Brownian Bridge for Coherent State Path Integral Monte Carlo

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We propose a new Brownian bridge construction for our newly devised Coherent States Path Integral Monte Carlo algorithm. We apply it to the numerically exact calculation of the thermodynamic properties of the Helium fluid on a plane at low non zero temperature. We find very good agreement with the conventional plane waves path integral Monte Carlo results.

Keywords: Quantum Many Body; Coherent States; Path Integral; Quantum Monte Carlo; Brownian Bridge; Helium; Thermodynamics

I. INTRODUCTION

We recently [1] constructed a new Path Integral Monte Carlo (PIMC) algorithm using Coherent States (CS), [2–7] in place of the more usual Plane Waves (PW), as the complete set over which to expand the thermal density matrix. We called this algorithm with the acronym CSPIMC. We proposed our new algorithm as an alternative to the more common Plane Waves PIMC of Ref. [8] to which we will refer with the acronym PWPIMC.

Although the mathematics of Ref. [1], where we proposed the new algorithm, is completely correct, the numerics in that paper was not complete. In particular it was lacking a justification of the Brownian bridges [8, 9] used in the CSPIMC scheme to sample the permutations sum necessary to calculate the properties of identical particles (being them bosons or fermions).

In the present work we will fill that gap proposing a correct realization of the Brownian bridge move within the CSPIMC algorithm. We will justify our new proposal and we will perform some new computer experiments with the new Browninan bridge move.

The CSPIMC numerical results that we obtain for Helium on a plane compare well with the results from the conventional PWPIMC. Within CSPIMC the continuum limit for the imaginary time must be taken simultaneously to the limit of an infinite elastic constant of the harmonic oscillator of unit mass subtending the coherent states. This was shown in Ref. [1]. Here we will refine the simulations carried out in that preliminary study.

II. PHYSICS MODEL

In Ref. [1] we performed several Path Integral Monte Carlo (PIMC) simulations for a two dimensional, $d = 2$, ^{4}He liquid [10] with either Boltzmann or Bose statistics.

The liquid has a surface number density $n = N/\Omega$ where N is the number of Helium atoms in an area Ω of a flat surface, at an inverse temperature $\beta = 1/k_B T$ with k_B Boltzmann constant. The Hamiltonian of the fluid is $\hat{H} = \hat{T} + \upsilon\hat{V} = \hat{P}^2/2m + \upsilon V(Q)$ with $\vec{Q} = (\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_N)$ the particles positions and $\vec{P} = (\hat{\boldsymbol{p}}_1, \hat{\boldsymbol{p}}_2, \ldots, \hat{\boldsymbol{p}}_N) = -i(\boldsymbol{\nabla}_{\boldsymbol{q}_1}, \boldsymbol{\nabla}_{\boldsymbol{q}_2}, \ldots, \boldsymbol{\nabla}_{\boldsymbol{q}_N})$ the particles momenta. The potential energy $V(Q)$ enters the Hamiltonian with a coupling constant υ.

The computer experiments [1] were done for for $N = 16$ ^{4}He atoms ($m = 0.0830594 \approx 1/12$ Å^{-2}K^{-1}) in two dimensions $d = 2$, in a square periodic cell of area $\Omega = L^2$, interacting with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556$ Å, $\varepsilon = 10.22$ K and a cutoff distance $r_{\rm cut} = 2.5$ Å (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a number density $n = N/L^2 = 0.05$ Å^{-2} and various temperatures T or timeslices number M, either with Boltzmann and Bose statistics. As we can see from the phase diagram of Ref. [10], at this density the fluid undergoes a phase transition from a fluid phase at high temperature to a superfluid phase at low temperatures.

In that work [1] we compared two different PIMC simulations: the conventional Plane Waves PIMC (**PW**PIMC) [8] and our newly devised Coherent States PIMC (**CS**PIMC) algorithm. The two PIMC differ for the expression of the hot kinetic density matrix at an imaginary timestep $\tau = \beta/M$ with M a large number of timeslices. The short imaginary time density matrix CSPIMC expression is reviewed in the next section. The PWPIMC requires a multidimensional integral over dNM coordinates whereas our CSPIMC requires $5dMN$ integrations, the usual dNM

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real particles coordinates, $2dNM$ ghost particles coordinates, and $2dNM$ ghost particles momenta. The coherent states are generated by a harmonic oscillator (h.o.) with mass $m_{h.o.}$ and elastic constant $k = m_{h.o.}\omega^2$. We introduced the parameter $\xi \equiv m_{h.o.}\omega/2$ and the adimensional one $\varphi \equiv \xi\tau/m = (\sigma_{p.w.}/\sigma_{c.s.})^2/2$ where $\sigma_{p.w.} \equiv \sqrt{2\lambda\tau}$ is the standard deviation in the plane wave scheme, with $\lambda = 1/2m$, and $\sigma_{c.s.} \equiv \sqrt{1/m_{h.o.}\omega}$ is the standard deviation in the coherent state scheme. As illustrated in Ref. [1] in order to compare PWPIMC and CSPIMC it is necessary to keep φ fixed.

