# Coherent State Path Integral Monte Carlo for Fermions

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We propose a new Quantum Simulation Method for a many Fermions liquid at finite (non-zero) temperature. The new scheme expands the high temperature density matrix on the overcomplete set of single particles coherent states of John Rider Klauder instead of plane waves as is usually done in conventional path integral methods. One is free to tune the elastic constant or the mass of the fiducial Harmonic Oscillator subtending the coherent states so as to maximize the computational efficiency of the numerical algorithm. We suggest that by choosing the oscillator extremely stiff could realize this maximization and thereby alleviate the Fermi sign problem of Feynman.

Keywords: Quantum Many-Body, Density Matrix, Coherent States, Fermions, Sign Problem, Monte Carlo

## I. INTRODUCTION

We describe a new algorithm able to simulate a quantum liquid at finite temperature through the cooperation of Coherent States (CS) [1–3] and the Path Integral Monte Carlo (PIMC) method [4]. The algorithm, that we will call Coherent States Path Integral Monte Carlo (CSPIMC), reconstructs the equilibrium hot thermal density matrix of a many body system of particles at each small imaginary time step thanks to the properties of the single particle coherent states that form an overcomplete set [1, 2]. The coherent state is a state of minimal uncertainty which is defined to be the (unique) eigenstate of the annihilation operator of a fiducial Harmonic Oscillator and as such it is described by a wave function whose probability distribution is a Gaussian. The information on the thermal density matrix after a sufficiently big number of sufficiently small time steps (so to reach the desired finite inverse temperature) is then reconstructed through the PIMC calculation.

We suggest that this way of simulating a Quantum Many Body (QMB) system of Fermions may overcome the infamous sign problem of Feynman [5, 6] which is still an open problem in statistical physics.

## II. THE ALGORITHM

Let us consider a many body system of $N$ Fermions with positions $Q = (\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_N)$ and momenta $P = (\boldsymbol{p}_1, \boldsymbol{p}_2, \ldots, \boldsymbol{p}_N)$ at thermal equilibrium at a finite temperature $T$.

The equilibrium statistical mechanic description of the many body Fermions requires the knowledge of the thermal density matrix operator $\hat{\rho} = \exp(-\beta \hat{H})$ where $\hat{H}$ is the Fermions Hamiltonian operator, $\beta = 1/k_B T$ is the "inverse temperature", and $k_B$ is the Boltzmann's constant.

The thermal density matrix satisfies to the Bloch equation

$$\frac{\partial \hat{\rho}}{\partial \beta} = -\hat{H}\hat{\rho}. \tag{2.1}$$

If we know the eigenstates and eigenvalues of the Hamiltonian, $|\Psi_i\rangle$ and $E_i$, we can use the completeness of this system of orthonormal states to write the position representation of the density matrix as follows

$$\rho(Q, Q'; \beta) = \langle Q|\hat{\rho}|Q'\rangle = \sum_i \langle Q|\Psi_i\rangle e^{-\beta E_i} \langle \Psi_i|Q'\rangle. \tag{2.2}$$

Otherwise, in the high temperature limit we can use the primitive approximation to the density matrix [4]

$$\rho(Q, Q'; \tau) = \langle Q|e^{-\tau \hat{H}}|Q'\rangle \approx \langle Q|e^{-\tau \hat{T}} e^{-\tau \hat{V}}|Q'\rangle, \tag{2.3}$$

where $\hat{H} = \hat{T} + \hat{V} = \hat{P}^2/2m + V(Q)$, $m$ is the particles mass, and $\hat{P} = -i(\nabla_{\boldsymbol{q}_1}, \nabla_{\boldsymbol{q}_2}, \ldots, \nabla_{\boldsymbol{q}_N})$, where here and in the following we choose $\hbar = 1$. In the last approximation we simply neglected the terms of order $\tau^2$ and higher in the Baker–Campbell–Hausdorff formula.

