Coherent State Path Integral Monte Carlo for Fermions

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(Dated: February 17, 2025)

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 we choose $\hbar = 1$. In the last approximation we simply neglected the terms of τ^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 α and the exponential containing the potential is diagonal in position space and just a multiplicative factor. Then the many body state $|\Psi_i\rangle$ factorizes into a product of single particle states $\prod_\alpha |\psi^i_\alpha\rangle$

$$|\Psi_a\rangle = \prod_{\alpha=1}^{N} |\psi^a_\alpha\rangle. \tag{2.5}$$

Antisymmetrizing so to satisfy Fermi statistics, we find

$$|\Psi_a\rangle\langle\Psi_a| = \sum_P (-)^P \prod_{\alpha,\beta=1}^{N} |\psi^a_\alpha\rangle\langle\psi^a_{P\beta}| = \det||\,|\psi^a_\alpha\rangle\langle\psi^a_\beta|\,||, \tag{2.6}$$

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

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

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

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

$$\psi^a_\alpha(\boldsymbol{q}_\alpha) \equiv \langle Q|\psi^a_\alpha\rangle \equiv \langle Q|\boldsymbol{q}_a,\boldsymbol{p}_a\rangle = \left(\frac{m_{h.o.}\omega}{\pi}\right)^{1/4} e^{-\frac{m_{h.o.}\omega}{2}\left[\boldsymbol{q}_\alpha - \sqrt{\frac{2}{m_{h.o.}\omega}}\mathrm{Re}(a_\alpha)\right]^2 + i\boldsymbol{q}\cdot\sqrt{2m_{h.o.}\omega}\mathrm{Im}(a_\alpha) - i\frac{3}{2}\mathrm{Re}(a_\alpha)\cdot\mathrm{Im}(a_\alpha)}, \tag{2.8}$$

where $\omega = \sqrt{k/m_{h.o.}}$ is the angular frequency of the Harmonic Oscillator of elastic constant k and mass $m_{h.o.}$ and i_α is given by Eq. (A6).

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

$$\rho(Q,Q';\tau) \approx e^{-K(Q,Q';\tau,m,k)}e^{-\tau V(Q')} \tag{2.9}$$

$$= e^{-\tau V(Q')}\sum_P (-)^P \prod_\alpha \zeta_\alpha\Big[\boldsymbol{q}_{P\alpha}|\boldsymbol{q}'_\alpha;\tau,m,k,m_{h.o.}\Big], \tag{2.10}$$

where K is the kinetic part of the semiclassical action depending on the expansion of $|\Psi_i\rangle$ on the single particle coherent states of Eq. (2.6), ζ is defined in Eq. (A9) in Appendix A, k is the elastic constant of the Harmonic Oscillator, and $m_{h.o.}$ 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, so that $k \to \infty$, or one with a big mass, $m_{h.o.} \to \infty$, then $\omega \to \infty$, then the Gaussian $\psi^i_\alpha(\boldsymbol{q})$ of Eq. (2.8) reduces to a Dirac δ centered on the position $\boldsymbol{q}_\alpha$ only. We think that this may solve the Fermi sign problem [5, 6] of Feynman. In fact in that case Eq. (2.4) reduces to a product formula with no spatial entanglement between the single electrons subject to Pauli exclusion principle. And we do not need Monte Carlo anymore.

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 $\Psi_i(Q,t) = \langle Q|\Psi_i\rangle = \Psi_i(Q,t+\beta)$.

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 $\Omega = L_1L_2L_3$ 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*.

For the *ground state* calculation, when $\beta \to \infty$, if L_i/L_j is irrational for $i \neq j$ then the ergodic hypothesis will become exact.

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.

In the limit of very high values of the angular frequency of the fiducial HO the ensemble thermal average $\langle\hat{\mathcal{O}}\rangle = \mathrm{tr}(\hat{\rho}\hat{\mathcal{O}})/\mathrm{tr}(\hat{\rho})$ reduces to .....

Appendix A: Determination of K in Eq. (2.9)

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 [7]

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

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

$$\begin{aligned}\rho(Q,Q';\tau) &\approx \sum_P(-)^P\sum_{a,b}\prod_{\alpha,\beta}\langle\boldsymbol{q}_{P1},\ldots,\boldsymbol{q}_{PN}|\psi^a_\alpha\rangle\langle\psi^a_\beta|e^{-\tau\hat{T}_\alpha}|\psi^b_\alpha\rangle\langle\psi^b_\beta|Q'\rangle e^{-\tau V(Q')}\\ &= \sum_P(-)^P\sum_{a,b}\prod_{\alpha}\langle\boldsymbol{q}_{P1},\ldots,\boldsymbol{q}_{PN}|\psi^a_\alpha\rangle\langle\psi^a_\alpha|e^{-\tau\hat{T}_\alpha}|\psi^b_\alpha\rangle\langle\psi^b_\alpha|Q'\rangle e^{-\tau V(Q')}, \qquad (A2)\\ & \qquad (A3)\end{aligned}$$

