No sign problem in one-dimensional path integral Monte Carlo simulation of fermions: A topological proof

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This paper shows that, in one dimension, due to its topology, a closed-loop product of short-time propagators is always positive, despite the fact that each antisymmetric free fermion propagator can be of either sign.

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I. INTRODUCTION

In their first path-integral Monte Carlo (PIMC) simulation of fermions in a one-dimensional harmonic oscillator, Takahashi and Imada were surprised that, "In the calculation of one-dimensional fermions, we do not find any cases of negative weight function in ten thousands Monte Carlo steps even at low temperature" [1]. They surmised that their situation maybe similar to the one-dimensional lattice fermions studies of Hirsch *et al.* [2]. The two are not similar. By a clever lattice arrangement, the matrix elements of the lattice fermions of Hirsch *et al.* can be chosen to be positive [2], whereas the free fermion propagator used by Takahashi and Imada [1] can have either sign. However, 24 yr earlier, Girardeau [3] has shown that, in one dimension, the ground state wave function of N impenetrable bosons $\{x_1, x_2 \cdots x_n\}$, which vanishes whenever $x_i = x_j$, is the same as the modulus of the ground state wave function of N *free* fermions,

$$\psi_0^B = \left|\psi_0^F\right|. \tag{1}$$

This means that, in one dimension, N *interacting* fermions can always be mapped into the ordered subspace,

$$x_1 < x_2 < \cdots < x_N, \tag{2}$$

with vanishing wave function at $x_i = x_{i+1}$. The ground state wave function in this subspace can then be taken to be positive, the same as that of N impenetrable, interacting bosons [4]. At any other subspace, corresponding to a permutation of (2), the fermion wave function is, then, this wave function multiplied by the sign of the permutation. Alternatively, one can view the subspace (2) as having the correct wave function nodes at $x_i = x_{i+1}$, thereby reduced a many-fermion problem to that of a many-boson problem in a single nodal region [5]. Since the determinant wave function $\det|\phi_i(x_j)|$ for any reasonable one-dimensional single particle state $\phi_i(x)$ has this nodal structure, diffusion Monte Carlo will also have no sign problem when *restricted* to any single subspace, such as (2). These views explain that fermions in one dimension do not have the sign problem because it is basically a boson problem.

However, these views do not explain why there is no sign problem *specifically* for PIMC simulations, despite the fact that the antisymmetric free fermion propagator can have either sign and that the simulation is not restricted to any particular nodal region.

This paper found that there is a surprisingly simple, but overlooked topological proof, that there is no sign problem for PIMC simulation of one-dimensional fermions. This topological explanation is related to the original insight of Girardeau [6], that any statistics is permissible in one dimension, but only Fermi-Dirac or Bose-Einstein statistics is mandated in more than one dimension.

II. FERMION PATH INTEGRAL MONTE CARLO

Consider the single particle imaginary time Schrödinger equation in one-dimension,

$$-\frac{\partial\psi(x,\tau)}{\partial\tau} = (\hat{T}+\hat{V})\psi(x,\tau) = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,\tau), \tag{3}$$

with dimensionless spatial variable x and imaginary time $\tau \propto \beta = (k_B T)^{-1}$. In PIMC, one is mostly interested in extracting the ground state wave function squared $\psi_0^2(x)$ and energy E_0 from the *diagonal* element of the imaginary time propagator (or the density matrix) at the large τ, zero temperature limit,

$$\lim_{\tau\to\infty} G(x,x;\tau) \longrightarrow \psi_0^2(x)e^{-\tau E_0} + \cdots, \tag{4}$$

where

$$G(x',x;\tau) = \langle x'|e^{-\tau(\hat{T}+\hat{V})}|x\rangle = \sum_n \psi_n^*(x')\psi_n(x)e^{-\tau E_n}. \tag{5}$$

