Formulas for HFB by the gradient method

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1. Basic Formulas

We mostly follow the notation of Ring and Schuck[1]. The basic definition of the Bogoliubov transformation is [1, Eq. 7.2]

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{bmatrix} U^\dagger & V^\dagger \\ V^t & U^t \end{bmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \tag{1}$$

The inverse transformation is

$$\begin{pmatrix} a \\ a^\dagger \end{pmatrix} = \begin{bmatrix} U & V^* \\ V & U^* \end{bmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \equiv \mathcal{W} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} . \tag{2}$$

Here $a^\dagger$ is a set of particle creation operators in an M-dimensional Fock space, and $b^\dagger$ is the set of HFB quasiparticle creation operators. We use the notation $\mathcal{W}$ for the $2M$-dimensional unitary matrix in Eq. 2 composed of blocks U, V and their complex conjugates.

The ordinary and anomalous density matrices ρ and κ matrices are constructed as

$$\rho = V^* V^t \tag{3}$$

$$\kappa = V^* U^t . \tag{4}$$

The density matrix ρ is obviously Hermitean, ($\rho = \rho^\dagger$). It may also be shown that κ is skew-symmetric, $\kappa = -\kappa^t$, as a consequence of the unitarity of $\mathcal{W}$.

We now come to the formulas for the physical operators. They are to be expressed in the quasiparticle basis, given their definition in the original basis. For a single particle operator $\hat{F} = F_{ij} a_i^\dagger a_j \equiv a^\dagger F a$, the quasiparticle representation is

$$F_{ij} a_i^\dagger a_j \equiv a^\dagger F a = F^{00} + \beta^\dagger F^{11} \beta + \tfrac{1}{2}(\beta^\dagger F^{20} \beta^\dagger + \beta F^{02} \beta). \tag{5}$$

Ordinary vector-matrix multiplication with the $\beta, \beta^\dagger$ vectors is implied by the ordering in Eq. (5). The formulas for the coefficients of the operators are obtained by expanding

$$a^\dagger F a = (U\beta + V^* \beta^\dagger)^\dagger F (U\beta + V^* \beta^\dagger) \tag{6}$$

and normal ordering. The results are

$$F^{00} = \mathrm{Tr}(F\rho) \tag{7}$$

TABLE I. Transformation of operator products to quasiparticle basis. Here $X = F$ is a Hermitean matrix and $X = G$ is a skew-symmetric matrix. The quasiparticle coefficients are defined in Eq. (5) and (11).

	Contraction	X^{00}	X^{11}	X^{20}
$a_i^\dagger a_j$	ρ_{ji}	$\mathrm{Tr}(F\rho)$	$U^\dagger F U - V^\dagger F^t V$	$U^\dagger F V^* - V^\dagger F^t U^*$
$a_i^\dagger a_j^\dagger$	κ_{ij}^*	$-\mathrm{Tr}(G\kappa^*)$	$2U^\dagger G V$	$2U^\dagger G U^*$
$a_i a_j$	$-\kappa_{ij}$	$\mathrm{Tr}(G^*\kappa)$	$2V^\dagger G^* U$	$2V^\dagger G^* V^*$

as in [1, Eq. (E.12)] and

$$F^{11} = U^\dagger F U - V^\dagger F^t V \tag{8}$$

as in [1, Eq. (E.13)]. For F^{20}, the transformation gives

$$F^{20} = 2U^\dagger F V^*. \tag{9}$$

However, only the skew-symmetric part of F^{20} has significance. If one demands skew-symmetry the formula becomes identical to RS Eq. (E.14),

$$F^{20} = U^\dagger F V^* - V^\dagger F^t U^*. \tag{10}$$

Assuming F is Hermitean, it follows that F^{00} is real, F^{11} is Hermitean, and $F^{02} = (F^{02})^\dagger$.

We also need to transform pair operators of the form

$$\tfrac{1}{2}(a^\dagger G a^\dagger - a G^* a) = G^{00} + \beta^\dagger G^{11}\beta + \tfrac{1}{2}(\beta^\dagger G^{20}\beta^\dagger + \beta G^{02}\beta) \tag{11}$$

where G is skew-symmetric. One obtains

$$G^{00} = -\tfrac{1}{2}\mathrm{Tr}(G\kappa^* + G^*\kappa) \tag{12}$$

$$G^{11} = U^\dagger G V - V^\dagger G^* U \tag{13}$$

and

$$G^{20} = U^\dagger G U^* - V^\dagger G^* V^*. \tag{14}$$

These formulas are identical to the corresponding terms in [1, Eq.(E.13)].

