A note on basic properties of f_{ij}

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In this note, we show relation between Pfaffian Slater determinant and single Slater determinant. We also discuss meaning of the singular value decomposition of coefficients f_{ij}.

1. Relation between f_{ij} and $\Phi_{in\sigma}$

Pfaffian Slater determinant [one-body part of the many-variable variational Monte Carlo (mVMC) method] is defined as

$$|\phi_{\mathrm{Pf}}\rangle = \Big(\sum_{i,j=1}^{N_s} f_{ij} c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger}\Big)^{N_{\mathrm{e}}/2} |0\rangle, \tag{1}$$

where N_s is number of sites, N_e is number of total particles, and f_{ij} are variational parameters. For simplicity, we assume that f_{ij} are real number. Single Slater determinant is defined as

$$|\phi_{\mathrm{SL}}\rangle = \Big(\prod_{n=1}^{N_e/2} \psi_{n\uparrow}^{\dagger}\Big)\Big(\prod_{m=1}^{N_e/2} \psi_{m\downarrow}^{\dagger}\Big)|0\rangle, \tag{2}$$

$$\psi_{n\sigma}^{\dagger} = \sum_{i=1}^{N_s} \Phi_{in\sigma} c_{i\sigma}^{\dagger}. \tag{3}$$

We note that Φ is the normalized orthogonal basis, i.e,

$$\sum_{i=1}^{N_s} \Phi_{in\sigma}\Phi_{im\sigma} = \delta_{nm}, \tag{4}$$

where δ_{nm} is the Kronecker's delta. Due to this normalized orthogonality, we obtain following relation:

$$[\psi_{n\sigma}^{\dagger}, \psi_{m\sigma}]_{+} = \delta_{nm}, \tag{5}$$

$$G_{ij\sigma} = \langle c_{i\sigma}^{\dagger} c_{j\sigma}\rangle = \frac{\langle\phi_{\mathrm{SL}}|c_{i\sigma}^{\dagger} c_{j\sigma}|\phi_{\mathrm{SL}}\rangle}{\langle\phi_{\mathrm{SL}}|\phi_{\mathrm{SL}}\rangle} \tag{6}$$

$$= \sum_{n} \Phi_{in\sigma}\Phi_{jn\sigma}. \tag{7}$$

Here, we rewrite ϕ_{SL} and obtain explicit relation between f_{ij} and $\Phi_{in\sigma}$. By using the

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commutation relation for $\psi^\dagger_{n\sigma}$, we rewrite $\phi_{\rm SL}$ as

$$|\phi_{\rm SL}\rangle \propto \prod_{n=1}^{N_e/2}\Big(\psi^\dagger_{n\uparrow}\psi^\dagger_{\mu(n)\downarrow}\Big)|0\rangle, \tag{8}$$

where $\mu(n)$ represents permutation of sequence of $n=1,2,\cdots,N_e/2$. For simplicity, we take identity permutation and obtain the relation

$$|\phi_{\rm SL}\rangle \propto \prod_{n=1}^{N_e/2}\Big(\psi^\dagger_{n\uparrow}\psi^\dagger_{n\downarrow}\Big)|0\rangle = \prod_{n=1}^{N_e/2} K^\dagger_n|0\rangle \tag{9}$$

$$\propto \Big(\sum_{n=1}^{\frac{N_e}{2}} K^\dagger_n\Big)^{\frac{N_e}{2}}|0\rangle = \Big(\sum_{i,j=1}^{N_s}\Big[\sum_{n=1}^{\frac{N_e}{2}}\Phi_{in\uparrow}\Phi_{jn\downarrow}\Big]c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}\Big)|0\rangle, \tag{10}$$

where $K^\dagger_n=\psi^\dagger_{n\uparrow}\psi^\dagger_{n\downarrow}$ and we use the relation $K^\dagger_nK^\dagger_m=K^\dagger_mK^\dagger_n$. This result shows that f_{ij} can be expressed by the coefficients of the single Slater determinant as

$$f_{ij}=\sum_{n=1}^{\frac{N_e}{2}}\Phi_{in\uparrow}\Phi_{jn\downarrow}. \tag{11}$$

We note that this is one of expression of f_{ij} for single Slater determinant, i.e, f_{ij} depend on the pairing degrees of freedom (choices of $\mu(n)$) and gauge degrees of freedom (we can arbitrary change the sign of Φ as $\Phi_{in\sigma}\to-\Phi_{in\sigma}$). This large degrees of freedom is the origin of huge redundancy of f_{ij}.

2. Singular value decomposition of f_{ij}

We define matrices F, $\Phi_\uparrow$, $\Phi_\downarrow$, and Σ as

$$(F)_{ij}=f_{ij},\quad (\Phi_\uparrow)_{in}=\Phi_{in\uparrow},\quad (\Phi_\downarrow)_{in}=\Phi_{in\downarrow}, \tag{12}$$

$$\Sigma={\rm diag}[1,\cdots,1,0,0,0]\quad (\#\text{ of }1=N_e/2). \tag{13}$$

By using these notations, we can describe the singular value decomposition of f_{ij} (or equivalently F) as

$$F=\Phi_\uparrow\Sigma\Phi^t_\downarrow. \tag{14}$$

This result indicates that f_{ij} can be described by the mean-field solutions if the number of nonzero singular values are $N_e/2$ and all the nonzero singular values of F are one. In other word, the singular values including their numbers offers the quantitative criterion how the Pfaffian Slater determinant deviates from the single Slate determinant.