Overlap Integrals of Fermionic Wave Functions

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Let $c_j^\dagger, c_j,\ j = 1, \dots, N$, be creation and annihilation operators of complex fermions satisfying the canonical anticommutation relations

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0. \tag{1}$$

1 M-Particle States

For $N \times M$ matrices A and B, define the M-particle states $|A\rangle$ and $|B\rangle$ by

$$|A\rangle = \left(\sum_i A_{i1} c_i^\dagger\right)\left(\sum_i A_{i2} c_i^\dagger\right)\cdots\left(\sum_i A_{iM} c_i^\dagger\right)|0\rangle, \tag{2}$$

$$|B\rangle = \left(\sum_i B_{i1} c_i^\dagger\right)\left(\sum_i B_{i2} c_i^\dagger\right)\cdots\left(\sum_i B_{iM} c_i^\dagger\right)|0\rangle. \tag{3}$$

In the following computation, it is not necessary to impose canonical anticommutation relations on the operators "$a_j^\dagger$"$= \sum_i A_{ij} c_i^\dagger$. We want to compute the inner product $\langle A|B\rangle$. Expanding it gives

$$\langle A|B\rangle = \sum_{i_1,\dots,i_M} \sum_{j_1,\dots,j_M} A^*_{i_1 1} \cdots A^*_{i_M M} B_{j_1 1} \cdots B_{j_M M} \langle 0| c_{i_M} \cdots c_{i_1} c_{j_1}^\dagger \cdots c_{j_M}^\dagger |0\rangle \tag{4}$$

$$= \sum_{i_1,\dots,i_M} \sum_P \operatorname{sgn}(P) A^*_{i_1 1} \cdots A^*_{i_M M} B_{P(i_1)1} \cdots B_{P(i_M)M}. \tag{5}$$

Here P is a permutation of $\{i_1, \dots, i_M\}$, and only terms in which $i_1, \dots, i_M$ are all distinct contribute. Notice that

$$B_{P(i_1)1} \cdots B_{P(i_M)M} = B_{i_{P(1)}1} \cdots B_{i_{P(M)}M}. \tag{6}$$

After reordering the factors, this becomes

$$B_{i_{P(1)}1} \cdots B_{i_{P(M)}M} = B_{i_1 P(1)} \cdots B_{i_M P(M)}. \tag{7}$$

Therefore

$$\langle A|B\rangle = \sum_P \operatorname{sgn}(P) \sum_{i_1,\dots,i_M} A^*_{i_1 1} \cdots A^*_{i_M M} B_{i_1 P(1)} \cdots B_{i_M P(M)} \tag{8}$$

$$= \sum_P \operatorname{sgn}(P) [A^\dagger B]_{1P(1)} \cdots [A^\dagger B]_{MP(M)} \tag{9}$$

$$= \det[A^\dagger B]. \tag{10}$$

2 BCS Ground States

For $N \times N$ antisymmetric matrices $A^T = -A$ and $B^T = -B$, define

$$|A\rangle = \exp\left(\frac{1}{2}\sum_{ij} A_{ij} c_i^\dagger c_j^\dagger\right)|0\rangle\,, \tag{11}$$

$$|B\rangle = \exp\left(\frac{1}{2}\sum_{ij} B_{ij} c_i^\dagger c_j^\dagger\right)|0\rangle\,. \tag{12}$$

The overlap $\langle A|B\rangle$ is given by [1]

$$\langle A|B\rangle = (-1)^{N(N+1)/2}\mathrm{Pf}\begin{pmatrix} B & -\mathbf{1} \\ \mathbf{1} & -A^* \end{pmatrix}. \tag{13}$$

Introduce fermionic coherent states $|\boldsymbol{z}\rangle$,

$$c_i|\boldsymbol{z}\rangle = z_i|\boldsymbol{z}\rangle\,, \quad \langle\boldsymbol{z}|c_i^\dagger = z_i^*\langle\boldsymbol{z}|\,, \quad i = 1,\ldots,N. \tag{14}$$

The variables z_i, z_i^*, $i = 1,\ldots,N$, are $2N$ independent Grassmann numbers. Explicitly,

$$|\boldsymbol{z}\rangle = e^{-\sum_i z_i c_i^\dagger}|0\rangle = \prod_i (1 - z_i c_i^\dagger)|0\rangle\,, \tag{15}$$

$$\langle\boldsymbol{z}| = \langle 0|e^{-\sum_i c_i z_i^*} = \langle 0|\prod_i (1 - c_i z_i^*). \tag{16}$$

One should keep track of anticommutation relations such as $\{c_i, z_j\} = 0$. We use the completeness relation

$$\int \prod_i dz_i^* dz_i\, e^{-\sum_i z_i^* z_i}|\boldsymbol{z}\rangle\langle\boldsymbol{z}| = 1, \tag{17}$$

and also note that

$$\langle 0|\boldsymbol{z}\rangle = \langle 0|0\rangle = 1. \tag{18}$$

Then the overlap integral is

$$\langle A|B\rangle = \int \prod_i dz_i^* dz_i\, e^{-\sum_i z_i^* z_i}\langle A|\boldsymbol{z}\rangle\langle\boldsymbol{z}|B\rangle \tag{19}$$

$$= \int \prod_i dz_i^* dz_i\, e^{-\sum_i z_i^* z_i} e^{\frac{1}{2}\sum_{ij} A_{ij}^* z_j z_i} e^{\frac{1}{2}\sum_{ij} B_{ij} z_i^* z_j^*}. \tag{20}$$

To perform the integral, introduce the antisymmetric matrix

$$M = \begin{pmatrix} B & -1 \\ 1 & -A^* \end{pmatrix} \tag{21}$$

and the vector of Grassmann variables $\eta = (z_1^*, \ldots, z_N^*, z_1, \ldots, z_N)$. Then

$$\langle A|B\rangle = s_N \int (d\eta_{2N}\cdots d\eta_1)\exp\left(\sum_{i<j} M_{ij}\eta_i\eta_j\right). \tag{22}$$

The sign coming from reordering the integration variables is

$$s_N = (-1)^{N(N-1)/2}(-1)^N = (-1)^{N(N+1)/2}. \tag{23}$$

For the Grassmann integral part, using $[\eta_i\eta_j, \eta_k\eta_l] = 0$, we have

$$\int (d\eta_{2N}\cdots d\eta_1) \exp\left(\sum_{i<j} M_{ij}\eta_i\eta_j\right) = \int (d\eta_{2N}\cdots d\eta_1) \prod_{i<j}(1 + M_{ij}\eta_i\eta_j). \tag{24}$$

Only the terms proportional to $\eta_1\cdots\eta_{2N}$ contribute. Let F_{2N} be the subset of S_{2N} consisting of permutations satisfying

$$F_{2N} = \{\sigma \in S_{2N} \mid \sigma(2i-1) < \sigma(2i),\ \sigma(1) < \sigma(3) < \cdots < \sigma(2N-1)\}. \tag{25}$$

Then

$$\int (d\eta_{2N}\cdots d\eta_1) \prod_{i<j}(1 + M_{ij}\eta_i\eta_j) = \sum_{\sigma\in F_{2N}} \operatorname{sgn}\sigma\, M_{\sigma(1)\sigma(2)}\cdots M_{\sigma(2N-1)\sigma(2N)}, \tag{26}$$

which is precisely $\operatorname{Pf} M$. This proves the formula above.

References

[1] L. M. Robledo, *Sign of the overlap of Hartree–Fock–Bogoliubov wave functions*, Phys. Rev. C **79**, 021302(R) (2009).