Quantum Molecular Dynamics for Fermions

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(Dated: February 12, 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 path integral methods. The coherent states evolve in imaginary time according to classical Hamilton dynamics. One is free to tune the elastic constant 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, Molecular Dynamics, Fermions, Sign Problem

I. INTRODUCTION

We describe a new algorithm able to simulate a quantum liquid at finite temperature through the cooperation of a Molecular Dynamics (MD) scheme and the Path Integral Monte Carlo (PIMC) method. The algorithm reconstructs the equilibrium thermal density matrix of a many body system of particles at each imaginary time step thanks to the properties of the single particle coherent states. These are particular states of the Hilbert space which evolve in imaginary time through a classical dynamics. 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 oscillating with fixed variance around the classical path of the particle as the particle moves in imaginary time according to the classical Hamilton's equations of motion with an Hamiltonian that is the classical counterpart of the quantum Hamiltonian. The MD scheme evolves the positions and momenta of each particle; these positions and momenta combine to determine the center around which the single particle coherent state oscillates. The coherent states of each particle combine their zig-zag dynamics to give rise to Gaussians with constant variance which connect the averaged positions of each particle at successive time steps as it moves along the classical paths determined by the MD simulation. The MD evolves the positions and momenta of the particles exactly as one would do in a conventional classical MD simulation. 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 with the paths wandering in their *zig-zag* motion.

We suggest that this way of simulating a quantum many body system of Fermions may overcome the infamous sign problem of Feynman which is still an open problems 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

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

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Otherwise, in the high temperature limit we can use the primitive approximation to the density matrix [1]

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

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

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 eigenstate $|\Psi_i\rangle$ factorizes into a product of single particle states $\prod_\alpha |\psi_\alpha\rangle$

$$|\Psi_i\rangle = \prod_{\alpha=1}^{N} |\psi_\alpha\rangle. \tag{2.5}$$

Antisymmetrizing so to satisfy Fermi statistics, we find

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

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

Now we can take as the single particle states $|\psi^i_\alpha\rangle$ the coherent states [2]

$$|\boldsymbol{q}_\alpha(t), \boldsymbol{p}_\alpha(t)\rangle = e^{-i\boldsymbol{q}_\alpha(t)\cdot\hat{\boldsymbol{p}}_\alpha} e^{i\boldsymbol{p}_\alpha(t)\cdot\hat{\boldsymbol{q}}_\alpha}|0\rangle, \tag{2.7}$$

where $|0\rangle$ is the ground state of the Harmonic Oscillator. These states evolve in imaginary time $0 \le t < \beta$ according to classical mechanics

$$|\boldsymbol{q}_\alpha(t+\tau), \boldsymbol{p}_\alpha(t+\tau)\rangle = |\boldsymbol{q}_\alpha(t) + \tau\nabla_{\boldsymbol{p}_\alpha}H, \boldsymbol{p}_\alpha(t) - \tau\nabla_{\boldsymbol{q}_\alpha}H\rangle, \tag{2.8}$$

where H is the classical Hamiltonian ($H = \lim_{\hbar\to 0}\hat{H}$).

We then can perform a Molecular Dynamics (MD) simulation on the single particles coherent states and reconstruct the thermal density matrix after $M\tau$ steps of the classical evolution in imaginary time, using Eqs. (2.3) and (2.4).

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

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

$$= e^{-\tau V(Q')}\sum_P (-)^P \prod_\alpha \zeta\Big[\langle\hat{\boldsymbol{q}}_\alpha(t)\rangle - \langle\hat{\boldsymbol{q}}'_{P\alpha}(t+\tau)\rangle;\tau,m,k\Big], \tag{2.10}$$

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 a Gaussian, $\langle\hat{\boldsymbol{q}}_\alpha(t)\rangle$ is the expectation value of the particle position at time t, and k is the elastic constant of the Harmonic Oscillator. These functions are made explicit in Appendix A.

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, following the evolution of the coherent states oscillating along their classical single particle paths. As shown by Eq. (2.9) this zig-zag dynamics gives rise to Gaussians with constant variance which connect the averaged positions of each particle at successive time steps as it move in phase space as is determined by the MD simulation [3].