2. The Hamiltonian

Ring and Schuck consider a Hamiltonian of the form

$$\hat{H} = a^\dagger \varepsilon a + \frac{1}{4}\sum_{1234} v_{1234} a_1^\dagger a_2^\dagger a_4 a_3 \tag{15}$$

This is to be expressed in the quasiparticle basis as

$$\hat{H} = H^{00} + \beta^\dagger H^{11}\beta + \tfrac{1}{2}\beta^\dagger H^{20}\beta^\dagger + ... \tag{16}$$

To convert from one basis to the other, RS define the mean-field matrix Γ and the pairing-field matrix Δ,

$$\Gamma_{ij} = \sum_{kl} v_{ikjl}\rho_{lk} \tag{17}$$

$$\Delta_{ij} = \tfrac{1}{2}\sum_{kl} v_{ijkl}\kappa_{kl} \tag{18}$$

Note that Γ is Hermitean and Δ is skew-symmetric. The formula for H^{00} is obtained by taking all possible contractions of the operators in Eq. (15). For the interaction term, the contractions are (13)(24) − (14)(23) + (12)(43). The result is [1, Eq. (E.20)]:

$$H^{00} = \mathrm{Tr}(\varepsilon\rho + \tfrac{1}{2}\Gamma\rho - \tfrac{1}{2}\Delta\kappa^*). \tag{19}$$

The formulas for H^{11} and H^{20} are obtained by taking single contractions of the operators in the interaction. The expression for the interaction summing over the 6 possible single contractions is

$$\tfrac{1}{2}\left(-a\Delta^* a + a^\dagger\Delta a^\dagger + 2a^\dagger\Gamma a\right) \tag{20}$$

Here the first two terms come from the contractions (12) and (34). The remain 4 contractions give identical expressions that are summed to give the third term. The transformation of the remaining operators in Eq. (15) is carried out according to Table I. The final result is

$$H^{11} = h^{11} + \Delta^{11} = U^\dagger h U - V^\dagger h^t V - V^\dagger\Delta^* U + U^\dagger\Delta V \tag{21}$$

and

$$H^{20} = h^{20} + \Delta^{20} = U^\dagger h V^* - V^\dagger h^t U^* - V^\dagger\Delta V^* + U^\dagger\Delta U^* \tag{22}$$

where we have written $h = \varepsilon + \Gamma$. These expressions agree with the corresponding equations in RS (E.21 and E.22).

The basic task is to minimize H^{00} subject to constraints. The constraints are treated by adding additional fields to the Hamiltonian with Lagrange mulipliers. We use the notation H' for the Hamiltonian including all the constraining fields Q_i,

$$H' = H - \sum_i \lambda_i Q_i \tag{23}$$

We discuss below how the Lagrange multipliers λ_i are chosen. For the iterative procedure described there, we shall need transform the operators to a basis that diagonalizes $(H')^{11}$. That basis gives the quasiparticle energies,

$$E_k = (H')^{11}_{kk}. \tag{24}$$

3. Conventional Formulation: the HFB equations

For completeness, we give the conventional HFB equations here. At an HFB minimum, the first M column vectors in $\mathcal{W}$ satisfy the HFB eigenvalue equations

$$\begin{bmatrix} h' & \Delta \\ -\Delta^* & -h'^* \end{bmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k \, . \tag{25}$$

The eigenvalues E_k are all nonnegative at an HFB minumum.

4. The Gradient Method

The gradient method is based on an iterative refinement of the HFB matrices U, V (ie. $\mathcal{W}$ in Eq. (2)) using an M-dimensional skew-symmetric matrix Z to carry out the refinement. The transformation from $\mathcal{W}$ to $\mathcal{W}'$ is carried out by the matrix product

$$\mathcal{W}' = \mathcal{W}\mathcal{Z} \tag{26}$$

where $\mathcal{Z}$ is the $2M$-dimensional matrix

$$\mathcal{Z} = \begin{bmatrix} 1 & Z \\ Z^* & 1 \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & D^* \end{bmatrix} \tag{27}$$

and $D = (1 - ZZ^*)^{-1/2}$. It is easy to show that $\mathcal{Z}$ is unitary using the property $Z = -Z^t$. Since $\mathcal{W}'$ is unitary and of the form Eq. 2, it is a legal HFB transformation no matter how the skew-symmetric Z was chosen.

We will derive the minimization algorithm from a series expansion of the HFB energy in powers of Z. It is useful to have the series expansions of the single-particle expectation values as well. For real matrices U, V, Z the operator expectation values are

$$Q^{00}_{i,new} = Q^{00}_i - \mathrm{Tr}(Q^{20}_i Z) - \mathrm{Tr}(Q^{11}_i Z^2) + \ldots \tag{28}$$

The power series expansion of $(H')^{00}$ can be carried out to first order in Z using only the previously derived quantities. At second order, there are contributions from the Z^2 terms in the densities and from products of two order-Z terms. Only the first contributions are easily evaluated. Keeping only those, $(H')^{00}_{new}$ is expanded as

$$(H')^{00}_{new} \approx (H')^{00} - \mathrm{Tr}((H')^{20} Z) - \mathrm{Tr}((H')^{11} Z^2)\,. \tag{29}$$

