
\end{aligned}
$$

Furthermore, for linear and quadratic operators of the form $\hat{q}$ and $\hat{q}^2$, the Matsubara observables are given by

$$
q_M = Q_0, \tag{50}
$$

and

$$
q_M^2 = \sum_{k=-\bar{M}}^{\bar{M}} Q_k^2, \tag{51}
$$

respectively.

To keep the notation simple, we will denote averages over the Matsubara density $e^{-\beta[H_M - i\theta_M]}$ as

$$
\langle \cdot \rangle_M \equiv \frac{Z_M^{-1}}{(2\pi\hbar)^M} \int d\mathbf{Q} \int d\mathbf{P}\ e^{-\beta[H_M(\mathbf{Q},\mathbf{P}) - i\theta_M(\mathbf{Q},\mathbf{P})]} \cdot, \tag{52}
$$

and averages over the ring-polymer distribution $e^{-\beta R_M}$ as

$$
\langle \cdot \rangle_{RP} \equiv \frac{Z_M^{-1}}{(2\pi\hbar)^M} \int d\mathbf{Q} \int d\mathbf{P}\ e^{-\beta R_M(\mathbf{Q},\mathbf{P})} \cdot . \tag{53}
$$

Notice that by performing the change of variables $P_k \to P_k + im\omega_k Q_{-k}$ and using the analytic continuation contour integration trick,[1, 4] one can express averages over the Matsubara density as averages over the ring-polymer distribution. Since for a harmonic oscillator the ring-polymer distribution is composed of decoupled Gaussians in $\mathbf{Q}$ and $\mathbf{P}$, it is straightforward to perform the integrals to show that

$$
\left\langle Q_k^2 \right\rangle_{RP} = \frac{1}{\beta m(\Omega^2 + \omega_k^2)}, \tag{54a}
$$

$$
\left\langle Q_k^4 \right\rangle_{RP} = \frac{3}{\beta^2 m^2 (\Omega^2 + \omega_k^2)^2}, \tag{54b}
$$

$$
\left\langle P_k^2 \right\rangle_{RP} = \frac{m}{\beta}, \tag{54c}
$$

and

$$\langle P_k^4 \rangle_{RP} = \frac{3m^2}{\beta^2}, \tag{54d}$$

whereas any average involving odd numbers of $\mathbf{Q}$ and/or $\mathbf{P}$ variables [such as $\langle Q_k \rangle_{RP}$, $\langle P_k Q_k \rangle_{RP}$ or $\langle Q_k Q_{-k} \rangle_{RP}$] vanishes.

Moreover, we will use the shorthand notation

$$\begin{aligned} f(t_2, t_1) &\equiv Q_k(t_2) \overleftrightarrow{\Lambda}_M Q_k(t_1) \\ &= Q_k(t_2) \overleftrightarrow{\Lambda}_k Q_k(t_1) \\ &= \frac{\partial Q_k(t_2)}{\partial P_k} \frac{\partial Q_k(t_1)}{\partial Q_k} - \frac{\partial Q_k(t_2)}{\partial Q_k} \frac{\partial Q_k(t_1)}{\partial P_k} \\ &= \frac{1}{m\Omega} \sin(\Omega t_2) \cos(\Omega t_1) - \cos(\Omega t_2) \frac{1}{m\Omega} \sin(\Omega t_1) \\ &= \frac{1}{m\Omega} \sin(\Omega(t_2 - t_1)). \end{aligned} \tag{55}$$

Notice that $f(t_2, t_1)$ does not depend on $\mathbf{Q}$ or $\mathbf{P}$.

A. Sine-Sine correlations

Here we provide results for Matsubara correlations of the form

$$\left\langle \left\{ C_M(t_2) \overleftrightarrow{\Lambda}_M B_M(t_1) \right\} \overleftrightarrow{\Lambda}_M A_M(t_0) \right\rangle_M, \tag{56}$$

that correspond to exact Sine-Sine correlations of the form

$$\left\langle \left\{ \hat{C}(t_2) \overleftrightarrow{s} \hat{B}(t_1) \right\} \overleftrightarrow{s} \hat{A}(t_0) \right\rangle_N. \tag{57}$$

1. $\hat{A} = \hat{B} = \hat{C} = \hat{q}$

Using Eq. (49) it is straightforward to check that

$$\begin{aligned} \left\langle \left\{ q_M(t_2) \overleftrightarrow{\Lambda}_M q_M(t_1) \right\} \overleftrightarrow{\Lambda}_M q_M(t_0) \right\rangle_M &= \left\langle \left\{ Q_0(t_2) \overleftrightarrow{\Lambda}_M Q_0(t_1) \right\} \overleftrightarrow{\Lambda}_M Q_0(t_0) \right\rangle_M \\ &= \left\langle f(t_2, t_1) \overleftrightarrow{\Lambda}_M Q_0(t_0) \right\rangle_M \\ &= 0, \end{aligned} \tag{58}$$

where the last equality follows from the independence of $f(t_2, t_1)$ on $\mathbf{Q}$ and $\mathbf{P}$.

2. $\hat{A} = \hat{q}^2$, $\hat{B} = \hat{C} = \hat{q}$

Using Eqs. (49) it is straightforward to check that

$$\begin{aligned}
\left\langle \left\{ q_M(t_2) \overleftrightarrow{\Lambda}_M q_M(t_1) \right\} \overleftrightarrow{\Lambda}_M q_M^2(t_0) \right\rangle_M &= \left\langle \left\{ Q_0(t_2) \overleftrightarrow{\Lambda}_M Q_0(t_1) \right\} \overleftrightarrow{\Lambda}_M \left(\sum_k Q_k^2(t_0) \right) \right\rangle_M \\
&= \left\langle f(t_2,t_1) \overleftrightarrow{\Lambda}_M \left(\sum_k Q_k^2(t_0) \right) \right\rangle_M \\
&= 0,
\end{aligned} \tag{59}$$

where the last equality follows from the independence of $f(t_2, t_1)$ on $\mathbf{Q}$ and $\mathbf{P}$.

3. $\hat{A} = \hat{B} = \hat{q}$, $\hat{C} = \hat{q}^2$

Using Eqs. (49) it is straightforward to check that

$$\begin{aligned}
\left\langle \left\{ q_M^2(t_2) \overleftrightarrow{\Lambda}_M q_M(t_1) \right\} \overleftrightarrow{\Lambda}_M q_M(t_0) \right\rangle_M &= \left\langle \left\{ \left(\sum_k Q_k^2(t_2) \right) \overleftrightarrow{\Lambda}_M Q_0(t_1) \right\} \overleftrightarrow{\Lambda}_M Q_0(t_0) \right\rangle_M \\
&= \left\langle \left\{ Q_0^2(t_2) \overleftrightarrow{\Lambda}_0 Q_0(t_1) \right\} \overleftrightarrow{\Lambda}_0 Q_0(t_0) \right\rangle_M \\
&= \left\langle 2Q_0(t_2) f(t_2,t_1) \overleftrightarrow{\Lambda}_0 Q_0(t_0) \right\rangle_M \\
&= 2f(t_2,t_1) f(t_2,t_0) \\
&= \frac{2}{m^2\Omega^2} \sin(\Omega(t_2-t_1)) \sin(\Omega(t_2-t_0)).
\end{aligned} \tag{60}$$