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

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

where δ is a Kronecker delta symbols and

$$\begin{aligned}G_{a_\alpha,b_\alpha} &= e^{-\frac{1}{2}(|a_\alpha|^2+|b_\alpha|^2)+a^*_\alpha\cdot b_\alpha}, &(A5)\\ a_\alpha &= \frac{1}{\sqrt{2m_{h.o.}\omega}}(m_{h.o.}\omega\boldsymbol{q}_a + i\boldsymbol{p}_a), &(A6)\\ b_\alpha &= \frac{1}{\sqrt{2m_{h.o.}\omega}}(m_{h.o.}\omega\boldsymbol{q}_b + i\boldsymbol{p}_b), &(A7)\end{aligned}$$

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. (2.9)

$$\begin{aligned}e^{-K(Q,Q';\tau,m,k)} &= \sum_P(-)^P\prod_\alpha\sum_{a,b}\langle\boldsymbol{q}_{P1},\ldots,\boldsymbol{q}_{PN}|\psi^a_\alpha\rangle\langle\psi^a_\alpha|e^{-\tau\hat{\boldsymbol{p}}^2_\alpha/2m}|\psi^b_\alpha\rangle\langle\psi^b_\alpha|\boldsymbol{q}'_1,\ldots,\boldsymbol{q}'_N\rangle &(A8)\\ &\equiv \sum_P(-)^P\prod_\alpha\zeta_\alpha\Big[\boldsymbol{q}_{P\alpha}|\boldsymbol{q}'_\alpha;\tau,m,k,m_{h.o.}\Big], &(A9)\end{aligned}$$

where $\langle Q|\psi^a_\alpha\rangle = \langle Q|\boldsymbol{q}_a,\boldsymbol{p}_a\rangle$ is the position representation of the single particle coherent states. The function ζ 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 τ 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).

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

$$\langle 0|e^{-i\boldsymbol{p}_a\cdot\hat{\boldsymbol{q}}_\alpha}e^{i\boldsymbol{q}_a\cdot\hat{\boldsymbol{p}}_\alpha}e^{-i\boldsymbol{q}_b\cdot\hat{\boldsymbol{p}}_\alpha}e^{i\boldsymbol{p}_b\cdot\hat{\boldsymbol{q}}_\alpha}|2\rangle = \tag{B7}$$

$$e^{i\boldsymbol{q}_a\cdot\boldsymbol{p}_a/4}e^{-|a_\alpha|^2/2}e^{-i\boldsymbol{q}_b\cdot\boldsymbol{p}_b/4}e^{-|b_\alpha|^2/2}\sum_{n,m=0}\frac{(a_\alpha^*)^n}{\sqrt{n!}}\frac{b_\alpha^m}{\sqrt{m!}}(\langle n|m+2\rangle-\langle n|m+1\rangle\sqrt{2}b_\alpha+\langle n|m\rangle\sqrt{2}b_\alpha^2/2) = \tag{B8}$$

$$e^{i\boldsymbol{q}_a\cdot\boldsymbol{p}_a/4}e^{-|a_\alpha|^2/2}e^{-i\boldsymbol{q}_b\cdot\boldsymbol{p}_b/4}e^{-|b_\alpha|^2/2}\sum_{n,m=0}\frac{(a_\alpha^*)^n}{\sqrt{n!}}\frac{b_\alpha^m}{\sqrt{m!}}(\delta_{n,m+2}-\delta_{n,m+1}\sqrt{2}b_\alpha+\delta_{n,m}\sqrt{2}b_\alpha^2/2) \tag{B9}$$

where we used the orthonormality of the Hermite polynomials $\langle n|m\rangle=\delta_{n,m}$.

Appendix C: Determination of ζ

We have from the definition in Eq. (A9)

$$\zeta_\alpha\Big[\boldsymbol{q}|\boldsymbol{q}';\tau,m,k,m_{h.o.}\Big]\equiv\sum_{a,b}\langle\boldsymbol{q}|\psi_\alpha^a\rangle\langle\psi_\alpha^a|e^{-\tau\hat{\boldsymbol{p}}_\alpha^2/2m}|\psi_\alpha^b\rangle\langle\psi_\alpha^b|\boldsymbol{q}'\rangle. \tag{C1}$$

ACKNOWLEDGMENTS

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$$\sum_{a,b} \dots \to \int \dots \frac{d\boldsymbol{q}_a \, d\boldsymbol{p}_a}{2\pi} \frac{d\boldsymbol{q}_b \, d\boldsymbol{p}_b}{2\pi}. \tag{C2}$$

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