Except for the constraints, this expression can be directly minimized by diagonalizing the quadratic form. This is carried out by appling an additional transformation

$$\mathcal{W}\text{"} = \mathcal{W}' \begin{bmatrix} U^{11} & 0 \\ 0 & U^{11} \end{bmatrix} \tag{30}$$

with U^{11} the unitary matrix that diagonalizes $(H')^{11}$. This tranformation does not affect operator expection values. The last trace in Eq. (29) then becomes

$$\mathrm{Tr}((H')^{11} Z^2) = \frac{1}{2} \sum_{kk'} (E_k + E_{k'}) Z^2_{kk'} \tag{31}$$

The resulting quadratic form can be minimized by setting $Z_{kk'}$ to

$$Z_{kk'} = \frac{(H')^{20}_{kk'}}{E_k + E_{k'}}. \tag{32}$$

Next we consider the problem of dealing with the constraints. We first define the parameters λ_i such that the tranformation Z in Eq. (32) leaves the expectation values of the fields unchanged. This is achieved to first order in Z by demanding that $\mathrm{Tr}(Q_i^{20} Z) = 0$ for each constraining field Q_i. This gives the following equations to be solved for λ_i:

$$\sum_{k,k'} \frac{H^{20}_{kk'} (Q^{20}_j)_{kk'}}{E_k + E_{k'}} - \sum_i \lambda_i \sum_{kk'} \frac{(Q^{20}_i)_{kk'} (Q^{20}_j)_{kk'}}{E_k + E_{k'}} = 0. \tag{33}$$

However, we also want to correct the error in the expectation values in the same step of the iteration. Call δq the deviation of the target value of the observable q^0 and the current value Q^{00}_i,

$$\delta q_i = Q^{00}_i - q^0_i. \tag{34}$$

Keeping only the first-order term in Eq. (29), the new expectation values will match the target values if we apply a transformation Z_c satisfying

$$\mathrm{Tr}(Q_i^{20} Z_c) = -\delta q_i\,. \tag{35}$$

Guided by Eq. (32), we take Z_c to be of the form

$$Z_{c,kk'} = \sum_i c_i \frac{Q^{20}_{i,kk'}}{E_k + E_{k'}}. \tag{36}$$

The cofficients c_i are found by solving the linear equations,

$$\sum_i c_i \sum_{kk'} \frac{(Q_i^{20})_{kk'}(Q_j^{20})_{kk'}}{E_k + E_{k'}} = -\delta q_j. \tag{37}$$

The iteration is then performed with the transformation Z_{it} given by

$$Z_{it} = Z_c + Z. \tag{38}$$

This algorithm is used [2] in the code `axialG2` [3], with some modifications to stabilize the iteration when the starting transformation is far from the minimum. In particular, the Z matrix is scaled by a factor η which is less than one, but can approach one when the HFB state is close to convergence.

5. Odd particle number

A variational energy can also be calculated for systems with odd particle numbers using the gradient method. We assume the wave function of the odd system can be expressed as a one-quasiparticle excitation of an HFB state of even particle number,

$$|k\rangle = b_k^\dagger |HFB\rangle \tag{39}$$

Here k labels the quasiparticle index. The expectation value of the Hamiltonian is given by

$$\langle k|H|k\rangle = H^{00} + H^{11}_{kk}. \tag{40}$$

As before, the gradient method is derived by applying a Z tranformation and expanding the energy in powers of Z. The expansion for the first term was given in Sect. 4 as Eq. (30). The expansion of the second term, H^{11}_{kk}, is more complicated. Eq. (21) defining H^{11} depends on the U, V matrices explicitly and also implicitly through h and Δ. Assuming that all quantities are real, the complete formula can be written

$$H^{11}_{kk}(\text{new}) = H^{11}_{kk}(\text{old}) - 2\left(H^{20}Z\right)_{kk} - \text{Tr}\left[(\delta_k\Gamma)^{20}Z\right] - \text{Tr}\left[(\delta_k\Delta)^{20}Z\right]. \tag{41}$$

The fields $\delta_k\rho$ and $\delta_k\Delta$ are obtained from quasiparticle densities defined by

$$(\delta_k\rho)_{ij} = U_{ik}U^\dagger_{kj} - V_{ik}V^\dagger_{kj} \tag{42}$$

$$(\delta_k\kappa)_{ij} = V_{ik}U^\dagger_{kj} - U_{ik}V^\dagger_{kj}$$

using formulas analogous to Eqs. (17,18):

$$(\delta_k\Gamma)_{ij} = \sum_{lm} v_{im,jl}(\delta_k\rho)_{lm} \tag{43}$$

$$(\delta_k \Delta)_{ij} = \frac{1}{2} \sum_{lm} v_{ij,ml} (\delta_k \kappa)_{lm}.$$

Note that the evaluation of the fields in Eq. (43) is more computationally demanding than the other operations required to calculate the gradient. This may be mitigated by a block structure of the U, V matrices; only one block will be active for a given quasiparticle.

[1] P. Ring and P. Schuck, "The Nuclear Many-Body Problem", (Springer, 1980).

[2] M. Warda, J.L. Egido, L.M. Robledo, and K. Pomorski, Phys. Rev. C **66** 014310 (2002).

[3] L.M. Robledo, unpublished.