Quantum Molecular Dynamics

Riccardo Fantoni*
Università di Trieste, Dipartimento di Fisica, strada Costiera 11, 34151 Grignano (Trieste), Italy
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We formulate a new quantum many body simulation method for a general quantum fluid at any given temperature. Unlike path integral Monte Carlo our method evolves in imaginary time the density matrix from its initial delta function condition to its final thermal form at time time equal to the inverse temperature. It does this with a molecular dynamics scheme on a classical Hamiltonian that has the same functional form as the one of the quantum mechanical Hamiltonian according to the properties of the continuous representation of John R. Klauder. We then end up with the thermal density matrix that can be used to extract thermal averages of observables using the Monte Carlo method equally well in any statistics.

Keywords: Quantum Many Body; Simulation; Quantum Molecular Dynamics; Monte Carlo; Continuous Representation; Density Matrix; Bloch Equation; Stationary Variational Principle; Hamilton Equations

I. INTRODUCTION

Many body simulations are of various kinds. There are the ones specific to classical, high temperature, fluids, like Monte Carlo (MC) or molecular dynamics (MD), [1] those specific to the ground state, zero temperature, of a quantum fluid, like variational (VMC) or diffusion Monte Carlo (DMC), [2] and then those that can treat a quantum fluid in full generality at finite non-zero temperature like the path integral Monte Carlo (PIMC) method [3, 4] which interpolates between the classical fluid and the ground state of the quantum fluid.

In this letter we propose a novel kind of a many body simulation that holds for a general quantum fluid and like PIMC can interpolate between high and low temperatures. It uses a MD scheme to evolve the density matrix of the statistical physical system from its initial condition at zero imaginary time $t=0$ to $t=\beta=1/k_BT$ with k_B Boltzmann constant and T the absolute temperature. And then a MC scheme to calculate the thermal average with the density matrix just obtained from its evolution up to the imaginary time equal to β.

We will call this new quantum many body simulation scheme a Quantum Molecular Dynamics (QMD) computer experiment. The idea hinges on the formulation of the *continuous representation* in quantum mechanics by John Rider Klauder in a sequel of 5 papers from 1963 to 1965 [5–10]. Of particular importance to us will be the paper II in this sequel [6]. Our merit lays just in performing a Wick rotation to imaginary time $t\to -i\hbar t$ which brings us from quantum mechanics to statistical mechanics and applying it to a many body system instead of a one body one like Klauder did in 1963.

We believe that this new algorithm may be of interest to the computer experiment community and certainly it enriches the panorama of algorithms at their disposal to treat a quantum fluid in full generality at any given temperature. We are not aware of any similar method able to treat any many body system irrespective of the statistics ruling the particles being them distinguishable, i.e. Boltzmann, or indistinguishable, i.e. Bose-Einstein or Fermi-Dirac.

II. DESCRIPTION OF THE ALGORITHM

Imagine to have a many body quantum system made of N particles of mass m, positions $Q=(\boldsymbol{q}_1,\boldsymbol{q}_2,\dots,\boldsymbol{q}_i,\dots,\boldsymbol{q}_N)$ and momenta $P=(\hat{\boldsymbol{p}}_1,\hat{\boldsymbol{p}}_2,\dots,\hat{\boldsymbol{p}}_i,\dots,\hat{\boldsymbol{p}}_N)=-i\hbar(\boldsymbol{\nabla}_{\boldsymbol{q}_1},\boldsymbol{\nabla}_{\boldsymbol{q}_2},\dots,\boldsymbol{\nabla}_{\boldsymbol{q}_N})$ [1] in thermal equilibrium at a finite temperature T, in a volume Ω, at a density $n=N/\Omega$, in d spatial dimensions.

