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A POSITIVE GENERATOR FOR THE FEYNMAN-KAC FUNCTIONAL OF FERMIONS

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Abstract

The propagator of N interacting fermions in a scalar potential can, in the coordinate space, be written as a Feynman-Kac functional over a symmetrized process, i.e., as a superposition of Euclidean-time path integrals over the diffusion process of N free fermions. Exploiting the properties of the permutation group allows to reduce the coordinate space by a factor $N!$, leading to a state space in which the propagator is positive. The expression for the state space is numerically inaccessible because of an intricate limit to be taken, reflecting the infamous fermion sign problem. However, by analytical methods the state space can be expressed in terms of standard, numerically tractable, $N \times N$ determinants. A well-defined Markov process is defined on the state space, namely Brownian motion with superimposed potential-dependent exponential weights and absorbing boundary conditions. This leads to a random process by stable diffusion of purely positive walkers which generate the Feynman-Kac functional in the state space.

1. Introduction

The Feynman-Kac functional [1, 2] as a Wiener integral with a well-defined

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measure is a mathematically sound formulation of the path-integral approach to quantum theory [3, 4]. Although the original derivation was limited to a restricted class of potentials, the formulation seems valid [5] for the most potentials of physical interest, including the Coulomb interaction.

Let $\bar{\mathbf{r}} = (\mathbf{r_1}, \mathbf{r_2}, \cdots, \mathbf{r}_N)$ be a *Nd* dimensional point in the coordinate space $(\mathbb{R}^d)^N$ of *N distinguishable* particles with dimension *d*, where $\mathbf{r}_j$ denotes the position vector of the j^{th} particle. The propagator (in Euclidean time τ)

$$K(\bar{\mathbf{r}}, \beta|\bar{\xi}) = \langle \bar{\mathbf{r}} \,| e^{-\beta H} |\bar{\xi}\rangle \tag{1}$$

of a stationary Hamiltonian of the form

$$H = \sum_j \left(\frac{\mathbf{p}_j^2}{2m} + U(\mathbf{r}_j) \right) + \sum_{j,k>j} v(\mathbf{r}_j, \mathbf{r}_k) \equiv \frac{\bar{\mathbf{p}}^2}{2m} + V(\bar{\mathbf{r}}), \tag{2}$$

is written as a Feynman-Kac functional

$$K(\bar{\mathbf{r}}, \beta|\bar{\xi}) = E_{\bar{R}(0)=\bar{\xi}}^{\bar{R}(\beta)=\bar{\mathbf{r}}} \left(e^{-\int_0^\beta V(\bar{\mathbf{R}}(\tau))d\tau} \right), \tag{3}$$

where $E_{\bar{R}(0)=\bar{\xi}}^{\bar{R}(\beta)=\bar{\mathbf{r}}}(\bullet)$ denotes an expectation value over all *Nd* dimensional Brownian paths $\{\bar{\mathbf{R}}(\tau \geq 0)\}$ between $\bar{\xi}$ at $\tau = 0$ and $\bar{\mathbf{r}}$ at $\tau = \beta$**.** The initial point $\bar{\xi}$ was explicitly introduced in the notation, keeping in mind the important analysis of the "reference point" in [6]. The propagator satisfies the equation of motion

$$\left(\frac{\partial}{\partial \beta} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial \bar{\mathbf{r}}^2} + V(\bar{\mathbf{r}}) \right) K(\bar{\mathbf{r}}, \beta|\bar{\xi}) = 0, \text{ with } K(\bar{\mathbf{r}}, \beta|\bar{\xi}) \xrightarrow[\beta \to 0^+]{} \delta(\bar{\mathbf{r}} - \bar{\xi}), \tag{4}$$

and the semigroup property

$$\int K(\bar{\mathbf{r}}, \beta - \tau|\bar{\mathbf{u}}) K(\bar{\mathbf{u}}, \tau|\bar{\xi}) d\bar{\mathbf{u}} = K(\bar{\mathbf{r}}, \beta|\bar{\xi}) \text{ for } 0 \leq \tau \leq \beta. \tag{5}$$