Since $G(x',x;\tau)$ is generally unknown, it is approximated by k short-time high temperature propagators via

$$G_k(x',x;\tau) = \langle x'|(e^{-\epsilon(\hat{T}+\hat{V})})^k|x\rangle = \int_{-\infty}^{\infty} dx_1\cdots dx_{k-1}\, G_1(x',x_1;\epsilon) \times G_1(x_1,x_2;\epsilon)\cdots G_1(x_{k-1},x;\epsilon), \tag{6}$$

where $\epsilon = \tau/k$ and $G_1(x',x,\epsilon)$ is usually the second-order short-time approximation of $\langle x'|e^{-\epsilon(\hat{T}+\hat{V})}|x\rangle$, the *primitive approximation* (PA) propagator,

$$G_1(x',x;\epsilon) = \langle x'|e^{-(\epsilon/2)\hat{V}}e^{-\epsilon\hat{T}}e^{-(\epsilon/2)\hat{V}}|x\rangle = \frac{1}{\sqrt{2\pi\epsilon}}e^{-(\epsilon/2)V(x')}e^{-(x'-x)^2/(2\epsilon)}e^{-(\epsilon/2)V(x)}. \tag{7}$$

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Since the PA propagator is only second order, it is accurate only at small ϵ. Therefore, many PA propagators are usually needed in (6) to extract the ground state properties at the large τ, zero temperature limit.

To generalize the above to N fermions, one replaces x by $\mathbf{x} = (x_1, x_2 \cdots x_N)$ and $G_1(x', x, \epsilon)$ by

$$G_1(\mathbf{x}', \mathbf{x}; \epsilon) = e^{-(\epsilon/2)V(\mathbf{x}')} G_0(\mathbf{x}', \mathbf{x}; \epsilon) e^{-(\epsilon/2)V(\mathbf{x})}, \qquad (8)$$

where $G_0(\mathbf{x}', \mathbf{x}; \epsilon)$ is the antisymmetric free-fermion propagator,

$$G_0(\mathbf{x}', \mathbf{x}; \epsilon) = \frac{1}{N!} \det\left(\frac{1}{\sqrt{2\pi\epsilon}} \exp\left[-\frac{1}{2\epsilon}(x_i' - x_j)^2 \right] \right). \qquad (9)$$

Note that any pair exchange $x_i' \leftrightarrow x_j'$ ($x_i \leftrightarrow x_j$) interchanges two rows (columns) of the determinant and, hence, the sign of $G_0(\mathbf{x}', \mathbf{x}; \epsilon)$, whereas $G_0(\mathbf{x}', \mathbf{x}; \epsilon) = G_0(\mathbf{x}, \mathbf{x}'; \epsilon)$.

When the fermion propagator (9) is negative, it cannot be directly sampled using Monte Carlo methods. One is then forced to sample its absolute value and attaches a sign to any observable when computing its expectation value. As one increases the number of propagators to reach the large τ limit, the sign of the product of fermion propagators tends equally likely to be negative as positive. The resulting cancellation then washes away any signal of the observable and one has the sign problem. However, as first noted by Takahashi and Imada [1], this does not happen for fermion propagators in one dimension. The goal of this work is to give a simple proof of this unexpected result.

III. NO SIGN PROBLEM IN ONE DIMENSION

The sign of the integrand in the discrete path integral (6) depends only on the product of k free-fermion propagators,

$$G_0(\mathbf{x}, \mathbf{x}_1; \epsilon) G_0(\mathbf{x}_1, \mathbf{x}_2; \epsilon) \cdots G_0(\mathbf{x}_{k-1}, \mathbf{x}; \epsilon). \qquad (10)$$

For extracting $\psi_0^2(\mathbf{x})$, the propagators must start at $\mathbf{x}$ and loop back to $\mathbf{x}$. The integral is that of a closed-end path integral. Consider first, the case of two (spinless) fermions. The antisymmetric free propagator is then,

$$\begin{aligned} G_0(x_1', x_2', x_1, x_2; \epsilon) &= \frac{1}{2} \frac{1}{2\pi\epsilon} \det \begin{pmatrix} e^{-\frac{1}{2\epsilon}(x_1'-x_1)^2} & e^{-\frac{1}{2\epsilon}(x_1'-x_2)^2} \\ e^{-\frac{1}{2\epsilon}(x_2'-x_1)^2} & e^{-\frac{1}{2\epsilon}(x_2'-x_2)^2} \end{pmatrix} \\ &= \frac{1}{2} \frac{1}{2\pi\epsilon} e^{-\frac{1}{2\epsilon}[(x_1'-x_1)^2 + (x_2'-x_2)^2]} \left(1 - e^{-\frac{1}{\epsilon}(x_1'-x_2')(x_1-x_2)}\right). \end{aligned} \qquad (11)$$

Thus, $G_0(x_1', x_2', x_1, x_2; \epsilon) < 0$ if and only if

$$(x_1' - x_2')(x_1 - x_2) < 0, \qquad (12)$$

i.e., either $x_1' > x_2'$ and $x_1 < x_2$ or vice versa. This means that the prime and unprime positions are on opposite sides of the line $x_1 = x_2$ dividing the x_1-x_2 plane.