In our quantum simulations we have to take care of two limiting procedures: The continuum limit where the ultraviolet cutoff $\tau \to 0$ or $M \to \infty$ at fixed absolute temperature T and the thermodynamic limit where $N \to \infty$ and $\Omega \to \infty$ at fixed density n. In particular in Ref. [1] we explicitly worried about the continuum limit and we proved that in the CSPIMC scheme it is necessary to keep φ constant as $\tau \to 0$ so that $\xi \to \infty$. To mimic the thermodynamic limit we simply used a periodic square cell which permeates the whole infinite space. This procedure gives rise to spurious finite size effects unavoidable on a computer.

We worked in units where $\hbar = k_B = 1$ so that the imaginary time has dimensions of temperature.

III. THE SHORT TIME DENSITY MATRIX FOR CSPIMC

The short imaginary time, τ, Green function for CSPIMC can be written as follows [1]:

$$\rho(Q, Q'; \tau) \approx e^{-\tau v V(Q)} \frac{1}{N!} \sum_P \prod_{\alpha=1}^{N} \zeta_\alpha\Big(\boldsymbol{q}_{P\alpha}|\boldsymbol{q}'_\alpha; \tau, m, \xi\Big), \tag{3.1}$$

with P a permutation of the N **real** identical particles and

$$\zeta_\alpha\Big(\boldsymbol{q}|\boldsymbol{q}'; \tau, m, \xi\Big) \approx \int \frac{d\boldsymbol{\mathcal{Q}}_\alpha\, d\boldsymbol{\mathcal{P}}_\alpha}{(2\pi)^d} \frac{d\boldsymbol{\mathcal{Q}}'_\alpha\, d\boldsymbol{\mathcal{P}}'_\alpha}{(2\pi)^d} \psi_\alpha(\boldsymbol{q}_\alpha, \boldsymbol{\mathcal{Q}}_\alpha, \boldsymbol{\mathcal{P}}_\alpha) {\psi_\alpha}^*(\boldsymbol{q}'_\alpha, \boldsymbol{\mathcal{Q}}'_\alpha, \boldsymbol{\mathcal{P}}'_\alpha) G_\alpha \exp\Big[-\tau(\boldsymbol{\mathcal{P}}_\alpha^2 + {\boldsymbol{\mathcal{P}}'}_\alpha^2)/4m\Big], \tag{3.2}$$

where $\psi_\alpha(\boldsymbol{q}_\alpha, \boldsymbol{\mathcal{Q}}_\alpha, \boldsymbol{\mathcal{P}}_\alpha)$ is the CS wave function with ghost canonical variables $\boldsymbol{\mathcal{Q}}_\alpha$ and $\boldsymbol{\mathcal{P}}_\alpha$, the **ghost** of the real particle α, namely

$$\psi_\alpha(\boldsymbol{q}_\alpha, \boldsymbol{\mathcal{Q}}_\alpha, \boldsymbol{\mathcal{P}}_\alpha) \equiv \langle \boldsymbol{q}_\alpha|\boldsymbol{\mathcal{Q}}_\alpha, \boldsymbol{\mathcal{P}}_\alpha\rangle = \left(\frac{2\xi}{\pi}\right)^{d/4} \exp\Big[-\xi\,(\boldsymbol{q}_\alpha - \boldsymbol{\mathcal{Q}}_\alpha)^2 + i\boldsymbol{\mathcal{P}}_\alpha \cdot (\boldsymbol{q}_\alpha - \boldsymbol{\mathcal{Q}}_\alpha)\Big], \tag{3.3}$$

$$G_\alpha = \exp\left[-\frac{1}{2}(|\boldsymbol{a}|^2 + |\boldsymbol{b}|^2) + \boldsymbol{a}^* \cdot \boldsymbol{b} + \frac{i}{2}(\boldsymbol{\mathcal{Q}}_\alpha \cdot \boldsymbol{\mathcal{P}}_\alpha - \boldsymbol{\mathcal{Q}}'_\alpha \cdot \boldsymbol{\mathcal{P}}'_\alpha)\right], \tag{3.4}$$