Obviously, the free-particle propagator $\rho(\bar{\mathbf{r}}, \beta|\bar{\xi})$ reads

$$\rho(\bar{\mathbf{r}}, \beta|\bar{\xi}) \equiv E_{\bar{R}(0)=\bar{\xi}}^{\bar{R}(\beta)=\bar{\mathbf{r}}}(1) = \sqrt{\frac{m}{2\pi\hbar^2\beta}}^{Nd} e^{-\frac{m}{2}\frac{(\bar{\mathbf{r}}-\bar{\xi})^2}{\hbar^2\beta}}. \tag{6}$$

The propagator is usually introduced to derive the wave function at Euclidean time β, given an initial wave function. But the propagator itself contains all necessary information to find the ground state and the ground state energy from the spectral representation (if stationary eigenstates $|E_n\rangle$ with eigenenergies E_n exist, and if the lower eigenenergies are discrete):

$$K(\bar{\mathbf{r}}, \beta|\bar{\xi}) = \sum_{n=0}^{\infty} \langle \bar{\mathbf{r}}|E_n\rangle\langle E_n|\bar{\xi}\rangle e^{-\beta E_n} \xrightarrow[\beta\to\infty]{} \langle \bar{\mathbf{r}}|E_0\rangle\langle E_n|\bar{\xi}\rangle e^{-\beta E_0}. \qquad (7)$$

An indirect estimator for the ground state energy E_0 is therefore associated with the expectation value of the path integral weights over the free diffusion Wiener process: $E_0 \simeq -\lim_{\beta\to\infty} \frac{1}{\beta} \ln(\int K(\bar{\mathbf{r}}, \beta|\bar{\xi}) d\bar{\mathbf{r}})$. In practice, however, the unbiased energy estimate as proposed in [7] is preferable. But the practical implementation of the algorithms is not the main concern in this paper.

If identical particles are involved, the antisymmetry under any permutation of two particles implies that there exists a state space which is reduced by a factor $N!$ as compared to the coordinate space $\mathbb{R}^{Nd}$. But if one wants to use the Feynman-Kac functional in the strict real-analysis sense, a Markov process on that state space has to be specified in order to describe how the sample paths are provided. The infamous sign problem for fermions is a manifestation of the lack of such a description so far, although a number of techniques have been developed to reduce the signal-to-noise ratio [6-16] arising from the changes in sign of the wave function, including the famous fixed-node approximation [9].

About twenty years ago, a promising calculation of the groundstate energy of a number of atoms was published [17], using the Feynman-Kac functional of real analysis. These authors constructed their sample paths using Bernoulli walks that got absorbed at a boundary but without an unambiguous definition of the state space and the Markov process. Neither the vivid discussion [18-20] on the validity of this approach, nor a more elaborate methodological paper [21], explicitly clarified this point.

In a few papers [22-27], I contributed to the formulation and implementation of random processes on an *ordered* state space. Although mathematically sound, practical applications had to be limited to some particular systems with additional

symmetry properties. Even for a relatively simple system as orthohelium, the technical bookkeeping turned out to be quite involved [27], because the processes and the state space were based on the Carthesian representation of the system.

In the present paper a positive generator for the Feynman-Kac functional of N *spin-polarized* fermions is constructed, which is polynomial convergent with the number of particles. (The treatment can easily be formulated for $N_\uparrow$ electrons with upward spin and $N_\downarrow$ electrons with downward spin along some direction, because the spin up electrons are "external charges" for the spin down electrons and vice versa. We prefer to avoid the cost in the notation.) One can construct a "fermion propagator" in the coordinate space $\mathbb{R}^{Nd}$

$$K_F(\bar{\mathbf{r}}, \beta|\bar{\xi}) = \frac{1}{N!}\sum_{\mathcal{P}} (-1)^p K(\bar{\mathbf{r}}, \beta|\mathcal{P}\bar{\xi}), \tag{8}$$

where the summation runs over all permutations $\mathcal{P}$ of the particles, with p the number of permutations. It clearly satisfies both the antisymmetry requirements and the equation of motion (4). Because $[\mathcal{P}, H] = 0$, it is irrelevant whether the permutations are applied on the initial or on the final points. But the initial condition in (4) implies

$$K_F(\bar{\mathbf{r}}, \beta|\bar{\xi}) \xrightarrow[\beta\to 0^+]{} \frac{1}{N!}\sum_{\mathcal{P}} (-1)^p \delta(\bar{\mathbf{r}} - \mathcal{P}\bar{\xi}), \tag{9}$$