Note that if we choose an extremely stiff Harmonic Oscillator, so that $k\to\infty$ and $\omega\to\infty$, then the Gaussian ζ reduces to a Dirac δ of the difference between the only positions (see Eq. (A9) in such limit) of the particle at two successive time steps. We think that this may solve the Fermi sign problem [4, 5] 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 $\Psi_i(Q,t) = \langle Q|\Psi_i\rangle = \Psi_i(Q,t+\beta)$. This can easily be obtained since Hamilton's equations of motion are second order ordinary differential equations that require fixing $\boldsymbol{q}_\alpha(0)$ and choosing $\boldsymbol{q}_\alpha(\beta) = \boldsymbol{q}_\alpha(0)$ so that the particle dynamics will have periodicity β in imaginary time.

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 dynamics of each particle will be quasi-periodic and its trajectory will explore Ω *ergodically*.

III. CONCLUSIONS

We propose a new Quantum Simulation Method for a many Fermions liquid. The method creates a bridge between a purely Quantum Molecular Dynamic (QMD) Simulation and a purely Path Integral Monte Carlo (PIMC) simulation. The idea hinges upon expanding the high temperature density matrix on the overcomplete set of single particles coherent states of John Rider Klauder. As the elastic constant of the subtending Harmonic Oscillator (HO) varies from very high values to very low values the simulation scheme changes from mainly QMD like to mainly PIMC like. We believe that going towards a more and more stiff fiducial HO the resulting extremely QMD like simulation could suffer less and less from the yet unsolved Fermi sign problem of Feynman that plagues Quantum Monte Carlo (QMC).

Note that thanks to the ergodic hypothesis we can usually substitute the ensemble thermal average $\langle\hat{\mathcal{O}}\rangle = \mathrm{tr}(\hat{\rho}\hat{\mathcal{O}})/\mathrm{tr}(\hat{\rho})$ with a time average $\langle\mathcal{O}\rangle = \lim_{\tau\to\infty}\int_0^\tau \mathcal{O}(Q(t),P(t))\,dt$. In the classical $\beta \to 0$ limit, this reduces to the well known equivalence between a MC strategy using for the density matrix the Boltzmann limit of the Fermi antisymmetrized expression, and a MD strategy where $Q(t), P(t)$ follow the corresponding Hamilton's classical dynamics. The QMD we propose in this work is an *extension* of this *equivalence* to the *quantum domain*.

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

$$\rho(Q,Q';\tau) \approx \sum_{i,j}\langle Q|\det||\,|\psi^i_\alpha\rangle\langle\psi^i_\beta|\,||e^{-\tau\hat{T}}\det||\,|\psi^j_\alpha\rangle\langle\psi^j_\beta|\,||\,|Q'\rangle e^{-\tau V(Q')}. \tag{A1}$$

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

$$\begin{aligned}\rho(Q,Q';\tau) &\approx \sum_P(-)^P\sum_{i,j}\prod_{\alpha,\beta}\langle\boldsymbol{q}_{P1},\ldots,\boldsymbol{q}_{PN}|\psi^i_\alpha\rangle\langle\psi^i_\beta|e^{-\tau\hat{T}_\alpha}|\psi^j_\alpha\rangle\langle\psi^j_\beta|Q'\rangle e^{-\tau V(Q')}\\ &= \sum_P(-)^P\sum_{i}\prod_{\alpha}\langle\boldsymbol{q}_{P1},\ldots,\boldsymbol{q}_{PN}|\psi^i_\alpha\rangle\langle\psi^i_\alpha|e^{-\tau\hat{T}_\alpha}|\psi^i_\alpha\rangle\langle\psi^i_\alpha|Q'\rangle e^{-\tau V(Q')}.\end{aligned} \tag{A2}$$

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

$$\langle\psi^i_\beta|\psi^j_\alpha\rangle = \delta_{i,j}\delta_{\alpha,\beta}, \tag{A3}$$

where these are Kronecker delta symbols.