The Hamiltonian of the fluid is made of a kinetic energy and a potential energy contribution $\hat{H}(Q,P)=\hat{K}(P)+\hat{V}(Q)=\hat{P}^2/2m+V(Q)$ where the potential energy is only function of the particles coordinates

$$V(Q)=\sum_{i<j}v(|\boldsymbol{q}_i-\boldsymbol{q}_j|), \tag{1}$$

and v is a pair potential. In position representation V is just a c-number. Since the potential V may not be quadratic in Q, the Klauder *continuous representation* for this Hamiltonian falls in the *inexact category* of Klauder [6].

Following Klauder work [6] we introduce a quantum action functional for the position representation of the many body density matrix $\varphi(Q,t)$,

$$I[\varphi]=\int\Big[(\varphi,\partial\varphi/\partial t)+(\varphi,\hat{H}\varphi)\Big]\,dt, \tag{2}$$

where $(\cdots,\cdots)$ is the scalar product of the Hilbert space. Extremizing this functional $\delta I=I[\varphi+\epsilon]-I[\varphi]=0$ over any vector ϵ obeying to Bloch equation with Hamilto-

[1] We are using here the coordinate representation. We will generally use a hat to denote an operator acting on the Hilbert space.

nian $\hat{H}$ [2], yields Bloch equation for the imaginary time evolution of φ,

$$\frac{\partial\varphi(Q,t)}{\partial t} = -\hat{H}\varphi(Q,t), \tag{3}$$

$$\varphi(Q,0) = \varphi_0(Q), \tag{4}$$

φ_0 is a *fiducial vector* that we will choose to be normalized $(\varphi_0,\varphi_0)=1$.

Now introduce a couple of *classical* c-vectors labels $\boldsymbol{\mathcal{Q}}_i, \boldsymbol{\mathcal{P}}_i$ for each particle $i=1,2,\ldots,N$. Assume that we have parametrized the coordinate representation of the many body density matrix with these $2Nd$ c-numbers labels so that

$$\varphi(Q,t) = e^{-t\hat{H}}\varphi_0(Q) = \varphi[\mathscr{Q}(t),\mathscr{P}(t);Q], \tag{5}$$

where $\mathscr{Q} = (\boldsymbol{\mathcal{Q}}_1,\boldsymbol{\mathcal{Q}}_2,\ldots,\boldsymbol{\mathcal{Q}}_N)$ and $\mathscr{P} = (\boldsymbol{\mathcal{P}}_1,\boldsymbol{\mathcal{P}}_2,\ldots,\boldsymbol{\mathcal{P}}_N)$ will be time dependent and will carry the information for the imaginary time evolution of φ.

Let us choose explicitly the following functional form

$$\begin{aligned}\varphi[\mathscr{Q},\mathscr{P};Q] &= e^{-i\alpha/\hbar}\prod_{i=1}^{N} e^{-i\boldsymbol{\mathcal{Q}}_i\cdot\hat{\boldsymbol{p}}_i/\hbar}e^{i\boldsymbol{\mathcal{P}}_i\cdot\hat{\boldsymbol{q}}_i/\hbar}\varphi_0,\\ &= e^{-i\alpha/\hbar}e^{-i\mathscr{Q}\cdot P/\hbar}e^{i\mathscr{P}\cdot Q/\hbar}\varphi_0(Q),\end{aligned} \tag{6}$$

where α is some c-number that may also be function of time, $\varphi_0(Q)$ is the initial condition of Eq. (4), and assume that

$$(\varphi_0, Q\varphi_0) = 0, \tag{7a}$$

$$(\varphi_0, P\varphi_0) = 0. \tag{7b}$$

Form (6) is called *continuous representation* by Klauder [5–10]. It is constructed so that the three exponential factors are such that the first one is just a phase, the second is a unitary operator that builds a translation in the positions according to $\exp(i\mathscr{Q}\cdot P/\hbar)f(Q)\exp(-i\mathscr{Q}\cdot P/\hbar) = f(Q+\mathscr{Q})$ for any infinitely differentiable function f [3], and the third builds a translation in the momenta according to $\exp(-i\mathscr{P}\cdot Q/\hbar)g(P)\exp(i\mathscr{P}\cdot Q/\hbar) = g(P+\mathscr{P})$ for any infinitely differentiable function g [3].