which is reminiscent of the image charge technique to study destructive interference. For N fermions, $N!$ "sources" are needed with alternating sign to determine the propagator in $\mathbb{R}^{Nd}$, with $N!/2$ domains with positive sign, and $N!/2$ domains with negative sign. Each one of these domains forms an irreducible representation of the permutation group. Because $e^{-\int V d\tau} > 0$, and because of the semigroup property (5), the potential affects the absolute value of the propagator in exactly the same way for all the contributing distinguishable propagators $K(\bar{\mathbf{r}}, \beta|\mathcal{P}\bar{\xi})$. But the sign of $K_F(\bar{\mathbf{r}}, \beta|\bar{\xi})$ is thus the same as that of the free fermion propagator

$$\rho_F(\bar{\mathbf{r}}, \beta|\bar{\xi}) = \sqrt{\frac{m}{2\pi\hbar^2\beta}}^{Nd} e^{-\frac{m}{2}\frac{\bar{\mathbf{r}}^2+\bar{\xi}^2}{\hbar^2\beta}} \frac{1}{N!}\sum_{\mathcal{P}} (-1)^p e^{\frac{m}{\hbar^2\beta}\bar{\mathbf{r}}\cdot P\bar{\xi}}, \tag{10}$$

to be examined in the limit $\beta \to \infty$. This result was obtained earlier (see, e.g., equation (4.4) in [24]), but it then was used to construct an ordered state space and Markov processes in the Carthesian representation of the system.

2. The State Space

For the fermionic ground state (which is an highly excited state in the state space of the distinguishable particles), one thus finds a state space $\Upsilon_{N,d}(\overline{\mathbf{r}}, \overline{\xi})$ for N fermions in d dimensions

$$\Upsilon_{N,d}(\overline{\mathbf{r}}, \overline{\xi}) \equiv \det(\mathbb{E}) > 0 \text{ for } \varepsilon \to 0^+, \quad \text{with } \mathbb{E}_{j,k} = e^{\varepsilon \mathbf{r}_j \cdot \xi_k}, \tag{11}$$

where the particle labels are restored. Since all permutations $\mathcal{P}\overline{\xi}$ of a particular initial point $\overline{\xi}$ generate the same distribution, the calculation is restricted to a fraction $1/N!$ of the coordinate space, which is a substantial gain factor. This state space is called the "reach of $\overline{\xi}$" in [6], obtained as a hyperplane from a trial density matrix. The above considerations show that it provides an exact state space for the fermion propagator, with boundaries at $\Upsilon_{N,d}(\overline{\mathbf{r}}, \overline{\xi}) = 0$. The problem of an absorbing boundary is solved in the theory of stochastic processes [29]. The basic ingredient is the first passage time. The process is made up from all sample paths obtained by a diffusion, with those paths that hit the boundary removed. (Bosonic eigenstates would require reflection at the boundary.) This is in essence a rejection method. Admittedly, as remarked in [19] this might not be the ideal way to simulate a distribution, because a lot of operations can take place before a sample path hits the boundary. However, I am unaware of a more efficient approach. It should be emphasized that we are not at all discussing a fixed node, but the boundary of a domain which in general might differ for any initial point $\overline{\xi}$.

Notice that the numerical evaluation of $\Upsilon_{N,d}(\overline{\mathbf{r}}, \overline{\xi})$ is bound to be inaccurate: the sign problem is accumulated here in a compact expression to be studied by analytical means. For two particles, $\Upsilon_{N=2,d}(\overline{\mathbf{r}}, \overline{\xi})$ is of order ε:

$$\begin{aligned} \Upsilon_{N=2,d}(\overline{\mathbf{r}}, \overline{\xi}) &= e^{\varepsilon(\mathbf{r}_1 \cdot \xi_1 + \mathbf{r}_2 \cdot \xi_2)} - e^{\varepsilon(\mathbf{r}_1 \cdot \xi_2 + \mathbf{r}_2 \cdot \xi_1)} \\ &\xrightarrow[\varepsilon \to 0]{} \varepsilon(\mathbf{r}_1 - \mathbf{r}_2) \cdot (\xi_1 - \xi_2). \end{aligned} \tag{12}$$

The requirement $\Upsilon_{N=2,d}(\bar{\mathbf{r}}, \bar{\xi}) > 0$, i.e., $(\mathbf{r}_1 - \mathbf{r}_2)\cdot(\xi_1 - \xi_2) > 0$ for 2 fermions, is precisely the condition for an antisymmetric solution under inversion symmetry in the relative coordinate system, as it should be. It is also the condition found in [6] from density matrix considerations. Although in [17] it is stated that they consider a different hyperplane, closer inspection reveals that their initial point is chosen such that $\xi_1 - \xi_2$ has equal components in the 3 Carthesian directions.

