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Supplementary Material

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1 OVERLAP BETWEEN NON-ORTHOGONAL CANONICAL BASES

In Haider and Gogny (1992) the norm overlap between two different HFB vacuua is expressed as a function of the single-particle overlap between the two respective sets of canonical wavefunctions and occupation numbers. This formula implicitly assumes that the canonical wavefunctions are orthornormal. When using canonical wavefunctions reconstructed by the AE, this property may not hold anymore and the Haider & Gogny formula should not be used 'as is' when evaluating the norm overlap. In this appendix, we show how to generalize it.

We recall that for a system with conserved time-reversal symmetry, the quasiparticle vacuum can be written Ring and Schuck (2004); Schunck (2019)

$$|\Phi\rangle = \prod_{\mu>} \beta^\dagger_\mu \beta^\dagger_{\bar{\mu}} |0\rangle , \tag{1}$$

where the quasiparticle operators $(\hat{\beta}, \hat{\beta}^\dagger)$ are obtained from a single-particle basis $(\hat{c}, \hat{c}^\dagger)$ by the Bogoliubov transformation W of (14) in Sec. 2.5. The Bloch-Messiah-Zumino decomposition of the matrix W is a consequence of the fact that the quasiparticle operators should obey the same anticommutation relations as the particle operators. In the resulting canonical basis, the quasiparticle vacuum can be written in the BCS form,

$$|\Phi\rangle = \prod_{\mu>} \left(u_\mu + v_\mu \hat{a}^\dagger_\mu \hat{a}^\dagger_{\bar{\mu}} \right) |0\rangle \,, \tag{2}$$

where $|0\rangle$ is the particle vacuum, $\bar{\mu}$ refers to the time-reversed partner of the state with index μ, and the summation runs only over "positive" indices μ. Implicit in this expression is the fact that the canonical wavefunctions associated with the operators $(\hat{a}, \hat{a}^\dagger)$ are orthonormal or, equivalently, that the operators $(\hat{a}, \hat{a}^\dagger)$ anticommute. If these conditions are not verified, the form (2) is not valid and the formulas for the norm overlap given in Haider and Gogny (1992) cannot apply. In our case, the fit of the AE gives a set of *reconstructed* canonical wavefunctions which we noted $\{\phi_\mu(\boldsymbol{r}, \sigma)\}_\mu$ and are associated with a set of single-particle creation and annihilation operators $(\hat{f}, \hat{f}^\dagger)$. Although we call these objects canonical orbitals, this is somewhat a misnomer since the wavefunctions are not necessarily orthonormal. As a consequence, one cannot define a BCS state (2) with these operators. Our goal is to find a transformation of these single-particle operators that allows us to define a BCS state.

Following the notations of Haider and Gogny (1992), we thus define the single-particle overlaps

$$\tilde{\tau}^{(ff)}_{\mu\nu} = \{\hat{f}^\dagger_\mu, \hat{f}_\nu\} = \sum_\sigma \int \mathrm{d}^3\boldsymbol{r}\, \phi^*_\mu(\boldsymbol{r}, \sigma)\phi_\nu(\boldsymbol{r}, \sigma). \tag{3}$$

The set of all such overlaps define the overlap matrix $\tilde{\tau}^{(ff)}$. This overlap matrix is block diagonal as it satisfies the relations

$$\tilde{\tau}^{(ff)}_{\mu\nu} = \tilde{\tau}^{(ff)^*}_{\bar{\mu}\bar{\nu}}, \qquad \tilde{\tau}^{(ff)}_{\mu\bar{\nu}} = \tilde{\tau}^{(ff)}_{\bar{\mu}\nu} = 0. \tag{4}$$

From the s.p. operators $(\hat{f}, \hat{f}^\dagger)$, we can introduce a new set of q.p. operators $(\hat{\chi}, \hat{\chi}^\dagger)$ through

$$\hat{\chi}_\mu = \tilde{u}_\mu \hat{f}_\mu - \tilde{v}_\mu \hat{f}^\dagger_{\bar{\mu}}, \tag{5a}$$

$$\hat{\chi}_{\bar{\mu}} = \tilde{u}_\mu \hat{f}_{\bar{\mu}} + \tilde{v}_\mu \hat{f}^\dagger_\mu. \tag{5b}$$