The key contribution of this paper is to rephrase the above condition in topological terms: the propagator is negative when the line connecting the prime and unprime position of the propagator crosses the line $x_1 = x_2$. This is shown in part A of Fig. 1. The trace, or the diagonal element of a single propagator is always non-negative,

$$G_0(\mathbf{x}, \mathbf{x}; \epsilon) \propto \left(1 - e^{-\frac{1}{\epsilon}(x_1 - x_2)^2}\right) \geqslant 0. \qquad (13)$$

So is the product of two propagators $G_0(\mathbf{x}, \mathbf{x}_1; \epsilon) G_0(\mathbf{x}_1, \mathbf{x}; \epsilon)$ since the line is either not crossed or crossed twice. The same is true for the product of three propagators $G_0(\mathbf{x}, \mathbf{x}_1; \epsilon) G_0(\mathbf{x}_1, \mathbf{x}_2; \epsilon) G(\mathbf{x}_2, \mathbf{x}; \epsilon)$ as shown in part B. More generally, any closed-loop product of propagators must be positive (or, at least, non-negative) as shown in part C since topologically, any planar closed curve must intersect an infinite straight line even a number of times.

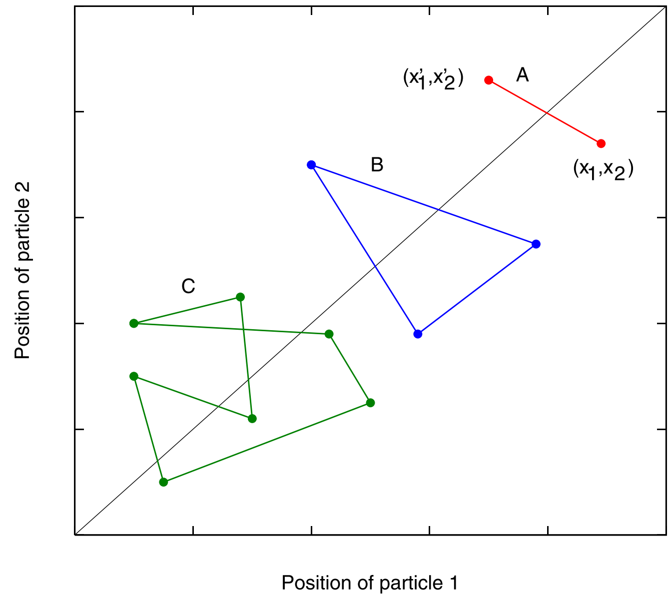

FIG. 1. Case A illustrates the sign change of the antisymmetric two-particle propagator when the line connecting its initial and final particle positions crosses the line $x_2 = x_1$. The propagator is *not* traced over. Cases B and C illustrate the tracing, or closed-loop products of three and seven antsymmetric propagators, respectively. They show that any closed-loop product of propagators must cross the line $x_2 = x_1$ an even number of times and, therefore, must remains positive.

For N fermions, the positions of the antisymmetric propagator are defined in a N-dimensional manifold. The propagator changes sign whenever its initial and final position cross any one of the $N(N-1)/2$, $(N-1)$-dimensional hyperplanes defined by $x_i = x_j$. Since each such $(N-1)$-dimensional hyperplanes completely divides the N-dimensional manifold into two halves, any closed curve in the N-dimensional manifold must pierce each such hyperplane even number of times. Thus, a closed-loop product of free-fermion propagators for N fermions is also always positive.

IV. SIGN PROBLEM IN MORE THAN ONE DIMENSION

In the d dimension, one replaces x_i by d-dimensional vectors $\mathbf{r}_i = (x_i, y_i, z_i, \dots)$ and set $\mathbf{x} = (\mathbf{r}_1, \mathbf{r}_2 \cdots \mathbf{r}_N)$. In this case, the antisymmetric two-fermion free propagator is

$$\begin{aligned} G_0(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2; \epsilon) &= \frac{1}{2} \frac{1}{(2\pi\epsilon)^d} e^{-\frac{1}{2\epsilon}[(\mathbf{r}_1'-\mathbf{r}_1)^2 + (\mathbf{r}_2'-\mathbf{r}_2)^2]} \\ &\quad \times \left(1 - e^{-\frac{1}{\epsilon}(\mathbf{r}_1'-\mathbf{r}_2')\cdot(\mathbf{r}_1-\mathbf{r}_2)}\right), \end{aligned} \qquad (14)$$

and vanishes whenever [5],

$$(\mathbf{r}_1' - \mathbf{r}_2') \cdot (\mathbf{r}_1 - \mathbf{r}_2) = 0. \tag{15}$$

