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 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 allow the use of larger timesteps.

I. INTRODUCTION

We describe a new algorithm able to simulate a quantum liquid at finite temperature through the cooperation of Coherent States (CS) [1–6] and the Path Integral Monte Carlo (PIMC) method [7]. 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 [1–6]. The coherent state is a state of minimal uncertainty which is defined to be the (unique) eigenstate of the annihilation operator of a Harmonic Oscillator (HO) 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 imaginary time steps τ, so to reach the desired finite inverse temperature β, is then reconstructed into a path integral through the PIMC calculation. As usual we take $\beta = 1/k_B T = M\tau$ with k_B Boltzmann's constant, T the absolute temperature, and M the number of time steps discretizations between 0 and β.

We suggest that this way of simulating a Quantum Many Body (QMB) system of Fermions may allow to choose larger timesteps τ which will make the Monte Carlo algorithm more efficient. This will not solve the sign problem of Feynman [8, 9] which is still an open problem in statistical physics. In particular we see, as is clearly shown in Appendix C, that choosing the HO mass big enough allows to work at larger timesteps.

Our novel Quantum Monte Carlo (QMC) algorithm adds to the rich variety of similar methods for a finite temperature numerical experiment starting from the conventional simulations of D. M. Ceperley [7], passing to the *worm-algorithm* of M. Boninsegni [10], to end to the *pair-product approximation* used by E. W. Brown [11]. All these Monte Carlo methods hinge on the Metropolis algorithm [12, 13].

If, from one side, we do not need to specify further the *primitive approximation* [7] for the potential energy action, on the other side, we will make a rather brute force approximation for the kinetic action that hinges on the peculiar properties of coherent states. We will worry about the mathematical rigor of the primitive approximation proposed here or about its refinements [7] in future works. This could be important also to further reduce the computational efficiency of the simulation.

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 mechanics 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

$$\frac{\partial\hat{\rho}}{\partial\beta} = -\hat{H}\hat{\rho}. \tag{1}$$

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

$$\rho(Q, Q'; \beta) = \langle Q|\hat{\rho}|Q'\rangle = \sum_i \langle Q|\Psi_i\rangle e^{-\beta E_i}\langle\Psi_i|Q'\rangle. \tag{2}$$

Otherwise, in the high temperature limit we can neglect terms of orders higher than one in the small τ in the Baker–Campbell–Hausdorff formula to find [7]

$$\rho(Q,Q';\tau) = \langle Q|e^{-\tau\hat{H}}|Q'\rangle \approx \langle Q|e^{-\tau\hat{T}}e^{-\tau\hat{V}}|Q'\rangle, \tag{3}$$

where $\hat{H} = \hat{T} + \hat{V} = \hat{P}^2/2m + V(Q)$, m is the particles mass, and $\hat{P} = -i(\nabla_{\boldsymbol{q}_1}, \nabla_{\boldsymbol{q}_2}, \ldots, \nabla_{\boldsymbol{q}_N})$; here and in the following we choose $\hbar = 1$.

Taking $\tau = \beta/M$ with M a large integer we can then reconstruct the finite temperature density matrix using Trotter formula in the following successive 'convolutions' [7, 14] as usual

$$\rho(Q,Q';\beta) = \int \rho(Q,Q_1;\tau)\cdots\rho(Q_{M-1},Q';\tau)\,dQ_1\cdots dQ_{M-1}. \tag{4}$$

Since $\hat{\rho} \approx e^{-\tau\hat{T}}e^{-\tau\hat{V}} = \prod_\alpha e^{-\tau\hat{T}_\alpha}e^{-\tau V}$, where $\hat{T}_\alpha$ is the kinetic energy of particle α 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 $\prod_\alpha |\psi^a_\alpha\rangle$

$$|\Upsilon_a\rangle = \prod_{\alpha=1}^{N} |\psi^a_\alpha\rangle, \tag{5}$$

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

Antisymmetrizing so to satisfy Fermi statistics, we find

$$|\Upsilon_a\rangle\langle\Upsilon_a| = \frac{1}{N!}\sum_{\mathcal{P}}(-)^{\mathcal{P}}\prod_{\alpha,\beta=1}^{N}|\psi^a_\alpha\rangle\langle\psi^a_{\mathcal{P}\beta}| = \frac{1}{N!}\det||\,|\psi^a_\alpha\rangle\langle\psi^a_\beta|\,||, \tag{6}$$