Then Klauder [6] proved that the quantum action functional of Eq. (2) reduces to the following *classical* action functional

$$\mathscr{I}[\mathscr{Q},\mathscr{P}] = \int\left[\sum_{i=1}^{N}\boldsymbol{\mathcal{P}}_i\cdot\dot{\boldsymbol{\mathcal{Q}}}_i + \dot{\alpha} - \mathscr{H}(\mathscr{Q},\mathscr{P})\right]dt, \tag{8}$$

where the dot denotes a derivative respect to imaginary time and

$$\begin{aligned}\mathscr{H}(\mathscr{Q},\mathscr{P}) &= -i\hbar(\varphi[\mathscr{Q},\mathscr{P};Q],\hat{H}(Q,P)\varphi[\mathscr{Q},\mathscr{P};Q])\\ &= -i\hbar(\varphi_0,\hat{H}(Q+\mathscr{Q},P+\mathscr{P})\varphi_0) \qquad (9)\\ &= -i\hbar\left[\hat{H}(\mathscr{Q},\mathscr{P}) + \mathscr{O}(\hbar;\varphi_0;\mathscr{Q},\mathscr{P})\right]. \qquad (10)\end{aligned}$$

According to Eq. (10), we see that $\mathscr{H}(\mathscr{Q},\mathscr{P})$ has the functional form of the quantum mechanical Hamiltonian with explicit c-number substitution, i.e., $\hat{H}(\mathscr{Q},\mathscr{P})$ plus an additional term $\mathscr{O}$ depending on $\hbar$, the fiducial vector φ_0 as well as on the coordinates and momenta classical labels. For nonpathological Hamiltonian operators, $\mathscr{O}$ depends only on positive powers of $\hbar$; hence in this case, $\mathscr{O}\to 0$ and $\mathscr{H}(\mathscr{Q},\mathscr{P})\to -i\hbar[\hat{K}(\mathscr{P})+\hat{V}(\mathscr{Q})]$ as $\hbar\to 0$. which is just the conventional relation in order that $\mathscr{H}(\mathscr{Q},\mathscr{P})$ be the appropriate classical Hamiltonian for the system under discussion. In this same limit, $\mathscr{Q}$ and $\mathscr{P}$ achieve their conventional, classical sharp physical significance since the equations of motion (13) obtained extremizing $\mathscr{I}$ are the usual ones for classical MD in real time $-i\hbar t$.

For our many body Hamiltonian we then find from Eq. (10)

$$\begin{aligned}\mathscr{O} &= (\varphi_0, P^2\varphi_0)/2m + (\varphi_0,[V(Q+\mathscr{Q})-V(\mathscr{Q})]\,\varphi_0)\\ &= c + w(\mathscr{Q}).\end{aligned} \tag{11}$$

Thus $\mathscr{Q}(t)$ is the only dynamical variable on which $\mathscr{O}$ depends. Following Klauder presentation in Ref. II [6], by choosing φ_0 sharp in Q space about zero we can make $w(\mathscr{Q})$ arbitrarily small. The price for reducing $w(\mathscr{Q})$ to a negligible quantity is that now $c=(\varphi_0,P^2\varphi_0)/2m$ becomes arbitrarily large. But we can cancel this constant by the choice of phase $\alpha = -i\hbar ct$ in Eq. (8), so that $\dot{\alpha} - \mathscr{H}(\mathscr{Q},\mathscr{P}) = i\hbar\hat{H}(\mathscr{Q},\mathscr{P})$.