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Taking $\tau = \beta/M$ with $M$ a large integer we can then reconstruct the finite temperature density matrix using Trotter formula as follows

$$\rho(Q, Q'; \beta) = \int \rho(Q, Q_1; \tau) \cdots \rho(Q_{M-1}, Q'; \tau) \, dQ_1 \cdots dQ_{M-1}. \tag{2.4}$$

Since for the high temperature density matrix we can neglect the commutator of the kinetic part of the Hamiltonian and the potential energy so that $\hat{\rho} \approx e^{-\tau \hat{T}} e^{-\tau \hat{V}} = \prod_\alpha e^{-\tau \hat{T}_\alpha} e^{-\tau V}$, where $\hat{T}_\alpha$ is the kinetic energy of particle $\alpha$ and the exponential containing the potential is diagonal in position space and just a multiplicative factor. Then the many body state $|\Upsilon_a\rangle$ factorizes into a product of single particle states $\prod_\alpha |\psi_\alpha^a\rangle$

$$|\Upsilon_a\rangle = \prod_{\alpha=1}^{N} |\psi_\alpha^a\rangle, \tag{2.5}$$

where $a$ labels the set of many body states which inherit the overcompleteness of the single particles coherent states.

Antisymmetrizing so to satisfy Fermi statistics, we find

$$|\Upsilon_a\rangle\langle\Upsilon_a| = \sum_P (-)^P \prod_{\alpha,\beta=1}^{N} |\psi_\alpha^a\rangle\langle\psi_{P\beta}^a| = \det|| \, |\psi_\alpha^a\rangle\langle\psi_\beta^a| \, ||, \tag{2.6}$$

where $P$ is any of the $N!$ permutations of the $N$ particles.

Now we can take as the single particle states $|\psi_\alpha^a\rangle$ the coherent states [1–3]

$$|\psi_\alpha^a\rangle \equiv |\boldsymbol{q}_a, \boldsymbol{p}_a\rangle = e^{-i\boldsymbol{q}_a \cdot \hat{\boldsymbol{p}}_a} e^{i\boldsymbol{p}_a \cdot \hat{\boldsymbol{q}}_a} |0\rangle, \tag{2.7}$$

where $|0\rangle$ is the ground state of the fiducial three dimensional Harmonic Oscillator of elastic constant $k$ along all three components. The coordinate representation of this state is

$$\psi_\alpha^a(\boldsymbol{q}_\alpha) \equiv \langle Q|\boldsymbol{q}_a, \boldsymbol{p}_a\rangle = \left(\frac{m_{h.o.}\omega}{\pi}\right)^{3/4} e^{-\frac{m_{h.o.}\omega}{2}\left[\boldsymbol{q}_a - \sqrt{\frac{2}{m_{h.o.}\omega}}\mathrm{Re}(a_\alpha)\right]^2 + i\boldsymbol{q}\cdot\sqrt{2m_{h.o.}\omega}\mathrm{Im}(a_\alpha) - i2\mathrm{Re}(a_\alpha)\cdot\mathrm{Im}(a_\alpha)}, \tag{2.8}$$

$$a_\alpha = \frac{1}{\sqrt{2m_{h.o.}\omega}}(m_{h.o.}\omega\boldsymbol{q}_a + i\boldsymbol{p}_a), \tag{2.9}$$

where $\omega = \sqrt{k/m_{h.o.}}$ is the angular frequency of the Harmonic Oscillator of elastic constant $k$ and mass $m_{h.o.}$.

This is an alternative way to obtain the thermal density matrix at an inverse temperature $\beta$ which still requires the convolution integral (2.4), but with

$$\rho(Q, Q'; \tau) \approx e^{-K(Q,Q';\tau,m,k)} e^{-\tau V(Q')} \tag{2.10}$$

$$= e^{-\tau V(Q')} \sum_P (-)^P \prod_\alpha \zeta_\alpha\left[\boldsymbol{q}_{P\alpha}|\boldsymbol{q}_\alpha'; \tau, m, k, m_{h.o.}\right], \tag{2.11}$$

where $K$ is the kinetic part of the semiclassical action depending on the expansion of $|\Upsilon_a\rangle$ on the single particle coherent states of Eq. (2.6), $\zeta$ is defined in Eq. (A9) in Appendix A, $k$ is the elastic constant of the Harmonic Oscillator, and $m_{h.o.}$ is its mass.

So that in the $M \to \infty$ limit the Trotter formula (2.4) becomes a path integral made of the $M$ high temperature density matrices at each time step.