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

Now we can take as the single particle states $|\psi^a_\alpha\rangle$ the coherent states [1–6]

$$|\psi^a_\alpha\rangle \equiv |\boldsymbol{q}_a,\boldsymbol{p}_a\rangle = e^{-i\boldsymbol{q}_a\cdot\hat{\boldsymbol{p}}_\alpha}e^{i\boldsymbol{p}_a\cdot\hat{\boldsymbol{q}}_\alpha}|0\rangle, \tag{7}$$

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

$$\psi^{\boldsymbol{a}}(\boldsymbol{q}_\alpha) \equiv \langle Q|\boldsymbol{q}_a,\boldsymbol{p}_a\rangle = \Big(\frac{m_{h.o.}\omega}{\pi}\Big)^{3/4} e^{-\frac{m_{h.o.}\omega}{2}\left[\boldsymbol{q}_\alpha - \sqrt{\frac{2}{m_{h.o.}\omega}}\mathrm{Re}(\boldsymbol{a})\right]^2 + i\boldsymbol{q}_\alpha\cdot\sqrt{2m_{h.o.}\omega}\mathrm{Im}(\boldsymbol{a}) - i2\mathrm{Re}(\boldsymbol{a})\cdot\mathrm{Im}(\boldsymbol{a})}, \tag{8}$$

$$\boldsymbol{a} = \frac{1}{\sqrt{2m_{h.o.}\omega}}(m_{h.o.}\omega\boldsymbol{q}_a + i\boldsymbol{p}_a), \tag{9}$$

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 way we obtain the thermal density matrix at a finite inverse temperature β through the multiple-'convolution' integral (4), but with

$$\rho(Q,Q';\tau) \approx e^{-K(Q,Q';\tau,m,k,m_{h.o.})}e^{-\tau V(Q')} \tag{10}$$

$$= e^{-\tau V(Q')}\frac{1}{N!}\sum_{\mathcal{P}}(-)^{\mathcal{P}}\prod_\alpha \zeta_\alpha\Big[\boldsymbol{q}_{\mathcal{P}\alpha}|\boldsymbol{q}'_\alpha;\tau,m,k,m_{h.o.}\Big], \tag{11}$$

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. (6), ζ is defined in Eq. (A8) in Appendix A and its *primitive* approximation is determined in Eqs. (C3), of Appendix C, 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 (4) becomes a path integral made of the M high temperature density matrices at each time step [14].

Note that if we choose an extremely stiff Harmonic Oscillator, i.e. one such that $m_{h.o.}\omega \to \infty$, then the Gaussian $|\psi^a_\alpha(\boldsymbol{q})|^2$ of Eq. (8) reduces to a Dirac δ centered on the position $\boldsymbol{q}$ only. We suggest that this may allow the use of larger timesteps in Eq. (4) that reduces to the path integral. And this will increase the efficiency of the MC algorithm.

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 Ω 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 taking the following infinite sum [15] at the end

$$\zeta_\alpha \to \zeta_\alpha^L = \sum_{i,j=-\infty}^{\infty} \zeta_\alpha \Big[\boldsymbol{q} + iL | \boldsymbol{q}' + jL; \tau, m, k, m_{h.o.} \Big], \tag{12}$$

where we assumed $L_1 = L_2 = L_3 = L$ for simplicity.

III. CONCLUSIONS

We propose a new Quantum Simulation Method for a many Fermions liquid. The method creates a bridge between Coherent States (CS) [1–6] and conventional Path Integral Monte Carlo (PIMC) [7] merged together into a Coherent State Path Integral Monte Carlo (CSPIMC) method. The idea hinges upon expanding the high temperature density matrix on the overcomplete set of single particles coherent states of John Rider Klauder [1–6]. As the *stiffness* 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 HO the resulting extremely spiked coherent states could render the Quantum Monte Carlo (QMC) simulation more and more efficient since one is allowed to work with larger timesteps.

