INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

H4.SMR/854-29

College on Computational Physics

15 May - 9 June 1995

Introduction to Path Integral Monte Carlo

C.J. Umrigar

Cornell University
Ithaca, USA

MAIN BUILDING STRADA COSTIERA, 11 TEL. 2240111 TELEFAX 224163 TELEX 460392 ADRIATICO GUEST HOUSE VIA GRIGNANO, 9 TEL. 224241 TELEFAX 224531 TELEX 460449
MICROPROCESSOR LAB. VIA BEIRUT, 31 TEL. 224471 TELEFAX 224600 TELEX 460392 GALILEO GUEST HOUSE VIA BEIRUT, 7 TEL. 22401 TELEFAX 2240310 TELEX 460392

International Center for Theoretical Physics, Trieste
College on Computational Physics, 15th May - 9th June 1995, Lecture Notes
Lecture 2, 6th June 1995

Introduction to Path Integral Monte Carlo

Cyrus J. Umrigar

Cornell Theory Center and Laboratory of Atomic and Solid State Physics,
Cornell University, Ithaca, NY 14853.

I. INTRODUCTION

This lecture provides an introduction to the path-integral Monte Carlo method. For further details the reader is referred to an excellent review by Ceperley [1].

Diffusion Monte Carlo and Green function Monte Carlo are used to calculate properties of pure states (mostly ground states, but some work has been done on excited states as well). On the other hand, path integral Monte Carlo is mostly used to calculate quantum statistical properties in the canonical ensemble. Some properties that have been studied are

- structure of atomic clusters and liquids and their pair-correlation functions,
- electron localization in various environments such as liquid rare gases, molten salts, atomic clusters, water and helium,
- properties of normal and superfluid ^{4}He, such as the pair-correlation function, specific heat near the λ-point, superfluid fraction (Ceperley and Pollock).

Properties of the ground state can be obtained by working at a sufficiently low temperature but this is computationally expensive. However, there exists a variant (Ye, Nightingale preprint) [3] of path integral Monte Carlo that is efficient for calculating pure states because it builds in information from approximate trial wavefunctions. They used it to calculate ground and excited states of a quantum spin chain.

II. DISCRETIZED PATH INTEGRAL MONTE CARLO

In quantum statistical mechanics the expectation value of an operator P is given by

$$\langle P \rangle = \frac{\mathrm{tr}(\rho \mathrm{P})}{\mathrm{tr}(\rho)} \tag{1}$$

where $\rho = e^{-\beta H}$ is the quantum density operator, $Z = \mathrm{tr}(\rho)$ is the partition function, H is the Hamiltonian and $\beta = 1/k_B T$. For example, if the trace is evaluated in the energy representation then the energy of the system is

$$E = \frac{\sum_{i=0}^{\infty} E_i e^{-\beta E_i}}{\sum_{i=0}^{\infty} e^{-\beta E_i}} \tag{2}$$

where E_i are the eigenvalues of H. For many-body systems it is in general impossible to find the energy eigenvalues and perform the above sum. However, path integral Monte Carlo provides us a means of evaluating the trace in the coordinate representation. The expectation value of P in coordinate representation is

$$\langle P\rangle = \frac{\int dx\ \langle x|Pe^{-\beta H}|x\rangle}{\int dx\ \langle x|e^{-\beta H}|x\rangle} \tag{3}$$

Introducing a complete set of states, we obtain,

$$\langle P\rangle = \frac{\int dx\ dx'\ \langle x|P|x'\rangle\langle x'|e^{-\beta H}|x\rangle}{\int dx\ \langle x|e^{-\beta H}|x\rangle} \tag{4}$$

If P is diagonal in the coordinate representation then this reduces to

$$\langle P\rangle = \frac{\int dx\ P(x)\ \rho(x,x,\beta)}{\int dx\ \rho(x,x,\beta)} \tag{5}$$

where $\rho(x',x,\beta) \equiv \langle x'|e^{-\beta H}|x\rangle$ is the density matrix in coordinate representation.