B. Sine-Cosine correlations

Here we provide results for Matsubara correlations of the form

$$\left\langle \left\{ C_M(t_2) \overleftrightarrow{\Lambda}_M B_M(t_1) \right\} A_M(t_0) \right\rangle_M, \tag{61}$$

that correspond to exact Sine-Cosine correlations of the form

$$\left\langle \left\{ \hat{C}(t_2) \overleftrightarrow{s} \hat{B}(t_1) \right\} \overleftrightarrow{c} \hat{A}(t_0) \right\rangle_N. \tag{62}$$

1. $\hat{A} = \hat{B} = \hat{C} = \hat{q}$

Using Eqs. (49) it is straightforward to check that

$$\left\langle \left\{ q_M(t_2) \overleftrightarrow{\Lambda}_M q_M(t_1) \right\} q_M(t_0) \right\rangle_M = \left\langle \left\{ Q_0(t_2) \overleftrightarrow{\Lambda}_M Q_0(t_1) \right\} Q_0(t_0) \right\rangle_M$$

$$
\begin{aligned}
&= \langle f(t_2,t_1) Q_0(t_0)\rangle_M \\
&= f(t_2,t_1)\left(\langle Q_0\rangle_M \cos(\Omega t_0) + \frac{\langle P_0\rangle_M}{m\Omega}\sin(\Omega t_0)\right) \\
&= f(t_2,t_1)\left(\langle Q_0\rangle_{RP} \cos(\Omega t_0) + \frac{\langle P_0\rangle_{RP}}{m\Omega}\sin(\Omega t_0)\right) \\
&= 0,
\end{aligned}
\tag{63}
$$

where we have used the contour integration trick with the change of variables $P_k \to P_k + im\omega_k Q_{-k}$ (note that since $\omega_0 = 0$, $P_0 \to P_0$) and where the last equality follows from the symmetry of the Gaussian integrals in the ring-polymer distribution.

2. $\hat{A} = \hat{q}^2$, $\hat{B} = \hat{C} = \hat{q}$

Using Eqs. (49) it is straightforward to check that

$$
\begin{aligned}
\left\langle \left\{ q_M(t_2) \overleftrightarrow{\Lambda}_M q_M(t_1)\right\} q_M^2(t_0)\right\rangle_M &= \left\langle \left\{ Q_0(t_2) \overleftrightarrow{\Lambda}_M Q_0(t_1)\right\} \left(\sum_k Q_k^2(t_0)\right)\right\rangle_M \\
&= \left\langle f(t_2,t_1)\left(\sum_k Q_k^2(t_0)\right)\right\rangle_M \\
&= f(t_2,t_1)\left(\sum_k \left\langle Q_k^2\right\rangle_M \cos^2(\Omega t_0) + \frac{\langle P_k^2\rangle_M}{m^2\Omega^2}\sin^2(\Omega t_0)\right. \\
&\quad \left. + \frac{2\left\langle Q_k P_k\right\rangle_M}{m\Omega}\cos(\Omega t_0)\sin(\Omega t_0)\right) \\
&= f(t_2,t_1)\left(\sum_k \left\langle Q_k^2\right\rangle_{RP} \cos^2(\Omega t_0)\right. \\
&\quad \left. + \left[\frac{\langle P_k^2\rangle_{RP}}{m^2\Omega^2} - \frac{\omega_k^2\left\langle Q_{-k}^2\right\rangle_{RP}}{\Omega^2}\right]\sin^2(\Omega t_0)\right),
\end{aligned}
\tag{64}
$$

where we have used the contour integration trick with the change of variables $P_k \to P_k + im\omega_k Q_{-k}$ in the last step and recognize that, since integrals are Gaussian in the ring-polymer distribution, terms of the form $\langle P_k Q_{\pm k}\rangle_{RP}$ and $\langle Q_k Q_{-k}\rangle_{RP}$ vanishes.

Using Eqs. (54), and noting that $\omega_{-k}^2 = \omega_k^2$, it is straightforward to check that

$$
\begin{aligned}
\sum_k \left\langle Q_k^2\right\rangle_{RP} &= \sum_k \frac{1}{\beta m(\Omega^2+\omega_k^2)}, \qquad (65)\\
\sum_k \frac{\langle P_k^2\rangle_{RP}}{m^2\Omega^2} - \frac{\omega_k^2\left\langle Q_{-k}^2\right\rangle_{RP}}{\Omega^2} &= \sum_k \frac{1}{\beta m\Omega^2} - \frac{\omega_k^2}{\beta m\Omega^2(\Omega^2+\omega_k^2)}
\end{aligned}
$$

$$= \sum_k \frac{1}{\beta m(\Omega^2+\omega_k^2)}. \tag{66}$$

Therefore, it follows that

$$\begin{aligned}
\left\langle \left\{ q_M(t_2)\overleftrightarrow{\Lambda}_M q_M(t_1)\right\} q_M^2(t_0)\right\rangle_M &= f(t_2,t_1)\left(\sum_k \frac{1}{\beta m(\Omega^2+\omega_k^2)}\right)\\
&= \frac{1}{m\Omega}\sin(\Omega(t_2-t_1))\left(\sum_k \frac{1}{\beta m(\Omega^2+\omega_k^2)}\right)\\
&\overset{M\to\infty}{=} \frac{\hbar}{2m^2\Omega^2}\coth\left(\beta\hbar\Omega/2\right)\sin(\Omega(t_2-t_1)),
\end{aligned} \tag{67}$$

where we have taken the $M\to\infty$ limit in the last equality and used the identity[5]

$$\lim_{\bar{M}\to\infty}\sum_{k=-\bar{M}}^{\bar{M}} \frac{1}{\beta m(\Omega^2+\omega_k^2)} = \sum_k \frac{1}{\beta m(\Omega^2+(\frac{2\pi k}{\beta\hbar})^2)} = \frac{\hbar}{2m\Omega}\coth\left(\beta\hbar\Omega/2\right). \tag{68}$$

3. $\hat{A}=\hat{B}=\hat{q}$, $\hat{C}=\hat{q}^2$

Using Eqs. (49) it is straightforward to check that

$$\begin{aligned}
\left\langle \left\{ q_M^2(t_2)\overleftrightarrow{\Lambda}_M q_M(t_1)\right\} q_M(t_0)\right\rangle_M &= \left\langle \left\{ \left(\sum_k Q_k^2(t_2)\right)\overleftrightarrow{\Lambda}_M Q_0(t_1)\right\} Q_0(t_0)\right\rangle_M\\
&= \left\langle \left\{ Q_0^2(t_2)\overleftrightarrow{\Lambda}_0 Q_0(t_1)\right\} Q_0(t_0)\right\rangle_M\\
&= \langle 2Q_0(t_2)f(t_2,t_1)Q_0(t_0)\rangle_M\\
&= 2f(t_2,t_1)\left(\left\langle Q_0^2\right\rangle_M \cos(\Omega t_0)\cos(\Omega t_2) + \frac{\langle P_0^2\rangle_M}{m^2\Omega^2}\sin(\Omega t_0)\sin(\Omega t_2)\right.\\
&\quad \left. + \frac{\langle Q_0P_0\rangle_M}{m\Omega}\sin(\Omega(t_0+t_2))\right)\\
&= 2f(t_2,t_1)\\
&\quad \times\left(\left\langle Q_0^2\right\rangle_{RP} \cos(\Omega t_0)\cos(\Omega t_2) + \frac{\langle P_0^2\rangle_{RP}}{m^2\Omega^2}\sin(\Omega t_0)\sin(\Omega t_2)\right)
\end{aligned} \tag{69}$$

where we have used the contour integration with the change of variables $P_k \to P_k + im\omega_k Q_{-k}$ in the last step (note that $P_0 \to P_0$) and recognize that since integrals are Gaussian in the ring-polymer distribution, the term $\langle Q_0P_0\rangle_{RP}$ vanishes.