It is easy to see that these q.p. operators do not obey the Fermion anticommutation relation. In other words, the q.p. *spinors* associated with these operators are not orthogonal. We thus introduce the overlap matrix $\tilde{\tau}^{(\chi\chi)}_{\mu\nu}$ between any two such spinors $\mu, \nu > 0$. Owing to (5a)-(5b) and (3) it is straightforward to show that it is given by

$$\tilde{\tau}^{(\chi\chi)}_{\mu\nu} = \tilde{u}_\mu \tilde{u}_\nu \tilde{\tau}^{(ff)}_{\mu\nu} + \tilde{v}_\mu \tilde{v}_\nu \tilde{\tau}^{(ff)^*}_{\mu\nu}, \tag{6}$$

and verify the same properties (4) as the single-particle overlap. We symmetrically orthogonalize the q.p. basis by eigendecomposing $\tilde{\tau}^{(\chi\chi)}_{\mu\nu}$ [1]

$$\tilde{\tau}^{(\chi\chi)}_{\mu\nu} = Q\Sigma^2 Q^\dagger, \tag{7}$$

[1] In fact, we can limit ourself to compute the Cholesky decomposition of $\tilde{\tau}^{(\chi\chi)}_{\mu\nu}$, but we use the eigenvalues to check the rank and invert the matrix.

where Q is unitary and $\Sigma = \mathrm{diag}(\sigma_0, \sigma_1, \dots)$ with $\sigma_\mu > 0$. We then construct a new orthogonal q.p. basis

$$\hat{\gamma}^\dagger_\mu = \sum_k \hat{\chi}^\dagger_k \left(Q\Sigma^{-1}\right)_{k\mu} \tag{8}$$

that satisfies the fermion commutation relations, $\{\hat{\gamma}^\dagger_\mu, \hat{\gamma}_\nu\} = \delta_{\mu\nu}$. We can associate with these new q.p. operators $(\hat{\gamma}^\dagger, \hat{\gamma})$ a quasiparticle vacuum of the type (1). We now need to find the Bogoliubov transformation $\tilde{W}$ (and its Bloch-Messiah decomposition) that relate the $(\hat{\gamma}^\dagger, \hat{\gamma})$ to a properly orthonormal s.p. basis. To this end, we first diagonalize the single-particle overlap matrix

$$\tilde{\tau}^{(ff)}_{\mu\nu} = R\tilde{\Sigma}^2 R^\dagger, \tag{9}$$

which defines a new set of *particle* operators $(\hat{b}, \hat{b}^\dagger)$ through the relations

$$\hat{b}^\dagger_i = \sum_k \hat{f}^\dagger_k \left(R\tilde{\Sigma}^{-1}\right)_{ki} \tag{10a}$$

$$\hat{b}_{\bar{i}} = \sum_k \hat{f}_{\bar{k}} \left(R\tilde{\Sigma}^{-1}\right)_{ki}, \tag{10b}$$

By construction these new particle operators also satisfy the Fermion anti-commutation relations, $\{\hat{b}^\dagger_i, \hat{b}_j\} = \delta_{ij}$. By inverting relations (10a)-(10b), using the expression (5a)-(5b) relating the $(\hat{\chi}^\dagger, \hat{\chi})$ to the $(\hat{f}^\dagger, \hat{f})$ and using (8), these new particle operators can be related to the q.p. operators $(\hat{\gamma}^\dagger, \hat{\gamma})$ through

$$\hat{\gamma}^\dagger_\mu = \sum_l \hat{b}^\dagger_l \left[\tilde{\Sigma}R^\dagger \tilde{u} Q \Sigma^{-1}\right]_{l\mu} - \hat{b}_{\bar{l}} \left[\tilde{\Sigma}R^\dagger \tilde{v} Q \Sigma^{-1}\right]_{l\mu} \tag{11a}$$

$$\hat{\gamma}^\dagger_{\bar{\mu}} = \sum_l \hat{b}^\dagger_{\bar{l}} \left[\tilde{\Sigma}R^\top \tilde{u} Q^* \Sigma^{-1}\right]_{l\mu} + \hat{b}_l \left[\tilde{\Sigma}R^\top \tilde{v} Q^* \Sigma^{-1}\right]_{l\mu}. \tag{11b}$$