We are often 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 β. Using the coordinate representation for the density matrix $\hat{\rho}$, as in Eq. (4), we find the sought for path integral expression. A key ingredient is the high temperature density matrix at a small inverse temperature τ. This is made up of two pieces: a kinetic energy operator and a potential energy factor. We find the explicit analytic primitive approximation form of the kinetic operator. Being this a product of single particles kinetic energy operators it is possible to expand it in the overcomplete set of single particles Klauder coherent states. The result is summarized into the ζ function of Eqs. (C3). In particular we see from that equation that is necessary to introduce some 'ghost variables' along the path integral that will become

$$\rho(Q, Q'; \beta) = \frac{1}{N!} \sum_{\mathcal{P}} (-)^{\mathcal{P}} \int_{\substack{Q(0) \to \mathcal{P}Q(\beta) \\ Q_a(0) \to Q_b(\beta) \\ P_a(0) \to P_b(\beta)}} e^{-\int_0^\beta \frac{P_a(t)^2}{2m} + V[Q(t)]\, dt} \prod_{t=0}^{\beta} \prod_{\alpha=1}^{N} \psi_\alpha^a(\boldsymbol{q}') \psi_\alpha^{b\,*}(\boldsymbol{q}) G_{a,b} \, \frac{\mathcal{D}Q_a \mathcal{D}P_a}{(2\pi)^{3N}} \, \mathcal{D}Q, \tag{13}$$

where $Q_a = (\boldsymbol{q}_{a1}, \ldots, \boldsymbol{q}_{aN})$ and $P_a = (\boldsymbol{p}_{a1}, \ldots, \boldsymbol{p}_{aN})$, $Q_b = (\boldsymbol{q}_{b1}, \ldots, \boldsymbol{q}_{b1})$ and $P_b = (\boldsymbol{p}_{b1}, \ldots, \boldsymbol{p}_{bN})$ are 'ghost variables', $G_{a,b}$ is the normalization factor of two coherent states as defined in Eq. (A4), and $\psi_\alpha^a(\boldsymbol{q})$ is the coherent state as defined in Eq. (8). Notice that the antisymmetrization is only necessary on the real variable.

Our calculation shows that for a very stiff HO the high temperature kinetic energy density matrix tend to become extremely peaked. We suggest that this could allow an improvement in the efficiency of the QMC algorithm where one can use larger timesteps.

I would like to thank prof. John Rider Klauder for transmitting me the passion for coherent states and all the 'family' of the Physics Department in Gainesville at the University of Florida which invited me to participate at the Memorial Conference held on 15 February 2025 in honor of the professor path in life and science. The professor passed away on 24 October 2024 at 92 years of age.

Appendix A: Determination of K in Eq. (10)

From Eq. (3) and inserting the resolution of the identity from Eq. (6) in terms of the complete set of coherent states two times we find [16]

$$\rho(Q, Q'; \tau) \approx \frac{1}{N!^2} \sum_{\boldsymbol{a},\boldsymbol{b}} \langle Q | \det || \, |\psi_\alpha^{\boldsymbol{a}}\rangle\langle\psi_\beta^{\boldsymbol{a}}| \, || e^{-\tau \hat{T}} \det || \, |\psi_\alpha^{\boldsymbol{b}}\rangle\langle\psi_\beta^{\boldsymbol{b}}| \, || \, |Q'\rangle e^{-\tau V(Q')}. \tag{A1}$$

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

$$\begin{aligned}\rho(Q,Q';\tau) &\approx \frac{1}{N!}\sum_{\mathcal{P}}(-)^{\mathcal{P}}\sum_{\boldsymbol{a},\boldsymbol{b}}\prod_{\alpha,\beta}\langle \boldsymbol{q}_{\mathcal{P}1},\ldots,\boldsymbol{q}_{\mathcal{P}N}|\psi_\alpha^{\boldsymbol{a}}\rangle\langle\psi_\beta^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle\langle\psi_\beta^{\boldsymbol{b}}|Q'\rangle e^{-\tau V(Q')} \\ &= \frac{1}{N!}\sum_{\mathcal{P}}(-)^{\mathcal{P}}\sum_{\boldsymbol{a},\boldsymbol{b}}\prod_{\alpha}\langle \boldsymbol{q}_{\mathcal{P}1},\ldots,\boldsymbol{q}_{\mathcal{P}N}|\psi_\alpha^{\boldsymbol{a}}\rangle\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle\langle\psi_\alpha^{\boldsymbol{b}}|Q'\rangle e^{-\tau V(Q')}, \qquad \text{(A2)}\end{aligned}$$

