The role of winding numbers in quantum Monte Carlo simulations

Patrik Henelius and S. M. Girvin

Department of Physics, Indiana University, Bloomington, Indiana 47405

Anders W. Sandvik

Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

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We discuss the effects of fixing the winding number in quantum Monte Carlo simulations. We present a simple geometrical argument as well as strong numerical evidence that one can obtain exact ground state results for periodic boundary conditions without changing the winding number. However, for very small systems the temperature has to be considerably lower than in simulations with fluctuating winding numbers. The relative deviation of a calculated observable from the exact ground state result typically scales as T^γ, where the exponent γ is model and observable dependent and the prefactor decreases with increasing system size. Analytic results for a quantum rotor model further support our claim.

One approach to numerical many-body physics is to stochastically sample the "world line" configurations of a real-space Euclidean path integral. The most common of these quantum Monte Carlo (QMC) methods[1,2] are based on the Trotter decomposition formula in discretized imaginary time,[3] with a resulting systematic error that vanishes as the discretization $\Delta\tau$ is decreased.[4,5] For lattice models, methods have recently been constructed for simulations in continuous imaginary time,[6–8] hence directly giving results exact to within statistical fluctuations. A related method is the stochastic series expansion technique[9] (a generalization of Handscomb's method[10]), which samples the power series expansion of the density matrix, and also is exact. For all these methods, the configurations for periodic systems can be labeled by a topological "winding number" w, which counts the net number of times the world lines wrap around the system in the course of propagation in imaginary time. In practice, it is often not possible to sample all winding number sectors, since changing w requires simultaneous modification of a number $\sim L$ world lines, where L is the linear size of the system, with a resulting low acceptance rate if L is large. Such non-ergodicity is clearly related to the boundary condition[5,11] (restricting to, e.g., $w = 0$ can be considered a particular boundary condition), and therefore results scaled to infinite system size are still correct, although there can be significant deviations from the exact periodic boundary condition results for any given small system size. The winding number is a consequence of the path integral formulation of quantum mechanics, and a fixed w is not related to the Hamiltonian in a simple way. In many cases it is of interest to obtain approximation-free results for periodic boundary conditions, specifically, and the restriction to fixed w can then be a practical limitation of the QMC method.

We here point out that the exact ground state can in fact be obtained in any winding number sector, even for the smallest possible systems. We base our claim on simple geometric considerations, and provide supporting simulation results for several many-body Hamiltonians (one- and two dimensional Heisenberg spin models) as well as analytic results for a quantum rotor. We expect our arguments to be generally valid for models for which the path integral is positive definite (i.e., there are no sign problems[5,12]), which is the case for, e.g., 1D fermion systems and non-frustrated spin and boson systems in any dimension.

In order to define the winding number, we first consider the standard path integral formulation of a continuous 1D system. The partition function for a single particle of mass M in a potential $V(x)$ is[13]

$$Z = \int_{x(\beta)=x(0)} D[x(\tau)]e^{-S}, \tag{1}$$

where the action is

$$S = \int_0^\beta d\tau \left[\frac{M}{2} \left(\frac{dx(\tau)}{d\tau} \right)^2 + V(x(\tau)) \right]. \tag{2}$$

The integral in (1) is over all paths (or world lines) starting at position x at imaginary time $\tau = 0$ and ending at the same position x at $\tau = \beta$, where β denotes the inverse temperature. For a periodic system, the paths can be divided into topologically distinct classes, characterized by a winding number w defined as the net number of times the world line spatially wraps around the system. For a many-particle system, the winding number is defined as the net total displacement to the "left" or the "right" of the world lines in the course of propagation between $\tau = 0$ and $\tau = \beta$, divided by the length of the system. In higher dimensions, there is a winding number associated with each dimension, and the definition of these is a direct generalization of the above definition in one dimension.

