Path Integral Monte Carlo and the Worm Algorithm in the Spatial Continuum

Adrian Del Maestro*
Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA and
Min H. Kao Department of Electrical Engineering and Computer Science,
University of Tennessee, Knoxville, TN 37996, USA
(Dated: November 29, 2021)

The goal of these lecture notes will be to describe a stochastically exact quantum Monte Carlo method for computing the expectation value of observables for systems of interacting particles in the spatial continuum described by a Hamiltonian which conserves particle number. The latest version of the notes can always be found online at `https://github.com/agdelma/pimc-notes` while instructions on how to obtain, install and run our groups continuous space worm algorithm code are located at `http://code.delmaestro.org`.

I. EXPECTATION VALUES AND THE PARTITION FUNCTION

We begin with the general definition for the expectation value of some operator $\hat{\mathcal{O}}$ in terms of a trace over configurations

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\, \hat{\mathcal{O}} \mathrm{e}^{-\beta \hat{\mathcal{H}}} \tag{1}$$

where $\beta = 1/k_\mathrm{B}T$ with k_B the Boltzmann constant and the partition function $\mathcal{Z}$ is given by

$$\mathcal{Z} = \mathrm{Tr}\, \mathrm{e}^{-\beta \hat{\mathcal{H}}} = \mathrm{Tr}\, \hat{\rho} \tag{2}$$

where

$$\hat{\rho} \equiv \mathrm{e}^{-\beta \hat{\mathcal{H}}} \tag{3}$$

is the density matrix. In order to compute the trace in Eq. (2) for a given system described by Hamiltonian $\hat{\mathcal{H}}$ we need to identify a set of convenient basis states $|\gamma\rangle$ that can be efficiently sampled allowing us to write the partition function as the direct sum

$$\begin{aligned} \mathcal{Z} &= \sum_\gamma \langle \gamma | \mathrm{e}^{-\beta \hat{\mathcal{H}}} | \gamma \rangle \\ &\approx \sum_\gamma W(\gamma) \end{aligned} \tag{4}$$

where $W(\gamma)$ is a positive real weight corresponding to configuration state $|\gamma\rangle$. In the next section we will introduce the specific form of $|\gamma\rangle$ in terms of the spatial positions of interacting particles and describe a method for computing the partition function as a sum of weights.

II. PATH INTEGRAL MONTE CARLO

The path-integral Monte Carlo method was first introduced by David Ceperley, and a comprehensive review can be found in Ref. [1]. Here we will attempt to provide an introduction to the method with sufficient details to allow for the creation of a simple code.

We are interested in a system of interacting particles described by the general many-body Hamiltonian:

$$\begin{aligned} \hat{\mathcal{H}} &= \hat{\mathcal{T}} + \hat{\mathcal{V}} \\ &= -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \hat{\boldsymbol{\nabla}}_i^2 + \sum_{i=1}^{N} \hat{V}_i + \sum_{i<j} \hat{U}_{ij}. \end{aligned} \tag{5}$$

It will be convenient to work in first quantized notation, where the N particles in the d-dimensional spatial continuum are located at positions $\boldsymbol{r}_i$ with $i = 1 \ldots N$. The first term in Eq. (5) corresponds to the kinetic energy $\hat{\mathcal{T}}$ where m_i

is the mass of the i^{th} particle. The external potential energy $V(\boldsymbol{r_i})$ only depends on the position of a single particle, while the two-body interaction potential $U(\boldsymbol{r}_i - \boldsymbol{r}_j)$ is in general a function of the vector displacement between them. We will most often work with spherically symmetric interaction potentials such that $U(\boldsymbol{r}_i - \boldsymbol{r}_j) = U(|\boldsymbol{r}_i - \boldsymbol{r}_j|)$ and we will neglect all self-interactions: $\hat{U}_{ii} = 0$. A physical system of interest could include trapped ultra-cold atoms, where $V(\boldsymbol{r}_i) \sim |\boldsymbol{r}_i|^2$ is a harmonic trapping potential and the particles interact via an induced dipole-dipole interaction $U(\boldsymbol{r}_i - \boldsymbol{r}_j) \sim |\boldsymbol{r}_i - \boldsymbol{r}_j|^{-3}$.

The most natural basis states $|\gamma\rangle$ are just a collection of the spatial locations of the N particles, where in the case of identical particles, the labels are fictitious. We will employ the convenient short-hand notation

$$|\boldsymbol{R}\rangle \equiv |\boldsymbol{r}_1, \cdots, \boldsymbol{r}_N\rangle \tag{6}$$

where particle conservation enforces the normalization constraint

$$\int \mathcal{D}\boldsymbol{R}\, |\boldsymbol{R}\rangle\langle\boldsymbol{R}| = \mathbb{1} \tag{7}$$

with

$$\int \mathcal{D}\boldsymbol{R} \equiv \prod_{i=1}^{N} \int d\boldsymbol{r}_i. \tag{8}$$

In the first-quantized spatial position basis, the partition function can be written as a $N \times d$ dimensional integral

$$\begin{aligned} \mathcal{Z} &= \operatorname{Tr} \mathrm{e}^{-\beta\hat{\mathcal{H}}} \\ &= \int d\boldsymbol{r}_1 \cdots \int d\boldsymbol{r}_N \langle \boldsymbol{r}_1, \cdots, \boldsymbol{r}_N | \mathrm{e}^{-\beta\hat{\mathcal{H}}} | \boldsymbol{r}_1, \cdots, \boldsymbol{r}_N \rangle \\ &\equiv \int \mathcal{D}\boldsymbol{R} \langle \boldsymbol{R} | \mathrm{e}^{-\beta\hat{\mathcal{H}}} | \boldsymbol{R} \rangle. \end{aligned} \tag{9}$$

As terms like this will appear quite frequently, it will be useful to define the elements of the density matrix at inverse temperature β in the spatial basis

$$\rho(\boldsymbol{R}, \boldsymbol{R}'; \beta) \equiv \langle \boldsymbol{R} | \mathrm{e}^{-\beta\hat{\mathcal{H}}} | \boldsymbol{R}' \rangle \tag{10}$$

where all matrix elements are real and positive. We note that in the spatial continuum, the Hilbert space is uncountably infinite, as the particles can take on any position in $\mathbb{R}^d$. This is an important observation that will guide the strategy we choose in the duration of these notes. Using the expression for $\rho(\boldsymbol{R}, \boldsymbol{R}'; \beta)$ we can write the partition function:

$$\mathcal{Z} = \int \mathcal{D}\boldsymbol{R}\, \rho(\boldsymbol{R}, \boldsymbol{R}; \beta). \tag{11}$$

As we have defined the potential operator $\hat{\mathcal{V}}$ to be diagonal in the position basis, it would be extremely convenient if we could decompose the density matrix into a product of terms containing $\hat{\mathcal{T}}$ and $\hat{\mathcal{V}}$. However, we know that $[\hat{\mathcal{T}}, \hat{\mathcal{V}}] \neq 0$ and thus

$$\begin{aligned} \hat{\rho} &= \mathrm{e}^{-\beta(\hat{\mathcal{T}} + \hat{\mathcal{V}})} \\ &\neq \mathrm{e}^{-\beta\hat{\mathcal{T}}} \mathrm{e}^{-\beta\hat{\mathcal{V}}}. \end{aligned} \tag{12}$$

In fact, by employing the Baker-Campbell-Hausdorff formula we know:

$$\mathrm{e}^{\epsilon(\hat{A}+\hat{B})} = \mathrm{e}^{\epsilon\hat{A}} \mathrm{e}^{\epsilon\hat{B}} \mathrm{e}^{-\frac{\epsilon^2}{2}[\hat{A},\hat{B}]} \tag{13}$$

where $\epsilon \in \mathbb{C}$ and thus

$$\hat{\rho} = \mathrm{e}^{-\beta\hat{\mathcal{T}}} \mathrm{e}^{-\beta\hat{\mathcal{V}}} + \mathrm{O}\left(\beta^2\right). \tag{14}$$

with the error diverging in the interesting (and quantum) low temperature limit $\beta \gg 1$. However, we may make the rather self-evident observation that the Hamiltonian must commute with itself, $[\hat{\mathcal{H}}, \hat{\mathcal{H}}] = 0$ thus

$$\begin{aligned} \hat{\rho} &= \mathrm{e}^{-\beta\hat{\mathcal{H}}} \\ &= \mathrm{e}^{-\frac{\beta}{2}\hat{\mathcal{H}} - \frac{\beta}{2}\hat{\mathcal{H}}} \\ &= \mathrm{e}^{-\frac{\beta}{2}\hat{\mathcal{H}}} \mathrm{e}^{-\frac{\beta}{2}\hat{\mathcal{H}}}. \end{aligned} \tag{15}$$