Note that if we choose an extremely stiff Harmonic Oscillator, one for which $k \to \infty$, or one with a big mass, $m_{h.o.} \to \infty$, then $m_{h.o.}\omega \to \infty$, and the Gaussian $|\psi_\alpha^i(\boldsymbol{q})|^2$ of Eq. (2.8) reduces to a Dirac $\delta$ centered on the position $\boldsymbol{q}$ only. We suggest that this may alleviate the Fermi sign problem [5, 6] of Feynman. In fact in that case Eq. (2.4) reduces to a path integral with no kinetic entanglement between the single electrons subject to Pauli exclusion principle. And *correlation* dominates over *exchange*.

As usual in order to measure an observable $\hat{\mathcal{O}}$ we need to calculate $\langle\hat{\mathcal{O}}\rangle = \mathrm{tr}(\hat{\rho}\hat{\mathcal{O}})/\mathrm{tr}(\hat{\rho})$. This requires to impose periodic boundary conditions on the imaginary time so that $\rho(Q, Q'; t) = \rho(Q, Q'; t + \beta)$.

Moreover in a simulation we want to mimic the thermodynamic limit as close as possible and this is usually obtained enforcing spatial periodic boundary conditions juxtaposing an infinite number of identical copies of the simulation box of volume $\Omega = L_1 L_2 L_3$ along the three dimensions. This can be easily obtained by taking for each particle $\boldsymbol{q}_\alpha + \boldsymbol{L} = \boldsymbol{q}_\alpha$, i.e a periodic box. Of course as $\Omega$ increases we will mimic the thermodynamic limit closer and closer. One usually refers to this feature of a computer experiment as the *finite size error*. This can be obtained with the expansion in coherent states by [7] .....................

## III. CONCLUSIONS

We propose a new Quantum Simulation Method for a many Fermions liquid. The method creates a bridge between conventional PIMC [4] and Coherent State Path Integral Monte Carlo (CSPIMC). The idea hinges upon expanding the high temperature density matrix on the overcomplete set of single particles coherent states of John Rider Klauder [1, 2]. As the angular frequency of the subtending Harmonic Oscillator (HO) varies from low values to very high values the coherent states probability distribution changes from Gaussian to Dirac delta like. We believe that going towards a more and more stiff fiducial HO the resulting extremely spiked coherent states could render the Quantum Monte Carlo (QMC) simulation less and less subject to the yet unsolved Fermi sign problem of Feynman.

We are interested in the ensemble thermal average $\langle \hat{\mathcal{O}} \rangle = \mathrm{tr}(\hat{\rho}\hat{\mathcal{O}})/\mathrm{tr}(\hat{\rho})$ of an observable $\mathcal{O}$ at a given finite inverse temperature $\beta$. Using the coordinate representation as in Eq. (2.4) we find the sought for path integral. In the limit of very high values of the angular frequency of the fiducial HO the $\zeta$ function of Eq. (C1) calculated at zero order in $\tau$ goes to zero. This could reduce the sign problem for Fermions since the kinetic coupling due to two exchanging Fermions is dumped and therefore each term in the alternating series in the path integral mainly feels the potential coupling. This means that *correlation* dominates over *exchange*. The loss in efficiency due to the Fermi-Dirac statistics could be reduced by tuning the fiducial HO so as to have a stiff one during the simulation (one for which $m_{h.o.}\omega = \sqrt{km_{h.o.}}$ is big). The stiffness can be obtained either choosing a high elastic constant $k$ or by choosing a high mass $m_{h.o.}$.

## Appendix A: Determination of $K$ in Eq. (2.10)

From Eq. (2.3) and inserting the resolution of the identity from Eq. (2.6) in terms of the complete set of coherent states two times we find [8]

$$\rho(Q, Q'; \tau) \approx \sum_{a,b} \langle Q | \det | | \psi_\alpha^a \rangle \langle \psi_\beta^a | | | e^{-\tau\hat{T}} \det | | \psi_\alpha^b \rangle \langle \psi_\beta^b | | | Q' \rangle e^{-\tau V(Q')}. \tag{A1}$$