$$\boldsymbol{a} \equiv \frac{1}{\sqrt{4\xi}}(2\xi\boldsymbol{\mathcal{Q}}_\alpha + i\boldsymbol{\mathcal{P}}_\alpha), \tag{3.5}$$

$$\boldsymbol{b} \equiv \frac{1}{\sqrt{4\xi}}(2\xi\boldsymbol{\mathcal{Q}}'_\alpha + i\boldsymbol{\mathcal{P}}'_\alpha), \tag{3.6}$$

where G_α is the scalar product of the two ghosts $\boldsymbol{\mathcal{Q}}$ and $\boldsymbol{\mathcal{Q}}'$.

We can then define a reduced high temperature density matrix

$$\tilde{\rho}(s, s'; \tau) \propto e^{-\tau v V(Q)} \prod_{\alpha=1}^{N} \psi_\alpha(\boldsymbol{q}_\alpha, \boldsymbol{\mathcal{Q}}_\alpha, \boldsymbol{\mathcal{P}}_\alpha) {\psi_\alpha}^*(\boldsymbol{q}'_\alpha, \boldsymbol{\mathcal{Q}}'_\alpha, \boldsymbol{\mathcal{P}}'_\alpha) G_\alpha e^{-\tau(\boldsymbol{\mathcal{P}}_\alpha^2 + {\boldsymbol{\mathcal{P}}'}_\alpha^2)/4m}, \tag{3.7}$$

with $s = (\vec{Q}, \vec{\mathscr{Q}}, \vec{\mathscr{P}}, P)$ the configurations space for a single link where $\vec{\mathscr{Q}} = (\boldsymbol{\mathcal{Q}}_1, \boldsymbol{\mathcal{Q}}_2, \ldots, \boldsymbol{\mathcal{Q}}_N)$ and $\vec{\mathscr{P}} = (\boldsymbol{\mathcal{P}}_1, \boldsymbol{\mathcal{P}}_2, \ldots, \boldsymbol{\mathcal{P}}_N)$.

Discretizing the imaginary time into M timeslices with $\tau = \beta/M$ we can use Trotter [12] identity to introduce M links $\tilde{\rho}(s_k, s_{k+1}; \tau)$ for $k = 0, 1, 2, \ldots, M-1$ to reconstruct the density matrix at an inverse temperature β as the following path integral

$$\begin{aligned}\rho(s_0, s'_M; \beta) \propto \sum_P \int \tilde{\rho}(s_0, s'_1; \tau)\tilde{\rho}(s_1, s'_2; \tau) \cdots \tilde{\rho}(s_{M-1}, s'_M; \tau) \times \\ \prod_{\alpha=1}^{N} \prod_{k=1}^{M-1} d\boldsymbol{q}_{\alpha,k} \frac{d\boldsymbol{\mathcal{Q}}^k_{\alpha,k-1} d\boldsymbol{\mathcal{P}}^k_{\alpha,k-1}}{(2\pi)^d} \frac{d\boldsymbol{\mathcal{Q}}^k_{\alpha,k} d\boldsymbol{\mathcal{P}}^k_{\alpha,k}}{(2\pi)^d} \frac{d\boldsymbol{\mathcal{Q}}^M_{\alpha,M-1} d\boldsymbol{\mathcal{P}}^M_{\alpha,M-1}}{(2\pi)^d} \frac{d\boldsymbol{\mathcal{Q}}^M_{\alpha,M} d\boldsymbol{\mathcal{P}}^M_{\alpha,M}}{(2\pi)^d}\end{aligned} \tag{3.8}$$

where $\boldsymbol{q}_{\alpha,k}$ are the coordinates of the real particle α at timeslice k, $\boldsymbol{\mathcal{Q}}^l_{\alpha,k}$ and $\boldsymbol{\mathcal{P}}^l_{\alpha,k}$ are respectively the canonical coordinates and momenta of the ghost of particle α at the timeslice k in the link $l-1 \to l$. In our notation $s_k = (\vec{Q}_k, \vec{\mathscr{Q}}^{k+1}_k, \vec{\mathscr{P}}^{k+1}_k, P)$ and $s'_k = (\vec{Q}_k, \vec{\mathscr{Q}}^k_k, \vec{\mathscr{P}}^k_k, P)$ with $\vec{Q}_k = (\boldsymbol{q}_{1,k}, \boldsymbol{q}_{2,k}, \ldots, \boldsymbol{q}_{N,k})$, $\vec{\mathscr{Q}}^l_k = (\boldsymbol{\mathcal{Q}}^l_{1,k}, \boldsymbol{\mathcal{Q}}^l_{2,k}, \ldots, \boldsymbol{\mathcal{Q}}^l_{N,k})$, and $\vec{\mathscr{P}}^l_k = (\boldsymbol{\mathcal{P}}^l_{1,k}, \boldsymbol{\mathcal{P}}^l_{2,k}, \ldots, \boldsymbol{\mathcal{P}}^l_{N,k})$.