The evaluation of $\Upsilon_{N,d}(\bar{\mathbf{r}}, \bar{\xi})$ becomes more involved if N increases, because the expansion of $e^{\varepsilon \mathbf{r}_j \cdot \xi_k}$ in powers of ε, introduces cancellations of low powers of ε if filled out in the determinant $\Upsilon_{N,d}(\bar{\mathbf{r}}, \bar{\xi})$.

2.1. One dimension

This cancellation problem is manifestly illustrated (and easily solved) in one dimension. Consider a $N \times N$ Vandermonde matrix $U(\bar{\mathbf{r}})$ and a related matrix $X(\bar{\mathbf{r}})$:

$$U_{j,k}(\bar{\mathbf{r}}) = x_k^{j-1},\ j,\ k = 1,\ 2,\ \cdots,\ N, \tag{13}$$

$$X_{j,k}(\bar{\mathbf{r}}) = \frac{U_{j,k}\left(\sqrt{\varepsilon}\bar{\mathbf{r}}\right)}{\sqrt{(j-1)!}}, \tag{14}$$

$$\det\left(U(\bar{\mathbf{r}})\right) = \prod_{j=1}^{N}\prod_{k=j+1}^{N}(x_j - x_k), \tag{15}$$

$$\det\left(X(\bar{\mathbf{r}})\right) = \sqrt{\frac{\varepsilon^{N(N-1)/2}}{\prod_{j=0}^{N-1} j!}}\,\det\left(U(\bar{\mathbf{r}})\right). \tag{16}$$

One then readily shows that the expansion of $e^{\varepsilon x_j \xi_k}$ to any order $(N-1)$ can be factorized:

$$\left[X(\bar{\mathbf{r}})^T\, X(\bar{\xi})\right]_{j,k} = \sum_{n=0}^{N-1}\frac{\varepsilon^n}{n!}(x_j\xi_k)^n. \tag{17}$$

Using $\det(AB) = \det(A)\det(B)$, the evaluation of $\Upsilon_{N,d=1}(\bar{\mathbf{r}}, \bar{\xi})$ for N fermions in 1

dimension thus gives the leading term

$$\Upsilon_{N,d=1}(\bar{\mathbf{r}},\bar{\xi}) \sim \left(\frac{\varepsilon^{N(N-1)/2}}{\prod_{j=0}^{N-1} j!}\right)\prod_{j=1}^{N}\prod_{k=j+1}^{N}(x_j - x_k)(\xi_j - \xi_k), \tag{18}$$

which defines the state space from the condition that the mutual initial ordering of all pairs of particles is never interchanged during the walk. We thus recover the state space, in contrast to the coordinate space $\mathbb{R}^N$, which Feynman defined [28] in order to introduce the concept of fermion statistics (in one dimension).

2.2. Two or three dimensions

For two and three dimensions, the analysis is substantially more complicated, physically because two particles can be interchanged without colliding, mathematically because the binomial expansion of $(\mathbf{r}_j \cdot \xi_k)^n$ invokes products of polynomials. Symbolic algebra is a helpful tool for a limited number of particles, but produces far from transparent results. For example, for 4 fermions in 2 dimensions, it turns out that $\Upsilon_{N=4,d=2}(\bar{\mathbf{r}},\bar{\xi})$ is of order ε^4, whereas for 4 fermions in 3 dimensions one finds that $\Upsilon_{N=4,d=3}(\bar{\mathbf{r}},\bar{\xi})$ is of order ε^3.

Instead of examining which leading power of ε survives for given *N* and *d*, we might revert the question and wonder how many particles *N* of dimension *d* can be described by a given leading power *n* of ε.