For interacting many-body systems, analogous real-space path-integrals (or related sums[9] based on series expanding the density matrix operator $e^{-\beta H}$) can be constructed, and are suitable for numerical simulations in cases where the weight associated with the paths is positive definite. Such QMC methods have been developed, e.g., for lattice fermions in one dimension[5], lattice[14] and

continuum[2] bosons, and quantum spin systems.[4] In the case of fermions in higher dimensions, the path integral cannot be efficiently sampled directly, due to the non-positive definiteness of the weight, which leads to the infamous "sign problem".[12,15]

Stochastic sampling of the bosonic paths within a sector of a fixed winding number can be accomplished by local modifications of the world lines, and is typically a relatively straight-forward task. The global modifications required in order to change the winding number are often practically impossible to carry out efficiently, however. Recently "loop-cluster" algorithms have been developed which in principle automatically sample all winding number sectors.[16] However, such algorithms do not perform well for all models, and therefore the restriction to a sector with fixed winding number remains the only option in many cases. We note that the winding number itself is related to long-range coherence in the system. For boson and spin systems, the winding number fluctuation $\langle w^2 \rangle$ is directly proportional to the superfluid density and the spin stiffness, respectively.[2] In some cases these quantities can, however, also be computed in a restricted simulation.[14,2]

We here argue that the exact ground state can actually be studied in any w sector. Consider first again a 1D periodic system with a single particle. A path integral configuration can be visualized as a string on the surface of a cylinder with periodic boundary conditions (i.e., a torus). As the temperature is lowered the length $\beta = 1/T$ of the system in the imaginary time direction becomes much larger than the spatial system size, and the string can then wrap around the cylinder multiple times in both directions between $\tau = 0$ and β. In the winding number w sector, the net number of revolutions has to be w. Nevertheless, locally, in an imaginary-time segment of length $\Delta\tau \ll \beta$, it would not be possible to detect the effects of this restriction. Hence, any quantity that can be defined on a finite segment of the cylinder should be the same in any winding number sector as $\beta \to \infty$. Since correlation functions decay exponentially with the imaginary-time separation in a finite system, due to the finite-size gap, all quantities which are not defined in terms of the global winding number itself should become exact as $\beta \to \infty$. This argument can clearly be generalized for a many-body system in any dimension, again of course provided that all paths have positive weights. In the case of mixed signs the positive and negative contributions to the partition function cancel as $\beta \to \infty$, and physical quantities are given by finite ratios of two vanishing numbers. It is then not clear that all the winding number sectors become equal as $\beta \to \infty$ (although we have not proved the contrary), and we will not consider this intricate issue further here.

We can rigorously prove that fixed w gives the correct ground state of a single particle in one dimension. This system (with $ML^2 = 2\pi^2$) is equivalent to the quantum rotor, described by the Hamiltonian

$$H = -\partial^2/\partial\theta^2. \tag{3}$$

The eigenfunctions labeled by the angular momentum m are

$$\Psi_m(\theta) = \exp(im\theta). \tag{4}$$

The partition function is

$$Z = \sum_{m=-\infty}^{+\infty} \exp(-\beta m^2), \tag{5}$$

and can be transformed from a sum over angular momenta to a sum over winding numbers in the following way: In the discrete path integral formulation with $\Delta\tau = \beta/N$ the partition function is

$$Z = \int D\theta \prod_{j=1}^{N} \langle\theta_{j+1}| \exp(-\Delta\tau H)|\theta_j\rangle$$

$$= \int D\theta \prod_{j=1}^{N} \left[\sum_m \exp(-\Delta\tau m^2) \exp[im(\theta_{j+1} - \theta_j)] \right], \tag{6}$$

where $\Delta\tau = \beta/N$ and $\theta_{N+1} = \theta_1$. Using Poisson's summation formula,

$$\sum_{m=-\infty}^{\infty} f(m) = \sum_{n=-\infty}^{\infty} F(2\pi n), \tag{7}$$

where $F(n)$ is the Fourier transform of $f(m)$, we obtain

$$Z = \int D\theta \prod_{j=1}^{N} \left[\sum_n \exp\left[-\frac{(\theta_{j+1} - \theta_j - 2\pi n)^2}{4\Delta\tau} \right] \right]. \tag{8}$$

