Path Integral Monte Carlo on a Sphere

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CONTENTS

I. INTRODUCTION

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II. MANY BODY PATH INTEGRAL ON A RIEMANNIAN MANIFOLD

A many body system is composed of N *distinguishable* particles of mass m with positions in $R = (\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) = (\{\boldsymbol{r}_i\})$ where each position vector $\boldsymbol{r}_i = (r_i^1, r_i^2, \ldots, r_i^d) = (\{r_i^\alpha\})$ in d dimensions. On a Riemannian manifold of dimension d and metric tensor $g_{\alpha\beta}(\boldsymbol{r})$, the geodesic distance between two infinitesimally close points R and R' is $d\tilde{s}^2(R,R') = \sum_{i=1}^N ds^2(\boldsymbol{r}_i, \boldsymbol{r}_i')$ where $ds^2(\boldsymbol{r},\boldsymbol{r}') = g_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')^\alpha(\boldsymbol{r}-\boldsymbol{r}')^\beta$. Moreover,

$$\tilde{g}_{\mu\nu}(R) = g_{\alpha_1\beta_1}(\boldsymbol{r}_1) \otimes \ldots \otimes g_{\alpha_N\beta_N}(\boldsymbol{r}_N), \tag{2.1}$$

$$\tilde{g}(R) = \prod_{i=1}^N \det ||g_{\alpha_i\beta_i}(\boldsymbol{r}_i)||, \tag{2.2}$$

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where $||\tilde{g}_{\mu\nu}||$ is a matrix made of N diagonal blocks $||g_{\alpha_i\beta_i}||$ with $i = 1, 2, \ldots, N$. The Laplace-Beltrami operator on the manifold of dimension dN is

$$\Delta_R = \tilde{g}^{-1/2}\nabla_\mu(\tilde{g}^{1/2}\tilde{g}^{\mu\nu}\nabla_\nu), \tag{2.3}$$

where $\nabla = \nabla_R$, $\tilde{g}^{\gamma\nu}$ is the inverse of $\tilde{g}_{\gamma\nu}$, i.e. $\tilde{g}_{\mu\gamma}\tilde{g}^{\gamma\nu} = \delta_\mu{}^\nu$ the Kronecker delta, and a sum over repeated indexes is tacitly assumed.

We will first assume *free*, non interacting bodies, with an Hamiltonian $\mathscr{H}$ that reduces to the one of the free gas in flat space. For the sake of simplicity [1] we will choose

$$\mathscr{H} = -\lambda\Delta_R, \tag{2.4}$$

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

For *interacting* bodies we will then have more generally

$$\mathscr{H} = -\lambda\Delta_R + V(R), \tag{2.5}$$

where V is the potential energy of the system, that we here assume only a function of the particles positions and bounded from below.

The density matrix ρ of the system obeys Bloch equation

$$\frac{\partial\rho(t)}{\partial t} = -\mathscr{H}\rho(t), \tag{2.6}$$

$$\rho(0) = \mathbb{1}, \tag{2.7}$$

where t is the imaginary time with the dimensions of an energy and $\mathbb{1}$ the identity matrix. The position representation of the density matrix is then obtained from $\rho(R, R'; t) = \langle R|\rho(t)|R'\rangle$ with $\langle R|R'\rangle = \delta(R - R')/\sqrt{\tilde{g}(R)}$ where δ is a dN dimensional Dirac delta function. In the small imaginary time τ limit the position representation of the density matrix is

$$\rho(R, R'; \tau) \propto \tilde{g}(R)^{-1/4}\sqrt{\mathscr{D}(R, R'; \tau)}\,\tilde{g}(R')^{-1/4}e^{\lambda\tau\mathscr{R}(R)/6}e^{-\mathscr{S}(R,R';\tau)}, \tag{2.8}$$

where $\mathscr{R}$ is the scalar curvature of the manifold [2], $\mathscr{S}$ the action, and $\mathscr{D}$ the van Vleck's determinant [3, 4]

$$\mathscr{D}_{\mu\nu} = \nabla_\mu\nabla'_\nu\mathscr{S}(R, R'; \tau), \tag{2.9}$$

$$\det||\mathscr{D}_{\mu\nu}|| = \mathscr{D}(R, R'; \tau), \tag{2.10}$$

where $\nabla = \nabla_R$ and $\nabla' = \nabla_{R'}$. This determinant is the Jacobian of the transformation from the initial conditions given by fixing the pair of momentum and coordinate to the boundary conditions given by specifying the pair of initial and final coordinates needed in the path integral formulation. For the density matrix (2.8) the volume element for integration is $\sqrt{\tilde{g}(R)}\,dR$. The two factors $\tilde{g}^{-1/4}$ are needed in order to have for the density matrix a bidensity for which the boundary condition to Bloch equation is simply a Dirac delta function $\rho(R, R'; 0) = \delta(R - R')$. The square root of the van Vleck determinant factor takes into account the density of paths among the minimum extremal region for the action (see Chapter 12 of Ref. [4]).