Eq. 5 is in a form that can be readily evaluated using the Metropolis method provided that we can devise a way to sample from the diagonal elements of the density matrix in coordinate space. This can be done by expressing the density matrix in the form of a path integral. We begin by trivially rewriting the density matrix as

$$\rho(x',x,\beta) = \langle x'|(e^{-\beta H/M})^M|x\rangle \tag{6}$$

where M is an integer. Introducing $M-1$ complete sets of position eigenstates we get

$$\rho(x',x,\beta) = \int dx_1 \ldots dx_{M-1}\langle x'|e^{-\epsilon H}|x_{M-1}\rangle\ldots\langle x_1|e^{-\epsilon H}|x\rangle \tag{7}$$

where $\epsilon = \beta/M$. We have reexpressed a density matrix at inverse reduced temperature β in terms of integrals of density matrices at inverse reduced temperature $\epsilon = \beta/M$. The reason for recasting the density matrix in this seemingly more complicated form is that approximate analytical expressions that become exact in the high-temperature limit can be derived for the density matrix.

The density operator in quantum statistical mechanics is identical to the quantum mechanical time evolution operator if we make the identification $t = -i\hbar\beta$. Hence Eq. 7 may be interpreted as the motion of a particle starting at position x at imaginary time 0, to a position x' at imaginary time $\hbar\beta$, through a sequence of $M-1$ intermediate steps that define a "path". The total amplitude for the particle to start at x and end up at x' is given by summing over all possible paths. The path becomes continuous in the limit $M \to \infty$, and Eq. 7 may be written as

$$\rho(x',x,\beta) = \int \mathcal{D}x\ \Phi[x(u)] \tag{8}$$

where $\mathcal{D}x = \lim_{M\to\infty} dx_1 \ldots dx_{M-1}$ and $\Phi[x(u)] = \lim_{M\to\infty}\rho(x',x_{M-1},\epsilon)\rho(x_{M-1},x_{M-2},\epsilon)\ldots\rho(x_1,x,\epsilon)$.

Now we derive an approximate expression for the high-temperature density matrix. First, we note that since the operators for the kinetic energy K and the potential energy V do not commute,

$$e^{-\epsilon H} = e^{-\epsilon K}\ e^{-\epsilon V}\ +\ \frac{\epsilon^2}{2}[V,K] = e^{-\epsilon K}\ e^{-\epsilon V}\ +\ \mathcal{O}(\epsilon^2). \tag{9}$$

or better

$$e^{-\epsilon H} = e^{-\epsilon V/2}\, e^{-\epsilon K}\, e^{-\epsilon V/2} \; + \; \mathcal{O}(\epsilon^3). \tag{10}$$

Since the potential energy is diagonal in position space, we can introduce 2 resolutions of the identity operator in coordinate representation to obtain

$$\langle x'|e^{-\epsilon H}|x\rangle = \langle x'|e^{-\epsilon K}|x\rangle e^{-\epsilon(V(x')+V(x))/2} \tag{11}$$

Since the kinetic energy is diagonal in momentum space, we can evaluate $\langle x'|e^{-\epsilon K}|x\rangle$ by introducing complete sets of momentum eigenstates

$$\begin{aligned}
\langle x'|e^{-\epsilon K}|x\rangle &= \frac{1}{2\pi\hbar}\int dp'\, dp\, \langle x'|p'\rangle\langle p'|e^{-\epsilon K}|p\rangle\langle p|x\rangle \\
&= \frac{1}{2\pi\hbar}\int dp\, dp'\, e^{\frac{-ip'x'}{\hbar}}\delta(p'-p)e^{\frac{-\epsilon p^2}{2m}}e^{\frac{ipx}{\hbar}} \\
&= \frac{1}{2\pi\hbar}\int dp\, e^{i\frac{p}{\hbar}(x-x')-\epsilon p^2/2m} \\
&= \frac{1}{2\pi\hbar}e^{\frac{-m}{2\hbar^2\epsilon}(x-x')^2}\int dp\, e^{\frac{\epsilon}{2m}(ip+\frac{m}{\hbar\epsilon}(x-x'))^2} \\
&= \left(\frac{m}{2\pi\hbar^2\epsilon}\right)^{\frac{1}{2}} e^{-(\frac{m}{2\hbar^2\epsilon})(x'-x)^2}.
\end{aligned} \tag{12}$$