Therefore choosing for the fiducial vector something as close as possible to a Dirac delta function in dN spatial dimensions [4]

$$\varphi_0 = \delta^{(dN)}(Q), \tag{12}$$

we can evolve the classical labels $\mathscr{Q},\mathscr{P}$ with a classical molecular dynamics simulation with the Hamiltonian $\mathscr{H}$ by extremising the classical action functional of Eq. (8) with $\dot{\alpha} = -i\hbar c = -i\hbar(\varphi_0,P^2\varphi_0)/2m$. The equations of motion stemming from extremising the functional (8)

[2] Note that in real time ϵ does not have this additional constraint and it is just *any* vector of the Hilbert space. In this case the action functional becomes [6] $I = \int\left[i\hbar(\varphi,\partial\varphi/\partial t) - (\varphi,\hat{H}\varphi)\right]dt$ and its Euler-Lagrange variational principle yields Schrödinger equation.

[3] This is a consequence of Hadamard lemma.

[4] It is rather gratifying to see how the choice of Eq. (12) that is here the necessary initial condition (4) to the Bloch equation for the coordinate representation of the many body density matrix was also found necessary by Klauder in his pioneering paper [6] at page 1064 of his section "Canonical Transformations and Inexact 'Classical' Action Functionals". Quoting his writing "*By choosing Φ_0 sharp in Q space about zero we can make $v(q)$ arbitrarily small*".

respect to variations in the classical labels of each particle $i = 1, 2, \ldots, N$ are

$$\dot{\boldsymbol{\mathcal{Q}}}_i = \frac{\partial \mathscr{H}(\mathscr{Q}, \mathscr{P})}{\partial \boldsymbol{\mathcal{P}}_i}, \tag{13a}$$

$$\dot{\boldsymbol{\mathcal{P}}}_i = -\frac{\partial \mathscr{H}(\mathscr{Q}, \mathscr{P})}{\partial \boldsymbol{\mathcal{Q}}_i}, \tag{13b}$$

as usual. Once we have the time evolution for $\mathscr{Q}(t), \mathscr{P}(t)$ we can reconstruct the many body density matrix imaginary time evolution from Eq. (5). Note that the condition of Eq. (12) coincides with the initial condition for the off diagonal coordinate representation of the density matrix operator, $\hat{\rho}(t) = \exp(-t\hat{H}) \to \hat{I}$ for $t \to 0$, where $\hat{I}$ is the identity operator, between positions Q and the origin 0 as reference point. This is not a coincidence and it is a consequence of Klauder continuous representation formalism where $\varphi(Q, t)$ should be considered as the off diagonal coordinate representation of the density matrix operator

$$\varphi(Q, t) = \langle Q|\hat{\rho}(t)|0\rangle = \rho(Q, 0; t), \tag{14}$$

where we used the notation of Ref. [3]. Conditions (7a) and (7b) will also be satisfied [5].

Eq. (12) holds for distinguishable, boltzmannons, particles. For identical particles it needs to be replaced with

$$\begin{aligned}\varphi_0 &= \frac{1}{N!}\sum_{\mathscr{C}} \mathrm{sgn}(\mathscr{C})\delta^{(dN)}(\boldsymbol{q}_{\mathscr{C}1}, \ldots, \boldsymbol{q}_{\mathscr{C}N}) \\ &= \frac{1}{N!}\sum_{\mathscr{C}} \mathrm{sgn}(\mathscr{C})\delta^{(dN)}(\mathscr{C}Q), \qquad (15) \\ \mathrm{sgn}(\mathscr{C}) &= (\pm 1)^{\sum_{\nu=1}^{N}(\nu-1)C_\nu},\end{aligned}$$

where $\mathscr{C}$ is any permutation of the N particles with sign $\mathrm{sgn}(\mathscr{C})$. Any permutations can be broken into cycles $\mathscr{C} = \{C_\nu\}$ where C_ν is the number of cycles of length ν in $\mathscr{C}$. In the sum over the permutation one should use a $+1$ for the symmetrization necessary for bosons and -1 for the antisymmetrization necessary for fermions, in $\mathrm{sgn}(\mathscr{C})$.

