Continuous representation of many-fermion systems over real Slater determinants

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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 taken[3] 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 $B_N=\{|n_1\rangle,\ldots,|n_N\rangle\}$:

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

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

$$|\Phi\rangle=\frac{1}{\sqrt{A!}}\det\{|\phi_1\rangle,|\phi_2\rangle,\ldots,|\phi_A\rangle\}\ , \tag{2}$$

we can introduce the operator

$$\hat{P}_N=\int|\Phi\rangle\langle\Phi|\prod_{i\geq j=1}^{A}\delta(\langle\phi_i|\phi_j\rangle-\delta_{ij})D[\phi]\ , \tag{3a}$$

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

$$D[\phi]=\prod_{i=1}^{A}\prod_{j=1}^{N}d\phi_i(n_j)\ . \tag{3b}$$

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 δ function in terms of a multidimensional Fourier transform on the variables k_{ij}:

$$\hat{P}_N=\sum_{\{n_i,n_i'\}}|n_1,\ldots,n_A\rangle\langle n_1',\ldots,n_A'|\int D[\phi]D[k]\exp\left\{i\left\{\sum_{i=1}^{A}k_{ii}-\sum_{\lambda=1}^{N}\sum_{i\geq j=1}^{A}\phi_i(n_\lambda)k_{ij}\phi_j(n_\lambda)\right\}\right\}$$
$$\times[\phi_1(n_1)\phi_1(n_1')]\cdots[\phi_A(n_A)\phi_A(n_A')]\ , \tag{4}$$

where $D[k]$ is the simple measure

$$D[k]=\prod_{i\geq j=1}^{A}\frac{dk_{ij}}{2\pi}\ , \tag{5}$$

and we sum over all possible sets of configurations $\{n_i\}$ and $\{n_i'\}$. Because of the Pauli principle, the contribution of each separate set $\{n_i\}$ and $\{n_i'\}$ to Eq. (4) is nontrivial only when their elements are distinct within each set. In addition, two sets $\{n_i\}$ and $\{n_i'\}$ 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 $P(n_i)P(n_i')$ where $P(n_i)$ is defined as

$$P(n_i)=\phi_1(n_1)\cdots\phi_A(n_A)\ . \tag{6}$$

Since n_1 can occur only once in the set $\{n_i\}$, $P(n_1)$ changes into $-P(n_1)$ and consequently n_1 must appear once in $P(n_i')$ in order to leave the integrand invariant. Applying successively the same transformation to $n_2,n_3,\ldots,n_A$ we conclude for a nonzero contribution to Eq. (4), only when the two sets $\{n_1,\ldots,n_A\}$ and $\{n_1',\ldots,n_A'\}$ are identical.

If we take into account all the possible permutations of both sets $\{n_1,\ldots,n_A\}$ and $\{n_1',\ldots,n_A'\}$, we can choose some particular lexicographic ordering and rewrite $\hat{P}_N$ as

$$\hat{P}_N=\sum_{n_1>\cdots>n_A}|n_1,\ldots,n_A\rangle\langle n_1,\ldots,n_A|I[n_i] \tag{7a}$$

and $I[n_i]$, defined for the set $\{n_1, \ldots, n_A\}$, is the integral

$$I[n_i]=\int \exp\left\{i\sum_{i=1}^{A}k_{ii}\right\}\int [\det M(n_i)]^2 \exp\left\{-i\sum_{\lambda=1}^{N}\sum_{i\geq j=1}^{A}\phi_i(n_\lambda)k_{ij}\phi_j(n_\lambda)\right\}D[\phi]D[k] \ , \tag{7b}$$

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

$$[M(n_i)]_{lm}=\phi_l(n_m) \ . \tag{7c}$$

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:

$$I[n_i]=I_N=\int [\det M(\phi)]^2\prod_{i\geq j=1}^{A}\delta(\langle\phi_i|\phi_j\rangle-\delta_{ij})D[\phi] \ , \tag{8}$$

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.[5]

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

$$I_N=\frac{A!(N-A)!}{N!}\int\prod_{i\geq j=1}^{A}\delta(\langle\phi_i|\phi_j\rangle-\delta_{ij})D[\phi] \ . \tag{9}$$

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

$$OO^T=I^{(A)} \ . \tag{10}$$

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

$$\begin{vmatrix} I^{(A)} & O \\ O & O_{N-A}\end{vmatrix} \ , \tag{11}$$

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

$$I_N=\frac{A!(N-A)!}{N!}(8\pi)^{(A/4)(2N-A-1)}\times\prod_{\nu=N-A+1}^{N}\frac{\Gamma[(\nu-1)/2]}{\Gamma(\nu-1)} \ . \tag{12}$$

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

$$D[\phi,\phi^*]=\prod_{i=1}^{A}\prod_{j=1}^{N}d\phi_i(n_j)d\phi_i^*(n_j) \ , \tag{13}$$

and the integration over the variables $\phi_i(n_j)$ would cover the entire complex plane.[7] As before, the volume of the manifold which consists of $A\times N$ matrices U satisfying the relation

$$UU^\dagger=I^{(A)} \tag{14}$$

is the ratio of the volumes of the corresponding unitary groups U_N and U_{N-A}, so that for the complex parametrization[6]

$$I_N=\frac{A!}{(N-A+1)!(N-A+2)!\cdots N!}(2\pi)^{(A/2)(2N-A+1)} \ . \tag{15}$$

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