Substituting this in Eq.7 we get

$$\begin{aligned}
&\rho(x',x,\beta) \\
&= \int dx_1 \ldots dx_{M-1}\left(\frac{m}{2\pi\hbar^2\epsilon}\right)^{(M-1)/2} \\
&\quad\times e^{-(\frac{m}{2\hbar^2\epsilon})[(x'-x_{M-1})^2+(x_{M-1}-x_{M-2})^2 \ldots (x_1-x)^2] \;-\; \epsilon(\frac{V(x')}{2}+V(x_{M-1})+\ldots+V(x_1)+\frac{V(x)}{2})} \\
&= \int dx_1 \ldots dx_{M-1}\left(\frac{m}{2\pi\hbar\tau}\right)^{(M-1)/2} \\
&\quad\times e^{(\frac{-\tau}{\hbar})[(\frac{m}{2})((\frac{x'-x_{M-1}}{\tau})^2+(\frac{x_{M-1}-x_{M-2}}{\tau})^2+\ldots+(\frac{x_1-x}{\tau})^2) \;+\; (\frac{V(x')}{2}+V(x_{M-1})+\ldots+V(x_1)+\frac{V(x)}{2})]} \qquad (13) \\
&= \int \mathcal{D}x\, e^{-S[x(u)]/\hbar} \qquad (14)
\end{aligned}$$

where $S[x(u)] = \int_0^{\hbar\beta} du\Big[\frac{m\dot{x}(u)^2}{2} + V(x(u))\Big]$ and $\tau = \hbar\epsilon$. $S[x(u)]$ is a classical action but with the sign of V reversed. Hence the most probable path is not the actual classical path that satisfies Newton's equations. Nevertheless, this path is referred to as the classical path. In classical mechanics the particle has a high velocity in low potential energy regions and consequently a low probability of being in those regions. In contrast, here the particle has a high probability of being in the low potential energy regions.

In Fig. 1 we show a representative path. The kinetic energy term favors smooth paths, whereas the original potential energy favors regions of low potential energy.

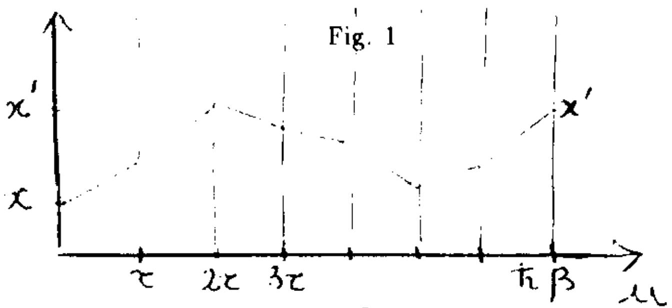


Fig. 1

Eq. 13 has the form of a Boltzman factor of a classical particle in $d+1$ dimensions (d being the dimensionality of the original quantum problem we wished to solve). We will refer to this extra dimension as the *time* direction or the *temperature* direction or the *Trotter* direction. Now that we have reduced the original quantum mechanical problem to an equivalent classical statistical mechanical problem, we can now use the Metropolis method to sample from the distribution and calculate various expectation values. The kinetic energy of the original quantum problem is now a potential energy of harmonic springs that connect a particle at a given time with the particle at adjacent times. Each of the original quantum particles is mapped onto a *polymer* consisting of *beads* that are connected by springs to adjacent beads of the same polymer. In addition we have the potential energy of the original problem. Hence, beads on one polymer interact with beads corresponding to the same time of other polymers, with the original inter-particle potential. All beads of all polymers interact with the external potential, if any. Expectation values of operators diagonal in the position representation require evaluation of a trace. In this case the polymers form closed loops.

The length of each polymer is set by the inverse temperature β. The length of each link $\tau = \beta/M$ is limited by the accuracy of the form of the approximate high-temperature density matrix relative to the discretization error that we are willing to tolerate. In the interest of computer efficiency, we wish to make M as small (τ as large) as possible. Ceperley and Pollock have developed techniques for constructing more accurate high-temperature density matrices than those in Eqs. 10 and 12.