Using Eqs. (54), and recognizing that $\omega_0=0$, it follows that

$$\left\langle \left\{ q_M^2(t_2)\overleftrightarrow{\Lambda}_M q_M(t_1)\right\} q_M(t_0)\right\rangle_M = \frac{2}{\beta m\Omega^2} f(t_2,t_1)\left(\cos(\Omega t_0)\cos(\Omega t_2)+\sin(\Omega t_0)\sin(\Omega t_2)\right)$$

$$\begin{aligned} &= \frac{2}{\beta m \Omega^2} f(t_2,t_1)\cos(\Omega(t_2-t_0)) \\ &= \frac{2}{\beta m^2 \Omega^3}\sin\left(\Omega(t_2-t_1)\right)\cos\left(\Omega(t_2-t_0)\right). \end{aligned} \tag{70}$$

C. Cosine-Cosine correlations

Here we provide results for Matsubara correlations of the form

$$\langle C_M(t_2) B_M(t_1) A_M(t_0)\rangle_M , \tag{71}$$

that correspond to exact Cosine-Cosine correlations of the form

$$\left\langle \hat{C}(t_2) \overleftrightarrow{c} \hat{B}(t_1) \overleftrightarrow{c} \hat{A}(t_0)\right\rangle_N . \tag{72}$$

1. $\hat{A} = \hat{B} = \hat{C} = \hat{q}$

Using Eqs. (49), it is straightforward to check that

$$\begin{aligned} \langle q_M(t_2) q_M(t_1) q_M(t_0)\rangle_M &= \langle Q_0(t_2) Q_0(t_1) Q_0(t_0)\rangle_M \\ &= 0, \end{aligned} \tag{73}$$

where we have recognize that averages involving an odd numbers of $\mathbf{Q}$ and/or $\mathbf{P}$ variables [namely $\langle Q_0^3\rangle_{RP}$, $\langle Q_0^2 P_0\rangle_{RP}$, $\langle Q_0 P_0^2\rangle_{RP}$ and $\langle P_0^3\rangle_{RP}$] vanish.

2. $\hat{A} = \hat{q}^2$, $\hat{B} = \hat{C} = \hat{q}$

Using Eqs. (49) it is straightforward to check that

$$\begin{aligned} \left\langle q_M(t_2) q_M(t_1) q_M^2(t_0)\right\rangle_M &= \left\langle Q_0(t_2) Q_0(t_1)\left(\sum_k Q_k^2(t_0)\right)\right\rangle_M \\ &= \left\langle Q_0(t_2) Q_0(t_1)\left(\sum_k Q_k^2 \cos^2(\Omega t_0) + \frac{P_k^2}{m^2\Omega^2}\sin^2(\Omega t_0)\right.\right. \\ &\quad \left.\left. + \frac{2 Q_k P_k}{m\Omega}\cos(\Omega t_0)\sin(\Omega t_0)\right)\right\rangle_M \\ &= \left\langle\left(Q_0^2 \cos(\Omega t_2)\cos(\Omega t_1) + \frac{P_0^2}{m^2\Omega^2}\sin(\Omega t_2)\sin(\Omega t_1)\right.\right. \end{aligned}$$

$$
\begin{aligned}
&+\frac{Q_0P_0}{m\Omega}\sin(\Omega(t_2+t_1))\Bigg)\left(\sum_k Q_k^2\cos^2(\Omega t_0)+\frac{P_k^2}{m^2\Omega^2}\sin^2(\Omega t_0)\right.\\
&\left.\left.+\frac{2Q_kP_k}{m\Omega}\cos(\Omega t_0)\sin(\Omega t_0)\right)\right\rangle_M\\
=&\sum_k \left\langle Q_0^2Q_k^2\right\rangle_M\cos(\Omega t_2)\cos(\Omega t_1)\cos^2(\Omega t_0)\\
&+\frac{\langle Q_0^2P_k^2\rangle_M}{m^2\Omega^2}\cos(\Omega t_2)\cos(\Omega t_1)\sin^2(\Omega t_0)\\
&+\frac{2\left\langle Q_0^2Q_kP_k\right\rangle_M}{m\Omega}\cos(\Omega t_2)\cos(\Omega t_1)\cos(\Omega t_0)\sin(\Omega t_0)\\
&+\frac{\langle P_0^2Q_k^2\rangle_M}{m^2\Omega^2}\sin(\Omega t_2)\sin(\Omega t_1)\cos^2(\Omega t_0)\\
&+\frac{\langle P_0^2P_k^2\rangle_M}{m^4\Omega^4}\sin(\Omega t_2)\sin(\Omega t_1)\sin^2(\Omega t_0)\\
&+\frac{2\left\langle P_0^2Q_kP_k\right\rangle_M}{m^3\Omega^3}\sin(\Omega t_2)\sin(\Omega t_1)\cos(\Omega t_0)\sin(\Omega t_0)\\
&+\frac{\langle Q_0P_0Q_k^2\rangle_M}{m\Omega}\sin(\Omega(t_2+t_1))\cos^2(\Omega t_0)\\
&+\frac{\langle Q_0P_0P_k^2\rangle_M}{m^3\Omega^3}\sin(\Omega(t_2+t_1))\sin^2(\Omega t_0)\\
&+\frac{2\left\langle Q_0P_0Q_kP_k\right\rangle_M}{m^2\Omega^2}\sin(\Omega(t_2+t_1))\cos(\Omega t_0)\sin(\Omega t_0)\\
=&\sum_k \left\langle Q_0^2Q_k^2\right\rangle_{RP}\cos(\Omega t_2)\cos(\Omega t_1)\cos^2(\Omega t_0)\\
&+\left(\frac{\langle Q_0^2P_k^2\rangle_{RP}}{m^2\Omega^2}-\frac{\omega_k^2\left\langle Q_0^2Q_{-k}^2\right\rangle_{RP}}{\Omega^2}\right)\cos(\Omega t_2)\cos(\Omega t_1)\sin^2(\Omega t_0)\\
&+\frac{\langle P_0^2Q_k^2\rangle_{RP}}{m^2\Omega^2}\sin(\Omega t_2)\sin(\Omega t_1)\cos^2(\Omega t_0)\\
&+\left(\frac{\langle P_0^2P_k^2\rangle_{RP}}{m^4\Omega^4}-\omega_k^2\frac{\left\langle P_0^2Q_{-k}^2\right\rangle_{RP}}{m^2\Omega^4}\right)\sin(\Omega t_2)\sin(\Omega t_1)\sin^2(\Omega t_0)\\
&+\frac{2\left\langle Q_0P_0Q_kP_k\right\rangle_{RP}}{m^2\Omega^2}\sin(\Omega(t_2+t_1))\cos(\Omega t_0)\sin(\Omega t_0),
\end{aligned}
\tag{74}
$$

where we have used the contour integration with the change of variables $P_k \to P_k + im\omega_k Q_{-k}$ (note that $\omega_0 = 0$ and $P_0 \to P_0$) and recognize that since the integrals are independent Gaussian in the ring-polymer distribution, terms with odd numbers of $\mathbf{Q}$ and/or $\mathbf{P}$ variables vanish.