Next we write the j (or τ) dependence of θ as

$$\theta_j = \mathrm{mod}[\theta_1 + \frac{2\pi w}{N}(j-1) + \delta\theta_j, 2\pi], \tag{9}$$

where w is the winding number. For the time being we neglect the fluctuations $\delta\theta_j$, which are the same for all w. As $\Delta\tau \to 0$, only the term $n = 0$ contributes in the above sum, unless θ crosses the boundary at $\theta = 0$, in which case $n = -1$ or $n = +1$ will give the contributing term. Hence the partition function can be expressed as

$$Z = f(\beta) \sum_{w=-\infty}^{\infty} \exp(-\pi^2 w^2/\beta), \tag{10}$$

where $f(\beta)$ is a function containing the effects of the fluctuations $\delta\theta_j$ which we have so far neglected. The easiest way to find $f(\beta)$ is to simply equate the above result with Eq. (5). This gives our final result for the partition function expressed as a sum over winding numbers:

$$Z = \sum_{w=-\infty}^{\infty} \sqrt{\pi/\beta} \exp(-\pi^2 w^2/\beta). \tag{11}$$

This result could have been directly obtained using Poisson's summation formula, Eq. (7), on Eq. (5). The above derivation shows that the new summation index indeed is the winding number, which hence can be thought of as a quantity conjugate to the angular momentum.

The energy $E = -(1/Z)\partial Z/\partial\beta$ given as a sum over angular momenta is

$$E = -\frac{1}{Z}\sum_m m^2 \exp(-\beta m^2), \qquad (12)$$

and expressed as a sum over winding numbers

$$E = -\frac{1}{Z}\sum_w \sqrt{\pi}(\frac{1}{2\beta^{3/2}} - \frac{\pi^2 w^2}{\beta^{5/2}})e^{-\pi^2 w^2/\beta}. \qquad (13)$$

In Fig. 1 the energy of the rotor is plotted versus β on a log-log scale. It decreases as β^{-1} at high temperatures, changing to an exponential decay around $\beta = 1$. In the same graph we also show the energy evaluated in the $w = 0$ sector. At high temperatures the results coincide with the full energy, but around $\beta = 1$ the behavior changes to be of the form $\beta^{-3/2}$, instead of exponential, as can be readily extracted from Eq. (13). Hence, we indeed get the correct energy (namely, zero) in the $w = 0$ sector, but the approach to the ground state is much slower than in the "ensemble" with fluctuating w.
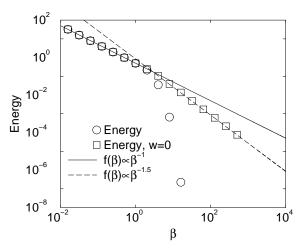

FIG. 1. Rotor model : The full energy and the energy for the $w = 0$ sector vs. β. The lines are the assymptotic high and low (for $w = 0$) temperature forms.

Next we present numerical results for several many-body models. We study the Heisenberg model, defined by the Hamiltonian

$$H = \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \qquad (14)$$

where $\langle i, j\rangle$ indicates a pair of nearest neighbors lattice sites, and $\mathbf{S}_i$ is a spin-S operator at site i. We consider the 1D model with $S = 1/2$ and $S = 1$, as well as the 2D model with $S = 1/2$. We note that these quantum spin models are formally equivalent to constrained boson systems.

For the simulations we use the stochastic series expansion algorithm,[9] which is based on a power series expansion of $e^{-\beta H}$, and hence is not a standard path integral method. The configuration space is nevertheless very strongly related to an Euclidean path integral,[8] and the winding number has exactly the same meaning. For systems of linear size $L \lesssim 16$ Monte Carlo updates changing the winding number can be easily carried out, but for larger systems a restriction to fixed w is necessary in practice. The advantage of the method is that there are no other sources of systematic errors. We present energy results both for $w = 0$ and fluctuating w, and compare with exact diagonalization data.