In the position basis, this corresponds to the elements of the density matrix satisfying a convolution relation

$$\begin{aligned}\rho(\boldsymbol{R},\boldsymbol{R}';\beta) &= \langle \boldsymbol{R}|\mathrm{e}^{-\beta\hat{\mathcal{H}}}|\boldsymbol{R}'\rangle \\ &= \langle \boldsymbol{R}|\mathrm{e}^{-\frac{\beta}{2}\hat{\mathcal{H}}}\mathrm{e}^{-\frac{\beta}{2}\hat{\mathcal{H}}}|\boldsymbol{R}'\rangle \\ &= \int \mathcal{D}\boldsymbol{R}''\,\langle \boldsymbol{R}|\mathrm{e}^{-\frac{\beta}{2}\hat{\mathcal{H}}}|\boldsymbol{R}''\rangle\langle \boldsymbol{R}''|\mathrm{e}^{-\frac{\beta}{2}\hat{\mathcal{H}}}|\boldsymbol{R}'\rangle \\ &= \int \mathcal{D}\boldsymbol{R}''\,\rho\left(\boldsymbol{R},\boldsymbol{R}'';\frac{\beta}{2}\right)\rho\left(\boldsymbol{R}'',\boldsymbol{R}';\frac{\beta}{2}\right)\end{aligned} \tag{16}$$

where have employed the normalization condition in Eq. (7) and we note that the individual density matrices are at a higher effective temperature: $\beta \to \beta/2 \Rightarrow T \to 2T$. Now, returning to Eq. (11), we can employ this convolution relation M times where $M \in \mathbb{Z} \gg 1$ to yield a new expression for the partition function

$$\begin{aligned}\mathcal{Z} &= \int \mathcal{D}\boldsymbol{R}\,\rho(\boldsymbol{R},\boldsymbol{R};\beta) \\ &= \int \mathcal{D}\boldsymbol{R}_0 \cdots \int \mathcal{D}\boldsymbol{R}_{M-1}\,\rho\left(\boldsymbol{R}_0,\boldsymbol{R}_1;\frac{\beta}{M}\right)\cdots\rho\left(\boldsymbol{R}_{M-1},\boldsymbol{R}_0;\frac{\beta}{M}\right)\end{aligned} \tag{17}$$

where we have introduced the new notation

$$|\boldsymbol{R}_\alpha\rangle \equiv |\boldsymbol{r}_{1,\alpha},\cdots,\boldsymbol{r}_{N,\alpha}\rangle. \tag{18}$$

Until now, we have not specified the symmetry of the particles, but for the duration of these notes we will consider systems of identical bosons and thus we can write Eq. (17) in a more compact form:

$$\mathcal{Z} = \frac{1}{N!}\sum_{\mathcal{P}}\prod_{\alpha=0}^{M-1}\int \mathcal{D}\boldsymbol{R}_\alpha\,\rho\left(\boldsymbol{R}_\alpha,\boldsymbol{R}_{\alpha+1};\frac{\beta}{M}\right) \tag{19}$$

where the sum is over all permutations $\mathcal{P}$ of the fictitious particle labels i, and we require

$$|\boldsymbol{R}_M\rangle = \hat{\mathcal{P}}|\boldsymbol{R}_0\rangle = \left|\boldsymbol{r}_{\mathcal{P}(1),0},\cdots\boldsymbol{r}_{\mathcal{P}(N),0}\right\rangle \tag{20}$$

to ensure the trace is non-zero.

Upon closer examination of the individual terms in the product, we may notice:

$$\langle \boldsymbol{R}_\alpha|\mathrm{e}^{-\frac{\beta}{M}\hat{\mathcal{H}}}|\boldsymbol{R}_{\alpha+1}\rangle = \left\langle \boldsymbol{R}_\alpha\left|\hat{\mathcal{U}}\left(-i\hbar\frac{\beta}{M}\right)\right|\boldsymbol{R}_{\alpha+1}\right\rangle \tag{21}$$

where

$$\hat{\mathcal{U}}(t) \equiv \mathrm{e}^{-it\hat{\mathcal{H}}/\hbar} \tag{22}$$

is the unitary time evolution operator of single particle quantum mechanics. Through the definition:

$$t = -i\hbar\tau \tag{23}$$

where

$$\tau \equiv \frac{\beta}{M} \tag{24}$$

we may identify Eq. (19) as the partition function of a N particle system which evolves in an *imaginary time* direction. The configurations of our system now correspond to M discrete classical configurations corresponding to the positions of the N particles: $|\boldsymbol{r}_{1,\alpha},\cdots,\boldsymbol{r}_{N,\alpha}\rangle$ where adjacent configurations in imaginary time at $\alpha\tau$ and $(\alpha+1)\tau$ are connected via an insertion of the short-imaginary-time propagator

$$\begin{aligned}\rho(\boldsymbol{R}_\alpha,\boldsymbol{R}_{\alpha+1};\tau) &= \langle \boldsymbol{R}_\alpha|\mathrm{e}^{-\frac{\beta}{2}\hat{\mathcal{H}}}|\boldsymbol{R}_{\alpha+1}\rangle \\ &= \langle \boldsymbol{R}_\alpha|\hat{\mathcal{U}}(-i\hbar\tau)|\boldsymbol{R}_{\alpha+1}\rangle.\end{aligned}$$

This is simply a re-statement of the discrete Feynman path integral formulation of quantum statistical mechanics[2], or equivalently the quantum-classical mapping, which says that a d-dimensional quantum system can be represented as a $(d+1)$-dimensional classical system, where the extra $(+1)^{th}$ dimension is potentially subject to an additional boundary condition.

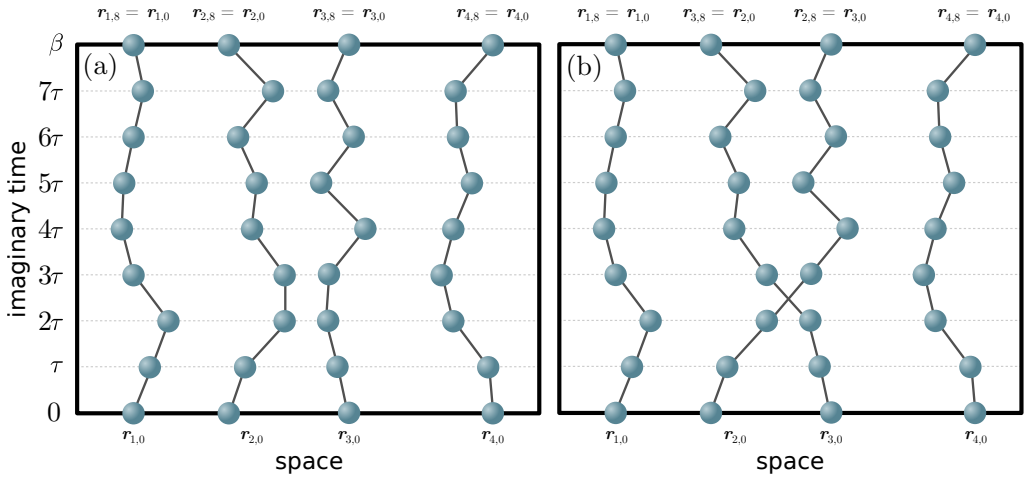

FIG. 1. A sample configuration $N = 4$ particles in d spatial dimensions ($d = 1$ here) where we have chosen $M = 8$ such that $\tau = \beta/8$. The actual spatial positions of the particles are identical in panels (a) and (b), however they differ by a reconnection between imaginary times 2τ and 3τ corresponding to a permutation of the particle labels $|R_8\rangle_{\mathrm{a}} = |R_0\rangle = |\boldsymbol{r}_{1,0}, \boldsymbol{r}_{2,0}, \boldsymbol{r}_{3,0}, \boldsymbol{r}_{4,0}\rangle$ while $|R_8\rangle_{\mathrm{b}} = \hat{\mathcal{P}}|R_0\rangle = |\boldsymbol{r}_{1,0}, \boldsymbol{r}_{3,0}, \boldsymbol{r}_{2,0}, \boldsymbol{r}_{4,0}\rangle$.