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

$$\langle\psi_\beta^{\boldsymbol{a}}|\psi_\alpha^{\boldsymbol{b}}\rangle = G_{\boldsymbol{a},\boldsymbol{b}}\delta_{\alpha,\beta}, \qquad \text{(A3)}$$

where δ is a Kronecker delta symbols and

$$\begin{aligned}G_{\boldsymbol{a},\boldsymbol{b}} &= e^{-\frac{1}{2}(|\boldsymbol{a}|^2+|\boldsymbol{b}|^2)+\boldsymbol{a}^*\cdot\boldsymbol{b}+\frac{i}{2}(\boldsymbol{q}_a\cdot\boldsymbol{p}_a-\boldsymbol{q}_b\cdot\boldsymbol{p}_b)}, \qquad \text{(A4)} \\ \boldsymbol{a} &= \frac{1}{\sqrt{2m_{h.o.}\omega}}(m_{h.o.}\omega\boldsymbol{q}_a+i\boldsymbol{p}_a), \qquad \text{(A5)} \\ \boldsymbol{b} &= \frac{1}{\sqrt{2m_{h.o.}\omega}}(m_{h.o.}\omega\boldsymbol{q}_b+i\boldsymbol{p}_b), \qquad \text{(A6)}\end{aligned}$$

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

We then find from Eq. (10)

$$\begin{aligned}e^{-K(Q,Q';\tau,m,k)} &= \frac{1}{N!}\sum_{\mathcal{P}}(-)^{\mathcal{P}}\prod_{\alpha}\sum_{\boldsymbol{a},\boldsymbol{b}}\langle \boldsymbol{q}_{\mathcal{P}1},\ldots,\boldsymbol{q}_{\mathcal{P}N}|\psi_\alpha^{\boldsymbol{a}}\rangle\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{\boldsymbol{p}}_\alpha^2/2m}|\psi_\alpha^{\boldsymbol{b}}\rangle\langle\psi_\alpha^{\boldsymbol{b}}|\boldsymbol{q}'_1,\ldots,\boldsymbol{q}'_N\rangle \qquad \text{(A7)} \\ &\equiv \frac{1}{N!}\sum_{\mathcal{P}}(-)^{\mathcal{P}}\prod_{\alpha}\zeta_\alpha\Big[\boldsymbol{q}_{\mathcal{P}\alpha}|\boldsymbol{q}'_\alpha;\tau,m,k,m_{h.o.}\Big], \qquad \text{(A8)}\end{aligned}$$

where $\langle Q|\psi^{\boldsymbol{a}}\rangle = \langle Q|\boldsymbol{q}_a,\boldsymbol{p}_a\rangle$ is the position representation of the single particle coherent state. The element $\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle$ is founs in Appendix B. The function ζ is defined in Eq. (A8) and determined in Appendix C.

Appendix B: Calculation of the element of Eq. (A7)

We want here calculate explicitly the matrix element of Eq. (A7). We can then think that we find

$$\begin{aligned}\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle &\approx \langle\psi_\alpha^{\boldsymbol{a}}|\psi_\alpha^{\boldsymbol{b}}\rangle e^{-\tau\boldsymbol{p}_b^2/2m} \qquad \text{(B1)} \\ &= G_{\boldsymbol{a},\boldsymbol{b}}e^{-\tau\boldsymbol{p}_b^2/2m}, \qquad \text{(B2)}\end{aligned}$$

where in the second equality we used the exact normalization factor of Eq. (A4). The approximation in Eq. (B1) is rather suggestive and extremely handy. We can think that it may be 'washed away' for small τ. In any case this is a rather subtle issue that still asks for mathematical rigor. We need to think that this high temperature matrix element should be able to reconstruct the finite temperature density matrix as an exact path integral [17].

Appendix C: Determination of ζ

We have from the definition in Eq. (A8)

$$\begin{aligned}&\zeta_\alpha\Big[\boldsymbol{q}|\boldsymbol{q}';\tau,m,k,m_{h.o.}\Big] \\ &\equiv \sum_{\boldsymbol{a},\boldsymbol{b}}\langle\boldsymbol{q}|\psi_\alpha^{\boldsymbol{a}}\rangle\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle\langle\psi_\alpha^{\boldsymbol{b}}|\boldsymbol{q}'\rangle \qquad \text{(C1)} \\ &= \int\frac{d\boldsymbol{q}_a\,d\boldsymbol{p}_a}{(2\pi)^3}\frac{d\boldsymbol{q}_b\,d\boldsymbol{p}_b}{(2\pi)^3}\psi_\alpha^{\boldsymbol{a}}(\boldsymbol{q})\psi_\alpha^{\boldsymbol{b}\,*}(\boldsymbol{q}')\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle \qquad \text{(C2)} \\ &\approx \int\frac{d\boldsymbol{q}_a\,d\boldsymbol{p}_a}{(2\pi)^3}\frac{d\boldsymbol{q}_b\,d\boldsymbol{p}_b}{(2\pi)^3}\psi_\alpha^{\boldsymbol{a}}(\boldsymbol{q})\psi_\alpha^{\boldsymbol{b}\,*}(\boldsymbol{q}')G_{\boldsymbol{a},\boldsymbol{b}}e^{-\tau\boldsymbol{p}_b^2/2m}, \qquad \text{(C3)}\end{aligned}$$