Using Eqs. (54), and recognizing that $\omega_{-k}^2 = \omega_k^2$ and that $\omega_0 = 0$, it is straightforward to show that

$$\begin{aligned}
\sum_k \left\langle Q_0^2 Q_k^2 \right\rangle_{RP} &= \left\langle Q_0^4 \right\rangle_{RP} + \sum_{k\neq 0} \left\langle Q_0^2 Q_k^2 \right\rangle_{RP} \\
&= \frac{3}{\beta^2 m^2 \Omega^4} + \sum_{k\neq 0} \frac{1}{\beta^2 m^2 \Omega^2 (\Omega^2+\omega_k^2)} \\
&= \frac{2}{\beta^2 m^2 \Omega^4} + \sum_{k} \frac{1}{\beta^2 m^2 \Omega^2 (\Omega^2+\omega_k^2)}, \qquad (75)
\end{aligned}$$

$$\begin{aligned}
\sum_k \frac{\langle Q_0^2 P_k^2 \rangle_{RP}}{m^2\Omega^2} - \frac{\omega_k^2 \left\langle Q_0^2 Q_{-k}^2 \right\rangle_{RP}}{\Omega^2} &= \sum_k \frac{1}{\beta^2 m^2 \Omega^4} - \frac{\omega_k^2}{\beta^2 m^2 \Omega^4 (\Omega^2+\omega_k^2)} \\
&= \sum_k \frac{1}{\beta^2 m^2 \Omega^2 (\Omega^2+\omega_k^2)}, \qquad (76)
\end{aligned}$$

$$\sum_k \frac{\langle P_0^2 Q_k^2 \rangle_{RP}}{m^2\Omega^2} = \sum_k \frac{1}{\beta^2 m^2 \Omega^2 (\Omega^2+\omega_k^2)}, \qquad (77)$$

$$\begin{aligned}
\sum_k \frac{\langle P_0^2 P_k^2 \rangle_{RP}}{m^4\Omega^4} - \omega_k^2 \frac{\left\langle P_0^2 Q_{-k}^2 \right\rangle_{RP}}{m^2\Omega^4} &= \frac{\langle P_0^4 \rangle_{RP}}{m^4\Omega^4} + \sum_{k\neq 0} \frac{\langle P_0^2 P_k^2 \rangle_{RP}}{m^4\Omega^4} - \omega_k^2 \frac{\left\langle P_0^2 Q_{-k} \right\rangle_{RP}}{m^2\Omega^4} \\
&= \frac{3}{\beta^2 m^2 \Omega^4} + \sum_{k\neq 0} \frac{1}{\beta^2 m^2 \Omega^4} - \frac{\omega_k^2}{\beta^2 m^2 \Omega^4 (\Omega^2+\omega_k^2)} \\
&= \frac{2}{\beta^2 m^2 \Omega^4} + \sum_{k} \frac{1}{\beta^2 m^2 \Omega^4} - \frac{\omega_k^2}{\beta^2 m^2 \Omega^4 (\Omega^2+\omega_k^2)} \\
&= \frac{2}{\beta^2 m^2 \Omega^4} + \sum_{k} \frac{1}{\beta^2 m^2 \Omega^2 (\Omega^2+\omega_k^2)}, \qquad (78)
\end{aligned}$$

$$\begin{aligned}
\sum_k \frac{2 \langle Q_0 P_0 Q_k P_k \rangle_{RP}}{m^2\Omega^2} &= \frac{2 \langle Q_0^2 P_0^2 \rangle_{RP}}{m^2\Omega^2} \\
&= \frac{2}{\beta^2 m^2 \Omega^4}. \qquad (79)
\end{aligned}$$

Therefore, it follows that

$$\begin{aligned}
\left\langle q_M(t_2) q_M(t_1) q_M^2(t_0) \right\rangle_M &= \frac{2}{\beta^2 m^2 \Omega^4} \left(\cos(\Omega t_2)\cos(\Omega t_1)\cos^2(\Omega t_0) + \sin(\Omega t_2)\sin(\Omega t_1)\sin^2(\Omega t_0) \right) \\
&\quad + \left(\sum_k \frac{1}{\beta^2 m^2 \Omega^2 (\Omega^2+\omega_k^2)} \right) \left(\cos(\Omega t_2)\cos(\Omega t_1) + \sin(\Omega t_2)\sin(\Omega t_1) \right) \\
&\quad + \frac{2}{\beta^2 m^2 \Omega^4} \sin(\Omega(t_2+t_1))\cos(\Omega t_0)\sin(\Omega t_0) \\
&= \frac{1}{\beta^2 m^2 \Omega^4} \left(\cos(\Omega(t_2+t_1)\cos(2\Omega t_0) + \cos(\Omega(t_2-t_1)) \right) \\
&\quad + \left(\sum_k \frac{1}{\beta^2 m^2 \Omega^2 (\Omega^2+\omega_k^2)} \right) \cos(\Omega(t_2-t_1))
\end{aligned}$$

$$
\begin{aligned}
& +\frac{1}{\beta^2 m^2 \Omega^4}\sin(\Omega(t_2+t_1))\sin(2\Omega t_0) \\
= \quad & \frac{1}{\beta^2 m^2 \Omega^4}\cos(\Omega(t_2+t_1-2t_0)) \\
& + \left(\frac{1}{\beta^2 m^2 \Omega^4} + \sum_k \frac{1}{\beta^2 m^2 \Omega^2(\Omega^2+\omega_k^2)}\right)\cos(\Omega(t_2-t_1)) \\
\overset{M\to\infty}{=} \quad & \frac{1}{\beta^2 m^2 \Omega^4}\cos(\Omega(t_2+t_1-2t_0)) \\
& + \left(\frac{1}{\beta^2 m^2 \Omega^4} + \frac{\hbar}{2\beta m^2 \Omega^3}\coth\left(\beta\hbar\Omega/2\right)\right)\cos(\Omega(t_2-t_1)),
\end{aligned}
\tag{80}
$$

where we have take the $M \to \infty$ limit in the last equality and used the identity[5]

$$
\lim_{\bar{M}\to\infty} \sum_{k=-\bar{M}}^{\bar{M}} \frac{1}{\beta^2 m^2 \Omega^2(\Omega^2+\omega_k^2)} = \frac{\hbar}{2\beta m^2 \Omega^3}\coth\left(\beta\hbar\Omega/2\right). \tag{81}
$$

IV. EXACT TCFS FOR HARMONIC OSCILLATOR

In this section, we will derive exact expressions for the three-point Sine/Cosine correlation functions in a harmonic potential of the form $V(\hat{q}) = \frac{1}{2}m\Omega^2\hat{q}^2$. To that end, it would be useful to work with the ladder operators

$$
\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle, \tag{82a}
$$

$$
\hat{a}^\dagger\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle, \tag{82b}
$$

where $|n\rangle$ is an eigenvector of the harmonic oscillator Hamiltonian, whose time dependence is given by

$$
\hat{a}(t) = \hat{a}e^{-i\Omega t}, \tag{83a}
$$

$$
\hat{a}^\dagger(t) = \hat{a}^\dagger e^{i\Omega t}. \tag{83b}
$$

Two observables will be considered, namely $\hat{q}$ and $\hat{q}^2$, whose time dependence in terms of the ladder operators is given by

$$
\hat{q}(t) = \sqrt{\frac{\hbar}{2m\Omega}}\left(\hat{a}^\dagger(t)+\hat{a}(t)\right), \tag{84a}
$$

$$
\hat{q}^2(t) = \frac{\hbar}{2m\Omega}\left(\hat{a}^\dagger(t)\hat{a}^\dagger(t)+\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a}+\hat{a}(t)\hat{a}(t)\right). \tag{84b}
$$

For ease of notation, in this section, we will denote traces over the density matrix $\hat{\rho}$ as

$$
\langle\cdot\rangle = Tr\left[\hat{\rho}\,\cdot\right]. \tag{85}
$$

Notice that quantum averages that do not involve the same number of raising and lowering operators (such as $\langle\hat{a}\rangle$, $\langle\hat{a}\hat{a}\rangle$,$\left\langle\hat{a}\hat{a}\hat{a}^{\dagger}\right\rangle$,...) vanish.