The simplest (but very inefficient) "bead pushing" way to evolve the system is to propose moves for individual beads with a uniform probability distribution in an interval around the current bead position, followed by a Metropolis accept/reject step. If a bead moves a considerable distance from either of its neighbours, then the move is unlikely to be accepted because of the increase in the kinetic energy. This is a particularly serious problem in those cases where there is more than one low-action path, separated by large regions of large action. In that case in order to have any reasonable probability for transitions from one low-action region to another one separated by a barrier it is necessary to propose moves that move a considerable section of the polymer in a single move. As discussed in the lecture on the Metropolis method, one has complete freedom in the nature of the proposed moves. In order to sample the correct distribution one just has to make sure that the acceptance probabilities are such that detailed balance is satisfied. Hence a variety of more intelligent ways of proposing moves have been presented in the literature, some of which we will now sketch.

We do not wish to propose multiparticle moves which consist of individual particles moving independently from each other, because such moves will for the most part have high kinetic energy and will consequently be rejected. One way is to grow sections of the polymer from one end to the other such that the probability distribution of each bead is a gaussian with its center of mass on a straight line from the previous bead to the far end of the section of polymer being grown.

We now describe two ideas, (due to Ceperley and co-workers) *bisection* and *multi-level Metropolis* that together lead to the most efficient method for evolving paths. We have a section of the path consisting of $m = 2^l - 1$ time slices that we wish to evolve. The fixed end-points are at times i and $i+m$. We will first evolve the midpoint $i + (m+1)/2$ of the path by sampling a gaussian of the width $\sqrt{m\tau/2}$ (about the point $(x_i + x_{i+m})/2$. Next we evolve the beads at the mid-points of each of the two segments of the path, *i.e.* at $i + (m+1)/4$ and $i + 3(m+1)/4$. by sampling gaussians of width $\sqrt{m\tau/4}$ and so on until all m beads in that section of path have been evolved. The advantage of this bisection method is that we can move a large section of the path by a large amount while at the same time growing a relatively smooth proposed path. The entire segment of path is then accepted or rejected with probabilities given by the Metropolis method. Most of the rejections occur because of unfavorable potential energies near the center of the path segment, because the beads in the center are furthest from the end-points which we know have acceptable potential energies. One can in fact make the method more efficient by performing Metropolis accept/reject steps at each of the l levels of the hierarchy. We define a *level density* ρ_k. The ideal ρ_k is the density matrix ρ with all the finer levels $k+1 \ldots l$ integrated out. ρ_l must equal ρ. For $k \neq l$ deviations from the ideal limit affect the efficiency of the method but do not compromise the correctness of the distribution sampled. $T_k(x'|x)$ is the proposal matrix for sampling the positions at level k contingent on the levels already sampled. The ideal $T_k(x'|x)$ is $\rho_k(x')/\rho_{k-1}(x')$. The detailed balance condition

$$A_k(x'|x)T_k(x'|x)\frac{\rho_k(x)}{\rho_{k-1}(x)} = A_k(x|x')T_k(x|x')\frac{\rho_k(x')}{\rho_{k-1}(x')} \tag{15}$$

is satisfied by choosing the acceptance probabilities to be

$$A_k(x'|x) = \min\left[1, \frac{T_k(x|x')\rho_k(x')\rho_{k-1}(x)}{T_k(x'|x)\rho_k(x)\rho_{k-1}(x')}\right]. \tag{16}$$

The total Markov matrix for the proposed move is

$$M(x'|x) = \prod_{k=1}^{l} A_k(x'|x)T_k(x'|x) \tag{17}$$

Multiplying Eq. 15 from $k = 1$ to l and using $\rho_l = \rho$ we obtain

$$M(x'|x)\rho(x) = M(x'|x)\rho(x'). \tag{18}$$

Hence we have shown that the algorithm satisfies detailed balance and must therefore converge to the distribution ρ. Since most of the rejections occur during the first few levels of the hierarchy, before much time has been spent on constructing the paths, this leads to a considerable gain in efficiency.