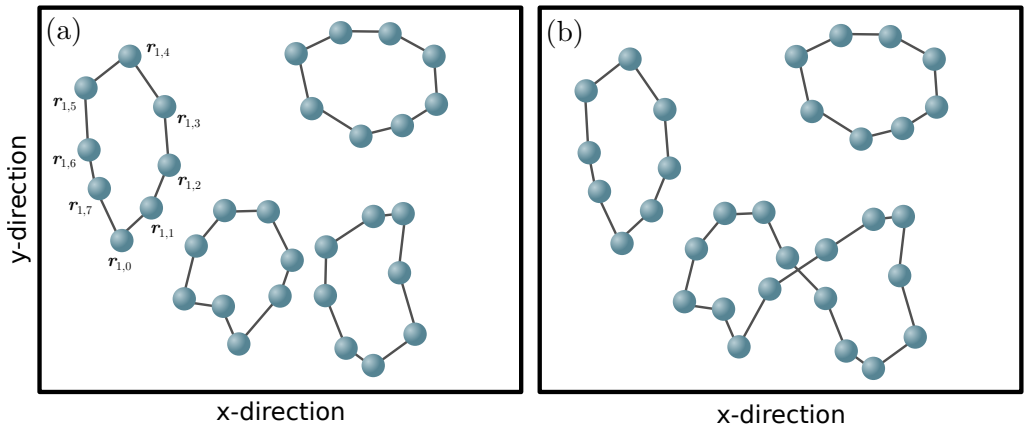

FIG. 2. Discrete particle worldlines can also be viewed as classical ring polymers where only beads on the same imaginary time slice interact between polymers. Here we have again chosen $N = 4$ and $M = 8$ with (a) and (b) differing by a particle permutation, which in this picture results in the "linking" of spatially adjacent polymers.

A. Configurations

We are now ready to unambiguously identify the configurations that will be sampled in our Monte Carlo. For a system of N particles, they will consist of N discrete *worldlines* as shown in Figure 1. These worldlines are composed of a series of "beads" which represent the spatial positions of the particles at a given imaginary time slice and a set of links which connect them and define a permutation of particle labels. Thus, the primary data structures used to store the configurations of the system include a $d \times N \times M$ tensor for the positions and a $2 \times N \times M$ tensor for the links allowing for the identification of any bead $\boldsymbol{r}_{i,\alpha}$ and its imaginary time neighbor at $\boldsymbol{r}_{i,\alpha+1}$.

Motivated by the imaginary time boundary condition $|\boldsymbol{R}_M\rangle = \hat{\mathcal{P}}|\boldsymbol{R}_0\rangle$, Chandler and Wolynes[3] introduced an alternative way to think about the worldlines in terms of an isomorphism to classical "ring polymers". Under the identity permutation, these polymers consist of M beads, but as permutations take place, the number of beads can grow to some nM where $1 \leq n \leq N$. This can be most easily visualized in two spatial dimensions as shown in Figure 2. We can now make a number of important observations:

1. A classical particle would consist of a "polymer" of zero radius.

2. The spatial extent of a polymer is related to the thermal de Broglie wavelength $\lambda_{\rm dB} = \sqrt{2\pi\hbar^2/mk_{\rm B}T}$.

3. For a finite size system with periodic boundary conditions, worldlines can *wind* around the cell as the number of beads per polymer grows via permutations which are more favorable at low temperatures. The width of the distribution of integer winding numbers is related to the superfluid fraction.

B. Weights

Now that we have identified our configurations, in order to devise a sampling scheme we must return to the partition function in Eq. (19) and attempt to compute the weights. Our construction thus far has been approximation free, and we have yet to utilize the fact that the new form of the partition function includes the elements of effective high temperature density matrices in the limit where $M \gg 1$. Consider a single transition amplitude:

$$\rho(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \tau) = \langle \boldsymbol{R}_\alpha | \mathrm{e}^{-\tau(\hat{T}+\hat{V})} | \boldsymbol{R}_{\alpha+1} \rangle \tag{25}$$

where we can now ignore the fact that $[\hat{\mathcal{T}}, \hat{\mathcal{V}}] \neq 0$ at the cost of an error that grows as τ^2. This is the *Primitive Approximation* and the error can be made arbitrarily small at a given temperature at the linear cost of increasing M. In practice, we can utilize various schemes to drastically improve the error by explicitly evaluating the commutator that appears in Eq. (13) and we have chosen to employ a fourth order scheme called the generalized Suzuki factorization[4]. For the purposes of these lecture notes, the primitive approximation will be sufficient to illustrate all concepts and we can write

$$\begin{aligned}
\rho(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \tau) &= \langle \boldsymbol{R}_\alpha | \mathrm{e}^{-\tau\hat{\mathcal{T}}} \mathrm{e}^{-\tau\hat{\mathcal{V}})} | \boldsymbol{R}_{\alpha+1} \rangle + \mathrm{O}(\tau^2) \\
&= \int \mathcal{D}\boldsymbol{R}' \, \langle \boldsymbol{R}_\alpha | \mathrm{e}^{-\tau\hat{\mathcal{T}}} | \boldsymbol{R}' \rangle \langle \boldsymbol{R}' | \mathrm{e}^{-\tau\hat{\mathcal{V}})} | \boldsymbol{R}_{\alpha+1} \rangle \\
&= \int \mathcal{D}\boldsymbol{R}' \, \langle \boldsymbol{R}_\alpha | \mathrm{e}^{-\tau\hat{\mathcal{T}}} | \boldsymbol{R}' \rangle \langle \boldsymbol{R}' | \boldsymbol{R}_{\alpha+1} \rangle \mathrm{e}^{-\tau\mathcal{V}(\boldsymbol{R}_{\alpha+1})} \\
&= \int \mathcal{D}\boldsymbol{R}' \, \langle \boldsymbol{R}_\alpha | \mathrm{e}^{-\tau\hat{\mathcal{T}}} | \boldsymbol{R}' \rangle \delta(\boldsymbol{R}' - \boldsymbol{R}_{\alpha+1}) \mathrm{e}^{-\tau\mathcal{V}(\boldsymbol{R}_{\alpha+1})} \\
&= \langle \boldsymbol{R}_\alpha | \mathrm{e}^{-\tau\hat{\mathcal{T}}} | \boldsymbol{R}_{\alpha+1} \rangle \mathrm{e}^{-\tau\mathcal{V}(\boldsymbol{R}_{\alpha+1})}
\end{aligned} \tag{26}$$

where we have inserted a complete set of states in line 2 and utilized the fact that the potential energy operator is diagonal in imaginary time. We have introduced a slight abuse of the set notation $\boldsymbol{R} = \{\boldsymbol{r}_1, \cdots, \boldsymbol{r}_N\}$ where, for example, the Dirac delta function is understood to mean

$$\delta(\boldsymbol{R} - \boldsymbol{R}') \equiv \prod_{i=1}^{N} \delta(\boldsymbol{r}_i - \boldsymbol{r}_i') \tag{27}$$

and

$$\mathcal{V}(\boldsymbol{R}) \equiv \sum_{i=1}^{N} V(\boldsymbol{r}_i) + \frac{1}{2} \sum_{i,j} U(\boldsymbol{r}_i - \boldsymbol{r}_j). \tag{28}$$

Since the kinetic energy operator $\hat{\mathcal{T}}$ is clearly not diagonal in the spatial position basis, in order to compute the first term in Eq. (26) we can write the position eigenstate in terms of free particle plane waves

$$\begin{aligned}
|\boldsymbol{R}\rangle &= |\boldsymbol{r}_1, \cdots, \boldsymbol{r}_N\rangle \\
&= \prod_{i=1}^{N} \int \frac{d\boldsymbol{k}_i}{(2\pi)^d} \mathrm{e}^{i\boldsymbol{k}_i \cdot \boldsymbol{r}_i} |\boldsymbol{k}_1, \cdots, \boldsymbol{k}_N\rangle.
\end{aligned} \tag{29}$$