In two dimensions, the two-fermion propagator is defined in the four-dimensional manifold (x_1, y_1, x_2, y_2), and vanishes at the *coincident* plane [5] given by $x_1 = x_2$ and $y_1 = y_2$. This is the direct generalization of the one-dimensional case. However, in this case, the coincident plane is only two dimensional, two dimensions less than the full manifold and, therefore, does not divide the four-dimensional manifold into disjoint regions [6]. (This is similar to the case of a line, which is two dimensions less than, and, therefore, cannot divide, the three-dimensional Euclidean space.) Therefore, in the four-dimensional manifold (x_1, y_1, x_2, y_2), a closed curve can either pierce the coincident plane or goes around it. Thus, a closed-loop product of antisymmetric propagators can be of either sign, and one has a sign problem. Generalizing this to N particles in the d dimension, the propagator is defined in a Nd-dimensional manifold. Any coincident plane is of dimension $(Nd - d)$ and cannot fully divide the Nd-dimensional manifold *except* for $d = 1$. Therefore, the sign problem is generally pervasive except in one dimension.

V. AN ALTERNATE PROOF

Although the topological proof for the absence of the sign problem in one dimension is obvious from Fig. 1, the proof's failure at higher dimensions as discussed in the last section is rather difficult to visualize. Here, we provide an alternate proof that traces the absence of the sign problem to the absence of angles in one dimension.

One observes that the sign of the two-fermion propagator (14) is determined by the sign of

$$1 - \exp\left(-\frac{1}{\epsilon}\mathbf{r}_{12}' \cdot \mathbf{r}_{12}\right), \tag{16}$$

where one has defined $\mathbf{r}_{12}' = \mathbf{r}_1' - \mathbf{r}_2'$ and $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$, which, in turn, is determined by the sign of $\mathbf{r}_{12}' \cdot \mathbf{r}_{12}$. Therefore, one has

$$\mathrm{sgn}[G_0(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2; \epsilon)] = \mathrm{sgn}(\mathbf{r}_{12}' \cdot \mathbf{r}_{12}). \tag{17}$$

This generalizes our earlier findings of (12) and (15). Since the trace of one and two propagators are always positive, we compare the trace of three propagators below.

In one dimension, one has

$$\mathrm{sgn}[G_0(x_{12}, x_{12}')G_0(x_{12}', x_{12}'')G_0(x_{12}'', x_{12})] = \mathrm{sgn}(x_{12}x_{12}'x_{12}'x_{12}''x_{12}''x_{12}) > 0, \tag{18}$$

since all displacements pair up to form a perfect square. This obviously generalizes to any number of two-fermion propagators.

In two dimensions, one has

$$\mathrm{sgn}[G_0(\mathbf{r}_{12}, \mathbf{r}_{12}')G_0(\mathbf{r}_{12}', \mathbf{r}_{12}'')G_0(\mathbf{r}_{12}'', \mathbf{r}_{12})] = \mathrm{sgn}[(\mathbf{r}_{12} \cdot \mathbf{r}_{12}')(\mathbf{r}_{12}' \cdot \mathbf{r}_{12}'')(\mathbf{r}_{12}'' \cdot \mathbf{r}_{12})]. \tag{19}$$

If the angle between two-dimensional vectors $\mathbf{r}_{12}$ and $\mathbf{r}_{12}'$ is θ, and that between $\mathbf{r}_{12}'$ and $\mathbf{r}_{12}''$ is θ', then the angle between $\mathbf{r}_{12}''$ and $\mathbf{r}_{12}$ must be either $\theta'' = \theta + \theta'$ or $\theta'' = \pi - \theta - \theta'$. The sign of three propagators is then,

$$\mathrm{sgn}[G_0(\mathbf{r}_{12}, \mathbf{r}_{12}')G_0(\mathbf{r}_{12}', \mathbf{r}_{12}'')G_0(\mathbf{r}_{12}'', \mathbf{r}_{12})] = |\mathbf{r}_{12}|^2|\mathbf{r}_{12}'|^2|\mathbf{r}_{12}''|^2\mathrm{sgn}(\cos\theta\,\cos\theta'\cos\theta''), \tag{20}$$

and can no longer be guaranteed to be positive. Generalizing this to any d dimension will involve the product of cosine functions which is not positive definite. Thus, there is no sign problem in one dimension because there is no angle in one dimension.