Another way to move all the beads of a polymer in a relatively smooth way is to propose the moves

$$x_i \to x_i + a_n \sin(n i \pi/M) \tag{19}$$

where $n = 1, 2, \ldots M/2$, with $x_0 = x$ and $x_M = x'$. The coefficients a_n are decreasing functions of n. Both these procedures ignore the effect of the potential, but it is possible to devise ways of favouring low potential energy regions.

III. FOURIER PATH INTEGRAL MONTE CARLO

The idea of the last section is taken a step further in Fourier path integral Monte Carlo, developed by Doll and Freeman. The Fourier components are themselves taken to be the dynamic variables (plus the coordinates of one of the beads of the closed polymer). The Fourier components define a continuous path, over which we can evaluate both the kinetic and the potential energies, so we no longer have a discretization approximation. However, in practice one must truncate the Fourier series somewhere, so this introduces an approximation that is akin to discretization. Most of the discretization error can be removed by "partial averaging" as we will discuss later. We can evaluate the free-particle action S_0 over the continuous path

$$x(u) = x + (x' - x)u/\hbar\beta + \sum_{k=1}^{k_{\max}} a_k \sin(\frac{k\pi u}{\hbar\beta}) \tag{20}$$

as follows:

$$\begin{aligned}
\frac{S_0}{\hbar} &= \frac{m}{2\hbar}\int_0^{\beta\hbar} du\, \dot{x}^2 \\
&= \frac{m}{2\hbar}\int_0^{\beta\hbar} du\Big[(\frac{x' - x}{\hbar\beta}) + \sum_{k=1}^{k_{\max}} a_k \frac{k\pi}{\hbar\beta}\cos(\frac{k\pi u}{\hbar\beta})\Big]^2 \\
&= \frac{m}{2\hbar}\int^{\hbar\beta} du\Big[(\frac{x' - x}{\hbar\beta})^2 + 2\frac{(x' - x)}{\hbar\beta}\sum_{k=1}^{k_{\max}} a_k \frac{k\pi}{\hbar\beta}\cos(\frac{k\pi u}{\hbar\beta}) + \sum_{k,k'=1}^{k_{\max}} a_k a'_k (\frac{k\pi}{\hbar\beta})^2 \cos(\frac{k\pi u}{\hbar\beta})\cos(\frac{k'\pi u}{\hbar\beta})\Big] \\
&= \frac{m}{2\hbar}\Big[\frac{(x' - x)^2}{\hbar\beta} + \sum_{k=1}^{k_{\max}} a_k^2 (\frac{k\pi}{\hbar\beta})^2 \frac{\hbar\beta}{2}\Big] \\
&= \frac{m}{2}\frac{(x' - x)^2}{\hbar^2\beta} + \sum_{k=1}^{k_{\max}} \frac{a_k^2}{2\sigma_k^2}
\end{aligned} \tag{21}$$

where $\sigma_k^2 = \frac{2\hbar^2\beta}{m(k\pi)^2}$. The density matrix $\rho(x', x, \beta)$ can then be written in terms of the free-particle density matrix $\rho_0(x', x, \beta)$ (the first term in Eq. 21 factors out of the numerator and denominator):

$$\rho(x', x, \beta) = \rho_0(x', x, \beta) \frac{\int d\mathbf{a} \, \exp\left(\sum_{k=1}^{k_{max}} \frac{a_k^2}{2\sigma_k^2} - \beta \langle V \rangle_{\mathbf{a}}\right)}{\int d\mathbf{a} \exp\left(\sum_{k=1}^{k_{max}} \frac{a_k^2}{2\sigma_k^2}\right)} \tag{22}$$

where

$$\langle V \rangle_{\mathbf{a}} = \frac{1}{\hbar\beta} \int_0^{\beta\hbar} du \; V(x(u)) \tag{23}$$

is the average potential over the particular path given by $\mathbf{a}$. The expectation value of the potential energy is then given by

$$\langle V \rangle = \frac{\int dx \;\; d\mathbf{a} \; w(x, x, \mathbf{a}, \beta) V(x)}{\int dx \;\; d\mathbf{a} \; w(x, x, \mathbf{a}, \beta)} \tag{24}$$

where

$$w(x', x, \mathbf{a}, \beta) = \rho_0(x', x, \beta) \exp\Big(\sum_{k=1}^{k_{max}} \frac{a_k^2}{2\sigma_k^2} - \beta \langle V \rangle_{\mathbf{a}}\Big). \tag{25}$$

(The denominator of Eq. 22 has cancelled out of the numerator and denominator of Eq. 24. $\rho_0(x', x, \beta)$ is constant that also cancels out.)