These two equations are the main result of this appendix. They show that we can extract from the non-orthogonal reconstructed, canonical wavefunctions a set of quasiparticle operators that obey the Fermion anticommutation relation, define a quasiparticle vacuum and are related to an orthonormal basis of the single-particle Hilbert space through the following Bogoliubov transformation

$$\tilde{W} = \begin{pmatrix} \tilde{\Sigma}R^\top \tilde{u} Q^* \Sigma^{-1} & \tilde{\Sigma}R^\dagger \tilde{v} Q \Sigma^{-1} \\ \tilde{\Sigma}R^\top \tilde{v} Q^* \Sigma^{-1} & \tilde{\Sigma}R^\dagger \tilde{u} Q \Sigma^{-1} \end{pmatrix} = \begin{pmatrix} \tilde{U} & \tilde{V}^* \\ \tilde{V} & \tilde{U}^* \end{pmatrix}. \tag{12}$$

This matrix only depends on the initial canonical occupations $\tilde{u}$ and $\tilde{v}$, as well as on the eigenvalues and eigenvectors of both the s.p. overlap matrix (3) and the q.p. overlap matrix (6).

From the new transformation $\tilde{W}$, we can define the one-body density matrix

$$\rho = \tilde{V}^* \tilde{V}^\top = \tilde{\Sigma}R^\dagger \tilde{v} \tilde{\tau}^{(\chi\chi)^{-1}} \tilde{v} R \tilde{\Sigma}. \tag{13}$$

and put it into canonical form by diagonalizing it

$$\rho = \tilde{D} v^2 \tilde{D}^\dagger. \tag{14}$$

The transformation $\tilde{D}$ defines the new canonical basis. By construction, these new canonical wavefunctions are expressed in the $(\hat{b}, \hat{b}^\dagger)$ basis, which is itself related to the original, non-orthogonal basis of the reconstructed wavefunctions $(\hat{f}, \hat{f}^\dagger)$ through (10a)-(10b). One can easily show that we have

$$\tilde{D}_n(\boldsymbol{r}, \sigma) = \sum_k \phi_k(\boldsymbol{r}, \sigma) \big(R\tilde{\Sigma}^{-1}\tilde{D}\big)_{kn} . \tag{15}$$

At this point, we have obtained a set of genuine canonical wavefunctions $\tilde{D}_n(\boldsymbol{r}, \sigma)$ that are orthonormal and are associated with the new occupations v_n defined by (14). The relation between these canonical wavefunctions and the wavefunctions reconstructed by the AE is given by (15). Thanks to this expression, we can now apply the Haider & Gogny formulas for the norm overlap between two many-body states $|\Phi\rangle$ and $|\Psi\rangle$. We find

$$\langle \Phi | \Psi \rangle = \det\big({\Sigma^{(\Phi)}}^{-1}\big) \det\big({\Sigma^{(\Psi)}}^{-1}\big) \det\big(\tau^{\Phi\Psi}\big) \det\big(\tilde{Z}^{(\Phi\Psi)}\big), \tag{16}$$

where

$$\tau_{mn}^{(\Phi\Psi)} = \sum_\sigma \int \mathrm{d}^3\boldsymbol{r}\, \tilde{D}_m^{(\Phi)*}(\boldsymbol{r}, \sigma) \tilde{D}_n^{(\Psi)}(\boldsymbol{r}, \sigma), \tag{17a}$$

$$Z^{(\Phi\Psi)} = u^{(\Phi)} \big(\tau^{(\Phi\Psi)\dagger}\big)^{-1} u^{(\Psi)} + v^{(\Phi)} \tau^{(\Phi\Psi)} v^{(\Psi)}, \tag{17b}$$

$$u^{(\Phi/\Psi)} = \sqrt{1 - v^{(\Phi/\Psi)2}}. \tag{17c}$$

2 METRIC INDUCED BY AN INNER PRODUCT

We present in this section the different notions of distance associated with an inner product. We note $\langle \boldsymbol{a} | \boldsymbol{b} \rangle$ the inner product between two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$. There are many examples of inner product in nuclear physics, such as the overlap $\langle \Phi | \Psi \rangle$ between two many-body states $|\Phi\rangle$ and $|\Psi\rangle$ or the overlap between single-particle orbitals $\varphi(\boldsymbol{r}, \sigma)$ and $\phi(\boldsymbol{r}, \sigma)$ defined as

$$\langle \varphi | \phi \rangle = \sum_\sigma \int \mathrm{d}^3\boldsymbol{r}\, \varphi^*(\boldsymbol{r}, \sigma) \phi(\boldsymbol{r}, \sigma). \tag{18}$$

