Simple proof that there is no sign problem in path integral Monte Carlo simulations of fermions in one dimension

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It is widely known that there is no sign problem in path integral Monte Carlo (PIMC) simulations of fermions in one dimension. As far as the author is aware, there is no direct proof of this in the literature. This work shows that the sign of the N-fermion antisymmetric free propagator is given by the product of all possible pairs of particle separations, or relative displacements. For a nonvanishing closed-loop product of such propagators, as required by PIMC, all relative displacements from adjacent propagators are paired into perfect squares, and therefore the loop product must be positive, but only in one dimension. By comparison, permutation sampling, which does not evaluate the determinant of the antisymmetric propagator exactly, remains plagued by a low-level sign problem, even in one dimension.

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I. INTRODUCTION

It is common knowledge since Takahashi and Imada's calculation [1] that there is no sign problem in path integral Monte Carlo (PIMC) simulations of fermions in one dimension. This conclusion is strongly supported by theoretical arguments by Girardeau [2], Negele and Orland [3], and Ceperley [4], but none of them are actual proofs specifically for PIMC. Only recently has the author given a proof [5] of this, based on Girardeau's [6] topological insight.

That topological idea is very simple in the case of two fermions in one dimension with coordinates x_1 and x_2. Since the propagator must change sign when the two positions are exchanged, the positive and negative regions of the propagator are completely separated by the nodal line $x_1 = x_2$ where the propagator vanishes. A closed-loop product of propagators in the plane of (x_1, x_2), as required in PIMC, must therefore cross this infinite nodal line, and changes sign, either zero, or even number of times. Hence, the sign of a nonvanishing closed loop product of propagators must be positive, with no sign problem.

At higher dimensions, say two dimension, the space of the propagator is four dimensional (x_1, y_1, x_2, y_2), but the coincidental nodal plane [4] given by $x_1 = x_2$ and $y_1 = y_2$ is only two dimensional. Just as a line, which is two dimensions less, cannot divide the three-dimensional space, a two-dimensional nodal plane, also cannot divide the four-dimensional space into two halves. Hence, the previous argument fails and there is a sign problem in more than one dimension.

Since this topological argument for the existence of the sign problem in more than one dimension is less intuitive, I alternately determined the sign of the two-fermion propagator directly in terms of their relative displacements [5]. Since only in one dimension can relative displacements from adjacent propagators be paired into pure squares, the sign problem is absent only in one dimension. For completeness, this important two fermion case, for understanding the dimensional dependence of the sign problem, is restated in Sec. III below. However, at the time of Ref. [5]'s publication, there was no known way of determining the sign of an arbitrary N-fermion propagator in one dimension, and hence no general proof by direct sign determination.

This work, by use of Mikhailov's expansion [7] in terms of Vandermonde determinants [8], can now compute the sign of the N-fermion propagator directly and present a much simpler proof. This work, which only computes the sign of the fermion propagator, is purely a technical achievement, filling a missing gap in the literature. However, as discussed in the conclusion, this proof can now explain why permutation sampling [9,10], which does not evaluate the fermion propagator's determinant completely, remains plagued by a low-level sign problem [10], even in one dimension.

This work will be concise in presenting only technical details; Ref. [5] can be consulted for more background discussions. After a brief summary of key PIMC equations and defining the sign problem in Sec. II, Sec. III answers the frequently asked question of why there is no sign problem only in one dimension. The sign of two, three, and N-fermion propagators is then determined in successive Secs. IV–VI. A concluding summary is given in Sec. VII, with a comparative discussion on permutation sampling.

II. FERMION PATH INTEGRAL MONTE CARLO

Let $\mathbf{x} = (\mathbf{r}_1, \mathbf{r}_2 \cdots \mathbf{r}_N)$ denote the coordinates of N fermions in d dimension. At the heart of PIMC is the Monte Carlo sampling of the closed-end, k-bead path integral

$$\begin{aligned} G_k(\mathbf{x}, \mathbf{x}; \tau) &= \langle \mathbf{x} | (\mathrm{e}^{-\epsilon(\hat{T}+\hat{V})})^k | \mathbf{x} \rangle \\ &= \int_{-\infty}^{\infty} d\mathbf{x}_1 \cdots d\mathbf{x}_{k-1}\, G_1(\mathbf{x}, \mathbf{x}_1; \epsilon) G_1(\mathbf{x}_1, \mathbf{x}_2; \epsilon) \cdots \\ &\quad \times G_1(\mathbf{x}_{k-1}, \mathbf{x}; \epsilon) \end{aligned} \tag{2.1}$$