For more than two fermions, one must determine the sign of the corresponding propagator individually, which is less powerful than the topological argument given in the last two sections.

VI. CONCLUDING REMARKS

The observation that a Nd-dimensional manifold remains connected, despite the existence of $(Nd - d)$-dimensional coincident hyperplanes, was Girardeau's [6] insight that the conventional proof for Fermi-Dirac or Bose-Einstein statistics only applies to $d > 1$. (The loop hole for anyon statistics in $d = 2$ was a later development [7,8].) For $d = 1$ since each coincident plane completely divides the manifold, statistics based any permutation symmetry is permissible [6]. Here, it provided a simple proof that there is no sign problem in PIMC simulations of fermions in one dimension. In its simplest form, this proof reflects the fact that there is no angle in one dimension.

Finally, as suggested by one of the reviewers, it is of interest to consider also the sign problem for fermions in a circle. The generalization of the topological proof to this case is given in the Appendix below.

APPENDIX: FERMIONS IN A CIRCLE

For fermions in a circle, periodic in [0,1], the single particle propagator is given by

$$g_p(x', x; \tau) = \langle x'|e^{-\tau H_0}|x\rangle,$$

$$= \sum_{k=-\infty}^{\infty} e^{ik2\pi(x-x')}e^{-\tau 2\pi^2 k^2}, \tag{A1}$$

$$= \frac{1}{\sqrt{2\pi\tau}}\sum_{n=-\infty}^{\infty} e^{-(x-x'-n)^2/2\tau}, \tag{A2}$$

where $\langle k|x\rangle = \exp(ikx2\pi)$ with energy $E_k = (k2\pi)^2/2 = 2\pi^2k^2$ and where the Poisson summation has been used to convert the sum from k to n. Propagators (A1) and (A2) are duals of each other; the first converges rapidly at large τ whereas the second converges rapidly at small τ.

At fixed values of $x_1' = 0.6$ and $x_2' = 0.3$, the two-fermion propagator,

$$G_p(x_1', x_2'; x_1, x_2; \tau) = \det\begin{pmatrix} g_p(x_1', x_1, \tau) & g_p(x_1', x_2, \tau) \\ g_p(x_2', x_1, \tau) & g_p(x_2', x_2, \tau)\end{pmatrix}, \tag{A3}$$

is evaluated numerically for 201×201 grid points of x_1 and x_2 inside the periodic box $[0,1] \times [0,1]$, using either propagator