In order to measure the thermal average at absolute temperature T for an observable $\hat{O}$ we need the diagonal coordinate representation of the density matrix

$$\varphi_d(Q, t) = \langle Q|\hat{\rho}(t)|Q\rangle = \rho(Q, Q; t), \tag{16}$$

so that one can write

$$\langle O\rangle = \frac{\int_{\Omega^N} O(Q, P)\varphi_d(Q, \beta)\, dQ}{\int_{\Omega^N} \varphi_d(Q, \beta)\, dQ}, \tag{17}$$

where $\beta = 1/k_B T$ with k_B Boltzmann constant and $O(Q, P) = \langle Q|\hat{O}|Q\rangle$ is the diagonal coordinate representation of the observable operator $\hat{O}$. In the quantum regime at small T we need to evolve the density matrix for a long imaginary time since β is large. The thermal average can then be computed with a Monte Carlo integration [2, 11]. Eq. (17) can also be rewritten in the more familiar form, $\langle O\rangle = \mathrm{tr}[\hat{O}\hat{\rho}(\beta)]/\mathrm{tr}[\hat{\rho}(\beta)]$, where $Z = \mathrm{tr}[\hat{\rho}(\beta)]$ is the canonical ensemble partition function of the statistical mechanics physical system. Note that $\varphi_d(Q, \beta) > 0$ for any Q, and therefore a well defined probability density, irrespective of the statistics. So assuming that the MD "classical" evolution is also able to find $\varphi_d(Q, \beta)$ equally well in any statistics, then our method would not suffer from the so called *fermions sign problem* [12–15].

Indeed one can determine φ_d at the cost of having a non-negligible $\mathscr{O}$ in Eq. (10). For a given $Q' = (\boldsymbol{q}'_1, \boldsymbol{q}'_2, \ldots, \boldsymbol{q}'_N)$ we choose an initial condition where

$$\varphi_0 = \delta^{(dN)}(Q - Q'). \tag{18}$$

Condition (7a) will now become $(\varphi_0, Q\varphi_0) = Q'$ and condition (7b) becomes $(\varphi_0, P\varphi_0) = P'$ where P' is an arbitrary momenta vector with arbitrarily large norm. Therefore the classical action functional now becomes

$$\begin{aligned}&\mathscr{I}'[\mathscr{Q}, \mathscr{P}] = \\ &\int \left\{ \sum_{i=1}^{N} \left[(\boldsymbol{\mathcal{P}}_i + \boldsymbol{p}'_i)\cdot \dot{\boldsymbol{\mathcal{Q}}}_i - \dot{\boldsymbol{\mathcal{P}}}_i \cdot \boldsymbol{q}'_i \right] + \dot{\alpha} \right. \\ &\left. - \mathscr{H}(\mathscr{Q}, \mathscr{P}) \right\} dt = \mathscr{I}[\mathscr{Q}, \mathscr{P}] + f + g, \qquad (19)\end{aligned}$$

where in the last equality we used the fact that the coordinates $\boldsymbol{q}'_i$ and $\boldsymbol{p}'_i$ are independent of time and $f = [\mathscr{P}(\beta) - \mathscr{P}(0)]\cdot Q'$ and $g = [\mathscr{Q}(\beta) - \mathscr{Q}(0)]\cdot P'$ are two constants which have no effect on the equations of motion stemming from the stationary variation of $\mathscr{I}'$. Moreover

$$\dot{\alpha} - \mathscr{H}(\mathscr{Q}, \mathscr{P}) = i\hbar \left[\hat{K}(\mathscr{P}) + \hat{V}(Q' + \mathscr{Q}) \right]. \tag{20}$$