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at imaginary time $\tau = k\epsilon$, where $\hat{T}$ and $\hat{V}$ are the kinetic and potential operators of the many-fermion system, and $G_1(\mathbf{x}', \mathbf{x}; \epsilon)$ is a short-time propagator, of which the simplest is the primitive second-order approximation

$$G_1(\mathbf{x}', \mathbf{x}; \epsilon) = \langle \mathbf{x}'|e^{-\epsilon(\hat{T}+\hat{V})}|\mathbf{x}\rangle \approx e^{-(\epsilon/2)V(\mathbf{x}')} G_0(\mathbf{x}', \mathbf{x}; \epsilon) e^{-(\epsilon/2)V(\mathbf{x})}, \quad (2.2)$$

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

$$G_0(\mathbf{x}', \mathbf{x}; \epsilon) = \frac{1}{N!} \det\left(\frac{1}{(2\pi\epsilon)^{d/2}} \exp\left[-\frac{1}{2\epsilon} (\mathbf{r}_i' - \mathbf{r}_j)^2 \right] \right). \quad (2.3)$$

Since $G_0(\mathbf{x}', \mathbf{x}; \epsilon)$ is not positive definite, the integrand in the loop integral (2.1) can be negative for some paths. This is the fermion sign problem in PIMC. The goal of this work is to show that, despite the fact that $G_0(\mathbf{x}', \mathbf{x}; \epsilon)$ can be of either sign, the integrand of (2.1) over any closed path

$$\mathbf{x} \to \mathbf{x}_1 \to \mathbf{x}_2 \to \cdots \mathbf{x}_{k-1} \to \mathbf{x}, \quad (2.4)$$

if it is non-vanishing, is always positive in one dimension.

The sign problem is due entirely to the fact that the free-fermion propagator (2.3) can be negative. The interacting potential $V(\mathbf{x})$ is exponentiated in (2.2) and the exponential function is always positive regardless whether the potential is attractive or repulsive. In one dimension, where there is no sign problem, the potential has no effect on sign of the integrand in (2.1). In more than one dimension, where there is a sign problem, it is possible that the exponentiated potential in (2.2) can further aggravate the sign problem by giving more weight to the negative region of the integrand.

III. WHY THERE IS NO SIGN PROBLEM ONLY IN ONE DIMENSION

In d dimension, the two-fermion free propagator from (2.3) is given by

$$G_0(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2; \epsilon) = \frac{1}{2} \frac{1}{(2\pi\epsilon)^d} \det \begin{pmatrix} e^{-(\mathbf{r}_1'-\mathbf{r}_1)^2/(2\epsilon)} & e^{-(\mathbf{r}_1'-\mathbf{r}_2)^2/(2\epsilon)} \\ e^{-(\mathbf{r}_2'-\mathbf{r}_1)^2/(2\epsilon)} & e^{-(\mathbf{r}_2'-\mathbf{r}_2)^2/(2\epsilon)} \end{pmatrix} \quad (3.1)$$

$$= \frac{1}{2} \frac{1}{(2\pi\epsilon)^d} e^{-\frac{1}{2\epsilon}[(\mathbf{r}_1'-\mathbf{r}_1)^2+(\mathbf{r}_2'-\mathbf{r}_2)^2]} (1 - e^{-\frac{1}{\epsilon}(\mathbf{r}_2'-\mathbf{r}_1')\cdot(\mathbf{r}_2-\mathbf{r}_1)}), \quad (3.2)$$

whose sign is determined by the sign of

$$1 - \exp\left(-\frac{1}{\epsilon} \mathbf{r}_{21}' \cdot \mathbf{r}_{21} \right), \quad (3.3)$$

where $\mathbf{r}_{21}' = \mathbf{r}_2' - \mathbf{r}_1'$ and $\mathbf{r}_{21} = \mathbf{r}_2 - \mathbf{r}_1$, which in turn is given by the sign of $\mathbf{r}_{21}' \cdot \mathbf{r}_{21}$. Therefore, one has

$$\mathrm{sgn}(G_0(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2; \epsilon)) = \mathrm{sgn}(\mathbf{r}_{21}' \cdot \mathbf{r}_{21}). \quad (3.4)$$

Note that the sign of the propagator is solely determined by particle positions and is independent of ϵ.

