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Article

Quantum Molecular Dynamics

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Abstract

We formulate a new quantum many-body simulation method for a general quantum fluid at any given temperature. Unlike the path integral Monte Carlo method, our method evolves, in imaginary time, the density matrix from its initial delta function condition to its final thermal form in an amount of time equal to the inverse temperature. It does this with a molecular dynamics scheme applied to a classical Hamiltonian that has the same functional form as the one for 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, which 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

1. Introduction

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

In this article, we propose a novel kind of many-body simulation that holds for a general quantum fluid and, like the PIMC method, 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 $t = \beta = 1/k_B T$, with k_B denoting the Boltzmann constant and T being the absolute temperature. And then a MC scheme to calculate the thermal average with the density matrix obtained from its evolution up to an 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 series of five papers written from 1963 to 1965 [5–10]. Of particular importance to us is paper II in this series [6]. The merit of our work lies in applying 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 it certainly enriches the panorama of algorithms at their disposal to treat

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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.

2. Description of the Algorithm

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

The Hamiltonian of the fluid is made up 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 a 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's work [6], we introduce a quantum action functional for the position representation of the many-body density matrix $\varphi(Q,t)$,

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

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 the Bloch equation with the Hamiltonian $\hat{H}$ (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 the Schrödinger equation) yields the 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, $(\varphi_0, \varphi_0) = 1$.

We 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 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 a function of time, and $\varphi_0(Q)$ is the initial condition of Equation (4). Additionally, we will 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 was developed so that the first of the three exponential factors is just a phase; the second is a unitary operator that generates a translation in the positions according to $\exp(i\mathcal{Q}\cdot P/\hbar)f(Q)\exp(-i\mathcal{Q}\cdot P/\hbar) = f(Q+\mathcal{Q})$ for any infinitely differentiable function f (this is a consequence of the Hadamard lemma); and the third generates a translation in the momenta according to $\exp(-i\mathcal{P}\cdot Q/\hbar)g(P)\exp(i\mathcal{P}\cdot Q/\hbar) = g(P+\mathcal{P})$ for any infinitely differentiable function g (this is also a consequence of the Hadamard lemma).

Klauder [6] proved that the quantum action functional of Equation (2) reduces to the following *classical* action functional:

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

where the dot denotes a derivative with respect to imaginary time and

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

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

For our many-body Hamiltonian, we then find from Equation (10) that

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

Thus, $\mathcal{Q}(t)$ is the only dynamical variable on which $\mathcal{O}$ depends. Following Klauder's presentation in Ref. II [6], by choosing a φ_0 that is sharp in Q space at about zero, we can make $w(\mathcal{Q})$ arbitrarily small. The price of reducing $w(\mathcal{Q})$ to a negligible quantity is that $c = (\varphi_0, P^2\varphi_0)/2m$ is now arbitrarily large. But we can cancel this constant by choosing phase $\alpha = -i\hbar ct$ in Equation (8) so that $\dot{\alpha} - \mathcal{H}(\mathcal{Q},\mathcal{P}) = i\hbar\hat{H}(\mathcal{Q},\mathcal{P})$.

Therefore, by choosing something as close as possible to a Dirac delta function in dN spatial dimensions for the fiducial vector

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

we can evolve the classical labels $\mathcal{Q},\mathcal{P}$ via a classical molecular dynamics simulation with the Hamiltonian $\mathcal{H}$ by extremising the classical action functional of Equation (8)

with $\dot{\alpha} = -i\hbar c = -i\hbar\langle\varphi_0, P^2\varphi_0\rangle/2m$. The equations of motion stemming from extremising functional (8) with respect to variations in the classical labels of each particle $i = 1, 2, \ldots, N$, namely,

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

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

as usual. Once we have determined the time evolution for $\mathscr{Q}(t)$, $\mathscr{P}(t)$, we can reconstruct the many-body density matrix imaginary-time evolution from Equation (5). Note that the condition of Equation (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 a reference point. This is not a coincidence, and it is a consequence of Klauder's continuous representation formalism, where $\varphi(Q,t)$ should be considered the off-diagonal coordinate representation of the density matrix operator

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

for which we used the notation employed in Ref. [3]. Conditions (7a) and (7b) will also be satisfied (Equation (7b) will be satisfied almost everywhere).