Now the two antisymmetrizations are redundant and one can safely keep just one of the two. Moreover the only left antisymmetrization can be transferred from the quantum numbers labeling the coherent single particle states to their positions. We then find

$$\rho(Q, Q'; \tau) \approx \sum_P (-)^P \sum_{a,b} \prod_{\alpha,\beta} \langle \boldsymbol{q}_{P1}, \ldots, \boldsymbol{q}_{PN} | \psi_\alpha^a \rangle \langle \psi_\beta^a | e^{-\tau\hat{T}_\alpha} | \psi_\alpha^b \rangle \langle \psi_\beta^b | Q' \rangle e^{-\tau V(Q')}$$

$$= \sum_P (-)^P \sum_{a,b} \prod_\alpha \langle \boldsymbol{q}_{P1}, \ldots, \boldsymbol{q}_{PN} | \psi_\alpha^a \rangle \langle \psi_\alpha^a | e^{-\tau\hat{T}_\alpha} | \psi_\alpha^b \rangle \langle \psi_\alpha^b | Q' \rangle e^{-\tau V(Q')}, \tag{A2}$$

$$\tag{A3}$$

where we decided to keep the antisymmetrization only on the left positions and in the last equality we used the following orthogonality condition among single particle coherent states

$$\langle \psi_\beta^a | \psi_\alpha^b \rangle = G_{a_\alpha, b_\beta} \delta_{\alpha,\beta}, \tag{A4}$$

where $\delta$ is a Kronecker delta symbols and

$$G_{a_\alpha, b_\alpha} = e^{-\frac{1}{2}(|a_\alpha|^2 + |b_\alpha|^2) + a_\alpha^* \cdot b_\alpha}, \tag{A5}$$

$$a_\alpha = \frac{1}{\sqrt{2m_{h.o.}\omega}}(m_{h.o.}\omega \boldsymbol{q}_a + i\boldsymbol{p}_a), \tag{A6}$$

$$b_\alpha = \frac{1}{\sqrt{2m_{h.o.}\omega}}(m_{h.o.}\omega \boldsymbol{q}_b + i\boldsymbol{p}_b), \tag{A7}$$

where $\omega = \sqrt{k/m_{h.o.}}$ is the angular frequency of the Harmonic Oscillator of elastic constant $k$ and mass $m_{h.o.}$.

where remember that $|0\rangle$ stands for the ground state of the Harmonic Oscillator of elastic constant $k$. This is calculated in Appendix B.

We then find from Eq. (2.10)

$$e^{-K(Q, Q'; \tau, m, k)} = \sum_P (-)^P \prod_\alpha \sum_{a,b} \langle \boldsymbol{q}_{P1}, \ldots, \boldsymbol{q}_{PN} | \psi_\alpha^a \rangle \langle \psi_\alpha^a | e^{-\tau\hat{\boldsymbol{p}}_\alpha^2/2m} | \psi_\alpha^b \rangle \langle \psi_\alpha^b | \boldsymbol{q}_1', \ldots, \boldsymbol{q}_N' \rangle \tag{A8}$$

$$\equiv \sum_P (-)^P \prod_\alpha \zeta_\alpha \Big[ \boldsymbol{q}_{P\alpha} | \boldsymbol{q}_\alpha'; \tau, m, k, m_{h.o.} \Big], \tag{A9}$$

where $\langle Q|\psi_\alpha^a\rangle = \langle Q|\boldsymbol{q}_a, \boldsymbol{p}_a\rangle$ is the position representation of the single particle coherent states. The function $\zeta$ is defined in Eq. (A9) and determined in Appendix C.

## Appendix B: Calculation of the element of Eq. (A8)

We want here calculate explicitly the matrix element of Eq. (A8). We then find

$$\langle \psi_\alpha^a | e^{-\tau \hat{T}_\alpha} | \psi_\alpha^b \rangle =$$

$$\langle 0 | e^{-i\boldsymbol{p}_a \cdot \hat{\boldsymbol{q}}_\alpha} e^{i\boldsymbol{q}_a \cdot \hat{\boldsymbol{p}}_\alpha} e^{-\tau \hat{\boldsymbol{p}}_\alpha^2/2m} e^{-i\boldsymbol{q}_b \cdot \hat{\boldsymbol{p}}_\alpha} e^{i\boldsymbol{p}_b \cdot \hat{\boldsymbol{q}}_\alpha} | 0 \rangle = \tag{B1}$$