For the *action* $\mathscr{S}$, the *kinetic-action* $\mathscr{K}$, and the *inter-action* $\mathscr{U}$ we have [3]

$$\mathscr{S}(R, R'; \tau) = \mathscr{K}(R, R'; \tau) + \mathscr{U}(R, R'; \tau), \tag{2.11}$$

$$\mathscr{K}(R, R'; \tau) = \frac{dN}{2}\ln(4\pi\lambda\tau) + \frac{d\tilde{s}^2(R, R')}{4\lambda\tau}. \tag{2.12}$$

In particular the kinetic-action is responsible for a diffusion of the random walk with a single particle variance on the α, β components equal to $\sigma^2_{\alpha\beta}(\boldsymbol{r}) = 2\lambda\tau/g_{\alpha\beta}(\boldsymbol{r})$. The inter-action is defined as $\mathscr{U} = \mathscr{S} - \mathscr{K}$ and for potential energies bounded from below one can resort to Trotter formula [5] to reach the *primitive approximation* [4]

$$\mathscr{U}(R, R'; \tau) = \tau[V(R) + V(R')]/2. \tag{2.13}$$

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[1] This is a delicate point and should be studied more carefully [1]. Especially for what concerns ordering ambiguities. We here appeal to simplicity.

[2] The factor depending on the curvature of the manifold is due to Bryce DeWitt [2]. For a space of constant curvature there is clearly no effect, as the term due to the curvature just leads to a constant multiplicative factor that has no influence on the measure of the various observables.

[3] The expression for $\mathscr{K}$ is the one of Eq. (24.16) of Ref. [4] to lowest order in $R - R'$.

[4] See Ref. [6] for a numerical analysis of the accuracy of this approximation and for possible its refinements.

For non interacting bodies $\mathscr{U} = 0$. Note that, even to lowest order in $R - R'$ [5], the path integral in the curved manifold for the non interacting system will not coincide with the one in flat space since it is not possible with a change of coordinates to simply remove the metric factor from both $d\tilde{s}^2$ and the volume element of integration, if not only locally. In fact this would require a *non coordinate basis* [8].

Given then an observable $\mathscr{O}$ we can determine its thermal average at an absolute temperature T from

$$\langle \mathscr{O} \rangle = \mathrm{tr}\{\rho(\beta)\mathscr{O}\}/Z_N, \tag{2.14}$$

$$Z_N = \mathrm{tr}\{\rho(\beta)\}, \tag{2.15}$$

where $\beta = 1/k_B T$ with k_B Boltzmann constant and Z_N the canonical partition function.

The position representation of the density matrix at an imaginary time $t = \beta$ is obtained through a path integral

$$\rho(R, R'; \beta) = \langle R|\rho(\beta)|R'\rangle = \int \prod_{k=0}^{M-1} \left[\rho(R_k, R_{k+1}; \tau)\, dR_k\right] \delta(R_0 - R)\delta(R_M - R')\, dR_M, \tag{2.16}$$

where we have discretized the imaginary time β into M *timeslices* with a small *timestep* $\tau = \beta/M$, a *bead* $R_k = (\{\boldsymbol{r}_{i,k}\}) = (\{r^\alpha_{i,k}\})$ at each timeslice $k = 1, 2, \ldots, M$. We will also call *link* a pair of contiguous beads.

For *identical* bodies if they satisfy to the Bose-Einstein statistics one needs to symmetrize the distinguishable density matrix, if they satisfy to the Fermi-Dirac statistics one needs to antisymmetrize it [9]. In these cases we can then write [6]

$$\rho_\pm(R, R'; \beta) = \frac{1}{N!} \sum_{\mathscr{P}} \mathrm{sgn}(\mathscr{P}) \rho(\mathscr{P}R, R'; \beta), \tag{2.17}$$

$$\mathrm{sgn}(\mathscr{P}) = (\pm 1)^{\sum_{\nu=1}^{N} (\nu-1) C_\nu}, \tag{2.18}$$

where $\mathscr{P}$ is any permutation of the N particles such that $\mathscr{P}R = (\boldsymbol{r}_{\mathscr{P}1}, \boldsymbol{r}_{\mathscr{P}2}, \ldots, \boldsymbol{r}_{\mathscr{P}N})$, with sign $\mathrm{sgn}(\mathscr{P})$. Any permutations can be broken into cycles $\mathscr{P} = \{C_\nu\}$ where C_ν is the number of cycles of length ν in $\mathscr{P}$. In the sum over the permutation one should use a $+1$ for the symmetrization necessary for bosons and -1 for the antisymmetrization necessary for fermions, in $\mathrm{sgn}(\mathscr{P})$.