Defining

$$\lambda \equiv \frac{\hbar^2}{2m} \tag{30}$$

we can write

$$\begin{aligned}
\langle \boldsymbol{R}|\mathrm{e}^{-\tau\hat{\mathcal{T}}}|\boldsymbol{R}'\rangle &= \prod_{i=1}^{N}\int\frac{d\boldsymbol{k}_i}{(2\pi)^d}\int\frac{d\boldsymbol{k}_i'}{(2\pi)^d}\mathrm{e}^{-i\boldsymbol{k}_i\cdot\boldsymbol{r}_i}\mathrm{e}^{i\boldsymbol{k}_i'\cdot\boldsymbol{r}_i'}\left\langle \boldsymbol{k}_1,\cdots,\boldsymbol{k}_N\left|\mathrm{e}^{\tau\lambda\sum_{j=1}^{N}\hat{\boldsymbol{\nabla}}_j^2}\right|\boldsymbol{k}_1',\cdots,\boldsymbol{k}_N'\right\rangle \\
&= \prod_{i=1}^{N}\int\frac{d\boldsymbol{k}_i}{(2\pi)^d}\int\frac{d\boldsymbol{k}_i'}{(2\pi)^d}\mathrm{e}^{-\lambda\tau|\boldsymbol{k}_i'|^2-i\boldsymbol{k}_i\cdot\boldsymbol{r}_i+i\boldsymbol{k}_i'\cdot\boldsymbol{r}_i'}\left\langle \boldsymbol{k}_1,\cdots,\boldsymbol{k}_N|\boldsymbol{k}_1',\cdots,\boldsymbol{k}_N'\right\rangle \\
&= \prod_{i=1}^{N}\int\frac{d\boldsymbol{k}_i}{(2\pi)^d}\int\frac{d\boldsymbol{k}_i'}{(2\pi)^d}\mathrm{e}^{-\lambda\tau|\boldsymbol{k}_i'|^2-i\boldsymbol{k}_i\cdot\boldsymbol{r}_i+i\boldsymbol{k}_i'\cdot\boldsymbol{r}_i'}(2\pi)^d\delta(\boldsymbol{k}_i-\boldsymbol{k}_i') \\
&= \prod_{i=1}^{N}\int\frac{d\boldsymbol{k}_i}{(2\pi)^d}\mathrm{e}^{-\lambda\tau|\boldsymbol{k}_i|^2+i\boldsymbol{k}_i\cdot(\boldsymbol{r}_i'-\boldsymbol{r}_i)} \\
&= (4\pi\lambda\tau)^{-Nd/2}\exp\left[-\frac{1}{4\lambda\tau}\sum_{i=1}^{N}|\boldsymbol{r}_i-\boldsymbol{r}_i'|^2\right]
\end{aligned} \tag{31}$$

which is just the free particle propagator that can be written in our set notation as

$$\begin{aligned}
\rho_0(\boldsymbol{R},\boldsymbol{R}';\tau) &= \left\langle \boldsymbol{R}\left|\mathrm{e}^{-\tau\hat{\mathcal{T}}}\right|\boldsymbol{R}'\right\rangle \\
&= (4\pi\lambda\tau)^{-Nd/2}\mathrm{e}^{-\frac{1}{4\lambda\tau}|\boldsymbol{R}-\boldsymbol{R}'|^2}.
\end{aligned} \tag{32}$$

We may now insert our complete expression for the primitive imaginary time propagator

$$\rho(\boldsymbol{R}_\alpha,\boldsymbol{R}_{\alpha+1};\tau) = \rho_0(\boldsymbol{R}_\alpha,\boldsymbol{R}_{\alpha+1};\tau)\mathrm{e}^{-\tau\mathcal{V}(\boldsymbol{R}_\alpha)} \tag{33}$$

into the partition function in Eq. (19) to find

$$\begin{aligned}
\mathcal{Z} &= (4\pi\lambda\tau)^{-NMd/2}\frac{1}{N!}\sum_{\mathcal{P}}\prod_{\alpha=0}^{M-1}\int\mathcal{D}\boldsymbol{R}_\alpha\,\mathrm{e}^{-\frac{1}{4\lambda\tau}|\boldsymbol{R}_\alpha-\boldsymbol{R}_{\alpha+1}|^2-\tau\mathcal{V}(\boldsymbol{R}_\alpha)} \\
&= (4\pi\lambda\tau)^{-NMd/2}\frac{1}{N!}\sum_{\mathcal{P}}\prod_{\alpha=0}^{M-1}\prod_{i=1}^{N}\int d\boldsymbol{r}_{i,\alpha}\exp\left\{-\sum_{\alpha=0}^{M}\sum_{i=1}^{N}\left[\frac{|\boldsymbol{r}_{i,\alpha+1}-\boldsymbol{r}_{i,\alpha}|^2}{4\lambda\tau}+\tau V(\boldsymbol{r}_{i,\alpha})+\frac{\tau}{2}\sum_{j=1}^{N}U(\boldsymbol{r}_{i,\alpha}-\boldsymbol{r}_{j,\alpha})\right]\right\}.
\end{aligned} \tag{34}$$

Because of the product of M copies of the primitive propagator, the finite Trotter error we make in the partition function is $\mathrm{O}(\tau)$. This partition function is then just a "path" integral over all possible configurations and permutations of particle worldlines where the weight of each configuration is just the exponentiated effective action.

C. Updates

In order to sample configurations we must devise a series of updates that can be proposed and accepted or rejected based on their weights. We are aided by the fact that it is possible to exactly sample the free density matrix $\rho_0(\boldsymbol{R},\boldsymbol{R}';\tau)$ since it is just a product of Gaussians. This will allow us to sample the kinetic part of the action in the ensemble and only consider the potential action in the weights. We will outline two types of simple updates, center-of-mass and staging moves, and briefly discuss a third permutation move that will present us with a difficult challenge.

1. Center of Mass

A center-of-mass update involves the spatial translation of an entire worldline, leaving the kinetic part of the action unchanged. It is shown schematically in Figure 3 and proceeds as follows:

1. Choose a random integer $i \in [0, N-1]$ fixing worldline i with beads located at $\boldsymbol{r}_{i,\alpha}$.

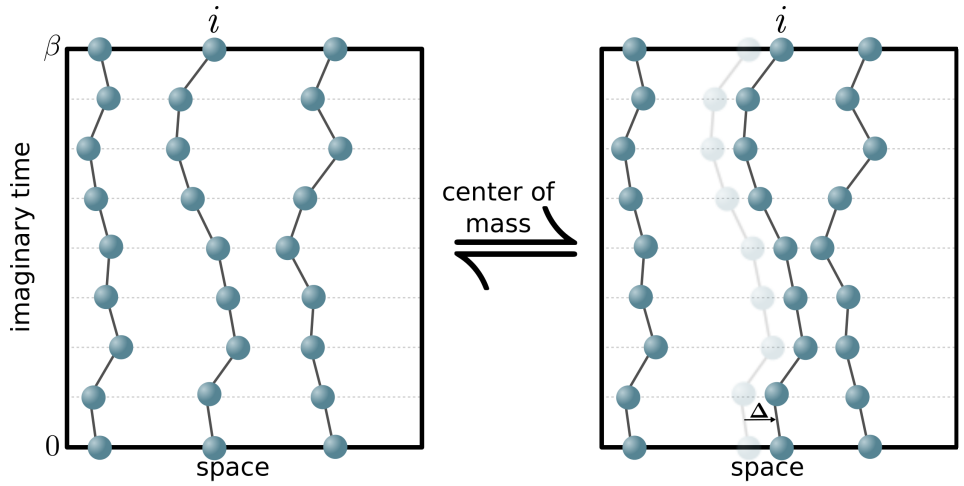

FIG. 3. A *center of mass* Monte Carlo update, which translates the entire worldline i by a vector displacement $\boldsymbol{\Delta}$ without modifying the connections between beads.

2. Generate uniformly distributed random numbers, Δ_a, where $a = 1, \ldots, d$ on $(-\delta/2, \delta/2)$ where δ is a small number that can be modified to optimize the acceptance rate. Construct the vector $\boldsymbol{\Delta} = (\Delta_1, \ldots, \Delta_d)$.

3. Translate the entire worldline by $\boldsymbol{\Delta}$ to obtain a new set of coordinates $\boldsymbol{r}'_{i,\alpha}$ where $\boldsymbol{r}'_{i,\alpha} = \boldsymbol{r}_{i,\alpha} + \boldsymbol{D}$ for $\alpha = 0, \ldots, M-1$.

4. Accept the update with probability

$$P_{\rm com} = \min\left\{1, \mathrm{e}^{-\tau[\mathcal{V}(\boldsymbol{r}'_i) - \mathcal{V}(\boldsymbol{r}_i)]}\right\} \tag{35}$$

where

$$\mathcal{V}(\boldsymbol{r}_i) \equiv \sum_{\alpha=0}^{M-1}\left[V(\boldsymbol{r}_{i,\alpha}) + \frac{1}{2}\sum_{j=1}^{N} U(\boldsymbol{r}_{i,\alpha} - \boldsymbol{r}_{j,\alpha})\right]. \tag{36}$$

2. *Staging*

A staging update[5] generates a new section of path between two fixed beads at time slices α and $\alpha + \overline{m}$ where $\overline{m} < M$ is an algorithmic parameter that can be tuned to optimize the acceptance rate. It utilizes the fact that the free particle density matrix in Eq. (32) is Gaussian and thus obeys a convolution relation. The problem is as follows: given two known spatial positions (beads) on worldline i, say $\boldsymbol{r}_{i,\alpha}$ and $\boldsymbol{r}_{i,\alpha+\overline{m}}$, how do we exactly sample the product of free particle density matrices:

$$\rho_0(\boldsymbol{r}_{i,\alpha}, \boldsymbol{r}_{i,\alpha+1}; \tau) \cdots \rho_0(\boldsymbol{r}_{i,\alpha+\overline{m}-1}, \boldsymbol{r}_{i,\alpha+\overline{m}}; \tau)\ ? \tag{37}$$