$$\langle 0 | e^{-i\boldsymbol{p}_a \cdot \hat{\boldsymbol{q}}_\alpha} e^{i\boldsymbol{q}_a \cdot \hat{\boldsymbol{p}}_\alpha} e^{-i\boldsymbol{q}_b \cdot \hat{\boldsymbol{p}}_\alpha} e^{i\boldsymbol{p}_b \cdot \hat{\boldsymbol{q}}_\alpha} e^{-\tau [\hat{\boldsymbol{p}}_\alpha + \boldsymbol{p}_b]^2/2m} | 0 \rangle = \tag{B2}$$

$$\langle 0 | e^{-i\boldsymbol{p}_a \cdot \hat{\boldsymbol{q}}_\alpha} e^{i\boldsymbol{q}_a \cdot \hat{\boldsymbol{p}}_\alpha} e^{-i\boldsymbol{q}_b \cdot \hat{\boldsymbol{p}}_\alpha} e^{i\boldsymbol{p}_b \cdot \hat{\boldsymbol{q}}_\alpha} e^{-\tau [\hat{\boldsymbol{p}}_\alpha^2 + 2\hat{\boldsymbol{p}}_\alpha \cdot \boldsymbol{p}_b + \boldsymbol{p}_b^2]/2m} | 0 \rangle = \tag{B3}$$

$$\sum_{n=0} \langle 0 | e^{-i\boldsymbol{p}_a \cdot \hat{\boldsymbol{q}}_\alpha} e^{i\boldsymbol{q}_a \cdot \hat{\boldsymbol{p}}_\alpha} e^{-i\boldsymbol{q}_b \cdot \hat{\boldsymbol{p}}_\alpha} e^{i\boldsymbol{p}_b \cdot \hat{\boldsymbol{q}}_\alpha} | n \rangle \langle n | 1 - \tau [\hat{\boldsymbol{p}}_\alpha^2 + 2\hat{\boldsymbol{p}}_\alpha \cdot \boldsymbol{p}_b + \boldsymbol{p}_b^2]/2m | 0 \rangle + o(\tau) = \tag{B4}$$

$$\left[ 1 - \tau \left( \frac{\boldsymbol{p}_b^2}{2m} + \frac{\omega}{4} \right) \right] G_{a_\alpha, b_\alpha} + \tau \sqrt{2} \frac{\omega}{4} \langle 0 | e^{-i\boldsymbol{p}_a \cdot \hat{\boldsymbol{q}}_\alpha} e^{i\boldsymbol{q}_a \cdot \hat{\boldsymbol{p}}_\alpha} e^{-i\boldsymbol{q}_b \cdot \hat{\boldsymbol{p}}_\alpha} e^{i\boldsymbol{p}_b \cdot \hat{\boldsymbol{q}}_\alpha} | 2 \rangle + o(\tau). \tag{B5}$$

where in the second equality we used Hadamard lemma

$$e^{-ip\hat{q}} e^{iq\hat{p}} f(\hat{q}, \hat{p}) e^{-iq\hat{p}} e^{ip\hat{q}} = f(\hat{q} + q, \hat{p} + p), \tag{B6}$$

valid for any function $f(\hat{q}, \hat{p})$. In the fourth equality we used the fact that $\tau$ is small and the completeness of the eigenstates $|n\rangle$ of the Harmonic Oscillator of angular frequency $\omega = \sqrt{k/m_{h.o.}}$, elastic constant $k$, and mass $m_{h.o.}$. In the last equality we used the orthogonality condition of Eq. (A5) for the coherent states.