Since the loop product of one and two propagators is always positive, the sign problem only appears for three or more propagators:

$$\begin{aligned} &\mathrm{sgn}(G_0(\mathbf{r}_{21}, \mathbf{r}_{21}')G_0(\mathbf{r}_{21}', \mathbf{r}_{21}'')G_0(\mathbf{r}_{21}'', \mathbf{r}_{21})) \\ &\quad = \mathrm{sgn}((\mathbf{r}_{21} \cdot \mathbf{r}_{21}')(\mathbf{r}_{21}' \cdot \mathbf{r}_{21}'')(\mathbf{r}_{21}'' \cdot \mathbf{r}_{21})), \\ &\quad = |\mathbf{r}_{21}|^2 |\mathbf{r}_{21}'|^2 |\mathbf{r}_{21}''|^2 \mathrm{sgn}(\cos\theta \cos\theta' \cos\theta''). \end{aligned} \quad (3.5)$$

Since the cosine functions can take both signs, the sign problems exist whenever the dot product produces a cosine function, i.e., at dimensions greater than one. At one dimension, there's no angles, no cosine functions and the sign is just

$$\begin{aligned} &\mathrm{sgn}(G_0(x_{21}, x_{21}')G_0(x_{21}', x_{21}'')G_0(x_{21}'', x_{21})) \\ &\quad = \mathrm{sgn}((x_{21}x_{21}')(x_{21}'x_{21}'')(x_{21}''x_{21})), \\ &\quad = \mathrm{sgn}((x_{21})^2(x_{21}')^2(x_{21}'')^2) \geqslant 0, \end{aligned} \quad (3.6)$$

where all displacements from adjacent propagators have paired up as perfect squares, and hence there is no sign problem. This is also true for a loop of any number of propagators. To prove the general case, one only needs to determine the sign of the N-fermion propagator in one dimension.

IV. THE SIGN OF THE TWO-FERMION PROPAGATOR

The method of computing the sign of the propagator by evaluating the determinant in (2.3) cannot be easily generalized to more than two fermions. Here, we first cast the one dimensional propagator into a form suggested in Ref. [5].

For two (spinless) fermions, the one dimensional form of (3.1) is just

$$G_0(x_1', x_2', x_1, x_2; \epsilon) = \frac{1}{2} \frac{1}{2\pi\epsilon} \det \begin{pmatrix} e^{-(x_1'-x_1)^2/(2\epsilon)} & e^{-(x_1'-x_2)^2/(2\epsilon)} \\ e^{-(x_2'-x_1)^2/(2\epsilon)} & e^{-(x_2'-x_2)^2/(2\epsilon)} \end{pmatrix}. \quad (4.1)$$

Since this work is not interested in the actual value of the propagator, but only its sign, all normalization factors and purely positive functions can be ignored.

By factoring out, from (4.1), $e^{-x_1'^2/(2\epsilon)}$, $e^{-x_2'^2/(2\epsilon)}$ from row one and two, respectively, and $e^{-x_1^2/(2\epsilon)}$, $e^{-x_2^2/(2\epsilon)}$ from column one and two, one has

$$G_0(x_1', x_2', x_1, x_2; \epsilon) \propto e^{-(x_1'^2+x_2'^2+x_1^2+x_2^2)/(2\epsilon)} \times \det \begin{pmatrix} e^{x_1'x_1/\epsilon} & e^{x_1'x_2/\epsilon} \\ e^{x_2'x_1/\epsilon} & e^{x_2'x_2/\epsilon} \end{pmatrix}. \quad (4.2)$$

The sign of G_0 is therefore just the sign of the above determinant. As noted in Sec. III, since the sign is fixed by the positions only, independent of ϵ, it can be determined in the limit of $\epsilon \to \infty$, yielding

$$\begin{aligned} &\mathrm{sgn}(G_0(x_1', x_2', x_1, x_2; \epsilon)) \\ &\quad = \mathrm{sgn}(e^{(x_1'x_1+x_2'x_2)/\epsilon} - e^{(x_1'x_2+x_2'x_1)/\epsilon}) \\ &\quad = \mathrm{sgn}((x_1'x_1 + x_2'x_2 - x_1'x_2 - x_2'x_1)/\epsilon) \\ &\quad = \mathrm{sgn}(x_{21}'x_{21}). \end{aligned} \quad (4.3)$$