The Monte Carlo used is the standard Metropolis algorithm [9, 13]. In our CSPIMC simulations we have two kinds of moves: a singleslice *displace move* and a multislice *Brownian bridge*.

In the displace move we choose as transition move a uniform displacement of each of the dMN real path coordinate $\boldsymbol{q}_{\alpha,k} \to \boldsymbol{q}_{\alpha,k} + (1/2-\eta)\boldsymbol{\Delta}$ for $\alpha = 1,\ldots,N$ and $k = 1,\ldots,M$, where η is a uniform pseudorandom number in $[0,1)$ and $\boldsymbol{\Delta}$ a fixed d-dimensional vector whose magnitude is chosen so to have acceptance ratios close to $1/2$. And of each of the $4dMN$ ghost path canonical variables $\boldsymbol{\mathcal{Q}}^k_{\alpha,k-1} \to \boldsymbol{\mathcal{Q}}^k_{\alpha,k-1} + (1/2-\eta)\boldsymbol{\Delta}$, $\boldsymbol{\mathcal{P}}^k_{\alpha,k-1} \to \boldsymbol{\mathcal{P}}^k_{\alpha,k-1} + (1/2-\eta)\boldsymbol{\Delta}$, and $\boldsymbol{\mathcal{Q}}^k_{\alpha,k} \to \boldsymbol{\mathcal{Q}}^k_{\alpha,k} + (1/2-\eta)\boldsymbol{\Delta}$, $\boldsymbol{\mathcal{P}}^k_{\alpha,k} \to \boldsymbol{\mathcal{P}}^k_{\alpha,k} + (1/2-\eta)\boldsymbol{\Delta}$. So that the transition probability density is just a constant and drops out of the acceptance probability.

The sum over permutations in Eq. (3.8) can be applied just to the real particles coordinates in the first (or last) timeslice. In order to sample the permutation sum we need to construct two Brownian bridges [8, 9] between the initial positions taken from the paths of two particles α and γ at the same timeslice and the final positions taken from the same two paths at a subsequent timeslice but exchaged, γ and α, so to connect particle α at the initial timeslice to particle γ at the final timeslice with one bridge and particle γ at the initial timeslice with particle α at the final timeslice. We accept or reject the move according to Metropolis algorithm [9, 13]. If the move is accepted one creates an exchange of two particles. Since any permutation of N particles can be obtained by composing a finite number of particles exchanges this is sufficient to simulate Bose-Einstein statistics in an exact numerical way. The Brownian bridge move is described in the next section.

In our simulations we measured the total potential energy $\mathscr{E}_P = v\langle V\rangle$ and the total kinetic energy

$$\mathscr{E}_K = \begin{cases} \dfrac{dN}{2\tau} - \dfrac{\langle(\vec{Q}_k - \vec{Q}_{k-1})^2\rangle}{4\lambda\tau^2} & \text{PWPIMC} \\ \dfrac{dN}{2\tau}\dfrac{\varphi}{1+\varphi} - \mu\dfrac{\langle\vec{\mathscr{P}}_k^2 + \vec{\mathscr{P}}_k'^2\rangle}{4m} & \text{CSPIMC} \end{cases} \tag{3.9}$$

where, given an observable $\mathscr{O}$, we denote with $\langle\mathscr{O}\rangle = \mathrm{tr}(\rho\mathscr{O})/\mathrm{tr}(\rho)$ the thermal average with 'tr' the trace operation. These expressions for $\mathscr{E}_K$ and $\mathscr{E}_P$ corresponds to the *thermodynamic* estimators of Ref. [8]. $\mathscr{E} = \mathscr{E}_K + \mathscr{E}_P$ is the total internal energy. The parameter μ, in the CSPIMC case, is necessary in order to find agreement with the kinetic energy of the PWPIMC, as explained in Ref. [1]. The kinetic energy from Eq. (3.9) is the small difference between two large quantities, infinite in the continuum $\tau \to 0$ limit. Note that in the $\xi \to \infty$ limit $\varphi/(1+\varphi) \to 1$ in agreement with the PWPIMC case.