The solution comes by choosing a single term in this product and constructing the probability distribution for propagation to that position, constrained by the endpoints. Let us drop the worldline index i for brevity:

$$\begin{aligned}
\pi_0(\boldsymbol{r}_\gamma | \boldsymbol{r}_\alpha, \boldsymbol{r}_{\alpha+\overline{m}}) &= \rho_0(\boldsymbol{r}_\alpha, \boldsymbol{r}_\gamma; (\gamma-\alpha)\tau)\rho_0(\boldsymbol{r}_\gamma, \boldsymbol{r}_{\alpha+\overline{m}}; (\alpha+\overline{m}-\gamma)\tau) \\
&\propto \exp\left[-\frac{|\boldsymbol{r}_\gamma - \boldsymbol{r}_\alpha|^2}{4\lambda(\gamma-\alpha)\tau}\right]\exp\left[-\frac{|\boldsymbol{r}_{\alpha+\overline{m}} - \boldsymbol{r}_\gamma|^2}{4\lambda(\alpha+\overline{m}-\gamma)\tau}\right] \\
&\propto \exp\left[-\frac{|\boldsymbol{r}_\gamma - \overline{\boldsymbol{r}}_\gamma|^2}{2\sigma^2}\right]
\end{aligned} \tag{38}$$

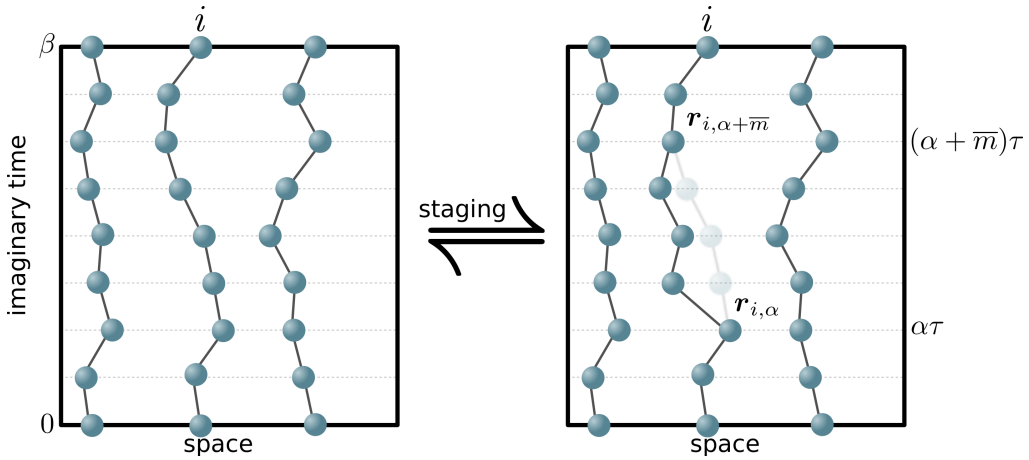

FIG. 4. A *staging* Monte Carlo update which uses the Lévy construction to exactly sample the product of $\overline{m}$ free particle density matrices connecting spatial positions $\boldsymbol{r}_{i,\alpha}$ and $\boldsymbol{r}_{i,\alpha+\overline{m}}$.

where

$$\overline{\boldsymbol{r}}_\gamma = \frac{1}{\overline{m}}\left[(\alpha+\overline{m}-\gamma)\boldsymbol{r}_\alpha + (\gamma-\alpha)\boldsymbol{r}_{\alpha+\overline{m}}\right]$$
$$\sigma^2 = \frac{2\lambda}{\frac{1}{(\alpha+\overline{m}-\gamma)\tau} + \frac{1}{(\gamma-\alpha)\tau}}. \tag{39}$$

As Eq. (38) is a simple Gaussian with mean $\overline{\boldsymbol{r}}_\gamma$ and variance σ^2, it can be exactly sampled. We are now ready to construct our staging move, which is shown in Figure 4:

1. Choose a random integer $i \in [0, N-1]$ which fixes a worldline.

2. Choose a random integer $\alpha \in [0, M-1]$ such that the start of the stage occurs at $\boldsymbol{r}_{i,\alpha}$ and it ends at $\boldsymbol{r}_{i,\alpha+\overline{m}}$. These beads are held fixed during the update.

3. Using $\boldsymbol{r}_{i,\alpha}$ and $\boldsymbol{r}_{i,\alpha+\overline{m}}$ construct the set of new positions $\{\boldsymbol{r}'_{i,\alpha+1}, \ldots, \boldsymbol{r}'_{i,\alpha+\overline{m}-1}\}$ by exactly sampling Eq. (38) for $\gamma = \alpha+1, \ldots, \alpha+\overline{m}-1$.

4. Accept the move with probability

$$P_{\text{staging}} = \min\left\{1, \mathrm{e}^{-\tau[\mathcal{V}(\boldsymbol{r}'_i)-\mathcal{V}(\boldsymbol{r}_i)]}\right\} \tag{40}$$

where

$$\mathcal{V}(\boldsymbol{r_i}) = \sum_{\gamma=\alpha+1}^{\alpha+\overline{m}-1}\left[V(\boldsymbol{r}_{i,\gamma}) + \frac{1}{2}\sum_{j=1}^{N} U(\boldsymbol{r}_{i,\gamma}-\boldsymbol{r}_{j,\gamma})\right]. \tag{41}$$

3. Permutation Sampling

We now address the point of how one can sample the sum over permutations of particle labels in Eq. (34). This is an onerous task, as for N particles there are $N!$ possible permutations. Historically this problem was addressed in a brute force manner, by explicitly sampling all possible reconnections of worldlines, between two fixed imaginary time slices as depicted in Figure 5 for $N = 3$. However this limited the total number of particles that could be efficiently simulated at low temperature to $N \sim 100$. In 2006, Boninsegni, Prokof'ev and Svistunov introduced a generalization of a previous path integral based lattice quantum Monte Carlo scheme[6] that has come to be known as the continuous space *worm* algorithm[7,8].

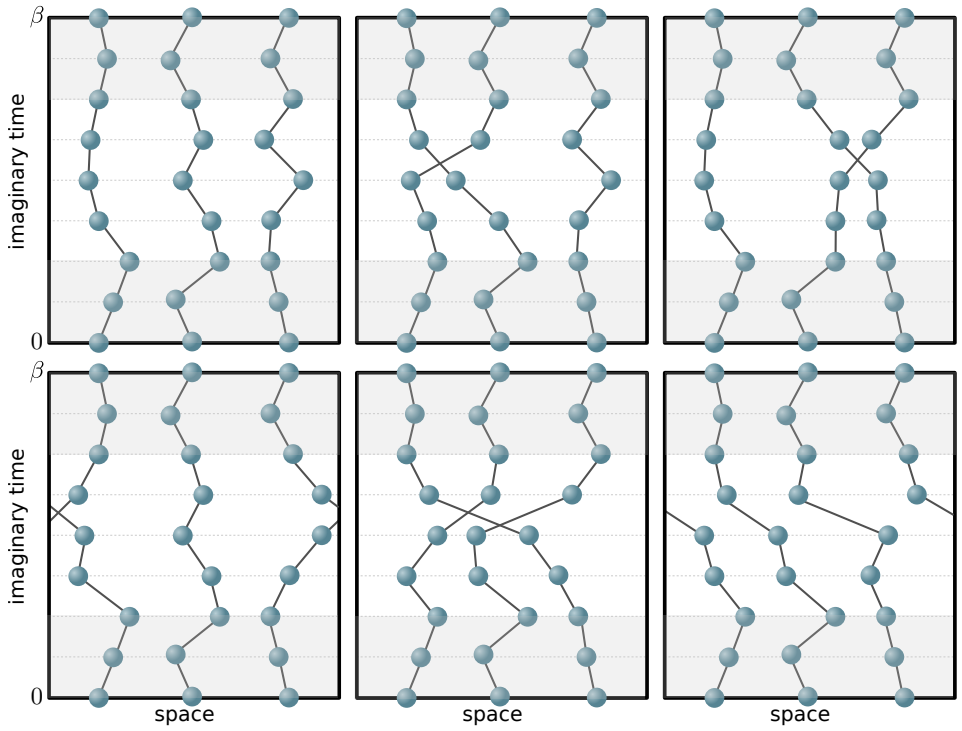

FIG. 5. A brute-force permutation update where 3! different connections of worldlines between two fixed imaginary time slices are directly sampled. The continuous space worm algorithm allows us to sample such permutations using only local updates.

III. CONTINUOUS SPACE WORM ALGORITHM

The worm algorithm[7,8] (WA) solves the following two problems:

1. Generalizes the configuration space to allow for simulations of interacting particles in the spatial continuum in the grand canonical ensemble.