The last term of Eq. (B5) can be calculated expanding on the Fock states

$$\langle 0 | e^{-i\boldsymbol{p}_a \cdot \hat{\boldsymbol{q}}_\alpha} e^{i\boldsymbol{q}_a \cdot \hat{\boldsymbol{p}}_\alpha} e^{-i\boldsymbol{q}_b \cdot \hat{\boldsymbol{p}}_\alpha} e^{i\boldsymbol{p}_b \cdot \hat{\boldsymbol{q}}_\alpha} | 2 \rangle =$$

$$e^{\frac{i}{2}(\boldsymbol{q}_a \cdot \boldsymbol{p}_a - \boldsymbol{q}_b \cdot \boldsymbol{p}_b) - \frac{1}{2}(|a_\alpha|^2 + |b_\alpha|^2)} \times$$

$$\sum_{n,m=0} \frac{(a_\alpha^*)^n}{\sqrt{n!}} \frac{b_\alpha^m}{\sqrt{m!}} (\langle n|m+2 \rangle - \langle n|m+1 \rangle \sqrt{2} b_\alpha + \langle n|m \rangle \sqrt{2} b_\alpha^2/2) = \tag{B7}$$

$$e^{\frac{i}{2}(\boldsymbol{q}_a \cdot \boldsymbol{p}_a - \boldsymbol{q}_b \cdot \boldsymbol{p}_b) - \frac{1}{2}(|a_\alpha|^2 + |b_\alpha|^2)} \times$$

$$\sum_{n,m=0} \frac{(a_\alpha^*)^n}{\sqrt{n!}} \frac{b_\alpha^m}{\sqrt{m!}} \left( \delta_{n,m+2} \sqrt{\frac{(m+1)(m+2)}{2}} - \delta_{n,m+1} \sqrt{2(m+1)} b_\alpha^* + \delta_{n,m} \frac{1}{\sqrt{2}} b_\alpha^{*2} \right) = \tag{B8}$$

$$e^{\frac{i}{2}(\boldsymbol{q}_a \cdot \boldsymbol{p}_a - \boldsymbol{q}_b \cdot \boldsymbol{p}_b) - \frac{1}{2}(|a_\alpha|^2 + |b_\alpha|^2) + a_\alpha^* \cdot b_\alpha} \frac{(a_\alpha^* - b_\alpha^*)^2}{\sqrt{2}} = \tag{B9}$$

$$e^{\frac{i}{2}(\boldsymbol{q}_a \cdot \boldsymbol{p}_a - \boldsymbol{q}_b \cdot \boldsymbol{p}_b)} \frac{(a_\alpha^* - b_\alpha^*)^2}{\sqrt{2}} G_{a_\alpha, b_\alpha}, \tag{B10}$$

where in the second equality we used the orthonormality of the Hermite polynomials $\langle n|m \rangle = \delta_{n,m}$ and in the last equality we used the definition of $G_{a,b}$ of Eq. (A5).

So putting all this together we finally find

$$\langle \psi_\alpha^a | e^{-\tau \hat{T}_\alpha} | \psi_\alpha^b \rangle = \left\{ 1 - \tau \left[ \frac{\boldsymbol{p}_b^2}{2m} + \frac{3\omega}{4} \left( 1 + e^{\frac{i}{2}(\boldsymbol{q}_a \cdot \boldsymbol{p}_a - \boldsymbol{q}_b \cdot \boldsymbol{p}_b)} (a_\alpha^* - b_\alpha^*)^2 \right) \right] \right\} G_{a_\alpha, b_\alpha} + o(\tau). \tag{B11}$$

## Appendix C: Determination of $\zeta$

We have from the definition in Eq. (A9)

$$\zeta_\alpha\left[\boldsymbol{q}|\boldsymbol{q}';\tau,m,k,m_{h.o.}\right] \equiv \sum_{a,b}\langle\boldsymbol{q}|\psi_\alpha^a\rangle\langle\psi_\alpha^a|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^b\rangle\langle\psi_\alpha^b|\boldsymbol{q}'\rangle \tag{C1}$$

$$= \int \frac{d\boldsymbol{q}_a\,d\boldsymbol{p}_a}{(2\pi)^3}\frac{d\boldsymbol{q}_b\,d\boldsymbol{p}_b}{(2\pi)^3}\psi_\alpha^a(\boldsymbol{q})\psi_\alpha^{b\,*}(\boldsymbol{q}')\langle\psi_\alpha^a|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^b\rangle \tag{C2}$$

$$= \sum_{n=0}\tau^n\zeta_\alpha^{(n)}\left[\boldsymbol{q}|\boldsymbol{q}';m,k,m_{h.o.}\right]. \tag{C3}$$

where $\psi_\alpha^a(\boldsymbol{q})$ is the coordinate representation of the single $\alpha$ particle coherent state of Eq. (2.8) and the propagator $\langle\psi_\alpha^a|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^b\rangle$ has been determined in Eq. (B11) of Appendix B.