The following identities would prove to be useful in order to evaluate traces over raising and lowering operators:

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} = \frac{1}{1-e^{-\beta\hbar\Omega}}, \tag{86a}$$

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} n = \frac{e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{86b}$$

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} n^2 = \frac{e^{-\beta\hbar\Omega}(1+e^{-\beta\hbar\Omega})}{(1-e^{-\beta\hbar\Omega})^3}, \tag{86c}$$

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n}(n+1)(n+2) = \frac{2}{(1-e^{-\beta\hbar\Omega})^3}, \tag{86d}$$

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} n(n-1) = \frac{2e^{-2\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^3}, \tag{86e}$$

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n}(n+1)^2 = \frac{1+e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^3}, \tag{86f}$$

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} n(n+1) = \frac{2e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^3}. \tag{86g}$$

A. Sine-Sine correlations

To compute exact Sine-Sine correlation functions we will use the fact that[6]

$$\left\langle \left\{ \hat{C}(t_2) \overleftrightarrow{s} \hat{B}(t_1) \right\} \overleftrightarrow{s} \hat{A}(t_0) \right\rangle_N = \left(\frac{i}{\hbar}\right)^2 \left\langle \left[\left[\hat{C}(t_2), \hat{B}(t_1) \right], \hat{A}(t_0) \right] \right\rangle, \tag{87}$$

and that

$$\left\langle \left[\left[\hat{C}(t_2), \hat{B}(t_1) \right], \hat{A}(t_0) \right] \right\rangle = 2\Re\left\{ \left\langle \hat{A}(t_0)\hat{B}(t_1)\hat{C}(t_2) \right\rangle - \left\langle \hat{B}(t_1)\hat{C}(t_2)\hat{A}(t_0) \right\rangle \right\}. \tag{88}$$

Additionally, explicitly computing the trace and using identities Eqs. (86) it is straightforward to show that

$$\left\langle \hat{a}\hat{a}\hat{a}^{\dagger}\hat{a}^{\dagger} \right\rangle = (1-e^{-\beta\hbar\Omega}) \sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n}(n+1)(n+2) = \frac{2}{(1-e^{-\beta\hbar\Omega})^2}, \tag{89a}$$

$$\left\langle \hat{a}^{\dagger}\hat{a}^{\dagger}\hat{a}\hat{a} \right\rangle = (1-e^{-\beta\hbar\Omega}) \sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} n(n-1) = \frac{2e^{-2\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{89b}$$

$$\left\langle \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\right\rangle = (1-e^{-\beta\hbar\Omega})\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} n(n+1) = \frac{2e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{89c}$$

$$\left\langle \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger\right\rangle = (1-e^{-\beta\hbar\Omega})\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} n(n+1) = \frac{2e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{89d}$$

$$\left\langle \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger\right\rangle = (1-e^{-\beta\hbar\Omega})\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} (n+1)^2 = \frac{1+e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{89e}$$

$$\left\langle \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\right\rangle = (1-e^{-\beta\hbar\Omega})\sum_{n=0}^{\infty} e^{-\beta\hbar\Omega n} n^2 = \frac{e^{-\beta\hbar\Omega}(1+e^{-\beta\hbar\Omega})}{(1-e^{-\beta\hbar\Omega})^2}. \tag{89f}$$

1. $\hat{A} = \hat{B} = \hat{C} = \hat{q}$

Noticing that upon expansion in terms of raising and lowering operators [i.e. Eqs. (84) and (83)] both $\langle \hat{q}(t_0)\hat{q}(t_1)\hat{q}(t_2)\rangle$ and $\langle \hat{q}(t_1)\hat{q}(t_2)\hat{q}(t_0)\rangle$ contains averages that do not involve the same number of raising and lowering operators (such as $\langle \hat{a}\hat{a}\hat{a}\rangle$, $\langle \hat{a}^\dagger\hat{a}\hat{a}\rangle$, $\langle \hat{a}\hat{a}^\dagger\hat{a}^\dagger\rangle$,...), it follows from Eqs. (87) and (88) that

$$\langle \{\hat{q}(t_2)\overleftrightarrow{s}\hat{q}(t_1)\}\overleftrightarrow{s}\hat{q}(t_0)\rangle_N = 0. \tag{90}$$

2. $\hat{A} = \hat{q}^2, \hat{B} = \hat{C} = \hat{q}$

Using Eqs. (84) and (83) it is straightforward to check that

$$\begin{aligned}
\Re\left\{\left\langle \hat{q}^2(t_0)\hat{q}(t_1)\hat{q}(t_2)\right\rangle\right\} &= \left(\frac{\hbar}{2m\Omega}\right)^2 \left\{\left[\left\langle \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger\right\rangle + \left\langle \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\right\rangle\right]\cos\left(\Omega(2t_0-t_1-t_2)\right)\right. \\
&\quad \left. + \left[\left\langle \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger\right\rangle + \left\langle \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\right\rangle + \left\langle \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\right\rangle + \left\langle \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger\right\rangle\right]\cos\left(\Omega(t_1-t_2)\right)\right\} \\
&= \Re\left\{\left\langle \hat{q}(t_1)\hat{q}(t_2)\hat{q}^2(t_0)\right\rangle\right\}.
\end{aligned} \tag{91}$$

It follows from Eqs. (87) and (88) that

$$\left\langle \{\{\hat{q}(t_2), \hat{q}(t_1)\}, \hat{q}^2(t_0)\}\right\rangle = 0. \tag{92}$$

3. $\hat{A} = \hat{B} = \hat{q}, \hat{C} = \hat{q}^2$

Using Eqs. (84) and (83) it is straightforward to check that

$$\Re\left\{\left\langle \hat{q}(t_0)\hat{q}(t_1)\hat{q}^2(t_2)\right\rangle\right\} = \left(\frac{\hbar}{2m\Omega}\right)^2 \left\{\left[\left\langle \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger\right\rangle + \left\langle \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\right\rangle\right]\cos\left(\Omega(t_0+t_1-2t_2)\right)\right.$$

$$+\left[\left\langle \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger\right\rangle + \left\langle \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\right\rangle + \left\langle \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\right\rangle + \left\langle \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger\right\rangle\right]\cos\left(\Omega(t_1-t_0)\right)\right\}, \tag{93}$$

and that

$$\begin{aligned}\Re\left\{\left\langle \hat{q}(t_1)\hat{q}^2(t_2)\hat{q}(t_0)\right\rangle\right\} &= \left(\frac{\hbar}{2m\Omega}\right)^2 \left\{\left[\left\langle \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\right\rangle + \left\langle \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger\right\rangle\right]\cos\left(\Omega(t_0+t_1-2t_2)\right)\right. \\ &\quad \left. +\left[\left\langle \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger\right\rangle + \left\langle \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\right\rangle + \left\langle \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger\right\rangle + \left\langle \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\right\rangle\right]\cos\left(\Omega(t_1-t_0)\right)\right\}.\end{aligned} \tag{94}$$