2. Solves the permutation problem by allowing for the sampling of topologically inequivalent winding sectors using only local updates.

This is accomplished by extending the configuration space of worldlines discussed in Section II A to include "worms" which are open worldlines containing a *head* at time slice α_h and *tail* at α_t with a variable imaginary time extent $(\alpha_h - \alpha_t)\tau$. The partition function governing the new system can be written as

$$\mathcal{Z}_W = \sum_{N=0}^{\infty} \mathcal{Z}(N) \mathrm{e}^{\beta\mu N} + C \sum_{\alpha_h,\alpha_t} \int d\boldsymbol{r}_h \int d\boldsymbol{r}_t \, g\left(\boldsymbol{r}_h, \boldsymbol{r}_t; \alpha_h\tau - \alpha_t\tau\right) \tag{42}$$

where $\mathcal{Z}(N)$ is the canonical partition function at fixed particle number N in Eq. (19), μ is the grand canonical chemical potential and $g(\boldsymbol{r}, \boldsymbol{r'}; \tau - \tau')$ is (up to a normalization constant) equal to the single particle Matsubara Green function

$$g(\boldsymbol{r}, \boldsymbol{r'}; \tau - \tau') \equiv \mathcal{Z}(N) \left\langle \hat{\mathsf{T}}_\tau \hat{\psi}(\boldsymbol{r}, \tau) \hat{\psi}^\dagger(\boldsymbol{r}', \tau') \right\rangle \tag{43}$$

with $\hat{\mathsf{T}}_\tau$ the imaginary time ordering operator. Working in this extended ensemble requires us to expand the configuration space to include open worldlines as shown in Figure 6. Such configurations are unphysical however, and we only make measurements of observables when there are no worms present in the simulation. We refer to the configurations of $\mathcal{Z}(N)$ as *diagonal*, while those containing worms are *off-diagonal*. The numerical constant C is of order one and can be tuned to change the relative amount of Monte Carlo time spent in each ensemble.

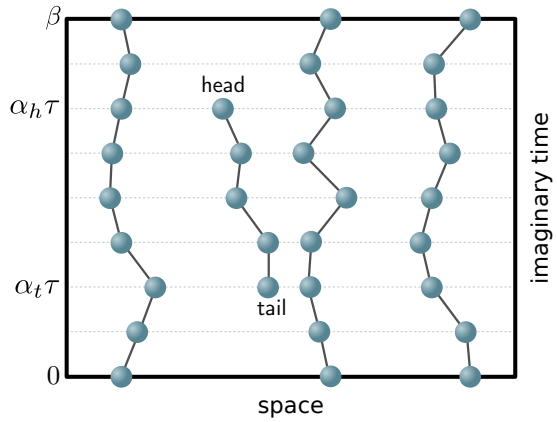

FIG. 6. A sample configuration $N = 3$ particles and one *worm* in d spatial dimensions ($d = 1$ here) where we have chosen $M = 8$ such that $\tau = \beta/8$. The worm *head* is located at imaginary time $\alpha_h\tau$ while the *tail* is at $\alpha_t\tau$. The imaginary time "length" of the worm is equal to $(\alpha_h - \alpha_\tau)\tau = 4\tau$ here.

A. Worm Updates

The worm updates come in complimentary pairs that satisfy detailed balance together except for the *swap* update, which provides the solution to the permutation sampling problem described above. Much of the notation in this section is taken directly from the original papers in Refs. [7] and [8]. In the following descriptions, when moving along worldlines, all addition of time slices is understood to be performed modulo M subject to the constraint that $\{\boldsymbol{r}_{1,0}, \ldots, \boldsymbol{r}_{N,0}\} = \{\boldsymbol{r}_{\mathcal{P}(1),M}, \ldots, \boldsymbol{r}_{\mathcal{P}(N),0}\}$.

1. *Open/Close*

An *open* update, depicted in Figure 7, moves the ensemble from diagonal to off-diagonal, and can only be attempted when there are no worms present. It proceeds as follows:

1. Choose a random integer $i \in [0, N-1]$ fixing worldline i with beads located at $\boldsymbol{r}_{i,\alpha}$.
2. Generate a random integer $\alpha_h \in [0, M-1]$; this will be the location of the head of the proposed worm.
3. Generate a random integer $m \in [1, \overline{m} - 1]$ where $\overline{m} < M$ is a parameter to be optimized. Starting at time slice α_h, find $\alpha_t = \alpha_h + m$, which will be the time slice of the tail.
4. Remove the set of $m-1$ beads $\{\boldsymbol{r}_{i,\alpha_h+1}, \ldots, \boldsymbol{r}_{,\alpha_h+m-1}\}$ where the addition is understood to be modulo M subject to the imaginary time boundary condition $\boldsymbol{r}_{i,M} = \boldsymbol{r}_{\mathcal{P}(i),0}$ for a given permutation of particle labels.
5. Accept the move with probability

$$P_{\text{open}} = \min\left[1, \frac{C\overline{m}MN}{\rho_0(\boldsymbol{r}_{i,\alpha_h}, \boldsymbol{r}_{i,\alpha_t}; m\tau)} \mathrm{e}^{-\tau\Delta\mathcal{V} - \mu m\tau}\right] \tag{44}$$

where $\Delta\mathcal{V}$ indicates the change in the total potential action, which in this case is

$$\Delta\mathcal{V} = -\sum_{\alpha=\alpha_h+1}^{\alpha_h+m-1}\left[V(\boldsymbol{r}_{i,\alpha}) + \frac{1}{2}\sum_{j=1}^{N} U(\boldsymbol{r}_{i,\alpha} - \boldsymbol{r}_{j,\alpha})\right] \tag{45}$$

and ρ_0 is the free particle propagator in Eq. (32).

If the move is accepted, the configuration now contains $N \to N-1$ physical particles and 1 worm.

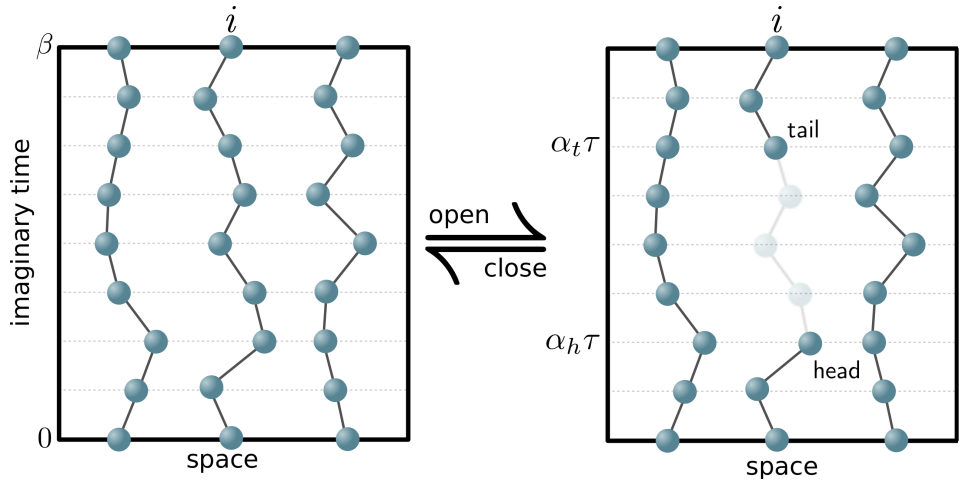

FIG. 7. The *open* and *close* complimentary Monte Carlo updates. For an open move, we select a worldline i and an imaginary time slice α_h. $\overline{m}$ beads are then removed from the configuration, moving to the off-diagonal ensemble and reducing the total number of physical particles by one. The close move operates in the reverse fashion, where a new portion of worldline is constructed between the head and the tail of a worm, resulting in a diagonal configuration with an additional particle.