A. Partial averaging

Freeman and Doll have shown that it is possible to take into account much of the effect of the omitted high-frequency Fourier components by a method called *partial averaging* [2]. The basic idea is that the path is mostly defined by the low-frequency components, but the high-frequency components have the effect of making this path fuzzy. The net effect of the high-frequency components can be approximately taken into account by replacing the path integral over the potential by a path-integral over a gaussian transform of the potential, when it exists. In practice the gaussian transform is performed by making a quadratic expansion of the potential at each point along the path. The result is to replace the potential $V(x_{\mathbf{a}}(u))$ by $V_{\text{eff}}(x_{\mathbf{a}}(u))$, where

$$V_{\text{eff}}(x_{\mathbf{a}}(u)) = V(x_{\mathbf{a}}(u)) + \frac{1}{2} V''((x_{\mathbf{a}}(u)) \; \sigma^2(u) \tag{26}$$

where

$$\sigma^2(u) = \frac{u}{\beta m}(\beta\hbar - u) - \sum_{k=1}^{k_{max}} \sigma_k^2 \sin^2\left(\frac{k\pi u}{\beta\hbar}\right). \tag{27}$$

IV. EVALUATION OF THE KINETIC ENERGY

Evaluation of the kinetic energy requires a little more thought than the potential energy because the kinetic energy operator is not diagonal in coordinate representation. However it is *semi-local* by which we mean that it requires evaluation of derivatives only at the point in question. Hence Eq. 5 becomes

$$\langle K \rangle = \frac{-\hbar^2}{2m} \frac{\int dx \ \nabla^2 \rho(x', x, \beta)|_{x'=x}}{\int dx \ \rho(x, x, \beta)} \tag{28}$$

There are two other methods that are used for calculating the kinetic energy but the tests in the literature seem to indicate that they yield larger statistical errors than the above. First, one can use the virial theorem to find the kinetic energy by evaluating an appropriate derivative of the potential energy. Second, one can use the relation

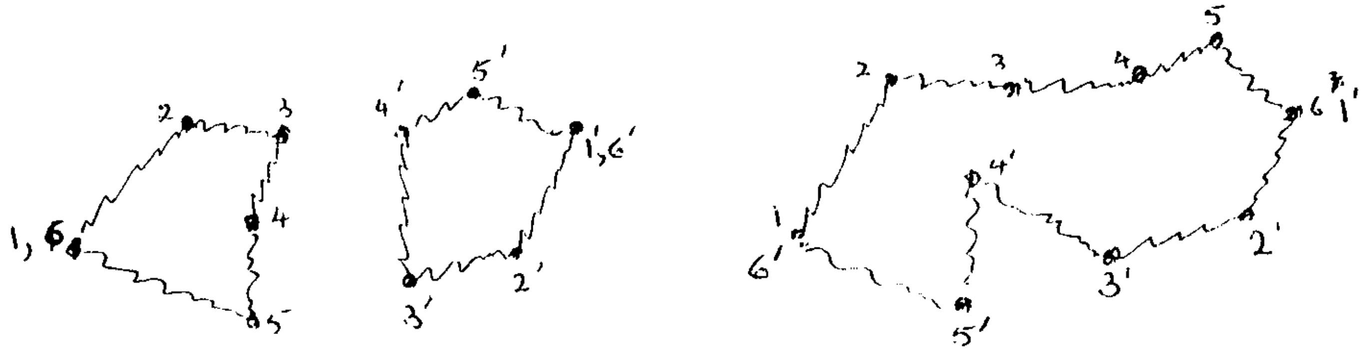
$$\langle E \rangle = -\frac{d \log Z}{d\beta}\bigg|_V \tag{29}$$

to evaluate the energy directly.