IV. THE BRIDGE MOVE

In order to take into account the particles permutations it is necessary to construct two Brownian bridges between two different [1] randomly chosen particles in two randomly chosen many body beads to generate an exchange between the two particles. With one bridge we connect a real particle 1 and its ghosts on timeslice i to particle 2 and its ghosts on timeslice j and with the other we connect particle 2 and its ghosts on timeslice i to particle 1 and its ghosts on timeslice j with $i < j$. This will produce an *exchange* of particles 1 and 2 and their respective ghosts.

The Brownian bridge between particle 1 at $\boldsymbol{q}_{1,i}$ and particle 2 at $\boldsymbol{q}_{2,j}$ is built through the following multislice transition move [8],

$$\boldsymbol{q}_{\mathrm{new},i} = \boldsymbol{q}_{1,i} \tag{4.1}$$

$$\boldsymbol{q}_{\mathrm{new},k} = \boldsymbol{q}_{\mathrm{new},k-1} + \frac{\boldsymbol{q}_{2,j} - \boldsymbol{q}_{\mathrm{new},k-1}}{j-k+1} + \xi \qquad k = i+1,\ldots,j \tag{4.2}$$

where ξ is a random number with a Gaussian probability distribution [2] with zero mean and variance $\sigma^2(j-k)/(j-k+1)$ where $\sigma^2 = 2\lambda\tau$ is the diagonal free particle variance. The same move (4.1)-(4.2) is also carried out on the ghosts coordinates $\boldsymbol{\mathcal{Q}}^k_{\alpha,k}$ and $\boldsymbol{\mathcal{Q}}^{k+1}_{\alpha,k}$ and we leave untouched the momenta of the two ghosts.

The Metropolis (rejection) method [13] can sample any probability distribution provided that the transition rule satisfies detailed balance and ergodicity. The Metropolis algorithm is a particular way of ensuring that the transition rule satisfies detailed balance. It does this by splitting the *transition probability* into an "a priori" *sampling distribution* $T(S_{\mathrm{old}} \to S_{\mathrm{new}})$ (which is a probability distribution that we already know) and an *acceptance probability* $A(S_{\mathrm{old}} \to S_{\mathrm{new}})$.

$$P(S_{\mathrm{old}} \to S_{\mathrm{new}}) = T(S_{\mathrm{old}} \to S_{\mathrm{new}})A(S_{\mathrm{old}} \to S_{\mathrm{new}}), \tag{4.3}$$

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[1] A bridge between the same particle can still be used to sample the density matrix of distinguishable particles as can be done with the displacement move.

[2] This can be generated with the Box-Muller algorithm [9] for example.

where we denote with $S \equiv (\{s_k\}, \{s'_k\})$, $S_{\rm old}$ is the state configuration before the Markov move and $S_{\rm new}$ the proposed configuration state after the move produced by the transition with probability P.

In the generalized Metropolis procedure [9], trial moves are accepted according to:

$$A(S_{\rm old} \to S_{\rm new}) = \min[1, q(S_{\rm old} \to S_{\rm new})], \tag{4.4}$$

where

$$q(S_{\rm old} \to S_{\rm new}) = \frac{\pi(S_{\rm new}) T(S_{\rm new} \to S_{\rm old})}{\pi(S_{\rm old}) T(S_{\rm old} \to S_{\rm new})}. \tag{4.5}$$

where $\pi \propto e^{-\mathscr{S}} \propto \rho(s_0, s'_1; \tau)\rho(s_1, s'_2; \tau) \cdots \rho(s_{M-1}, s'_M; \tau)$ is the action probability distribution in the $s = (\{s_k\})$ configurations space. The transition probability corresponding to the move of Eqs. (4.1)-(4.2) is then given by

$$\frac{T(S_{\rm new} \to S_{\rm old})}{T(S_{\rm old} \to S_{\rm new})} \propto \exp\left\{ \frac{1}{4\lambda\tau} \sum_{k=i+1}^{j} \Big[(\boldsymbol{q}_{{\rm new},k} - \boldsymbol{q}_{{\rm new},k-1})^2 + (\boldsymbol{\mathcal{Q}}^k_{{\rm new},k} - \boldsymbol{\mathcal{Q}}^k_{{\rm new},k-1})^2 + (\boldsymbol{\mathcal{Q}}^{k+1}_{{\rm new},k} - \boldsymbol{\mathcal{Q}}^{k+1}_{{\rm new},k-1})^2 \right.$$
$$\left. - (\boldsymbol{q}_{{\rm old},k} - \boldsymbol{q}_{{\rm old},k-1})^2 - (\boldsymbol{\mathcal{Q}}^k_{{\rm old},k} - \boldsymbol{\mathcal{Q}}^k_{{\rm old},k-1})^2 - (\boldsymbol{\mathcal{Q}}^{k+1}_{{\rm old},k} - \boldsymbol{\mathcal{Q}}^{k+1}_{{\rm old},k-1})^2 \Big] \right\}. \tag{4.6}$$