Now using the property of coherent states that for any given function of phase space $f(\hat{q},\hat{p})$

$$e^{-ip\hat{q}}e^{ip\hat{p}}f(\hat{q},\hat{p})e^{-iq\hat{p}}e^{ip\hat{q}} = f(\hat{q}+q,\hat{p}+p), \tag{A4}$$

which immediately follows from Hadamard lemma, we readily find

$$\langle\psi^i_\alpha|e^{-\tau\hat{T}_\alpha}|\psi^i_\alpha\rangle = \langle 0|e^{-\tau[\hat{\boldsymbol{p}}_\alpha+\boldsymbol{p}_\alpha(t+\tau)]^2/2m}|0\rangle, \tag{A5}$$

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)

$$e^{-K(Q,Q';\tau,m,k)} = \sum_P (-)^P \sum_i \prod_\alpha \langle \boldsymbol{q}_{P1},\ldots,\boldsymbol{q}_{PN}|\psi_\alpha^i\rangle\langle 0|e^{-\tau[\hat{\boldsymbol{p}}_\alpha+\boldsymbol{p}_\alpha(t+\tau)]^2/2m}|0\rangle\langle\psi_\alpha^i|\boldsymbol{q}'_1,\ldots,\boldsymbol{q}'_N\rangle \tag{A6}$$

$$= \sum_P (-)^P \prod_\alpha \zeta\Big[\langle\hat{\boldsymbol{q}}_\alpha(t)\rangle - \langle\hat{\boldsymbol{q}}'_{P\alpha}(t+\tau)\rangle;\tau,m,k\Big], \tag{A7}$$

where

$$\prod_\alpha \langle Q|\psi_\alpha^i\rangle = \langle \boldsymbol{q}_1|\boldsymbol{q}_1(t),\boldsymbol{p}_1(t)\rangle\cdots\langle\boldsymbol{q}_N|\boldsymbol{q}_N(t),\boldsymbol{p}_N(t)\rangle, \tag{A8}$$

is the position representation of the N-particle product state of the single particle coherent states. Each one of these single particle coherent states is a Gaussian centered around the expectation value of the position of the particle. The convolution (subtended by the $\sum_i$) of two of those states each centered around the expectation value of the position of the same particle at different time steps gives rise to the Gaussian ζ of variance $\sigma^2 = 2\hbar/m\omega$, where the expectation value of the particle position is given by

$$\langle\hat{\boldsymbol{q}}(t)\rangle = \mathrm{Re}\left\{e^{i\omega t}\left[\boldsymbol{q}(t) + i\frac{\boldsymbol{p}(t)}{m\omega}\right]\right\}, \tag{A9}$$

where $\omega = \sqrt{k/m}$ is the angular frequency of the Harmonic Oscillator of elastic constant k.

Appendix B: Calculation of the element of Eq. (A5)

We want here calculate explicitly the matrix element of Eq. (A5). We then find

$$\begin{aligned}
\langle 0|e^{-\tau[\hat{\boldsymbol{p}}+\boldsymbol{p}_0]^2/2m}|0\rangle &= \langle 0|e^{-\tau[\hat{\boldsymbol{p}}^2+2\hat{\boldsymbol{p}}\cdot\boldsymbol{p}_0+\boldsymbol{p}_0^2]/2m}|0\rangle \\
&= e^{-\tau\boldsymbol{p}_0^2/2m}\langle 0|e^{-\tau\hat{p}^2/2m}e^{-\tau\hat{\boldsymbol{p}}\cdot\boldsymbol{p}_0/m}|0\rangle \\
&= e^{-\tau\boldsymbol{p}_0^2/2m}\sum_{n=0}\langle 0|e^{-\tau\hat{p}^2/2m}|n\rangle\langle n|e^{-\tau\hat{\boldsymbol{p}}\cdot\boldsymbol{p}_0/m}|0\rangle \\
&= \left(1-\frac{\tau}{2m}\boldsymbol{p}_0^2\right)\left[1-\frac{\tau}{2m}\left(\langle 0|\hat{\boldsymbol{p}}^2|0\rangle + 2\langle 0|\hat{\boldsymbol{p}}\cdot\boldsymbol{p}_0|0\rangle\right)\right] + o(\tau) \\
&= 1-\tau\left(\frac{\boldsymbol{p}_0^2}{2m}+\frac{\hbar\omega}{4}\right)+o(\tau).
\end{aligned} \tag{B1}$$

where $\omega = \sqrt{k/m}$ is the angular frequency of the Harmonic Oscillator of elastic constant k and in the last two steps we used the fact that τ is small.

ACKNOWLEDGMENTS

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