The *close* move, shown in Figure 7, provides a detailed balance compliment to *open* and moves the ensemble from off-diagonal back to diagonal. It is only possible when a worm and N particles are present and contains the following steps:

1. Identify the "particle" label i of the worm and the integer number of time steps, m between α_h and α_τ between the head and tail where we assume $\alpha_h > \alpha_t$ modulo M.
2. If $m = 0$ or $m > \overline{m}$ reject the move immediately.
3. Otherwise, generate a new partial worldline containing $m-1$ particle positions connecting $\boldsymbol{r}_{i,\alpha_h}$ and $\boldsymbol{r}_{i,\alpha_t}$: $\{\boldsymbol{r}'_{i,\alpha_h+1}, \ldots, \boldsymbol{r}'_{,\alpha_h+m-1}\}$ where the individual positions are sampled from the product of m free particle propagators $\prod_{\alpha=\alpha_h}^{\alpha_h+m-1} \rho_0(\boldsymbol{r}_{i,\alpha}, \boldsymbol{r}_{i,\alpha+1}; \tau)$.
4. Accept the move with probability

$$P_{\text{close}} = \min\left[1, \frac{\rho_0(\boldsymbol{r}_{i,\alpha_h}, \boldsymbol{r}_{i,\alpha_t}; m\tau)}{C\overline{m}M(N+1)} \mathrm{e}^{-\tau\Delta\mathcal{V}+\mu m\tau}\right] \tag{46}$$

where

$$\Delta\mathcal{V} = \sum_{\alpha=\alpha_h+1}^{\alpha_h+m-1} \left[V(\boldsymbol{r}'_{i,\alpha}) + \frac{1}{2}\sum_{j=1}^{N} U(\boldsymbol{r}'_{i,\alpha} - \boldsymbol{r}_{j,\alpha})\right]. \tag{47}$$

If the move is accepted, we are now in a configuration with $N \to N+1$ particles and no worms.

2. *Insert/Remove*

An *insert* move (Figure 8) involves the addition to the ensemble of an entire worm and moves the configuration from diagonal to off-diagonal. It is only possible if there are no worms present in the system and proceeds as follows:

1. Choose a random integer $\alpha_t \in [0, M-1]$; this will be the location of the worm tail.
2. Choose a random integer $m \in [1, \overline{m}]$, this will be the length of the worm.
3. Randomly choose a position inside the simulation cell of volume V and label it $\boldsymbol{r}'_{i,\alpha_t}$ where i is the particle label of the proposed worm.

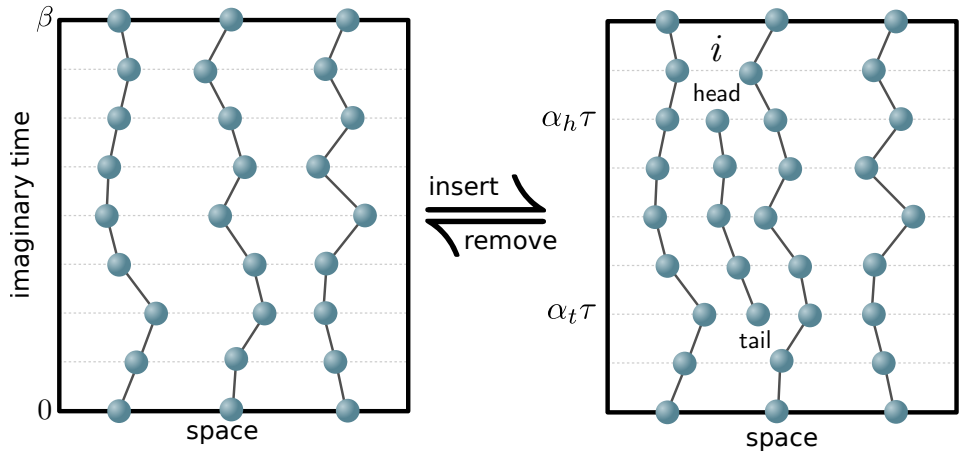

FIG. 8. The *insert* and *remove* pair of Monte Carlo updates. For an insert move, a worm of imaginary time extent $m\tau = (\alpha_h - \alpha_t)\tau$ is placed at a random set of positions in the simulation cell, moving the configuration space to the off-diagonal ensemble. The remove update deletes all beads on worm, moving the simulation to the diagonal ensemble.

4. Generate a new partial worldline containing $m-1$ particle positions starting at position $\boldsymbol{r}'_{i,\alpha_t}$: $\{\boldsymbol{r}'_{i,\alpha_t+1}, \ldots, \boldsymbol{r}'_{,\alpha_t+m}\}$ where the individual positions are sampled from the product of m free particle propagators $\prod_{\alpha=\alpha_t}^{\alpha_t+m-1} \rho_0(\boldsymbol{r}_{i,\alpha}, \boldsymbol{r}_{i,\alpha+1}; \tau)$.

5. Accept the move with probability

$$P_{\text{insert}} = \min\left[1, CV\overline{m}M\mathrm{e}^{-\tau\Delta\mathcal{V}+\mu m\tau}\right] \tag{48}$$

where

$$\Delta\mathcal{V} = \sum_{\alpha=\alpha_t}^{\alpha_t+m}\left[V(\boldsymbol{r}'_{i,\alpha}) + \frac{1}{2}\sum_{j=1}^{N} U(\boldsymbol{r}'_{i,\alpha} - \boldsymbol{r}_{j,\alpha})\right]. \tag{49}$$

If the move is accepted, the simulation cell will contain N particles and 1 worm.

The *remove* update deletes a worm from the configuration, moving the ensemble from off-diagonal to diagonal. It is only possible if there is a worm present and is undertaken as follows:

1. Find the particle label of the worm, call it i, and the positions of the head and tail: $\boldsymbol{r}_{i,\alpha_h}$ and $\boldsymbol{r}_{i,\alpha_h}$.

2. Determine $m = \alpha_h - \alpha_t$, the length of the worm.

3. If $m > \overline{m}$ reject the move.

4. Otherwise, delete the set of m beads $\{\boldsymbol{r}_{i,\alpha_t}, \ldots, \boldsymbol{r}'_{,\alpha_t+m}\}$.

5. Accept the move with probability

$$P_{\text{remove}} = \min\left[1, \frac{1}{CV\overline{m}M}\mathrm{e}^{-\tau\Delta\mathcal{V}-\mu m\tau}\right] \tag{50}$$

where

$$\Delta\mathcal{V} = -\sum_{\alpha=\alpha_t}^{\alpha_t+m}\left[V(\boldsymbol{r}_{i,\alpha}) + \frac{1}{2}\sum_{j=1}^{N} U(\boldsymbol{r}_{i,\alpha} - \boldsymbol{r}_{j,\alpha})\right]. \tag{51}$$

If the move is accepted, the simulation cell will contain N particles and 0 worms.

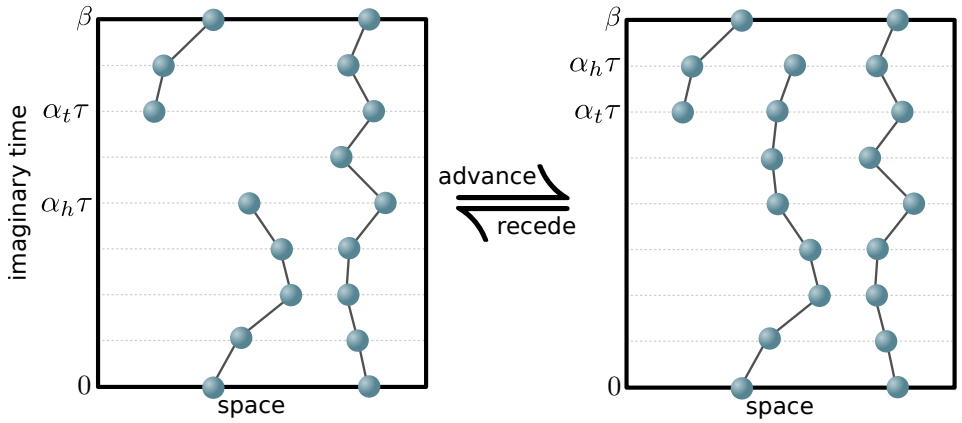

FIG. 9. The *advance* and *recede* Monte Carlo updates. The advance move propagates the head of the worm forwards in imaginary time by generating a set of new spatial positions. The recede move does the opposite, deleting beads and reducing the length of the worm.

