Continuous representation of many-fermion systems over real Slater determinants

T. Troudet and S. E. Koonin
W. K. Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, California 91125
(Received 11 July 1983)

We derive a resolution of unity over real Slater determinants using simple symmetry arguments. The resulting simplification of the measure with respect to the previous representations makes it a good candidate for stochastic evaluations.

There has been recent interest in functional and path-integral representations of many-fermion systems. These provide a natural framework for semiclassical approximations and have already proven useful for emphasizing the role of static and dynamic mean-field theories in the nuclear many-body problem. A recent review of the subject can be found in Ref. 1.

The Monte-Carlo evaluation of fermion path integrals is therefore a natural issue in connection with nuclear structure physics,2 and so it is of interest to consider compact path-integral representations with as few redundant degrees of freedom as possible. One step in this direction was recently taken3 with the coherent state representation by integrating out the imaginary part of the complex variables of the resolution of unity proposed in Ref. 4. The purpose of this note is to propose an alternative to the real coherent state resolution of unity using a simple real Slater determinant (RSD) representation.

One advantage of this new resolution of unity is its straightforward construction through elementary symmetry arguments; complex and real parametrizations appear on equal footing. This is of some pedagogical interest. In addition, the RSD resolution of unity has a trivial measure on a domain of integration which is the surface of a many-dimensional hypersphere. The sampling of paths in numerical simulations is thus greatly simplified.

We introduce $A$ arbitrary single-particle wave functions $|\phi_i\rangle$ that we expand in the truncated single-particle basis

$$B_N = \{|n_1, \ldots , n_N\rangle\} ,$$

$$|\phi_i\rangle = \sum_{j=1}^N \phi_j(n_j)|n_j\rangle ,$$

where the coefficients $\phi_j(n_j) = \langle n_j | \phi_i \rangle$ are arbitrary real numbers. Upon defining $|\Phi\rangle$ as a Slater determinant of the $A$ orbitals $|\phi_i\rangle$:

$$|\Phi\rangle = \frac{1}{\sqrt{A!}} \text{det}(|\phi_1\rangle, |\phi_2\rangle, \ldots , |\phi_A\rangle) ,$$

we can introduce the operator

$$\hat{P}_N = \int |\Phi\rangle \langle \Phi| \prod_{\beta \neq \alpha} \delta(\langle \phi_\beta | \phi_\alpha \rangle - \delta_{\alpha \beta}) D[\phi] ,$$

where the measure $D[\phi]$ is a simple product of Riemann differential elements

$$D[\phi] = \prod_{i=1}^A \prod_{j=1}^N d\phi_i(n_j) .$$

Equation (3a) shows that $\hat{P}_N$ is a linear superposition of Slater determinants, the only constraint being that the single-particle orbitals are orthonormal. We now show that $\hat{P}_N$ is proportional to the identity operator in the subspace of $A$-particle antisymmetric wave functions generated by $B_N$. To do so, we expand Eq. (3a) in the basis of Slater determinants $|n_1, n_2, \ldots , n_A\rangle$ and express the $\delta$ function in terms of a multidimensional Fourier transform on the variables $k_\alpha$:

$$\hat{P}_N = \sum_{\{|n_1, \ldots , n_A\rangle\}} \prod_{i=1}^A \frac{d k_\alpha}{2\pi} ,$$

and we sum over all possible sets of configurations $|n_\alpha\rangle$ and $|n_\alpha'\rangle$. Because of the Pauli principle, the contribution of each separate set $|n_\alpha\rangle$ and $|n_\alpha'\rangle$ to Eq. (4) is nontrivial only when their elements are distinct within each set. In addition, two sets $|n_\alpha\rangle$ and $|n_\alpha'\rangle$ contribute only when they are globally identical. To prove this last point, change all the variables $\phi_i(n_j)$ of the integrand (4) into $-\phi_i(n_j)$. Under this transformation, the sign of the whole integrand is given by the sign of the product $P(n_\alpha)P(n_\alpha')$ where $P(n_\alpha)$ is de-
and $I[n_i]$, defined for the set $[n_1, \ldots, n_A]$, is the integral

$$I[n_i] = \int \exp \left[ i \sum_{i=1}^{A} k_i \right] \int \left| \det M(n_i) \right|^2 \exp \left[ -i \sum_{\lambda=1}^{N} L \sum_{\lambda=1}^{A} \phi_i(n_{\lambda}) k_{\lambda} \phi_j(n_{\lambda}) \right] D[\phi_i] D[k_i] ,$$