In order to produce an exchange of two particles 1 and 2 one needs a combination of two bridge transitions as described above. Together with the real particles we propose also the exchange of the relative ghosts. Any permutation can be reached through a two particles exchange so the bridge transition move allows to sample the sum in Eq. (3.8).

In order to increase the acceptance ratios of this bridge and swap moves it is necessary to diminish ξ and the number $j - i$ of its timeslices. Of course our kinetic energy estimator is left unchanged by this bridge move since the ghosts momenta are not moved at all. But the potential energy obtained with only the bridge move converges to the same value obtained with the displace and the bridge moves together, as it should. Moreover the potential energy becomes more negative as ξ increases at constant φ, as expected.

V. NUMERICAL RESULTS

We here compare the conventional PWPIMC with our CSPIMC algorithm on specific simulations.

Our PWPIMC simulations (see Tables I, II and III, IV) confirm that at high temperature (classical regime) the nature of the statistics is not important. Whereas it becomes important at low temperatures (quantum regime). The zero temperature (ground state) limit can only be reached through an extrapolation of the PIMC results. In Tables I and II we use PWPIMC at constant $\tau = 0.025$ K^{-1} (same as Ref. [10]) and various temperatures. In Tables III and V we compare the PWPIMC with the CSPIMC for Boltzmann statistics at fixed $M = 250$ and various temperatures. In Tables IV and VI we do the same for Bose statistics. We found favorable match between PWPIMC and CSPIMC results for $\varphi = 0.7 \approx 2^{-1/2}$. [3] Each run has no less than 2×10^6 MC steps where one step is made of a displace move of all the timeslices of a single particle path and their associated ghost paths and a bridge move.

TABLE I. Results from **PW**PIMC for $N = 16$ ^{4}He atoms ($m = 0.0830594$) in two dimensions, with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556, \varepsilon = 10.22$ and a cutoff distance $r_{\rm cut} = 2.5$ (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a density $N/L^2 = 0.05$ and various temperatures T with $\tau = 0.025$, with **Boltzmann statistics**. In the Table $\mathscr{E}_K$ and $\mathscr{E}_P$ are the total kinetic and potential energies respectively. $\mathscr{E} = \mathscr{E}_K + \mathscr{E}_P$ is the total internal energy.

T (K)	$\mathscr{E}_K$ (K)	$-\mathscr{E}_P$ (K)	$-\mathscr{E}$ (K)
1.0	66.6(2)	94.4(1)	27.8
0.5	60.8(2)	92.9(1)	32.1
0.2	59.0(2)	93.00(8)	34.0
0.1	58.2(2)	93.23(8)	35.0

[3] Note that in Ref. [1] we fixed $\varphi = \pi/2$ but the comparison between CSPIMC and PWPIMC results was not very good. Moreover here we changed the acceptance probabilities of both the displace and the bridge moves.

TABLE II. Results from **PW**PIMC for $N = 16$ ^{4}He atoms ($m = 0.0830594$) in two dimensions, with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556, \varepsilon = 10.22$ and a cutoff distance $r_{\rm cut} = 2.5$ (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a density $N/L^2 = 0.05$ and various temperatures T with $\tau = 0.025$, with **Bose statistics**. In the Table $\mathscr{E}_K$ and $\mathscr{E}_P$ are the total kinetic and potential energies respectively. $\mathscr{E} = \mathscr{E}_K + \mathscr{E}_P$ is the total internal energy.