3. Advance/Recede

The *advance* and *recede* updates, shown in Figure 9 do not change the nature of the ensemble and operate only in the off-diagonal case in the presence of a worm. For advance:

1. Determine the time slice α_h and spatial location $\boldsymbol{r}_{i,\alpha_h}$ of the worm head.
2. Choose a random integer $m \in [1, \overline{m}]$.
3. Generate a partial worldline composed of the set of new particle positions $\{\boldsymbol{r}'_{i,\alpha_h+1}, \ldots, \boldsymbol{r}'_{i,\alpha_h+m}\}$ which are sampled from $\prod_{\alpha=\alpha_h}^{\alpha_h+m-1} \rho_0(\boldsymbol{r}_{i,\alpha}, \boldsymbol{r}_{i,\alpha+1}; \tau)$.
4. Accept the move with probability

$$P_{\text{advance}} = \min\left[1, \mathrm{e}^{-\tau\Delta\mathcal{V}+\mu m\tau}\right] \tag{52}$$

where

$$\Delta\mathcal{V} = \sum_{\alpha=\alpha_t+1}^{\alpha_t+m} \left[V(\boldsymbol{r}'_{i,\alpha}) + \frac{1}{2}\sum_{j=1}^{N} U(\boldsymbol{r}'_{i,\alpha} - \boldsymbol{r}_{j,\alpha}) \right]. \tag{53}$$

For recede:

1. Determine the time slice α_h and spatial location $\boldsymbol{r}_{i,\alpha_h}$ of the worm head.
2. Choose a random integer $m \in [1, \overline{m}]$.
3. Reject if $m > |\alpha_h - \alpha_t|$.
4. Delete the partial worldline containing the set of particle coordinates: $\{\boldsymbol{r}_{i,\alpha_h-(m-1)}, \ldots, \boldsymbol{r}_{i,\alpha_h}\}$.
5. Accept the move with probability

$$P_{\text{recede}} = \min\left[1, \mathrm{e}^{-\tau\Delta\mathcal{V}-\mu m\tau}\right] \tag{54}$$

where

$$\Delta\mathcal{V} = -\sum_{\alpha=\alpha_h-(m-1)}^{\alpha_h} \left[V(\boldsymbol{r}'_{i,\alpha}) + \frac{1}{2}\sum_{j=1}^{N} U(\boldsymbol{r}'_{i,\alpha} - \boldsymbol{r}_{j,\alpha}) \right]. \tag{55}$$

We note that similar copies of these updates could also be performed at the tail of the worm, but such moves should be unnecessary for ergodicity in the presence of imaginary time translation symmetry.

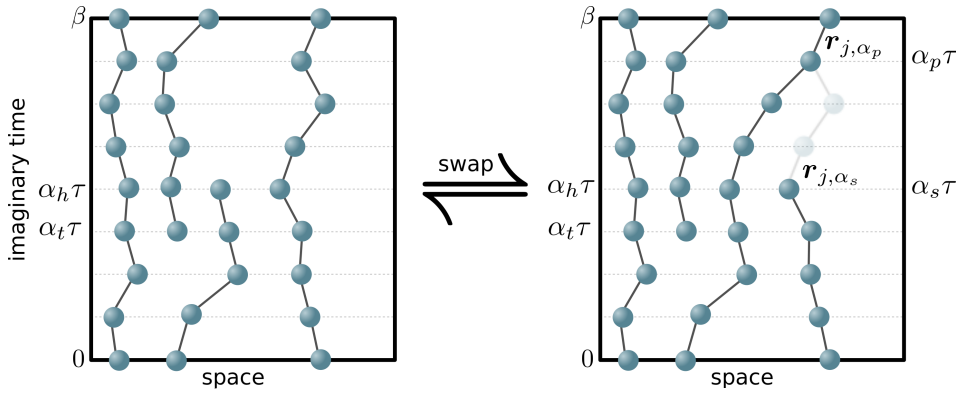

FIG. 10. The *swap* Monte Carlo update, which does not change the nature of the ensemble, but allows for the sampling of different topological sectors. A new partial worldline is generated between the head of the worm and a neighboring particle worldline position at an advanced time slice. The original portion of the particle worldline is then erased, "swapping" the head of the worm and increasing the imaginary time extent of the worm.

4. Swap

The *swap* update, shown in Figure 10 is behind the huge speedup inherent in the worm algorithm, as it allows us to sample different topological winding sectors (permutations) using only local updates. It does not, therefore, suffer from the horrendous $N!$ scaling of brute-force permutation sampling. It only operates on off-diagonal configurations, in the presence of a worm, and does not change the ensemble. It provides a method by which a single worm grows by nM time slices where $1 \leq n \leq N$ by "swapping" its head with a proximate unbroken particle worldline. To perform a swap move:

1. Determine the time slice α_h and spatial location $\boldsymbol{r}_{i,\alpha_h}$ of the worm head.

2. Advance to the time slice of the *pivot* bead $\alpha_p = \alpha_h + \overline{m}$ where the addition is modulo M and find the set of all beads $\ell_h \equiv \{\boldsymbol{r}_{k,\alpha_p}\}$ such that $|\boldsymbol{r}_{i,\alpha_h} - \boldsymbol{r}_{k,\alpha_p}| < R$ where $R \in \mathbb{R}$ is a simulation parameter to be optimized.

3. Use tower sampling to select a single bead $\boldsymbol{r}_{j,\alpha_p} \in \{\boldsymbol{r}_{k,\alpha_p}\}$ from the list with probability

$$P_{\text{pivot}} = \frac{1}{\Sigma_h}\rho_0(\boldsymbol{r}_{i,\alpha_h}, \boldsymbol{r}_{j,\alpha_p}; \overline{m}\tau) \tag{56}$$

   where the normalization factor is

$$\Sigma_h = \sum_{\boldsymbol{r}\in\ell_h} \rho_0(\boldsymbol{r}_{i,\alpha_h}, \boldsymbol{r}; \overline{m}\tau). \tag{57}$$

4. Recede $\overline{m}$ time steps along worldline j from α_p to identify the *swap* bead at $\alpha_s = \alpha_h = \alpha_p - \overline{m}$: $\boldsymbol{r}_{j,\alpha_s}$. If the tail of the worm, $\boldsymbol{r}_{i,\alpha_t}$, is encountered during this process, immediately reject the move.

5. If $|\boldsymbol{r}_{j,\alpha_p} - \boldsymbol{r}_{j,\alpha_s}| \geq R$ reject the move.

6. Otherwise, create a second list $\ell_s \equiv \{\boldsymbol{r}_{k,\alpha_p}\}$ such that $|\boldsymbol{r}_{j,\alpha_s} - \boldsymbol{r}_{k,\alpha_p}| < R$ and form the sum

$$\Sigma_s = \sum_{\boldsymbol{r}\in\ell_s} \rho_0(\boldsymbol{r}_{j,\alpha_s}, \boldsymbol{r}; \overline{m}\tau). \tag{58}$$

7. Delete the set of $\overline{m} - 1$ beads $\{\boldsymbol{r}_{j,\alpha_s+1}, \ldots, \boldsymbol{r}_{j,\alpha_s+\overline{m}-1}\}$.

8. Construct a new partial worldline containing the set of particle positions $\{\boldsymbol{r}'_{i,\alpha_h+1}, \ldots \boldsymbol{r}'_{i,\alpha_h+\overline{m}-1}\}$ connecting $\boldsymbol{r}_{i,\alpha_h}$ and $\boldsymbol{r}_{j,\alpha_p}$ sampled from the product of $\overline{m}$ free particle propagators $\prod_{\alpha=\alpha_h}^{\alpha_h+\overline{m}-1} \rho_0(\boldsymbol{r}_{i,\alpha}, \boldsymbol{r}_{i,\alpha+1}; \tau)$ where $\boldsymbol{r}_{i,\alpha_h+\overline{m}} = \boldsymbol{r}_{j,\alpha_p}$.

9. The head of the worm is now located at $\boldsymbol{r}_{j,\alpha_s}$ and its length has increased by the number of beads contained in the particle that was labeled by j.

10. Accept the move with probability

$$P_{\text{swap}} = \min\left[1, \frac{\Sigma_p}{\Sigma_s} \mathrm{e}^{-\tau \Delta \mathcal{V}}\right] \tag{59}$$

where

$$\Delta \mathcal{V} = \sum_{\alpha=\alpha_h+1}^{\alpha_h+\overline{m}-1} \left\{ V(\boldsymbol{r}'_{i,\alpha}) - V(\boldsymbol{r}_{j,\alpha}) + \frac{1}{2} \sum_{k=1}^{N} \left[U(\boldsymbol{r}'_{i,\alpha} - \boldsymbol{r}_{k,\alpha}) - U(\boldsymbol{r}_{j,\alpha} - \boldsymbol{r}_{k,\alpha}) \right] \right\}. \tag{60}$$

---

* Adrian.DelMaestro@utk.edu

[1] D. M. Ceperley, Review Modern Physics **67**, 279 (1995).
[2] R. Feynman and A. Hibbs, *Quantum mechanics and path integrals*, International series in pure and applied physics (McGraw-Hill, 1965).
[3] D. Chandler and P. G. Wolynes, The Journal of Chemical Physics **74**, 4078 (1981).
[4] S. Jang, S. Jang, and G. A. Voth, The Journal of Chemical Physics **115**, 7832 (2001).
[5] M. Sprik, M. Klein, and D. Chandler, Physical Review B **31**, 4234 (1985).
[6] N. Prokof'ev, Svistunov, B.V., and I. Tupitsyn, Physics Letters A **238**, 253 (1998).
[7] M. Boninsegni, N. Prokof'ev, and B. Svistunov, Physical Review Letters **96**, 070601 (2006).
[8] M. Boninsegni, N. V. Prokof'ev, and B. V. Svistunov, Physical Review E **74**, 036701 (2006).