Extremising now $\mathscr{I}'$ we find other "classical" equations of motion for the labels $\mathscr{Q}, \mathscr{P}$ which are in form equivalent to (13) but with a different "classical" Hamiltonian (20). Choosing as initial conditions $\mathscr{Q}(0) = \mathscr{Q}_0$ and $\mathscr{P}(0) = \mathscr{P}_0$ these equations allow to evolve in imaginary time the continuous representation of Eq. (6), $\bar{\varphi}$, that will now also depend on Q'. We may then write

$$\begin{aligned}\bar{\varphi}[\mathscr{Q}(t), \mathscr{P}(t); Q, Q'] &= \bar{\varphi}(Q, Q', t) \\ &= \langle Q|\hat{\rho}(t)|Q'\rangle \\ &= \rho(Q, Q'; t), \qquad (21)\end{aligned}$$

for the general off diagonal position representation of the density matrix at time t. So that $\varphi(Q, t) = \bar{\varphi}(Q, 0, t)$ and $\varphi_d(Q, \beta) = \bar{\varphi}(Q, Q, \beta) > 0$. In the Appendix we show this for the ideal gas case.

Imagine we solved the MD imaginary time evolution. It is convenient to choose Neumann initial conditions as

[5] Eq. (7b) will be satisfied almost everywhere.

$\mathscr{Q}_0 = \mathscr{P}_0 = 0$ so that

$$\bar{\varphi}(Q,Q',0) = e^{-i\alpha(0)/\hbar} e^{-i\mathscr{Q}(0)\cdot P/\hbar} e^{i\mathscr{P}(0)\cdot Q/\hbar} \varphi_0 = \varphi_0 = \delta^{(dN)}(Q-Q'), \quad (22)$$

then at the end of the evolution we will have

$$\bar{\varphi}(Q,Q',\beta) = e^{-i\alpha(\beta)/\hbar} e^{-i\mathscr{Q}(\beta)\cdot P/\hbar} e^{i\mathscr{P}(\beta)\cdot Q/\hbar} \varphi_0 = e^{-\beta(\varphi_0, P^2\varphi_0)/2m} e^{-i\mathscr{Q}(\beta)\cdot P/\hbar} e^{i\mathscr{P}(\beta)\cdot Q/\hbar} \delta^{(dN)}(Q-Q') = e^{-\beta(\varphi_0, P^2\varphi_0)/2m} e^{i\mathscr{P}(\beta)\cdot Q'/\hbar} \delta^{(dN)}(Q-\mathscr{Q}(\beta)-Q') \propto, (4\lambda\beta\pi)^{-dN/2} e^{-\beta(Q-\mathscr{Q}(\beta)-Q')^2/4\lambda\beta} e^{i\mathscr{P}(\beta)\cdot Q'/\hbar}, \quad (23)$$

where $\lambda = \hbar^2/2m$. This correctly reduces to (22) in the $\beta \to 0$ limit and gives the desired off diagonal thermal density matrix that can be used to estimate the thermal average (17).

III. CONCLUSIONS

In conclusions we described a new algorithm that can be used to perform a computer experiment on a general quantum many body system with only pairwise interactions dependent on positions only at any given temperature. The algorithm evolves in imaginary time the system density matrix from its initial delta function form to its final thermal density matrix form at an imaginary time equal to the inverse temperature. The evolution follows a molecular dynamics scheme (13) guided by a "classical" Hamiltonian that has the same functional form as the quantum mechanical Hamiltonian (10) thanks to the properties of the *continuous representation* of John R. Klauder (6). Klauder carefully proved the equivalence between the "classical" stationary variational principle (8) extremized by the solutions to Hamilton equations of motion and the quantum stationary variational principle (2) extremized by the solutions to Bloch equation.