We immediately see that to order zero in $\tau$ we find for $\zeta_\alpha^{(0)}$,

$$\zeta_\alpha^{(0)}\left[\boldsymbol{q}|\boldsymbol{q}';m,k,m_{h.o.}\right] =$$
$$\int \frac{d\boldsymbol{q}_a\,d\boldsymbol{p}_a}{(2\pi)^3}\frac{d\boldsymbol{q}_b\,d\boldsymbol{p}_b}{(2\pi)^3}\psi_\alpha^a(\boldsymbol{q})\psi_\alpha^{b\,*}(\boldsymbol{q}')G_{a_\alpha,b_\alpha} =$$
$$\left(\frac{1}{\pi^2}\sqrt{\frac{m_{h.o.}\omega}{13\pi}}\right)^3 e^{-\frac{m_{h.o.}\omega}{26}(33\boldsymbol{q}^2-64\boldsymbol{q}\cdot\boldsymbol{q}'+33\boldsymbol{q}'^2)}. \tag{C4}$$

To first order in $\tau$ we find for $\zeta_\alpha^{(1)}$,

$$\zeta_\alpha^{(1)}\left[\boldsymbol{q}|\boldsymbol{q}';m,k,m_{h.o.}\right] =$$
$$-\int \frac{d\boldsymbol{q}_a\,d\boldsymbol{p}_a}{(2\pi)^3}\frac{d\boldsymbol{q}_b\,d\boldsymbol{p}_b}{(2\pi)^3}\psi_\alpha^a(\boldsymbol{q})\psi_\alpha^{b\,*}(\boldsymbol{q}')G_{a_\alpha,b_\alpha}\left[\frac{\boldsymbol{p}_b^2}{2m}+\frac{3\omega}{4}\left(1+e^{\frac{i}{2}(\boldsymbol{q}_a\cdot\boldsymbol{p}_a-\boldsymbol{q}_b\cdot\boldsymbol{p}_b)}(a_\alpha^*-b_\alpha^*)^2\right)\right].$$

In the high $m_{h.o.}$ limit at fixed $k$ we have $\omega\to0$ and one finds

$$\zeta_\alpha^{(1)}\left[\boldsymbol{q}|\boldsymbol{q}';m,k,m_{h.o.}\right] \to$$
$$-\int \frac{d\boldsymbol{q}_a\,dp_a}{(2\pi)^3}\frac{d\boldsymbol{q}_b\,d\boldsymbol{p}_b}{(2\pi)^3}\psi_\alpha^a(\boldsymbol{q})\psi_\alpha^{b\,*}(\boldsymbol{q}')G_{a_\alpha,b_\alpha}\frac{\boldsymbol{p}_b^2}{2m} =$$
$$\frac{m_{h.o.}\omega}{m}\left(\frac{1}{(13\pi)^2}\sqrt{\frac{m_{h.o.}\omega}{13\pi}}\right)^3 e^{-\frac{m_{h.o.}\omega}{26}(33\boldsymbol{q}^2-64\boldsymbol{q}\cdot\boldsymbol{q}'+33\boldsymbol{q}'^2)}[-1053+m_{h.o.}\omega(800\boldsymbol{q}^2-1520\boldsymbol{q}\cdot\boldsymbol{q}'+722\boldsymbol{q}'^2)]. \tag{C5}$$

To a first approximation for the high temperature density matrix we will neglect higher orders in $\tau$.

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[7] Given any function $f(x)$ it can always be made periodic of period $L$ by choosing $f_L(x) = \sum_{n=-\infty}^{\infty} f(x + nL)$.
[8] Here

$$\sum_{a,b} \cdots \to \int \cdots \frac{d\boldsymbol{q}_a \, d\boldsymbol{p}_a}{(2\pi)^3} \frac{d\boldsymbol{q}_b \, d\boldsymbol{p}_b}{(2\pi)^3}. \tag{C6}$$

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