(7b)

where $M(n_i)$ is the square $A \times A$ matrix

$$[M(n_i)]_{nm} = \phi_i(n_m) .$$

(7c)

From Eq. (7b) it is straightforward to see that $I[n_i]$ is independent of the choice of the set $[n_i]$ and is identical to a positive definite constant $I_N$:

$$I[n_i] = I_N = \int \left| \det M(\phi) \right|^2 \prod_{i \leq j=1}^{A} \delta(\langle \phi_i | \phi_j \rangle - \delta_{ij}) D[\phi] ,$$

(8)

where $M(\phi)$ is an arbitrary $A \times A$ matrix of the type (7c).

We have thus proved that the operator $\hat{P}_N$ introduced in (3a) is directly proportional to the projector on the subspace of antisymmetric many-body wave functions built from $B_N$. It is therefore a resolution of unity constructed from real Slater determinants. A numerical simulation using Eq. (3a) is conveniently accomplished by sampling randomly $A$ orthonormal vectors $|\phi_i\rangle$ on the $N$-dimensional unit hypersphere.  

In order to calculate the normalization constant $I_N$ defined in Eq. (8), it is advantageous to express the trace of the operator $\hat{P}_N$ in both representations (3a) and (7a), which leads to

$$I_N = \frac{A!((N-A)!)!}{N!} \int \prod_{i \leq j=1}^{A} \delta(\langle \phi_i | \phi_j \rangle - \delta_{ij}) D[\phi] .$$

(9)

The latter integral is simply the volume of the manifold $O_{A,N}$ which consists of the $A \times N$ rectangular matrices $O$ satisfying the relation

$$OO^T = I^4 .$$

(10)

This manifold $O_{A,N}$ coincides with the set of the cosets of the orthogonal group $O_N$ with respect to its subgroup $O_{N-A}$ consisting of matrices of the form

$$\begin{pmatrix} I^{(4)} & 0 \\ 0 & O_{N-A} \end{pmatrix} ,$$

(11)

where $O_{N-A}$ is any real orthogonal matrix of dimension $N-A$. Therefore, the integral (9) is the ratio of the volumes of the orthogonal groups $O_N$ and $O_{N-A}$. These volumes have been computed in Ref. 6 by direct integration of the matrix elements of the real orthogonal matrices. This leads to

$$I_N = \frac{A!((N-A)!)! }{N!} (8\pi)^{A/4(2N-A-1)} \prod_{\nu=N-A+1}^{N} \frac{\Gamma((\nu-1)/2)}{\Gamma(\nu-1)} .$$

(12)

It is obvious that the symmetry arguments we have used also can be applied to a complex parametrization of the wave functions. This leads to a resolution of unity of the form (3a) where the measure $D[\phi]$ is

$$D[\phi, \phi^*] = \prod_{i \neq j=1}^{A} \prod_{\nu=N-A+1}^{N} d\phi_i(n_{\nu}) d\phi^*_j(n_{\nu}) ,$$

(13)

and the integration over the variables $\phi_i(n_{\nu})$ would cover the entire complex plane. As before, the volume of the manifold which consists of $A \times N$ matrices $U$ satisfying the relation

$$UU^* = I^4 ,$$

(14)

is the ratio of the volumes of the corresponding unitary groups $U_N$ and $U_{N-A}$, so that for the complex parametrization

$$I_N = \frac{A!}{(N-A+1)!(N-A+2)! \cdots N!} (2\pi)^{A/2(2N-A+1)} .$$

(15)

1J. W. Negele, Rev. Mod. Phys. 54, 913 (1982).