where $\psi_\alpha^{\boldsymbol{a}}(\boldsymbol{q})$ is the coordinate representation of the single α particle coherent state of Eq. (8) and the propagator $\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle$ has been approximated in Eq. (B2) of Appendix B. Eq. (C3) can be integrated with a simple Monte Carlo scheme (see Fig. 1) and this will give us a primitive approximation for ζ. These additional integrations over $(\boldsymbol{q}_a, \boldsymbol{p}_a)$ and $(\boldsymbol{q}_b, \boldsymbol{p}_b)$ must be carried out at each timestep but Monte Carlo will not suffer critically since it is able to treat highly multidimensional integrals. We will then reach a path integral both on the particles positions and on *ghost variables* at two next time steps. The ghost variables are the canonical pair of labels from the continuous representation of Klauder. As it should be, in the $\tau \to 0$ limit, also within the approximation (B1) we will have,

$$\zeta_\alpha\Big[\boldsymbol{q}|\boldsymbol{q}';\tau,m,k,m_{h.o.}\Big] \xrightarrow{\tau\to 0} \langle\boldsymbol{q}|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q}-\boldsymbol{q}'), \tag{C4}$$

where δ is a Dirac delta function. The $\tau \to 0$ limit washes away the $k, m_{h.o.}$ dependence. On the other hand choosing a stiff harmonic oscillator, i.e. one with an high mass, the ζ function width diminishes, as is shown in Fig. 1. This will allow to choose bigger timesteps in the path integral, thereby reducing the computational cost.

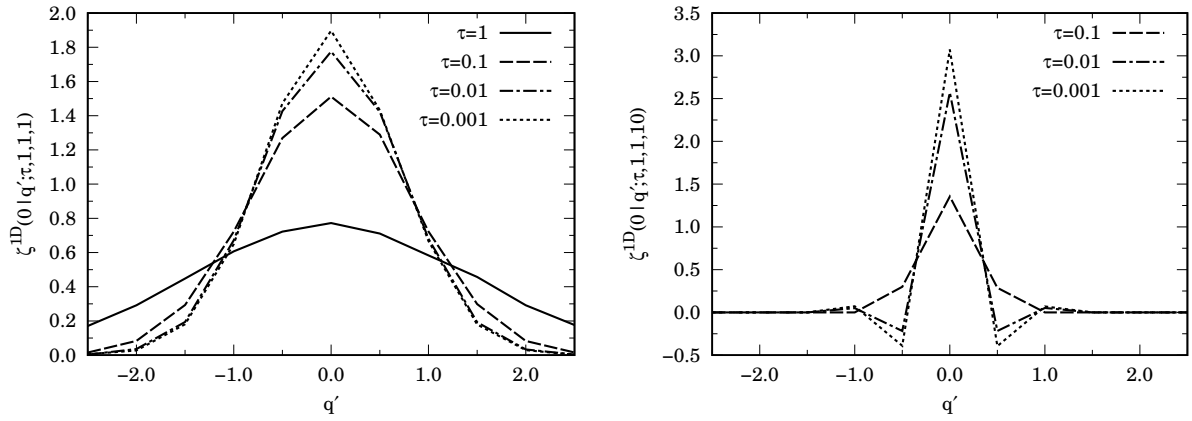

FIG. 1. We show the one dimensional $\zeta^{1D}(q|q';\tau,m,k,m_{h.o.})$ calculated with a Monte Carlo scheme using 10^7 (with the related statistical error) sampling points and choosing smaller and smaller timestep τ. All the four integrations over the ghost variables (q_a, p_a) and (q_b, p_b) were chosen in the interval $[-10, 10]$ (with the related finite size error). On the left $m_{h.o.} = 1$ on the right $m_{h.o.} = 10$.

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

$$\sum_{\boldsymbol{a},\boldsymbol{b}} \ldots \to \int \ldots \frac{d\boldsymbol{q}_a\, d\boldsymbol{p}_a}{(2\pi)^3} \frac{d\boldsymbol{q}_b\, d\boldsymbol{p}_b}{(2\pi)^3}. \tag{C5}$$

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