2.3. Two dimensions

In 2 dimensions, the binomial expansion $(\mathbf{r}_j \cdot \xi_k)^n = (x_j\xi_k + y_j\eta_k)^n$ yields $(n+1)$ terms. Let $N_2(n)$ denote the number of 2-dimensional fermions for which all available polynomials of degree $0, 1$ up to *n* are activated:

$$N_2(n) = \sum_{j=1}^{n+1} j = \frac{(n+2)(n+1)}{2}. \tag{19}$$

Note that $N_2(1) = 3$, $N_2(2) = 6$, $N_2(3) = 10$ and so on, reflecting the cylindrical symmetry of the free diffusion, which in the case of a cylindrical symmetric potential would result in closed shells. For given *n*, construct two $N_2(n)\times N_2(n)$ matrices

$V^{(n)}(\bar{\mathbf{r}})$ and $Y^{(n)}(\bar{\mathbf{r}})$ as follows:

$$\text{for } \begin{matrix}\nu = 0, \cdots, n, \\ m = 0, \cdots, \nu,\end{matrix} : \begin{matrix} V^{(n)}_{m+1+N_2(\nu-1),\,k}(\bar{\mathbf{r}}) = x_k^{\nu-m} y_k^m, \\ Y^{(n)}_{m+1+N_2(\nu-1),\,k}(\bar{\mathbf{r}}) = \sqrt{\frac{\binom{\nu}{m}\varepsilon^\nu}{\nu!}} x_k^{\nu-m} y_k^m. \end{matrix} \tag{20}$$

For instance, the $Y^{(2)}$ matrix for 6 two-dimensional fermions is

$$Y^{(2)}(\bar{\mathbf{r}}) = \begin{bmatrix} 1 & \cdots & 1 \\ \sqrt{\varepsilon}x_1 & \cdots & \sqrt{\varepsilon}x_6 \\ \sqrt{\varepsilon}y_1 & \cdots & \sqrt{\varepsilon}y_6 \\ \varepsilon x_1^2/\sqrt{2} & \cdots & \varepsilon x_6^2/\sqrt{2} \\ \varepsilon x_1 y_1 & \cdots & \varepsilon x_6 y_6 \\ \varepsilon y_1^2/\sqrt{2} & \cdots & \varepsilon y_6^2/\sqrt{2} \end{bmatrix}.$$

Some algebra reveals that

$$\left[\left(Y^{(n)}(\bar{\mathbf{r}})\right)^T Y^{(n)}(\bar{\xi})\right]_{j,k} = \sum_{\nu=0}^{n} \frac{\varepsilon^\nu (x_j\xi_k + y_j\eta_k)^\nu}{\nu!}.$$

Because

$$\det\left(Y^{(n)}(\bar{\mathbf{r}})\right) = \det\left(V^{(n)}(\bar{\mathbf{r}})\right) \frac{\varepsilon^{n(n+1)(n+2)/6}}{\prod_{\nu=0}^{n}\prod_{m=0}^{\nu}\sqrt{m!(\nu-m)!}^{\nu+1}}, \tag{21}$$

the state space $\Upsilon_{N_2(n),\,d=2}(\bar{\mathbf{r}},\,\bar{\xi})$ for $N_2(n)$ fermions in 2 dimensions is thus determined by the factorized condition

$$\det\left(V^{(n)}(\bar{\mathbf{r}})\right)\det\left(V^{(n)}(\bar{\xi})\right) > 0, \tag{22}$$

and absorption at a boundary at the first hitting time is easily imposed numerically.

If the number of fermions differs from the numbers $N_2(n)$, the state space condition does not factorize, and linear combinations of products of determinants have to be considered. For example, for 4 two-dimensional fermions one finds

$$\Upsilon_{N=4,\,d=2}(\bar{\mathbf{r}},\,\bar{\xi}) \sim \begin{matrix} \det(A_1(\bar{\mathbf{r}}))\det(A_1(\bar{\xi})) \\ +\,2\det(A_2(\bar{\mathbf{r}}))\det(A_2(\bar{\xi})) \\ +\,\det(A_3(\bar{\mathbf{r}}))\det(A_3(\bar{\xi})) \end{matrix} > 0,$$

$$A_1(\bar{\mathbf{r}}) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ x_1^2 & x_2^2 & x_3^2 & x_4^2 \end{bmatrix}, \quad A_2(\bar{\mathbf{r}}) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ x_1y_1 & x_2y_2 & x_3y_3 & x_4y_4 \end{bmatrix},$$

$$A_3(\bar{\mathbf{r}}) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ y_1^2 & y_2^2 & y_3^2 & y_4^2 \end{bmatrix}, \tag{23}$$

where the factors before the products of determinants derive from the binomial expansion of $(x+y)^2$. But the detailed treatment for general N is rather lengthy and cumbersome, and lies beyond the scope of this paper.