Using Eqs. (89), it follows from Eqs. (87) and (88) that

$$\begin{aligned}\left\langle\left\{\left\{\hat{q}^2(t_2),\hat{q}(t_1)\right\},\hat{q}(t_0)\right\}\right\rangle &= -\frac{2}{\hbar^2}\left(\frac{\hbar}{2m\Omega}\right)^2\left\{2\cos\left(\Omega(t_0+t_1-2t_2)\right)\right. \\ &\quad \left.-2\cos\left(\Omega(t_1-t_0)\right)\right\} \\ &= -\left(\frac{1}{m^2\Omega^2}\right)\left\{\cos\left(\Omega(t_0+t_1-2t_2)\right)\right. \\ &\quad \left.-\cos\left(\Omega(t_1-t_0)\right)\right\} \\ &= \left(\frac{2}{m^2\Omega^2}\right)\sin\left(\Omega(t_2-t_1)\right)\sin\left(\Omega(t_2-t_0)\right).\end{aligned} \tag{95}$$

B. Sine-Cosine correlation functions

To compute exact Sine-Cosine correlation functions we will use the fact that[6]

$$\left\langle\left\{\hat{C}(t_2)\overleftrightarrow{s}\hat{B}(t_1)\right\}\overleftrightarrow{c}\hat{A}(t_0)\right\rangle_N = \left(\frac{i}{\hbar}\right)\left\langle\left[\hat{C}(t_2),\hat{B}(t_1)\right]\bullet\hat{A}(t_0)\right\rangle, \tag{96}$$

where the Kubo transformed correlation function is defined as[6, 7]

$$\begin{aligned}\left(\frac{i}{\hbar}\right)\left\langle\left[\hat{C}(t_2),\hat{B}(t_1)\right]\bullet\hat{A}(t_0)\right\rangle &= \left(\frac{i}{\hbar}\right)\frac{1}{\beta}\int_0^\beta d\lambda\,\left\langle e^{+\lambda\hat{H}}[\hat{C}(t_2),\hat{B}(t_1)]e^{-\lambda\hat{H}}\hat{A}(t_0)\right\rangle \\ &= -\frac{2}{\hbar}\Im\left\{\frac{1}{\beta}\int_0^\beta d\lambda\,\left\langle e^{+\lambda\hat{H}}\hat{C}(t_2)\hat{B}(t_1)e^{-\lambda\hat{H}}\hat{A}(t_0)\right\rangle\right\} \\ &= -\frac{2}{\hbar}\Im\left\{\left\langle\hat{C}(t_2)\hat{B}(t_1)\bullet\hat{A}(t_0)\right\rangle\right\}.\end{aligned} \tag{97}$$

Additionally, explicitly computing the trace and using Eqs. (89) it is straightforward to show that

$$\left\langle\hat{a}^\dagger\hat{a}\bullet\hat{a}^\dagger\hat{a}\right\rangle = \left\langle\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\right\rangle = \frac{e^{-\beta\hbar\Omega}(1+e^{-\beta\hbar\Omega})}{(1-e^{-\beta\hbar\Omega})^2}, \tag{98a}$$

$$\left\langle \hat{a}\hat{a}^\dagger \bullet \hat{a}\hat{a}^\dagger \right\rangle = \left\langle \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger \right\rangle = \frac{1+e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{98b}$$

$$\left\langle \hat{a}^\dagger\hat{a}^\dagger\hat{a} \bullet \hat{a} \right\rangle = \frac{(e^{\beta\hbar\Omega}-1)}{\beta\hbar\Omega}\left\langle \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} \right\rangle = \frac{(e^{\beta\hbar\Omega}-1)}{\beta\hbar\Omega}\frac{2e^{-2\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{98c}$$

$$\left\langle \hat{a}^\dagger\hat{a}\hat{a}^\dagger \bullet \hat{a} \right\rangle = \frac{(e^{\beta\hbar\Omega}-1)}{\beta\hbar\Omega}\left\langle \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a} \right\rangle = \frac{(e^{\beta\hbar\Omega}-1)}{\beta\hbar\Omega}\frac{e^{-\beta\hbar\Omega}(1+e^{-\beta\hbar\Omega})}{(1-e^{-\beta\hbar\Omega})^2}, \tag{98d}$$

$$\left\langle \hat{a}\hat{a}^\dagger\hat{a}^\dagger \bullet \hat{a} \right\rangle = \frac{(e^{\beta\hbar\Omega}-1)}{\beta\hbar\Omega}\left\langle \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a} \right\rangle = \frac{(e^{\beta\hbar\Omega}-1)}{\beta\hbar\Omega}\frac{2e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{98e}$$

$$\left\langle \hat{a}\hat{a}\hat{a}^\dagger \bullet \hat{a}^\dagger \right\rangle = \frac{(1-e^{-\beta\hbar\Omega})}{\beta\hbar\Omega}\left\langle \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger \right\rangle = \frac{(1-e^{-\beta\hbar\Omega})}{\beta\hbar\Omega}\frac{2}{(1-e^{-\beta\hbar\Omega})^2}, \tag{98f}$$

$$\left\langle \hat{a}\hat{a}^\dagger\hat{a} \bullet \hat{a}^\dagger \right\rangle = \frac{(1-e^{-\beta\hbar\Omega})}{\beta\hbar\Omega}\left\langle \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger \right\rangle = \frac{(1-e^{-\beta\hbar\Omega})}{\beta\hbar\Omega}\frac{1+e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{98g}$$

$$\left\langle \hat{a}^\dagger\hat{a}\hat{a} \bullet \hat{a}^\dagger \right\rangle = \frac{(1-e^{-\beta\hbar\Omega})}{\beta\hbar\Omega}\left\langle \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger \right\rangle = \frac{(1-e^{-\beta\hbar\Omega})}{\beta\hbar\Omega}\frac{2e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}. \tag{98h}$$

1. $\hat{A} = \hat{B} = \hat{C} = \hat{q}$

Noticing that upon expansion in terms of raising and lowering operators [i.e. Eqs. (84) and (83)] $\langle \hat{q}(t_2)\hat{q}(t_1) \bullet \hat{q}(t_0)\rangle$ contains averages that do not involved the same number of raising and lowering operators (such as $\langle \hat{a}\hat{a} \bullet \hat{a}\rangle$, $\left\langle \hat{a}^\dagger\hat{a} \bullet \hat{a}\right\rangle$, $\left\langle \hat{a}\hat{a}^\dagger \bullet \hat{a}^\dagger\right\rangle$,...), it follows from Eq. (96) that

$$\langle \{\hat{q}(t_2)\overleftrightarrow{s}\hat{q}(t_1)\}\overleftrightarrow{c}\hat{q}(t_0)\rangle_N = 0. \tag{99}$$

2. $\hat{A} = \hat{q}^2, \hat{B} = \hat{C} = \hat{q}$

Using Eqs. (84) and (83) it is straightforward to check that

$$\begin{aligned}\Im\left\{\left\langle \hat{q}(t_2)\hat{q}(t_1) \bullet \hat{q}^2(t_0)\right\rangle\right\} = \left(\frac{\hbar}{2m\Omega}\right)^2 &\left\{\left[\left\langle \hat{a}^\dagger\hat{a}^\dagger \bullet \hat{a}\hat{a}\right\rangle - \left\langle \hat{a}\hat{a} \bullet \hat{a}^\dagger\hat{a}^\dagger\right\rangle\right]\sin\left(\Omega(t_2+t_1-2t_0)\right)\right. \\ &\left.+\left[\left\langle \hat{a}^\dagger\hat{a} \bullet \hat{a}^\dagger\hat{a}\right\rangle + \left\langle \hat{a}^\dagger\hat{a} \bullet \hat{a}\hat{a}^\dagger\right\rangle - \left\langle \hat{a}\hat{a}^\dagger \bullet \hat{a}^\dagger\hat{a}\right\rangle - \left\langle \hat{a}\hat{a}^\dagger \bullet \hat{a}\hat{a}^\dagger\right\rangle\right]\sin\left(\Omega(t_2-t_1)\right)\right\},\end{aligned} \tag{100}$$

where we have used the fact that averages involving not the same number of raising and lowering operators vanish.