The simulation scheme is formulated in the standard basis where the operators S_i^z are diagonal. The internal energy per spin can be calculated in two different ways in the simulation; from the nearest-neighbor correlation function $\langle S_i^z S_{i+1}^z\rangle$ as well as from a manifestly rotationally invariant estimator giving the full $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1}\rangle$.[9] We define

$$E_z = 3\langle S_i^z S_{i+1}^z\rangle, \qquad (15a)$$
$$E_s = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1}\rangle. \qquad (15b)$$

The agreement between the two estimates can serve as a good internal check of the spherical spin symmetry in the simulation. With w fixed in a finite system, the spin-rotational symmetry is broken since only the xy-terms are involved in the spatial propagation (spin flipping) of the path and the estimates will therefore not agree completely.

In Fig. 2 E_s and E_z are graphed versus the inverse temperature β used in simulations of an 8-site $S = 1/2$ chain, both in the $w = 0$ sector and with fluctuating winding numbers. In the $w = 0$ sector, the rotationally invariant and diagonal estimates approach the exact ground state result from above, and below, respectively. For fluctuating winding numbers the exact ground state energy is obtained within statistical errors already for $\beta \approx 8$ for this system size, reflecting the large finite-size gap and the exponential approach to the ground state with increasing β.

In Fig. 3 the difference between Monte Carlo data obtained in the $w = 0$ sector and the exact temperature-dependent energy is graphed on a log-log scale for $L = 4, 8$ and 16. At high temperatures the difference tends to vanish rapidly since the system is too short in the imaginary time dimension to allow for the winding number to change from zero. At low temperatures the deviation decreases as $\beta^{-\gamma}$, with $\gamma = 1$ within the numerical precision, and there is a maximum at an intermediate value β^*. As expected, the maximum difference decreases rapidly with system size. The relative error decreases roughly as $1/L$ at a given temperature, and β^* increases roughly as L. β^* hence reflects the inverse finite-size gap.
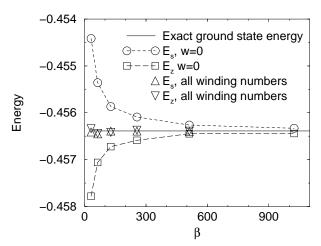
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FIG. 2. 1D spin-1/2 model: The energy estimators E_s and E_z vs. β for L=8.

FIG. 4. 1D spin-1 model: The deviation from the ground state energy of E_s vs. β for L=4 and 8. The lines have slope -1.

These results confirm that for a given desired accuracy of the energy at a given temperature, there will be some system size beyond which it is not necessary to sample different winding number sectors. Furthermore, the exact ground state is always obtained as $\beta \to \infty$. However, for small systems we have to use higher values of β in order to achieve a certain accuracy if we do not sample all winding number sectors.
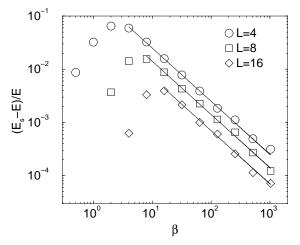

FIG. 3. 1D spin-1/2 model: The deviation from the exact energy of E_s vs. β for L=4,8 and 16. The lines have slope -1.

Next we consider the 1D $S = 1$ model and the 2D $S = 1/2$ model. The relative deviation of the $w = 0$ energies from the exact ground state values are graphed versus β for different system sizes in Fig. 4 and Fig. 5 (for the 2D systems with $L > 4$ "exact" results were obtained in simulations with fluctuating w). Again we see that at low temperatures the ground state is approached as β^{-1}, instead of the exponential approach expected for the exact energy.
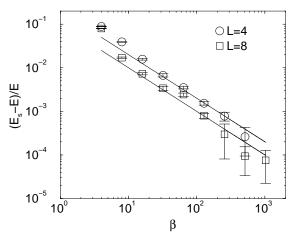
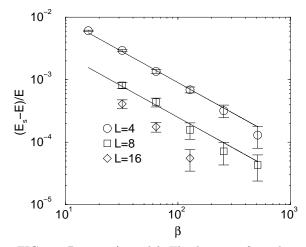To summarize we have given an intuitive argument why