T (K)	$\mathscr{E}_K$ (K)	$-\mathscr{E}_P$ (K)	$-\mathscr{E}$ (K)
1.0	57.1(1)	94.8(3)	37.7
0.5	55.0(5)	93.4(2)	38.4
0.2	55.8(1)	93.55(5)	37.7
0.1	55.9(1)	93.46(5)	37.6

TABLE III. Results from **PW**PIMC for $N = 16$ ^{4}He atoms ($m = 0.0830594$) in two dimensions, with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556, \varepsilon = 10.22$ and a cutoff distance $r_{\rm cut} = 2.5$ (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a density $N/L^2 = 0.05$ and various temperatures T with $M = 250$, with **Boltzmann statistics**. The runs are 2×10^6 steps long. In the Table $\mathscr{E}_K$ and $\mathscr{E}_P$ are the total kinetic and potential energies respectively. $\mathscr{E} = \mathscr{E}_K + \mathscr{E}_P$ is the total internal energy (note that unlike Ref. [10] we fix M and not τ).

T (K)	$\mathscr{E}_K$ (K)	$-\mathscr{E}_P$ (K)	$-\mathscr{E}$ (K)
1.0	82.3(6)	83.6(1)	1.3(6)
0.5	74.6(4)	84.8(1)	10.2(4)
0.2	62.5(4)	90.5(1)	28.0(4)
0.1	49.0(2)	101.1(1)	52.1(2)

In Tables VII and VIII we performed simulations at fixed $\varphi = 0.7$, and fixed temperatures $T = 1$ (K) and $T = 0.2$ (K) respectively, at increasing numbers M of timeslices. We see that it is necessary to keep φ constant upon taking the continuum limit, $\tau \to 0$, in order to find agreement between the results for the CSPIMC and the ones for the PWPIMC for both the kinetic and potential energies. We find that, in the continuum limit, μ tends to ≈ 0.4.

VI. CONCLUSIONS

In this short work we proposed and tested a possible realization of the Brownian bridge move in the CSPIMC algorithm presented in our recent work of Ref. [1]. As discussed in that work in the CSPIMC algorithm is necessary to take the continuum limit at fixed $\varphi = \xi\tau/m$ by letting $\tau \to 0$ and $\xi \to \infty$. For non zero τ, we found agreement

TABLE IV. Results from **PW**PIMC for $N = 16$ ^{4}He atoms ($m = 0.0830594$) in two dimensions, with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556, \varepsilon = 10.22$ and a cutoff distance $r_{\rm cut} = 2.5$ (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a density $N/L^2 = 0.05$ and various temperatures T with $M = 250$, with **Bose statistics**. The runs are 2×10^6 steps long. In the Table $\mathscr{E}_K$ and $\mathscr{E}_P$ are the total kinetic and potential energies respectively. $\mathscr{E} = \mathscr{E}_K + \mathscr{E}_P$ is the total internal energy (note that unlike Ref. [10] we fix M and not τ).

T (K)	$\mathscr{E}_K$ (K)	$-\mathscr{E}_P$ (K)	$-\mathscr{E}$ (K)
1.0	77(1)	84.1(4)	7.1(4)
0.5	69.7(7)	84.6(4)	14.9(7)
0.2	60.0(5)	90.6(1)	30.6(5)
0.1	49.3(3)	101.1(2)	51.8(3)

TABLE V. Results from **CS**PIMC with $\varphi = 0.7$ for $N = 16$ ^{4}He atoms ($m = 0.0830594$) in two dimensions, with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556, \varepsilon = 10.22$ and a cutoff distance $r_{\rm cut} = 2.5$ (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a density $N/L^2 = 0.05$ and various temperatures T with $M = 250$, with **Boltzmann statistics**. The runs are 2×10^6 steps long. In the Table $\mathscr{E}_K$ is taken from Table III and used to determine μ. $\mathscr{E}_P$ is the total potential energy.

T (K)	$\langle \vec{\mathscr{P}}_k^2 + \vec{\mathscr{P}}_k'^2 \rangle / 4m$ (K)	$\mathscr{E}_K$ (K)	$-\mathscr{E}_P$ (K)	μ
1.0	3550(6)	82.3	84.4(4)	0.44
0.5	1608(3)	74.6	85.4(2)	0.47
0.2	607(1)	62.5	90.3(2)	0.44
0.1	293.3(1)	49.0	99.1(1)	0.40

TABLE VI. Results from **CS**PIMC with $\varphi = 0.7$ for $N = 16$ ^{4}He atoms ($m = 0.0830594$) in two dimensions, with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556, \varepsilon = 10.22$ and a cutoff distance $r_{\rm cut} = 2.5$ (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a density $N/L^2 = 0.05$ and various temperatures T with $M = 250$, with **Bose statistics**. The runs are 2×10^6 steps long. In the Table $\mathscr{E}_K$ is taken from Table IV and used to determine μ. $\mathscr{E}_P$ is the total potential energy.