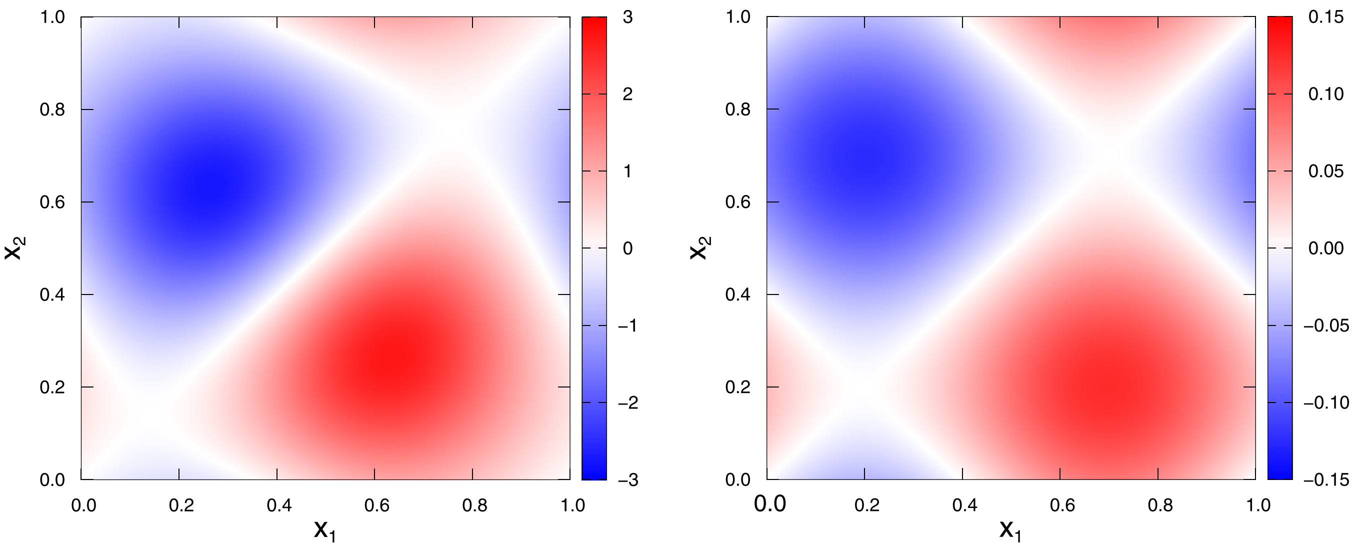

FIG. 2. Intensity plot of $G_0(x_1', x_2'; x_1, x_2; \tau)$ as a function of x_1 and x_2 for $x_1' = 0.6$, $x_2' = 0.3$. Left: $\tau = 0.05$. Right: $\tau = 0.2$. The nodal lines no longer change at $\tau \geqslant 0.2$.

(A1) or (A2), summed over the lowest 11 terms including zero. The resulting intensity plots for $\tau = 0.05$ and $\tau = 0.2$ are as shown in Fig. 2. The positive (red) and negative (blue) regions are now separated by *two* nodal lines (white), preventing any propagator loop from returning to its initial position by crossing the nodal line $x_2 = x_1$ only once.

The two straight nodal lines at $\tau \geqslant 0.2$ for the ground state of two free fermions have been previously derived by Ceperley [5]. Since the ground and two degenerate first excited states are 1, $e^{i2\pi x}$ and $e^{-i2\pi x}$, the resulting two degenerate antisymmetric wave functions can only be

$$\det\begin{pmatrix} 1 & e^{i2\pi x_1} \\ 1 & e^{i2\pi x_2} \end{pmatrix} = e^{i2\pi x_2} - e^{i2\pi x_1}$$
$$\text{and} \quad \det\begin{pmatrix} 1 & e^{-i2\pi x_1} \\ 1 & e^{-i2\pi x_2} \end{pmatrix} = e^{-i2\pi x_2} - e^{-i2\pi x_1}. \quad \text{(A4)}$$

The most general two-fermion wave function is then,

$$\begin{aligned}\psi(x_1, x_2) &\propto A(e^{i2\pi x_2} - e^{i2\pi x_1}) + B(e^{-i2\pi x_2} - e^{-i2\pi x_1}) \\ &\propto e^{-i2\pi\theta}(e^{i2\pi x_2} - e^{i2\pi x_1}) + e^{i2\pi\theta}(e^{-i2\pi x_2} - e^{-i2\pi x_1}) \\ &\propto \cos[2\pi(x_2 - \theta)] - \cos[2\pi(x_1 - \theta)] \\ &= -2\,\sin[\pi(x_2 + x_1 - 2\theta)]\sin[\pi(x_2 - x_1)], \quad \text{(A5)}\end{aligned}$$

where θ is an arbitrary phase. There are, thus, two nodal lines,

$$x_2 = x_1 \quad \text{and} \quad x_2 = 2\theta - x_1, \quad \text{(A6)}$$

with 2θ as the "y intercept" at $x_1 = 0$. Ceperley's diagram [5] illustrating (A6), exactly matches the nodal lines on the $\tau = 0.2$ plot of Fig. 2. However, in his derivation, there is no way of knowing the intercept 2θ.

At large τ, propagator (A1) is well approximated by keeping only the $k = -1, 0, 1$ terms, giving,

$$g_p(x', x, \tau) = 1 + a\,\cos[2\pi(x' - x)], \quad \text{(A7)}$$

where $a = 2e^{-\pi^2 2\tau}$ is a very small number even for $\tau \approx 1$. Keeping only the first order term in a gives