On a surface, $d = 2$, for *impenetrable* identical bodies, one can also have anyonic statistics [10]. In this case it is necessary to consider, more generally,

$$\rho_\nu(R, R'; \beta) = \sum_{\alpha \in B_N} \chi(\alpha) \rho_\alpha(R, R'; \beta), \tag{2.19}$$

$$\chi(\text{paths with } n \text{ braids among the pairs of single particle paths}) = e^{-i\nu n\pi}, \tag{2.20}$$

where B_N is the infinite braid group which admits an infinite number of unitary one dimensional representations parametrized by an arbitrary number ν which determine the statistics and ρ_α is the distinguishable density matrix obtained from paths of kind α only.

III. THE SPHERE

A sphere of radius a is the surface, $d = 2$ [7], with metric $ds^2 = g_{\alpha\beta} dr^\alpha dr^\beta = s^2(d\theta^2 + \sin^2\theta\, d\varphi^2)$, of constant positive scalar curvature $2/a^2$ so that $\mathscr{R} = 2N/a^2$. The polar angle $r^1 = \theta \in]0, \pi]$ and the azimuthal angle $r^2 = \varphi \in]-\pi, \pi]$ are the contravariant coordinates of the position vector $\boldsymbol{r}$ and $g(\boldsymbol{r}) = |\sin\theta|$. In the small $\tau \to 0$ limit $\tilde{g}(R)^{-1/4} \sqrt{D(R, R'; \tau)}\, \tilde{g}(R')^{-1/4} \to (1/2\lambda\tau)^N$. So we see how both the curvature term and the van Vleck factor, being constant, simply drop off from the measure of the various observables of Eq. (2.14).

The position of a particle on the sphere in the three dimensional Euclidean space embedding the sphere is

$$\begin{cases} x = a \sin\theta \cos\varphi \\ y = a \sin\theta \sin\varphi \\ z = a \cos\theta \end{cases} \tag{3.1}$$

and the particle path in it is $\boldsymbol{q}(t) = (x(t), y(t), z(t))$.

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[5] For next orders corrections see for example Ref. [7].

[6] One can symmetrize or antisymmetrize respect to the first, the second or both the arguments of the distinguishable density matrix. We here choose the first case.

[7] So it is conformally flat as any Riemannian manifold of dimension $d \leq 3$.

We use the Metropolis algorithm [11, 12] to evaluate the average of Eq. (2.14). In order to explore ergodically the configuration space $\boldsymbol{r} = (\theta, \varphi) \in]0, \pi] \times] - \pi, \pi]$ we choose the transition displacement move described in Appendix A. In order to sample the permutation sum of Eq. (2.17) needed for identical bodies we use the transition bridge move described in Appendix B.

IV. DISTINGUISHABLE BODIES

V. IDENTICAL BODIES

Bosons

Fermions

VI. ANYONIC BODIES

Appendix A: The transition displacement move

In order to explore the θ and φ configuration space on the sphere it is convenient to propose the following transition move for each particle in a randomly chosen bead

$$\begin{aligned} &0 < \theta_{\rm old} \leq \pi \quad \theta_0 = \theta_{\rm old} + \Delta_\theta(\eta - 1/2) \\ &\theta_{\rm new} = 2\pi\ \texttt{ABS}[\theta_0/2\pi - \texttt{FLOOR}(\theta_0/2\pi + 1/2)] \quad 0 < \theta_{\rm new} \leq \pi, \end{aligned} \tag{A1}$$

$$\begin{aligned} &-\pi < \varphi_{\rm old} \leq \pi \quad \varphi_0 = \varphi_{\rm old} + \Delta_\varphi(\eta - 1/2) \\ &\varphi_1 = \varphi_0 - \pi\ \{\texttt{INT}(\theta_0/\pi) + [\texttt{SGN}(\theta_0) - 1]/2\} \\ &\varphi_{\rm new} = \varphi_1 - 2\pi\ \texttt{NINT}(\varphi_1/2\pi) \quad -\pi < \varphi_{\rm new} \leq \pi \end{aligned} \tag{A2}$$