Let us first recall some standard mathematics notations. The norm induced by the inner product $\langle \boldsymbol{a} | \boldsymbol{b} \rangle$ is defined in the usual way as

$$\|\boldsymbol{a}\| = \sqrt{\langle \boldsymbol{a} | \boldsymbol{a} \rangle}. \tag{19}$$

We can then introduce the distance induced by the inner product as

$$d_{\mathrm{I}}(\boldsymbol{a}, \boldsymbol{b}) = \|\boldsymbol{a} - \boldsymbol{b}\|. \tag{20}$$

Note that this distance depends on the possible phase and norm of $\boldsymbol{a}$ and $\boldsymbol{b}$. However, quantum-mechanical observables do not depend on either of them. The norm-independent distance thus reads

$$d_\circ(\boldsymbol{a}, \boldsymbol{b}) = \left\| \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} - \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|} \right\|, \tag{21}$$

which can be rewritten as a function of the inner product between the two normed vectors

$$d_\circ(\boldsymbol{a},\boldsymbol{b}) = \sqrt{2}\sqrt{1-\Re\left[\left\langle \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} \,\middle|\, \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|}\right\rangle\right]} = \sqrt{2}\sqrt{1-\left|\left\langle \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} \,\middle|\, \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|}\right\rangle\right|\cos\Theta}, \tag{22}$$

where $\Theta = \arg\langle \boldsymbol{a}|\boldsymbol{b}\rangle$. Another choice for a norm-invariant distance is the Great-Circle distance, also known as orthodromic or spherical distance, that is defined as Deza and Deza (2009)

$$d_\perp(\boldsymbol{a},\boldsymbol{b}) = \arccos\left(\Re\left[\left\langle \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} \,\middle|\, \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|}\right\rangle\right]\right) = \arccos\left(\left|\left\langle \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} \,\middle|\, \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|}\right\rangle\right|\cos\Theta\right) \tag{23}$$

The orthodromic distance is defined on the manifold of unit vectors. In the case of real vector spaces, it can be interpreted as the angle between $\boldsymbol{a}$ and $\boldsymbol{b}$. Equations (22) and (23) clearly show that both distances $d_\circ$ and $d_\perp$ still depend on the phase Θ between $\boldsymbol{a}$ and $\boldsymbol{b}$. To remove this dependency, we minimize each distance $d_\circ$ and $d_\perp$ over Θ. This gives the following two norm- and phase-independent distances [2],

$$D(\boldsymbol{a},\boldsymbol{b}) = \sqrt{2}\sqrt{1-\left|\left\langle \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} \,\middle|\, \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|}\right\rangle\right|}, \tag{24a}$$

and

$$D_\perp(\boldsymbol{a},\boldsymbol{b}) = \arccos\left|\left\langle \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|} \,\middle|\, \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|}\right\rangle\right|. \tag{25a}$$

The distance $D_\perp$ is an intrinsic metric and is named the Fubini–Study metric. It is a generalization of the Bloch sphere. Table 1 presents all the distances on the 1-body Hilbert space between orbitals that we have considered in this work.

Notation	**Space**	**Invariance**		**Definition**
		Norm	**Phase**	
d_{I}	$\mathcal{H}$	No	No	(20)
$d_\circ$	Unit vectors of $\mathcal{H}$	Yes	No	(21)
$d_\perp$	Unit vectors of $\mathcal{H}$	Yes	No	(23)
D	Riemann sphere of $\mathcal{H}$	Yes	Yes	(24)
$D_\perp$	Riemann sphere of $\mathcal{H}$	Yes	Yes	(25)

Table 1. Different metrics can be defined on the set of orbitals.

All these distances are defined on the one-body Hilbert space of s.p. wavefunctions. As a result, they do not depend on the occupation probability of canonical orbitals, in contrast to the many-body state which takes the BCS form. As already mentioned in the main text, determining such a dependency exactly from (32) in Sec. 4.1.3 is not trivial and computationally demanding. Instead, we can adopt the approximation that the dependency should be proportional to some power p of the occupation number v_μ^2 associated with the current orbital,

$$d^{(p)}(\varphi,\phi) = \left(v_\mu^2\right)^p \times d(\varphi,\phi). \tag{26}$$

[2] Note that they are distances over the projective space $P(\mathcal{H})$, not over the 1-body Hilbert space $\mathcal{H}$

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