$$\begin{aligned}&G_p(x_1', x_2'; x_1, x_2; \tau) \\ &\quad \propto \cos[2\pi(x_1' - x_1)] + \cos[2\pi(x_2' - x_2)] \\ &\qquad - \cos[2\pi(x_1' - x_2)] - \cos[2\pi(x_2' - x_1)] \\ &\quad = -2\,\sin[\pi(2x_1' - x_1 - x_2)]\sin[\pi(x_2 - x_1)] \\ &\qquad - 2\,\sin[\pi(2x_2' - x_1 - x_2)]\sin[\pi(x_1 - x_2)] \\ &\quad = 2\,\sin[\pi(x_2 - x_1)](\sin[\pi(2x_2' - x_1 - x_2)] \\ &\qquad - \sin[\pi(2x_1' - x_1 - x_2)]) \\ &\quad = 2\,\sin[\pi(x_2 - x_1)]2\,\cos[\pi(x_1' + x_2' - x_1 - x_2)] \\ &\qquad \times\,\sin[\pi(x_2' - x_1')]. \quad \text{(A8)}\end{aligned}$$

At fixed x_1' and x_2', the nodal lines are exactly Ceperley's (A6) but now with the phase determined as

$$2\theta = x_1' + x_2' \pm \tfrac{1}{2}, \quad \text{(A9)}$$

so that for $x_1' = 0.6$, $x_2' = 0.3$, the intercept 2θ equals 0.4 as shown in Fig. 2.

Since the periodic box is a torus, one can always shift the view so that the intercept is at 1. This is shown in Fig. 3 with $x_1' = 0.1$ and $x_2' = 0.4$. The two nodal lines are the two Villarceau circles on the torus, dividing its surface into two equal halves. Starting at $x_1' = 0.1$ and $x_2' = 0.4$ in the positive red region on the left if one were to return to the same starting point, one must either go through no nodal lines, two nodal lines, four nodal lines or through the nodal crossing point. Since there is no sign change when crossing through the nodal crossing point, it is equivalent to no crossing. Thus, any closed loop of the two-fermion propagator must cross an even number of nodal lines and remains positive.

For the N-fermion propagator, the positions are defined on the manifold T^N, where T is a circle. This manifold is completely divided into two halves by each $N(N-1)/2$ pairs of perpendicular Villarceau hyperplanes $x_i - x_j = 0$ and

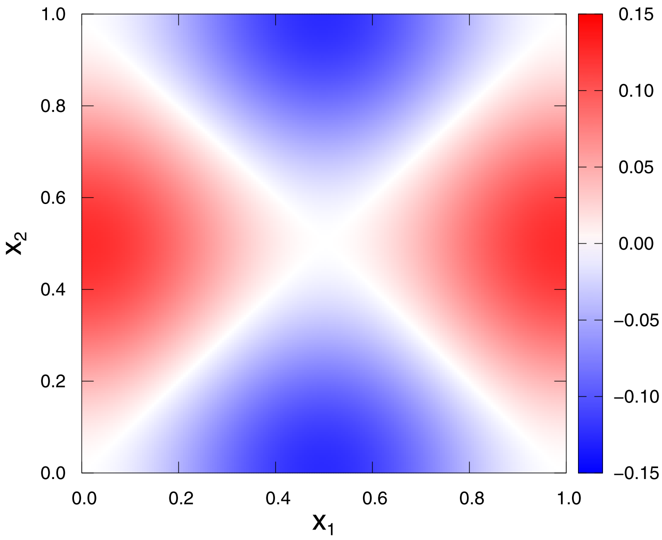

FIG. 3. Intensity plot of $G_0(x_1', x_2'; x_1, x_2; 0.2)$ as a function of x_1 and x_2 for $x_1' = 0.1, x_2' = 0.4$.

$x_i + x_j = 0$. Any closed curve on this manifold must pierce each hyperplane an even number of times thereby ensuring that a closed loop of N-fermion propagators remains positive. Hence, there is also no sign problem for fermions in a circle.

Postscript: Ceperley's motivation for deriving (A5) was to claim that nodal lines are somewhat arbitrary because the phase 2θ is arbitrary. However, it was never explained how such an arbitrary phase can be acquired by a physical wave function. Here, we have shown an instance where this phase only appears in an intermediate state. Whereas the square of Ceperley's wave function (A5) retains both nodal lines (A6), the square of the wave function by setting $x_1' = x_1$ and $x_2' = x_2$ in (A8) only yields $\sin^2[\pi(x_2 - x_1)]$. That is, if one were to extract the ground state wave function of two free fermions using PIMC, one can never obtain Ceperley's wave function (A5). The reason for this is clear. Ceperley's phase is the relative phase between $e^{i2\pi x}$ and $e^{-i2\pi x}$, such a phase is excluded from the fundamental definition of the propagator in (A1).

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