Coherent State Path Integral Monte Carlo for Fermions

Riccardo Fantoni*
Università di Trieste, Dipartimento di Fisica, strada Costiera 11, 34151 Grignano (Trieste), Italy
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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, Quantum Monte Carlo; Density Matrix, Coherent States, Path Integral; Fermions, Sign Problem

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 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 overcome the infamous sign problem of Feynman [5, 6] which is still an open problem in statistical physics. In particular we see that choosing the product of the HO mass and its angular frequency big we will increase the importance of *correlation* effects over the *exchange* effects in the numerical experiment.

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 [4], passing to the *worm-algorithm* of M. Boninsegni [7], to end to the *pair-product approximation* used by E. W. Brown [8]. All these Monte Carlo methods hinge on the Metropolis algorithm [9, 10].

If, from one side, we do not need to specify further the *primitive approximation* [4] for the potential energy action 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 refinements of the primitive approximation [4] in future works. This could be important mainly to reduce the computational cost of the simulation.

As is clearly shown in Appendix C it is convenient to work with a stiff HO, i.e. one for which the angular frequency is small but the product of its mass and its angular frequency is big. In this limit in fact the kinetic hot density matrix tends to become small. So that the effect of the *correlation* will dominate over the effect due to the *exchange*.

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.

* riccardo.fantoni@scuola.istruzione.it

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 neglect terms of order higher than one in the small τ in the Baker–Campbell–Hausdorff formula to find [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 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 state $|\Upsilon_a\rangle$ factorizes into a product of single particle states $\prod_\alpha |\psi^a_\alpha\rangle$

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

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

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

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]

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

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

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

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

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 β which still requires the convolution integral (2.4), but with

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

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

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), ζ is defined in Eq. (A9) in Appendix A and its *primitive* approximation is determined in Eq. (C3) of Appendic 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 (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, i.e. one with a big mass, $m_{h.o.} \to \infty$, so that $\omega \to 0$ and $m_{h.o.}\omega \to \infty$, then the Gaussian $|\psi^a_\alpha(\boldsymbol{q})|^2$ of Eq. (2.8) reduces to a Dirac δ 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 $\Omega = L_1L_2L_3$ 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*. This can be obtained with the expansion in coherent states by taking the following infinite sum [11] at the end

$$\zeta_\alpha \to \zeta^L_\alpha = \sum_{i,j=-\infty}^{\infty} \zeta_\alpha\Big[\boldsymbol{q} + iL|\boldsymbol{q}' + jL; \tau, m, k, m_{h.o.}\Big], \tag{2.12}$$

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, 2] and conventional Path Integral Monte Carlo (PIMC) [4] 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, 2]. 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 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 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. (2.4), 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 factors: a kinetic energy factor and a potential energy factor. We find the explicit analytic form (up to order one in τ) of the kinetic factor. Being this a product of single particles kinetic energy factors 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 Eq. (C2).

Our calculation shows that for a very stiff HO the high temperature kinetic energy factor tend to become exponentially small. We suggest that 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 energy 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, i.e. one for which $m_{h.o.}$ is big so that ω is small and $m_{h.o.}\omega = \sqrt{km_{h.o.}}$ is big.

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 [12]

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

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

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

$$\qquad \text{(A3)}$$

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

$$\langle\psi_\beta^{\boldsymbol{a}}|\psi_\alpha^{\boldsymbol{b}}\rangle = G_{\boldsymbol{a},\boldsymbol{b}}\delta_{\alpha,\beta}, \qquad \text{(A4)}$$

where δ is a Kronecker delta symbols and

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

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. (2.10)

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

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 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

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

where in the second equality we used the normalization factor of Eq. (A5). We can think that the inherent approximation used holds for small τ.

Appendix C: Determination of ζ

We have from the definition in Eq. (A9)

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

$$= \int \frac{d\boldsymbol{q}_a\,d\boldsymbol{p}_a}{(2\pi)^3}\frac{d\boldsymbol{q}_b\,d\boldsymbol{p}_b}{(2\pi)^3}\psi_\alpha^{\boldsymbol{a}}(\boldsymbol{q})\psi_\alpha^{\boldsymbol{b}\,*}(\boldsymbol{q}')\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle \tag{C1}$$

$$\approx \left(4\sqrt{\frac{m_{h.o.}\omega}{5\pi}}\right)^3 e^{-\frac{m_{h.o.}\omega}{10}(33\boldsymbol{q}^2-64\boldsymbol{q}\cdot\boldsymbol{q}'+33\boldsymbol{q}'^2)}e^{-\tau\boldsymbol{p}'^2/2m} \tag{C2}$$

$$\approx \left(4\sqrt{\frac{m_{h.o.}\omega}{5\pi}}\right)^3 e^{-\frac{m_{h.o.}\omega}{10}(33\boldsymbol{q}^2-64\boldsymbol{q}\cdot\boldsymbol{q}'+33\boldsymbol{q}'^2)}e^{-m(\boldsymbol{q}'-\boldsymbol{q})^2/2\tau}, \tag{C3}$$

where $\psi_\alpha^{\boldsymbol{a}}(\boldsymbol{q})$ is the coordinate representation of the single α particle coherent state of Eq. (2.8) and the propagator $\langle\psi_\alpha^{\boldsymbol{a}}|e^{-\tau\hat{T}_\alpha}|\psi_\alpha^{\boldsymbol{b}}\rangle$ has been determined in Eq. (B2) of Appendix B. In the last approximation we just write the discretized version of the kinetic energy.

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

$$\sum_{\boldsymbol{a},\boldsymbol{b}}\cdots \to \int \cdots \frac{d\boldsymbol{q}_a\,d\boldsymbol{p}_a}{(2\pi)^3}\frac{d\boldsymbol{q}_b\,d\boldsymbol{p}_b}{(2\pi)^3}. \tag{C4}$$

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