It then follows that for $\mathbf{x} = (x_1, x_2)$, the sign of a loop product of n propagator is given by

$$\mathrm{sgn}(G_0(\mathbf{x}, \mathbf{x}'; \epsilon)G_0(\mathbf{x}', \mathbf{x}''; \epsilon)G_0(\mathbf{x}'', \mathbf{x}'''; \epsilon) \cdots \times G_0(\mathbf{x}^{\{n-1\}}, \mathbf{x}; \epsilon))$$

$$= \mathrm{sgn}\big(x_{21}x'_{21}x'_{21}x''_{21}x''_{21}\cdots x_{21}^{\{n-1\}}x_{21}\big) \tag{4.4}$$

$$= \mathrm{sgn}\big((x_{21})^2(x'_{21})^2(x''_{21})^2\cdots\big(x_{21}^{\{n-1\}}\big)^2\big) \geqslant 0. \tag{4.5}$$

Thus, for a product of any number of two-fermion propagators, if it is nonvanishing, then its sign must be positive because for a closed loop, relative displacements from adjacent propagators will always pair up to a perfect square.

The determinant in (4.2) can now be evaluated by an alternative method generalizable to N fermions. Since the $\epsilon \to \infty$ limit is the same as the $x, x' \to 0$ limit, one can just do the latter and suppress the appearance of ϵ. For notational clarity, we will also replace x' by s in the discussion below and evaluate the determinant as follows:

$$\begin{aligned}
\det\begin{pmatrix} e^{x_1 s_1} & e^{x_1 s_2} \\ e^{x_2 s_1} & e^{x_2 s_2} \end{pmatrix} &= e^{x_1 s_1}e^{x_2 s_2} - e^{x_2 s_1}e^{x_1 s_2} \\
&= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\frac{1}{n_1!n_2!}\big(x_1^{n_1}s_1^{n_1}x_2^{n_2}s_2^{n_2} - x_2^{n_1}s_1^{n_1}x_1^{n_2}s_2^{n_2}\big) \\
&= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\frac{1}{n_1!n_2!}s_1^{n_1}s_2^{n_2}\big(x_1^{n_1}x_2^{n_2} - x_2^{n_1}x_1^{n_2}\big) \\
&= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\frac{1}{n_1!n_2!}s_1^{n_1}s_2^{n_2}\det\begin{pmatrix} x_1^{n_1} & x_1^{n_2} \\ x_2^{n_1} & x_2^{n_2} \end{pmatrix}.
\end{aligned} \tag{4.6}$$

Since n_i serve as a column index, the determinant above vanishes for $n_1 = n_2$. Therefore, the sum is over $n_1 < n_2$ and $n_2 < n_1$ only. The latter case can be viewed as the former case with n_1 interchanged with n_2. This changes the column of the determinant, corresponding to the original determinant with a negative sign, hence,

$$\begin{aligned}
\det\begin{pmatrix} e^{x_1 s_1} & e^{x_1 s_2} \\ e^{x_2 s_1} & e^{x_2 s_2} \end{pmatrix} &= \sum_{n_1<n_2}\frac{1}{n_1!n_2!}\left[s_1^{n_1}s_2^{n_2}\det\begin{pmatrix} x_1^{n_1} & x_1^{n_2} \\ x_2^{n_1} & x_2^{n_2} \end{pmatrix} - s_1^{n_2}s_2^{n_1}\det\begin{pmatrix} x_1^{n_1} & x_1^{n_2} \\ x_2^{n_1} & x_2^{n_2} \end{pmatrix}\right] \\
&= \sum_{n_1<n_2}\frac{1}{n_1!n_2!}\big(s_1^{n_1}s_2^{n_2} - s_1^{n_2}s_2^{n_1}\big)\det\begin{pmatrix} x_1^{n_1} & x_1^{n_2} \\ x_2^{n_1} & x_2^{n_2} \end{pmatrix} \\
&= \sum_{n_1<n_2}\frac{1}{n_1!n_2!}\det\begin{pmatrix} s_1^{n_1} & s_1^{n_2} \\ s_2^{n_1} & s_2^{n_2} \end{pmatrix}\det\begin{pmatrix} x_1^{n_1} & x_1^{n_2} \\ x_2^{n_1} & x_2^{n_2} \end{pmatrix}.
\end{aligned} \tag{4.7}$$

The above is the simplest 2×2 version of of Mikhailov's method [7] of expanding a determinant of mixed variable into a product of two determinants of separated variables.