FIG. 5. 2D spin-1/2 model: The deviation from the ground state energy of E_s vs. β for L=4,8 and 16. The lines have slope -1

restricting the winding number in QMC simulations number should not affect calculated ground state properties of even the smallest lattices. We have given strong numerical evidence to support this statement, in addition to rigorous results for a simple quantum rotor model. Typically, the asymptotic deviations from the exact periodic boundary condition results scale as $\beta^{-\gamma}$ at low temperatures, with a prefactor that goes to zero as the system size increases. Hence, in terms of the β needed to obtain the ground state, to the statistical precision possible in QMC simulations, there does not appear to be any advantage of fluctuating numbers for moderate and large systems.

Our considerations are closely related to the imaginary-time boundary conditions recently discussed by Täuber and Nelson.[17] They showed that the condition that the world line configurations at $\tau = 0$ and $\tau = \beta$

being equal can be relaxed, still giving the same result as the periodic imaginary time boundary condition when $\beta \to \infty$. In analogy with our discussion above, the reason for this is that the changed boundary condition does not affect the behavior of the world lines in a segment of length $\ll \beta$.

[1] For reviews of QMC methods for lattice models, see, e.g., D. Scalapino in *Frontiers and border lines in many-particle physics*, edited by R. A. Broglia and J. R. Schrieffer (Elsevier, 1988); W. Von Der Linden, Phys. Rep. **220**, 53 (1992); A. W. Sandvik in *Strongly Correlated magnetic and superconducting systems*, edited by G. Sierra and M. A. Martin Delgado (Springer, Berlin, 1997).

[2] For a review of QMC methods for continuum bosons, see D. Ceperley, Rev. Mod. Phys. **67**, 279 (1995).

[3] H. F. Trotter, Proc. Am. Math. Soc. **10**, 545 (1959); M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976).

[4] M. Suzuki, S. Miyashita, and A. Kuroda, Prog. Theor. Phys. **58**, 1377 (1977); M. Barma and B. S. Shastry, Phys. Rev. B **18**, 3351 (1977); J. J. Cullen and D. P. Landau, Phys. Rev. B **27**, 297 (1983).

[5] J. E. Hirsch, R. L. Sugar, D. J. Scalapino, and R. Blankenbecler, Phys. Rev. B **26**, 5033 (1982).

[6] B. B. Beard and U.-J. Wiese, Phys. Rev. Lett. **77**, 5130 (1996).

[7] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn, Zh. Eks. Teor. Fiz. **64**, 853 (1996); preprint (cond-mat/9703200).

[8] A. W. Sandvik, R. R. P. Singh, and D. K. Campbell, to appear in Phys. Rev. B (preprint cond-mat/9706046).

[9] A. W. Sandvik and J. Kurkijärvi, Phys. Rev. B **43**, 5950 (1991); A. W. Sandvik, J. Phys. A **25**, 3667 (1992).

[10] D. C. Handscomb, Proc. Cambridge Philos. Soc. **58**, 594 (1962); **60**, 115 (1964); D. H. Lee, J. D. Joannopoulos, and J. W. Negele, Phys. Rev. B **30**, 1599 (1984).

[11] M. Marcu, in *Quantum Monte Carlo methods in equilibrium and nonequilibrium systems*, edited by M. Suzuki (Springer, Berlin, 1987).

[12] E. Y. Loh Jr. *et al.*, Phys. Rev. B **41**, 9301 (1990).

[13] For an introduction to path integrals, see, e.g., R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals*, (McGraw-Hill, New York, 1965).

[14] G. G. Batrouni, R. T. Scalettar and G. T. Zimanyi, Phys. Rev. Lett. **65**, 1765 (1990).

[15] Alternative methods have been developed that are better suited for studies of fermions in higher dimensions; R. Blankenbecler, D. J. Scalapino and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).

[16] H. G. Evertz, G. Lana, and M. Marcu, Phys. Rev. Lett. **70**, 875 (1993).

[17] U. C. Täuber and D. R. Nelson, to appear in Phys. Rep. (1997) (cond-mat/9608057).