V. BOSONS AND FERMIONS

If the particles obey Fermi or Bose statistics then it is necessary to sum over all the permutations of the particles (with the appropriate sign) in evaluating $\rho(x', x, \beta)$. In the Fermi case $\rho(x', x, \beta)$ is no longer positive everywhere. This results in the "Fermion sign problem" to which there is no general solution as yet. We will discuss the Fermion sign problem further in the lecture on diffusion Monte Carlo. In the Bose case, Ceperley and Pollock have devised efficient ways of summing over the permutations. The permuted paths result in polymers that link up to form larger polymers. In the figure below we show both the permuted and the unpermuted paths for a 2-particle system. In a many-body system one needs to sum over all the $n!$ permutations.

Fig. 2



non-exchanging path

exchanging path

VI. EFFICIENT GROUND STATE ENERGY EVALUATION

Evaluation of ground state properties requires us to use a large value of β and therefore polymers with large numbers of beads resulting in computationally expensive calculations. If a good trial wavefunction $\psi_{\rm T}$ is known then the length of the projection time (the value of β) can be greatly reduced since one just has to project away only a relatively small amount of contamination from the higher states. Further, for operators that commute with the Hamiltonian

$$\langle H \rangle = \frac{\langle \psi_{\rm T} | H | \psi \rangle}{\langle \psi_{\rm T} | \psi \rangle}. \tag{30}$$

Hence

$$\begin{aligned} \langle H \rangle &\approx \frac{\langle \psi_{\rm T} | H e^{-\beta H} | \psi_{\rm T} \rangle}{\langle \psi_{\rm T} | \psi \rangle} \\ &= \frac{\int dx \;\, dx' \;\, \langle \psi_{\rm T} | H | x' \rangle \langle x' | e^{-\beta H} | x \rangle \langle x | \psi_{\rm T} \rangle}{\int dx \;\, dx' \;\, \langle \psi_{\rm T} | x' \rangle \langle x' | e^{-\beta H} | x \rangle \langle x | \psi_{\rm T} \rangle} \\ &= \frac{\int dx \;\, dx' \;\, \frac{\langle \psi_{\rm T} | H | x' \rangle}{\langle \psi_{\rm T} | x' \rangle} \langle \psi_{\rm T} | x' \rangle \langle x' | e^{-\beta H} | x \rangle \langle x | \psi_{\rm T} \rangle}{\int dx \;\, dx' \;\, \langle \psi_{\rm T} | x' \rangle \langle x' | e^{-\beta H} | x \rangle \langle x | \psi_{\rm T} \rangle} \\ &= \frac{\int dx \;\, dx' \;\, E_{\rm L}(x') \; \psi_{\rm T}(x') \langle x' | e^{-\beta H} | x \rangle \psi_{\rm T}(x)}{\int dx \;\, dx' \;\, \psi_{\rm T}(x') \langle x' | e^{-\beta H} | x \rangle \psi_{\rm T}(x)} \end{aligned} \tag{31}$$

In order to evaluate Eq. 31 one needs to propagate an open polymer whose ends are subjected to a field given by $\psi_{\rm T}$. This method was (to the best of my knowledge) introduced in condensed matter applications of path integral Monte Carlo by Ye and Nightingale [3], though it is commonly used in lattice gauge theory and is closely analogous to diffusion Monte Carlo. As $\psi_{\rm T} \to \psi$, $E_{\rm L}(x')$ aproaches a constant independent of x'. Hence this is a "zero variance estimator" for the energy, *i.e.*, as $\psi_{\rm T} \to \psi$ the variance of the energy estimate goes to zero. Hence, in this unattainable limit, the exact energy can be obtained in a single Monte Carlo time step!

---

[1] D.M. Ceperley, Rev. Mod. Phys. xx, xxx, 1995.

[2] J.D. Doll, D.L. Freeman and T.L. Beck, *Adv. Chem. Phys.* , 78, 61 (1990).

[3] Y. Ye and M.P. Nightingale, preprint (1993).