2.4. Three dimensions

The bookkeeping of the case of N three-dimensional fermions is still more involved than in two dimensions because the binomial expansion of $(x\xi + y\eta + z\zeta)^n$ contains $(n+1)(n+2)/2$ terms. As a consequence the factorization of the state space $\Upsilon_{N,d=3}(\bar{\mathbf{r}}, \bar{\xi})$ is only possible if $N = N_3(n)$ with

$$N_3(n) = \sum_{j=0}^{n} \frac{(j+1)(j+2)}{2} = \frac{(n+3)(n+2)(n+1)}{6}. \tag{24}$$

The resulting numbers $N_3(1) = 4$, $N_3(2) = 10$, $N_3(3) = 20$ and so on reflect the spherical symmetry of the free diffusion, which in the case of a spherical symmetric potential would result in the familiar filled shells as in atoms. The analysis follows the same line as in the two-dimensional case, but now an additional z component enters the calculation. The state space $\Upsilon_{N_3(n),d=3}(\bar{\mathbf{r}}, \bar{\xi})$ for $N_3(n)$ fermions in 3 dimensions is determined form the condition

$$\det(W^n(\bar{\mathbf{r}}))\det(W^n(\bar{\xi})) > 0, \tag{25}$$

where $W^{(n)}(\bar{\mathbf{r}})$ is a $N_3(n)\times N_3(n)$ matrix. For 4 particles it is given by

$$W^{(1)}(\bar{\mathbf{r}}) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ z_1 & z_2 & z_3 & z_4 \end{bmatrix}. \tag{26}$$

For 10 fermions, $W^{(2)}(\bar{\mathbf{r}})$ is obtained by adding 6 rows and columns. The additional columns are for the particle labels. The extra rows contain the 6 quantities $x_k^2, y_k^2, z_k^3, x_k y_k, x_k z_k, y_k z_k$ from the binomial expansion of $(x_k + y_k + z_k)^2$. If one would go further to find $W^{(3)}(\bar{\mathbf{r}})$ for 20 fermions, also the binomial expansion of $(x_k + y_k + z_k)^3$ has to be taken into account.

If N is not one of the numbers $N_3(n)$, the factorization of the state space into a single product of determinants fails and linear combinations have to be considered. For 2 three-dimensional fermions, this linear combination is not complicated

$$\Upsilon_{2,d=3}(\bar{\mathbf{r}}, \bar{\xi}) \sim \begin{vmatrix} 1 & 1 \\ x_1 & x_2 \end{vmatrix} \begin{vmatrix} 1 & 1 \\ \xi_1 & \xi_2 \end{vmatrix} + \begin{vmatrix} 1 & 1 \\ y_1 & y_2 \end{vmatrix} \begin{vmatrix} 1 & 1 \\ \eta_1 & \eta_2 \end{vmatrix} + \begin{vmatrix} 1 & 1 \\ z_1 & z_2 \end{vmatrix} \begin{vmatrix} 1 & 1 \\ \zeta_1 & \zeta_2 \end{vmatrix} > 0, \tag{27}$$

consistent with the condition (12) found above. The rather intricate derivation of the appropriate linear combinations for general N is not further elaborated in the present paper.

3. Conclusions

In summary, for N spin-polarized fermions, a state space was derived on which the fermion propagator is positive for systems with scalar potentials. This state space is obtained by reducing the coordinate space by a factor $N!$, utilizing the permutation (anti) symmetry. The price to pay is the evaluation of well-defined $N \times N$ determinants with $O(N^3)$ operations. A sign-problem-free algorithm is obtained, because a diffusion process with superimposed potential-dependent exponential weights is defined on this state space with absorbing boundary conditions. In order to avoid unobserved border crossings, Bernouilli walks provide the safest and most transparent algorithm. The resulting random process can be realized by stable diffusion of purely positive walkers.

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