In the limit of $s_i, x_i \to 0$, the single leading order term in the above sum is given by $n_1 = 0$ and $n_2 = 1$:

$$\det\begin{pmatrix} e^{x_1 s_1} & e^{x_1 s_2} \\ e^{x_2 s_1} & e^{x_2 s_2} \end{pmatrix} \to \det\begin{pmatrix} 1 & s_1 \\ 1 & s_2 \end{pmatrix}\det\begin{pmatrix} 1 & x_1 \\ 1 & x_2 \end{pmatrix} = (s_2 - s_1)(x_2 - x_1) = s_{21}x_{21}, \tag{4.8}$$

reproducing the sign of the two-fermion propagator (4.3).

V. THE SIGN OF THE THREE-FERMION PROPAGATOR

For three fermions,

$$\begin{aligned}
\det\begin{pmatrix} e^{x_1 s_1} & e^{x_1 s_2} & e^{x_1 s_3} \\ e^{x_2 s_1} & e^{x_2 s_2} & e^{x_2 s_3} \\ e^{x_3 s_1} & e^{x_3 s_2} & e^{x_3 s_3} \end{pmatrix} &= \det\begin{pmatrix} e^{x_1 s_1} & e^{x_1 s_2} \\ e^{x_2 s_1} & e^{x_2 s_2} \end{pmatrix}e^{x_3 s_3} - \det\begin{pmatrix} e^{x_1 s_1} & e^{x_1 s_2} \\ e^{x_3 s_1} & e^{x_3 s_2} \end{pmatrix}e^{x_2 s_3} + \det\begin{pmatrix} e^{x_2 s_1} & e^{x_2 s_2} \\ e^{x_3 s_1} & e^{x_3 s_2} \end{pmatrix}e^{x_1 s_3} \\
&= \det\begin{pmatrix} e^{x_1 s_1} & e^{x_1 s_2} \\ e^{x_2 s_1} & e^{x_2 s_2} \end{pmatrix}e^{x_3 s_3} - (x_2 \leftrightarrow x_3) + (x_2 \leftrightarrow x_3 \text{ then } x_1 \leftrightarrow x_2),
\end{aligned} \tag{5.1}$$

corresponding to

$$\begin{aligned}
&= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_3=0}^{\infty}\frac{1}{n_1!n_2!n_3!}s_1^{n_1}s_2^{n_2}s_3^{n_3}\big[\,\big(x_1^{n_1}x_2^{n_2} - x_2^{n_1}x_1^{n_2}\big)x_3^{n_3} - \big(x_1^{n_1}x_3^{n_2} - x_3^{n_1}x_1^{n_2}\big)x_2^{n_3} + \big(x_2^{n_1}x_3^{n_2} - x_3^{n_1}x_2^{n_2}\big)x_1^{n_3}\big] \\
&= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_3=0}^{\infty}\frac{1}{n_1!n_2!n_3!}s_1^{n_1}s_2^{n_2}s_3^{n_3}\det\begin{pmatrix} x_1^{n_1} & x_1^{n_2} & x_1^{n_3} \\ x_2^{n_1} & x_2^{n_2} & x_2^{n_3} \\ x_3^{n_1} & x_3^{n_2} & x_3^{n_3} \end{pmatrix}.
\end{aligned} \tag{5.2}$$

This is the three fermion generalization of (4.6). As in the two-fermion case, the sign changes in permuting the unrestricted sum $\sum_{n_1,n_2,n_3}$ into the ordered sum $\sum_{n_1<n_2<n_3}$ result in a determinant for s_i:

$$\det\begin{pmatrix} e^{x_1 s_1} & e^{x_1 s_2} & e^{x_1 s_3} \\ e^{x_2 s_1} & e^{x_2 s_2} & e^{x_2 s_3} \\ e^{x_3 s_1} & e^{x_3 s_2} & e^{x_3 s_3} \end{pmatrix} = \sum_{n_1<n_2<n_3}^{\infty} \frac{1}{n_1! n_2! n_3!} \det\begin{pmatrix} s_1^{n_1} & s_1^{n_2} & s_1^{n_3} \\ s_2^{n_1} & s_2^{n_2} & s_2^{n_3} \\ s_3^{n_1} & s_3^{n_2} & s_3^{n_3} \end{pmatrix} \det\begin{pmatrix} x_1^{n_1} & x_1^{n_2} & x_1^{n_3} \\ x_2^{n_1} & x_2^{n_2} & x_2^{n_3} \\ x_3^{n_1} & x_3^{n_2} & x_3^{n_3} \end{pmatrix}. \tag{5.3}$$

This is the 3×3 version of Mikhailov's method [7] of expanding a mixed variable determinant.