In other words we evolve the many body density matrix according to Bloch equation starting from the delta function initial configuration by means of a "classical" molecular dynamics simulation which evolves in imaginary time a set of canonical variables (13) for each particle according to a "classical" Hamiltonian (10) that has the same functional form of the quantum many body Hamiltonian of the fluid. This set of "classical canonical variables" then plays the role of c-number labels for the continuous representation of the density matrix (6). We stop the evolution at an imaginary time equal to the inverse temperature $\beta = 1/k_B T$ which gives us the thermal density matrix at a temperature T.

Once the diagonal thermal density matrix has been reached it can be used to extract thermal averages of observables with the Monte Carlo method as usual (17). Since the diagonal thermal density matrix is always a good probability density our new method continues to hold for any kind of particles either distinguishable or identical and any kind of statistics: Boltzmann, Bose-Einstein, or Fermi-Dirac.

We are not aware of any similar simulation algorithm in the community and we will worry about its implementation in a near future. This should not be too complicated since it requires as ingredients the interplay of two of the most well established simulation schemes in the community of classical computer experiments, i.e. MD and MC [1].

In particular it should be carefully assessed the efficiency of the algorithm since in order to extract the diagonal density matrix it requires a different MD simulation for each MC sampling according to (20). This could become heavy from a computational cost point of view especially at low temperatures when the MD time evolution takes a long time $\hbar\beta$.

This new method goes together with a recent newly proposed path integral Monte Carlo algorithm that uses coherent states instead of the usual plane waves to expand the hot kinetic density matrix [4].

Upon a necessary discretization of the time evolution our algorithm will depend on an imaginary-time-step τ. At low temperature one needs to evolve the density matrix on a long imaginary time. For a fixed large β one has to find the optimal balance between the maximum accuracy in the final density matrix and the minimum number of necessary time-steps.

Our formal computational algorithm solves the fermions sign problem for the measurement of observables diagonal in their position representation. For non diagonal observables like the momentum distribution or dynamical properties some more work is necessary.

Unlike PIMC our method will not suffer from the requirement of dealing with interactions bounded from below since the interaction is not "integrated" but is "evolved" in the imaginary time dynamics.

Appendix A: The ideal gas

For an ideal gas $V = 0$ and the Hamiltonian is quadratic. So according to the analysis of Klauder [6] the continuous representation falls in the *exact category*.

In this case Bloch equation reduces to the usual diffusion equation which, with the initial condition

$$\bar{\varphi}(Q,Q',0) = \delta^{(dN)}(Q-Q'), \quad (A1)$$

has the following solution

$$\bar{\varphi}(Q,Q',\beta) = (4\lambda\beta\pi)^{-dN/2} e^{-(Q-Q')^2/4\lambda\beta}, \quad (A2)$$

where $\lambda = \hbar^2/2m$.

On the other hand if we choose $\varphi_d(Q,0) = \delta^{(dN)}(0) = \text{constant} \to \infty$, from the equations of motion (13) follows $\dot{\mathscr{P}} = 0$ and $\dot{\mathscr{Q}} = -i\hbar\mathscr{P}/m$ which can be rewritten as

$\mathscr{P}(\beta) = \mathscr{P}(0)$ and $\mathscr{Q}(\beta) = \mathscr{Q}(0) - i\hbar\beta\mathscr{P}(0)/m$. We will then have

$$\begin{aligned}
&\varphi_d(Q,\beta) = e^{-\beta\hat{H}}\varphi_d(Q,0) = \\
&e^{-\beta\hat{H}}e^{-i\alpha(0)/\hbar}e^{-i\mathscr{Q}(0)\cdot P/\hbar}e^{i\mathscr{P}(0)\cdot Q/\hbar}\varphi_0 = \\
&e^{-i\alpha(\beta)/\hbar}e^{-i\mathscr{Q}(\beta)\cdot P/\hbar}e^{i\mathscr{P}(\beta)\cdot Q/\hbar}\varphi_0 = \\
&e^{-\beta\mathscr{P}(0)\cdot P/m}e^{-\beta c}e^{-i\mathscr{Q}(0)\cdot P/\hbar}e^{i\mathscr{P}(0)\cdot Q/\hbar}\varphi_0 = \\
&e^{-\beta(\varphi_0,P^2\varphi_0)/2m}e^{-\beta\mathscr{P}(0)\cdot P/m}\varphi_d(Q,0) = \\
&e^{-\beta(\varphi_0,P^2\varphi_0)/2m}\varphi_d(Q+i\hbar\beta\mathscr{P}(0)/m,0). \qquad \text{(A3)}
\end{aligned}$$