Noticing that

$$\left\langle \hat{a}^\dagger\hat{a}^\dagger \bullet \hat{a}\hat{a}\right\rangle = \left\langle \hat{a}\hat{a} \bullet \hat{a}^\dagger\hat{a}^\dagger\right\rangle, \tag{101}$$

$$\left\langle \hat{a}^\dagger\hat{a}\bullet\hat{a}\hat{a}^\dagger\right\rangle = \left\langle \hat{a}\hat{a}^\dagger\bullet\hat{a}^\dagger\hat{a}\right\rangle, \tag{102}$$

and using Eqs. (98), it follows from Eq. (96) that

$$\begin{aligned}\left\langle\{\hat{q}(t_2)\overleftrightarrow{s}\hat{q}(t_1)\}\overleftrightarrow{c}\hat{q}^2(t_0)\right\rangle_N &= -\frac{\hbar}{2m^2\Omega^2}\left[\left\langle\hat{a}^\dagger\hat{a}\bullet\hat{a}^\dagger\hat{a}\right\rangle-\left\langle\hat{a}\hat{a}^\dagger\bullet\hat{a}\hat{a}^\dagger\right\rangle\right]\sin\left(\Omega(t_2-t_1)\right)\\ &= \frac{\hbar}{2m^2\Omega^2}\left[\frac{1+e^{-\beta\hbar\Omega}}{1-e^{-\beta\hbar\Omega}}\right]\sin\left(\Omega(t_2-t_1)\right)\\ &= \frac{\hbar}{2m^2\Omega^2}\coth(\frac{\beta\hbar\Omega}{2})\sin\left(\Omega(t_2-t_1)\right).\end{aligned} \tag{103}$$

3. $\hat{A}=\hat{B}=\hat{q}$, $\hat{C}=\hat{q}^2$

Using Eqs. (84) and (83) it is straightforward to check that

$$\begin{aligned}\Im\left\{\left\langle\hat{q}^2(t_2)\hat{q}(t_1)\bullet\hat{q}(t_0)\right\rangle\right\} &= -\frac{2}{\hbar}\left(\frac{\hbar}{2m\Omega}\right)^2\left\{\left[\left\langle\hat{a}^\dagger\hat{a}^\dagger\hat{a}\bullet\hat{a}\right\rangle-\left\langle\hat{a}\hat{a}\hat{a}^\dagger\bullet\hat{a}^\dagger\right\rangle\right]\sin\left(\Omega(2t_2-t_1-t_0)\right)\right.\\ &\left.+\left[\left\langle\hat{a}^\dagger\hat{a}\hat{a}^\dagger\bullet\hat{a}\right\rangle-\left\langle\hat{a}^\dagger\hat{a}\hat{a}\bullet\hat{a}^\dagger\right\rangle+\left\langle\hat{a}\hat{a}^\dagger\hat{a}^\dagger\bullet\hat{a}\right\rangle-\left\langle\hat{a}\hat{a}^\dagger\hat{a}\bullet\hat{a}^\dagger\right\rangle\right]\sin\left(\Omega(t_1-t_0)\right)\right\},\end{aligned} \tag{104}$$

where we have used the fact that averages involving not the same number of raising and lowering operators vanish.

Using Eqs. (98), it follows from Eq. (96) that

$$\begin{aligned}\left\langle\{\hat{q}^2(t_2)\overleftrightarrow{s}\hat{q}(t_1)\}\overleftrightarrow{c}\hat{q}(t_0)\right\rangle_N &= \frac{1}{\beta m^2\Omega^3}\left\{\sin\left(\Omega(2t_2-t_1-t_0)\right)-\sin\left(\Omega(t_1-t_0)\right)\right\}\\ &= \frac{2}{\beta m^2\Omega^3}\sin\left(\Omega(t_2-t_1)\right)\cos\left(\Omega(t_2-t_0)\right).\end{aligned} \tag{105}$$

C. DKT

To compute exact DKT correlation functions we will use the fact that[6, 8]

$$\begin{aligned}\left\langle\hat{C}(t_2)\overleftrightarrow{c}\hat{B}(t_1)\overleftrightarrow{c}\hat{A}(t_0)\right\rangle_N &= \left\langle\hat{C}(t_2)\bullet\hat{B}(t_1)\bullet\hat{A}(t_0)\right\rangle\\ &\equiv \frac{1}{\beta^2}\int_0^\beta d\lambda_0\int_0^\beta d\lambda_1\ \left\langle\hat{T}_\beta\hat{C}(t_2-i\hbar\lambda_0)\hat{B}(t_1-i\hbar\lambda_1)\hat{A}(t_0)\right\rangle\\ &= 2\Re\left\{\frac{1}{\beta^2}\int_0^\beta d\lambda_0\int_0^{\lambda_0} d\lambda_1\ \left\langle\hat{C}(t_2-i\hbar\lambda_0)\hat{B}(t_1-i\hbar\lambda_0)\hat{A}(t_0)\right\rangle\right\}\\ &= 2\Re\left\{\left\langle\hat{C}(t_2)\bullet\hat{B}(t_1)\bullet\hat{A}(t_0)\right\rangle^{ns}\right\},\end{aligned} \tag{106}$$

where in the last line we have defined the non-symmetric (ns superscript) DKT.

Additionally, explicitly computing the trace and using Eqs. (89) it is straightforward to show that

$$\left\langle \hat{a}^\dagger \bullet \hat{a}^\dagger \bullet \hat{a}\hat{a} \right\rangle^{ns} = \frac{(e^{\beta\hbar\Omega}-1)^2}{2(\beta\hbar\Omega)^2} \left\langle \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} \right\rangle = \frac{1}{(\beta\hbar\Omega)^2}, \tag{107a}$$

$$\left\langle \hat{a} \bullet \hat{a} \bullet \hat{a}^\dagger\hat{a}^\dagger \right\rangle^{ns} = \frac{(e^{-\beta\hbar\Omega}-1)^2}{2(\beta\hbar\Omega)^2} \left\langle \hat{a}\hat{a}\hat{a}^\dagger\hat{a}^\dagger \right\rangle = \frac{1}{(\beta\hbar\Omega)^2}, \tag{107b}$$

$$\left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a}^\dagger\hat{a} \right\rangle^{ns} = \frac{(e^{\beta\hbar\Omega}-1-\beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \left\langle \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a} \right\rangle = \frac{(e^{\beta\hbar\Omega}-1-\beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \frac{e^{-\beta\hbar\Omega}(1+e^{-\beta\hbar\Omega})}{(1-e^{-\beta\hbar\Omega})^2}, \tag{107c}$$