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

$$\begin{aligned} \varphi_0 &= \frac{1}{N!}\sum_{\mathscr{C}}\mathrm{sgn}(\mathscr{C})\delta^{(dN)}(\boldsymbol{q}_{\mathscr{C}1},\ldots,\boldsymbol{q}_{\mathscr{C}N}) \\ &= \frac{1}{N!}\sum_{\mathscr{C}}\mathrm{sgn}(\mathscr{C})\delta^{(dN)}(\mathscr{C}Q), \\ \mathrm{sgn}(\mathscr{C}) &= (\pm1)^{\sum_{\nu=1}^{N}(\nu-1)C_\nu}, \end{aligned} \tag{15}$$

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 with a length of ν in $\mathscr{C}$. In the sum over the permutation, one should use $+1$ 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 to determine 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 $\beta = 1/k_BT$, with k_B denoting the 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 values of T, we need to evolve the density matrix for a long stretch of imaginary time since β is large. The thermal average can then be computed with a Monte Carlo integration [2,11]. Equation (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 can also be used 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 Equation (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) will become $(\varphi_0, P\varphi_0) = P'$, where P' is an arbitrary momenta vector with an arbitrarily large norm. Therefore, the classical action functional now becomes

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

where, in the last equality, we use 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,

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

Now, by extremising $\mathscr{I}'$, we can 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). With $\mathscr{Q}(0) = \mathscr{Q}_0$ and $\mathscr{P}(0) = \mathscr{P}_0$ chosen as initial conditions, these equations allow the evolution, in imaginary time, of the continuous representation of Equation (6), $\bar{\varphi}$, which will now also depend on Q'. We may thus write

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

for the general off-diagonal position representation of the density matrix at time t. Thus, $\varphi(Q,t) = \bar{\varphi}(Q,0,t)$ and $\varphi_d(Q,\beta) = \bar{\varphi}(Q,Q,\beta) > 0$. In Appendix A, 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 $\mathscr{Q}_0 = \mathscr{P}_0 = 0$ so that

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

Then, at the end of the evolution, we will have

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

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).

3. Conclusions

In conclusion, we have 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 the Hamilton equations of motion and the quantum stationary variational principle (2) extremized by the solutions to the Bloch equation.

In other words, we evolve the many-body density matrix according to the 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 will 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, the efficiency of the algorithm should be carefully assessed since a different MD simulation is required for each MC sampling, according to (20), in order to extract the diagonal density matrix. This could become extensive 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 temperatures, one needs to evolve the density matrix over a long period of 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 fermion sign problem for the measurement of observables that are diagonal in their position representation. For non-diagonal observables like the momentum distribution or dynamical properties, some more work is necessary.

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Unlike the PIMC, our method does not suffer from a need to deal with interactions bounded from below since the interaction is not "integrated" but "evolved" in the imaginary time dynamics.

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Appendix A. The Ideal Gas

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

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

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

has the following solution:

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

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

On the other hand, if we set $\varphi_d(Q, 0) = \delta^{(dN)}(0) = \text{constant} \to \infty$, from the equation of motion (13), it follows that $\dot{\mathscr{P}} = 0$ 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 would then have

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

Then, we can set $\mathscr{Q}(0) = \mathscr{P}(0) = 0$ 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 that is arbitrarily large. Then, $e^{-\beta(\varphi_0, P^2\varphi_0)/2m}$ is arbitrarily small, and when it is multiplied by the arbitrarily large constant $\delta^{(dN)}(0)$, it gives the finite result of (A2). (When 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 $Q = Q'$.)

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

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

so that

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

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

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

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

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

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

$$\lim_{\tau\to 0^+} e^{-\mathscr{N}(\tau)} \bar{\varphi}\left(Q, Q, \beta e^{-2\mathscr{N}(\tau)}\right) =$$

$$\varphi_d(Q;\beta) = (4\lambda\beta\pi)^{-1/2}. \tag{A8}$$

Since 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.

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