Then we may choose $\mathscr{Q}(0) = \mathscr{P}(0) = 0$ to find

$$\varphi_d(Q,\beta) = e^{-\beta(\varphi_0,P^2\varphi_0)/2m}\delta^{(dN)}(0),$$

where $(\varphi_0, P^2\varphi_0)$ is a positive quantity arbitrarily large. Then $e^{-\beta(\varphi_0,P^2\varphi_0)/2m}$ is arbitrarily small and when multiplied by the arbitrarily large constant $\delta^{(dN)}(0)$ gives the finite result of (A2). [6]

For a concrete realization of the Dirac delta in one dimension for one particle we can for example take

$$\begin{aligned}
\varphi_0 &= \delta(Q-Q') \\
&= \lim_{\tau\to 0^+}(4\lambda\tau\pi)^{-1/2}e^{-(Q-Q')^2/4\lambda\tau}, \\
&= \lim_{\tau\to 0^+}\bar{\varphi}(Q,Q',\tau) \qquad \text{(A4)}
\end{aligned}$$

so that

$$\beta(\varphi_0,P^2\varphi_0)/2m = \lim_{\tau\to 0^+}\mathscr{N}(\tau), \qquad \text{(A5)}$$

$$\mathscr{N}(\tau) = \beta\lambda/(\tau\lambda)^{3/2}8\sqrt{2\pi}, \qquad \text{(A6)}$$

which is arbitrarily large for arbitrarily small $\tau > 0$.

Then $\varphi_d(Q;\beta)$ must be given by

$$\lim_{\substack{\tau\to 0^+\\ \tau'\to 0^+}} e^{-\mathscr{N}(\tau)}\bar{\varphi}\left(Q,Q,\tau'\right). \qquad \text{(A7)}$$

This is possible if one chooses in the limit above, $\tau' = \beta e^{-2\mathscr{N}(\tau)}$ like so

$$\begin{aligned}
&\lim_{\tau\to 0^+} e^{-\mathscr{N}(\tau)}\bar{\varphi}\left(Q,Q,\beta e^{-2\mathscr{N}(\tau)}\right) = \\
&\varphi_d(Q;\beta) = (4\lambda\beta\pi)^{-1/2}. \qquad \text{(A8)}
\end{aligned}$$

Since the limit (A7) must exist this has to be unique.

This proves that the imaginary time evolution of the initial continuous representation of (6), $\bar{\varphi}[\mathscr{Q}(0),\mathscr{P}(0);Q,Q]$, is still of the continuous representation kind, $\bar{\varphi}[\mathscr{Q}(\beta),\mathscr{P}(\beta);Q,Q]$, at the end of the "classical" MD evolution.

[6] Working with the off diagonal density matrix $\bar{\varphi}(Q,Q',\beta)$ the fiducial vector $\varphi_0 = \delta^{(dN)}(Q-Q')$ in momentum representation will be an arbitrary oscillating function $e^{iQ'\cdot P/\hbar}$ and $(\varphi_0,P^2\varphi_0)/2m = \int dP\, P^2/2m$ will be arbitrarily large. The infinitesimally small quantity $\exp[-\beta(\varphi_0,P^2\varphi_0)/2m]$ when multiplied by the Dirac delta φ_0 will give rise to zero unless $Q = Q'$.

AUTHOR DECLARATIONS

Conflicts of interest

None declared.

Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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* riccardo.fantoni@scuola.istruzione.it

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