where ABS is the function absolute value, SGN is the sign function, INT is the function integer part, NINT is the nearest integer function and FLOOR is the floor function. $\eta \in [0, 1]$ is a uniform pseudo random number. Δ_θ and Δ_φ are two positive quantities measuring the θ-displacement and the φ-displacement respectively in the transition move. When the path $\boldsymbol{r}(t) = (\theta(t), \varphi(t))$ crosses a pole φ changes by π. One can easily convince himself that starting from an arbitrary $\boldsymbol{r}(t_0)$ and generating $\boldsymbol{r}(t_{\rm new})$ from $\boldsymbol{r}(t_{\rm old})$ through the recipe of Eqs. (A1) and (A2) the generated points cover $]0, \pi] \times] - \pi, \pi]$ uniformly independently of the chosen $\boldsymbol{r}(t_0)$ and Δ_θ, Δ_φ. In the simulation we choose Δ_θ and Δ_φ so to have acceptance ratios close to 1/2 in the acceptance/rejection choices for the random walk transition displacement moves of the Metropolis algorithm.

Appendix B: The transition bridge move

In order to take into account of the particles permutations it is necessary to construct two Brownian bridges between two randomly chosen particles in two randomly chosen beads to generate an exchange between the two particles. With one bridge we connect particle 1 on bead R_i to particle 2 on bead R_j and with the other we connect particle 2 on bead R_i to particle 1 on bead R_j with $i < j$.

The Brownian bridge between particle 1 at $\boldsymbol{r}_{1,i}$ and particle 2 at $\boldsymbol{r}_{2,j}$ is built like so [6],

$$\boldsymbol{r}_{{\rm new},i} = \boldsymbol{r}_{1,i} \tag{B1}$$

$$\boldsymbol{r}_{{\rm new},k} = \boldsymbol{r}_{{\rm new},k-1} + \frac{(\boldsymbol{r}_{2,j} - \boldsymbol{r}_{{\rm new},k-1})}{j - k + 1} + \boldsymbol{\xi}(\boldsymbol{r}_{{\rm new},k-1}) \quad k = i + 1, \ldots, j - 1 \tag{B2}$$

where ξ^α is a random number with a Gaussian probability distribution with variance $\sigma^2_{\alpha\alpha}(\boldsymbol{r})(j-k)/(j-k+1)$ where $\sigma^2_{\alpha\alpha}(\boldsymbol{r}) = 2\lambda\tau/g_{\alpha\alpha}(\boldsymbol{r})$ is the diagonal free particle variance. Note that the metric enters the free particle variance since it is not possible by a change of coordinates to remove it both from the kinetic-action and from the integration measure $\sqrt{g(\boldsymbol{r})}\, d\boldsymbol{r}$, if not only locally.

Any permutation can be reached through a two particles exchange so the bridge transition move allows to sample the sum in Eq. (2.17). Moreover, even for the non interacting system, one would still need to adopt Metropolis algorithm in order to sample additionally the metric factor in the integration measure that can be seen as giving rise to an effective potential $\ln \sqrt{g(\boldsymbol{r})}$.

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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[1] J. R. Klauder and R. Fantoni, The Magnificent Realm of Affine Quantization: valid results for particles, fields, and gravity, Axioms **12**, 911 (2023).
[2] B. S. DeWitt, Dynamical Theory in Curved Spaces. I. A Review of the Classical and Quantum Action Principles, Rev. Mod. Phys. **29**, 377 (1957).
[3] J. H. V. Vleck, The Correspondence Principle in the Statistical Interpretation of Quantum Mechanics, Proc Natl Acad Sci U S A **14**, 178 (1928).
[4] L. S. Schulman, *Techniques and Applications of Path Integration* (John Wiley & Sons, Technion, Haifa, Israel, 1981) chapter 24.
[5] H. F. Trotter, On the Product of Semi-Groups of Operators, Proc. Am. Math. Soc. **10**, 545 (1959).
[6] D. M. Ceperley, Path integrals in the theory of condensed Helium, Rev. Mod. Phys. **67**, 279 (1995).
[7] F. Bastianelli and O. Corradini, On the simplified path integral on spheres, Eur. Phys. J. C **77**, 731 (2017).
[8] C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation* (W. H. Freeman, San Francisco, 1973).
[9] D. M. Ceperley, Path integral Monte Carlo methods for fermions, in *Monte Carlo and Molecular Dynamics of Condensed Matter Systems*, edited by K. Binder and G. Ciccotti (Editrice Compositori, Bologna, Italy, 1996) page 4.
[10] A. Lerda, *Anyons. Quantum Mechanics of Particles with Fractional Statistics* (Springer-Verlag, Berlin, 1992).
[11] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. M. Teller, and E. Teller, Equation of state calculations by fast computing machines, J. Chem. Phys. **1087**, 21 (1953).
[12] M. H. Kalos and P. A. Whitlock, *Monte Carlo Methods* (John Wiley & Sons Inc., New York, 1986).