T (K)	$\langle \vec{\mathscr{P}}_k^2 + \vec{\mathscr{P}}_k'^2 \rangle / 4m$ (K)	$\mathscr{E}_K$ (K)	$-\mathscr{E}_P$ (K)	μ
1.0	3721(5)	77	82.6(2)	0.42
0.5	1611(3)	69.7	86.4(2)	0.48
0.2	606.8(8)	60.0	89.8(1)	0.44
0.1	293.0(1)	49.3	100.42(6)	0.40

between our CSPIMC and the conventional PWPIMC for $\varphi \approx 2^{-1/2}$. [4] So that

$$\text{CSPIMC} \xrightarrow{\varphi \to 1/\sqrt{2}} \text{PWPIMC},$$

where the CSPIMC is the PIMC proposed in Ref. [1] and PWPIMC is the PIMC defined in Ref. [8].

Since in the bridge move we do not move the two ghosts momenta it is always necessary to use this move together with the displace move. For Boltzmann statistics we will only construct bridges between two timeslices of the same particle path. Whereas in the Bose-Einstein statistics the bridges are between two timeslices of two different particles paths allowing therefore the two particles exchange. Clearly for Boltzmann statistics we can just use the displace move even if the use of both the displace and the bridge moves allows faster equilibration of the random walk. [5]

TABLE VII. Results from **CS**PIMC with $\varphi = 0.7$ for $N = 16$ ^{4}He atoms ($m = 0.0830594$) in two dimensions, with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556, \varepsilon = 10.22$ and a cutoff distance $r_{\rm cut} = 2.5$ (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a density $N/L^2 = 0.05$ and a temperature $T = 0.2$ with various values of M, with **Boltzmann statistics**. In the Table $\mathscr{E}_K \approx 62.5$ is used to determine μ. $\mathscr{E}_P$ is the total potential energy. The PWPIMC at $M = 1000$ gives an $\mathscr{E}_P = -83.64(7)$.

M	$\langle \vec{\mathscr{P}}_k^2 + \vec{\mathscr{P}}_k'^2 \rangle / 4m$ (K)	μ	$-\mathscr{E}_P$ (K)
250	607(1)	0.44	90.3(2)
500	1268(1)	0.47	86.7(1)
750	2208(3)	0.42	88.0(1)
1000	4156(4)	0.30	86.0(3)

[4] This corrects the value $\approx \pi/2$ used in Ref. [1].

[5] Note that for distinguishable particles we may use just the displace move without the bridge move but not the bridge move without the displace move.

TABLE VIII. Results from **CS**PIMC with $\varphi = 0.7$ for $N = 16$ ^{4}He atoms ($m = 0.0830594$) in two dimensions, with a Lennard-Jones pair potential with parameters [11] $\sigma = 2.556, \varepsilon = 10.22$ and a cutoff distance $r_{\rm cut} = 2.5$ (so that $v(r) = 0$ for $r > r_{\rm cut}\sigma$ without long range corrections), at a density $N/L^2 = 0.05$ and a temperature $T = 0.2$ with various values of M, with **Bose statistics**. In the Table $\mathscr{E}_K \approx 60.0$ is used to determine μ. $\mathscr{E}_P$ is the total potential energy. The PWPIMC at $M = 1000$ gives an $\mathscr{E}_P = -84.0(1)$.

M	$\langle \vec{\mathscr{P}}_k^2 + \vec{\mathscr{P}}_k'^2 \rangle / 4m$ (K)	μ	$-\mathscr{E}_P$ (K)
250	606.8(8)	0.44	89.8(1)
500	1272(1)	0.47	86.2(1)
750	2241(5)	0.41	87.8(2)
1000	4193(3)	0.30	85.2(2)

The necessary relation

$$\xi = \frac{m}{\sqrt{2}\tau},$$

tells that in the continuum limit $\tau \to 0$ the unit mass, $m_{h.o.} = 1$, harmonic oscillator underlying the coherent states tends to become infinitely stiff with a diverging elastic constant $k = 4\xi^2 \to \infty$.

But we see that in the pure CSPIMC we are free to change φ. This is made possible since the two ghosts for each particle are given a role before integrating them out. CSPIMC with different φ will have different continuum limits $\tau \to 0$. This freedom allows to explore domains different from the one of conventional PWPIMC. And this is the main novelty of our CSPIMC method. Clearly, in the continuum limit $\tau \to 0$, the CSPIMC becomes independent of ξ, i.e. of the properties of the harmonic oscillator generating the coherent states.

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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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