The leading order term in the above sum is $n_1 = 0$, $n_2 = 1$, and $n_3 = 2$,

$$\to \frac{1}{2} \det\begin{pmatrix} 1 & s_1 & s_1^2 \\ 1 & s_2 & s_2^2 \\ 1 & s_3 & s_3^2 \end{pmatrix} \det\begin{pmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{pmatrix} = \frac{1}{2} s_{21} s_{31} s_{32} x_{21} x_{31} x_{32}, \tag{5.4}$$

which correctly changes sign whenever any pair of particles is exchanged. All relative displacements will again pair up as perfect squares for any closed loop product of propagators.

VI. THE SIGN OF THE N-FERMION PROPAGATOR

The two determinants in (4.8) and (5.4) are simple cases of the general $N \times N$ Vandermonde determinant [8]:

$$\det\begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{N-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{N-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{N-1} \\ 1 & \cdots & \cdots & \cdots & \cdots \\ 1 & x_N & x_n^2 & \cdots & x_N^{N-1} \end{pmatrix} = \prod_{1 \leqslant i < j \leqslant N} (x_j - x_i). \tag{6.1}$$

The generalization of (5.4) to N fermions then follows from (6.1) immediately as

$$G_0(s_1, s_2, \cdots s_N, x_1, x_2, \cdots x_N, \epsilon) \propto \left(\prod_{i<j} s_{ji}\right)\left(\prod_{i<j} x_{ji}\right), \tag{6.2}$$

which changes sign whenever any pair of s_i or x_i is exchanged. This then again entails that a nonvanishing closed-loop product of propagators (6.2) will have paired displacements as squares and its sign will always be positive.

VII. CONCLUSIONS

This work has proved that fermion PIMC using antisymmetric free propagators has no sign problem in one dimension. This proof is based solely on determining the sign of the N-fermion free propagator, without referencing anything external, such as equivalent bosons [2], a preferred subspace [3], restricted nodal regions [4], or even topology [5]. The proof gives insight into why there is no sign problem in one dimension by showing that in a closed loop of propagators, all relative displacements are paired up as squares. However, the proof depends crucially on knowing the sign of the determinant exactly, as dictated by (6.2). This implies that if fermion PIMC is implemented by sampling permutations [9,10] only, then the determinant's sign is not exactly determined, with displacements not precisely paired up as squares. Permutation sampling (PS) refers to the fact that the antisymmetric free-fermion propagator (2.3) can be expanded as a sum over permutations,

$$\begin{aligned} G_0(\mathbf{x}', \mathbf{x}; \epsilon) &= \frac{1}{N!} \det\left(\frac{1}{(2\pi\epsilon)^{d/2}} \exp\left[-\frac{1}{2\epsilon} (\mathbf{r}_i' - \mathbf{r}_j)^2 \right] \right), \\ &= \frac{1}{N!} \sum_P (-1)^P \frac{1}{(2\pi\epsilon)^{Nd/2}} \exp\left[-\frac{1}{2\epsilon} (\mathbf{x}' - \mathbf{x}_P)^2 \right], \end{aligned} \tag{7.1}$$

but only a single random permutation is sampled for each propagator. This clearly then does not determine the sign of each propagator exactly but only on the average. The result is a lingering low-level sign problem, yielding poorer results than that of evaluating the determinant of the antisymmetric propagator (AP), as reported by Lyubartsev [10]:

> "In the case of the PS scheme, it was only possible to evaluate the density of the first excited state of the one-dimensional harmonic oscillator with a few percent precision. However, in the case of the AP scheme applied to the same system, very accurate estimations of the densities of up to at least the eighth excited state become possible. The key to success lies in the fact that the AP scheme solves the sign problem completely, providing a strictly positive weight function for fermions in one dimension."

The fundamental reason why the AP scheme should provide "a strictly positive weight function for fermions in one dimension" can now be understood, according to this work, as due to the fact that all relative displacements from adjacent propagators can be paired up as pure squares only in one dimension.

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