$$\left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a}\hat{a}^\dagger \right\rangle^{ns} = \frac{(e^{\beta\hbar\Omega}-1-\beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \left\langle \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger \right\rangle = \frac{(e^{\beta\hbar\Omega}-1-\beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \frac{2e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{107d}$$

$$\left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}^\dagger\hat{a} \right\rangle^{ns} = \frac{(e^{-\beta\hbar\Omega}-1+\beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \left\langle \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a} \right\rangle = \frac{(e^{-\beta\hbar\Omega}-1+\beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \frac{2e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}, \tag{107e}$$

$$\left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}\hat{a}^\dagger \right\rangle^{ns} = \frac{(e^{-\beta\hbar\Omega}-1+\beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \left\langle \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger \right\rangle = \frac{(e^{-\beta\hbar\Omega}-1+\beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \frac{1+e^{-\beta\hbar\Omega}}{(1-e^{-\beta\hbar\Omega})^2}. \tag{107f}$$

1. $\hat{A} = \hat{B} = \hat{C} = \hat{q}$

Noticing that upon expansion in terms of raising and lowering operators [i.e. Eqs. (84) and (83)] $\langle \hat{q}(t_2) \bullet \hat{q}(t_1) \bullet \hat{q}(t_0) \rangle$ contains averages that do not involve the same number of raising and lowering operators (such as $\langle \hat{a} \bullet \hat{a} \bullet \hat{a} \rangle$, $\left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a} \right\rangle$, $\left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}^\dagger \right\rangle$,...), it follows from Eq. (106) that

$$\langle \hat{q}(t_2) \overleftrightarrow{c} \hat{q}(t_1) \overleftrightarrow{c} \hat{q}(t_0) \rangle_N = 0. \tag{108}$$

2. $\hat{A} = \hat{q}^2, \hat{B} = \hat{C} = \hat{q}$

Using Eqs. (84) and (83) it is straightforward to check that

$$\begin{aligned} \Re\left\{ \left\langle \hat{q}(t_2) \bullet \hat{q}(t_1) \bullet \hat{q}^2(t_0) \right\rangle^{ns} \right\} &= \left(\frac{\hbar}{2m\Omega}\right)^2 \left\{ \left[\left\langle \hat{a}^\dagger \bullet \hat{a}^\dagger \bullet \hat{a}\hat{a} \right\rangle^{ns} + \left\langle \hat{a} \bullet \hat{a} \bullet \hat{a}^\dagger\hat{a}^\dagger \right\rangle^{ns} \right] \cos\left(\Omega(t_2+t_1-2t_0)\right) \right. \\ &\quad + \left[\left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a}^\dagger\hat{a} \right\rangle^{ns} + \left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a}\hat{a}^\dagger \right\rangle^{ns} + \left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}^\dagger\hat{a} \right\rangle^{ns} + \left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}\hat{a}^\dagger \right\rangle^{ns} \right] \\ &\quad \left. \times \cos\left(\Omega(t_2-t_1)\right) \right\}, \end{aligned} \tag{109}$$

where we have used the fact that averages involving not the same number of raising and lowering operators vanish.

Using Eqs. (107) it is straightforward to check that

$$\left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a}^\dagger \hat{a} \right\rangle^{ns} + \left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a}\hat{a}^\dagger \right\rangle^{ns} = \frac{(e^{\beta\hbar\Omega} - 1 - \beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \frac{(3e^{-\beta\hbar\Omega} + e^{-2\beta\hbar\Omega})}{(1 - e^{-\beta\hbar\Omega})^2}, \tag{110}$$

$$\left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}^\dagger \hat{a} \right\rangle^{ns} + \left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}\hat{a}^\dagger \right\rangle^{ns} = \frac{(e^{-\beta\hbar\Omega} - 1 + \beta\hbar\Omega)}{(\beta\hbar\Omega)^2} \frac{(1 + 3e^{-\beta\hbar\Omega})}{(1 - e^{-\beta\hbar\Omega})^2}, \tag{111}$$

and, therefore,

$$\begin{aligned} &\left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a}^\dagger \hat{a} \right\rangle^{ns} + \left\langle \hat{a}^\dagger \bullet \hat{a} \bullet \hat{a}\hat{a}^\dagger \right\rangle^{ns} + \left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}^\dagger \hat{a} \right\rangle^{ns} + \left\langle \hat{a} \bullet \hat{a}^\dagger \bullet \hat{a}\hat{a}^\dagger \right\rangle^{ns} \\ &\qquad = \frac{2}{(\beta\hbar\Omega)^2} + \frac{(1 - e^{-2\beta\hbar\Omega})}{(\beta\hbar\Omega)(1 - e^{-\beta\hbar\Omega})^2} \\ &\qquad = \frac{2}{(\beta\hbar\Omega)^2} + \frac{1}{\beta\hbar\Omega} \coth\left(\frac{\beta\hbar\Omega}{2}\right). \end{aligned} \tag{112}$$

Using Eq. (106), it follows that

$$\begin{aligned} \left\langle \hat{q}(t_2) \overleftrightarrow{c} \hat{q}(t_1) \overleftrightarrow{c} \hat{q}^2(t_0) \right\rangle_N &= 2 \left(\frac{\hbar}{2m\Omega}\right)^2 \left\{ \left(\frac{2}{(\beta\hbar\Omega)^2}\right) \cos\left(\Omega(t_2 + t_1 - 2t_0)\right) \right. \\ &\quad \left. + \left[\frac{2}{(\beta\hbar\Omega)^2} + \frac{1}{\beta\hbar\Omega} \coth\left(\frac{\beta\hbar\Omega}{2}\right)\right] \cos\left(\Omega(t_2 - t_1)\right) \right\} \\ &= \left(\frac{1}{\beta^2 m^2 \Omega^4}\right) \left(\cos\left(\Omega(t_2 + t_1 - 2t_0)\right) + \cos\left(\Omega(t_2 - t_1)\right)\right) \\ &\quad + \left(\frac{\hbar}{2\beta m^2 \Omega^3}\right) \coth\left(\frac{\beta\hbar\Omega}{2}\right) \cos\left(\Omega(t_2 - t_1)\right). \end{aligned} \tag{113}$$

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[1] T. J. H. Hele, M. J. Willatt, A. Muolo, and S. C. Althorpe, The Journal of Chemical Physics **142**, 134103 (2015), https://doi.org/10.1063/1.4916311.

[2] H. Goldstein, C. Poole, and J. Safko, *Classical Mechanics* (Addison Weslet, 2002).

[3] M. E. Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation* (Oxford University Press, 2010).

[4] K. A. Jung, P. E. Videla, and V. S. Batista, The Journal of Chemical Physics **153**, 124112 (2020), https://doi.org/10.1063/5.0021843.

[5] I. Gradshteyn and I. Ryzhik, *Table of Integrals, Series, and Products* (Elsevier Academic Press, 2007).

[6] P. E. Videla and V. S. Batista, J. Chem. Phys. , (in press) (2023).

[7] R. Kubo, Journal of the Physical Society of Japan **12**, 570 (1957).

[8] K. A. Jung, P. E. Videla, and V. S. Batista, The Journal of Chemical Physics **148**, 244105 (2018), https://doi.org/10.1063/1.5036768.