Notes on HFB for systems with odd particle number

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I. INTRODUCTION

This is a pedagogical note explaining how the HFB formalism works for systems with an odd number of particles. I start with the basic properties of the HFB matrix. This is just a reminder; I assume that everybody knows these already. The HFB matrix has form

$$\begin{bmatrix} H & \Delta \\ -\Delta^* & -H \end{bmatrix} \tag{1}$$

The submatrices H and Δ are Hermitian and antisymmetric respectively, making the HFB matrix Hermitian. A elementary consequence of the structure (1) is that all eigenvalues come in pairs $\pm E$. The matrix can be transformed to a canonical basis. In that basis the matrix is block-diagonal in blocks of 4×4 matrices. They have the form

$$\begin{bmatrix} h_1 & 0 & 0 & \Delta_{12} \\ 0 & h_2 & -\Delta_{12} & 0 \\ 0 & -\Delta_{12}^* & -h_1 & 0 \\ \Delta_{12}^* & 0 & 0 & -h_2 \end{bmatrix} \tag{2}$$

Here h_1, h_2 are real numbers and Δ_{12} is a complex number. These block can be split into the subblocks A and B as

$$\begin{aligned} \mathrm{A}: \quad & \begin{bmatrix} h_1 & \Delta_{12} \\ \Delta_{12}^* & -h_2 \end{bmatrix} \\ \mathrm{B}: \quad & \begin{bmatrix} h_2 & -\Delta_{12} \\ -\Delta_{12}^* & -h_1 \end{bmatrix}. \end{aligned} \tag{3}$$

Most often one sees the HFB theory applied to even-particle systems that are invariant under time reversal, in which case $h_1 = h_2$. But more generally h_1 can differ from h_2 and we will see that this is necessary to construct and odd-particle HFB ground state.

I now turn to the quasiparticle representation, obtained from the eigenvectors of the HFB matrix. The eigenvectors give the coefficients of the fermion creation and annihilation operators in the definition of the quasiparticle operators. The rule is to take all of the eigenvectors that have positive eigenvalues. The usual situation is that there is one positive eigenvalue from the block A and one from block B. Let the eigenvector of block A be written (u, v). Then the quasiparticle annihilation operator associated with it is [1]

$$\alpha_A = (u a_1^\dagger + v a_2)^\dagger = v a_2^\dagger + u a_1 \tag{4}$$

The block B eigenvector is $(-u, v)$ and its quasiparticle annihilation operator is

$$\alpha_B = v a_1^\dagger - u a_2. \tag{5}$$

With the quasiparticle operators in hand, one can transform the Hamiltonian and other operators to the quasiparticle representation, and normal order the operators. Then one takes expectation values in the quasiparticle vacuum to calculate properties of the ground state.

One usually doesn't need to know what the ground state looks like in the ordinary particle representation. But it is useful to exhibit it here to see whether the wave function has an even or odd number of particles. I will work in the canonical representation and call the quasiparticle vacuum $|HFB\rangle$. The most general state in the A+B Fock space has the form

$$|wxyz\rangle = (w + x a_1^\dagger + y a_2^\dagger + z a_2^\dagger a_1^\dagger |\rangle \tag{6}$$

I shall determine the coefficients w, x, y, z by demanding that $\alpha_A |wxyz\rangle = 0$ and similarly for α_B. Carrying out the operator algebra for α_A, one finds

$$(vw - uz) a_2^\dagger |\rangle + x u a_1^\dagger a_2^\dagger |\rangle + x v |\rangle = 0 \tag{7}$$

This can only be satisfied if $x = 0$ and $(w, z) \sim (u, v)$. Carrying out the same algebra for α_B, one finds the same condition for (w, z) together with the condition $y = 0$. Apart from an overall factor, the conditions can only be satisfied by

$$(u + v a_2^\dagger a_1^\dagger)|\rangle \tag{8}$$

which therefore must be the quasiparticle vacuum state $|HFB\rangle$.

A time-odd field that splits the degeneracy between h_1 and h_2 can change the situation completely. For definiteness, let us write the new values as $h_{1,2} = \bar{h} \pm \delta h$ The eigenvalues of the A matrix are

$$\pm\sqrt{\bar{h}^2 + \Delta_{12}^2} + \delta h \tag{9}$$

and those of the B matrix are

$$\pm\sqrt{\bar{h}^2 + \Delta_{12}^2} - \delta h. \tag{10}$$

The δh has no effect on the eigenvalues: it just shifts the eigenenergies of each submatrix up or down. Now imagine starting from the time-even system and gradually increasing δh. At first nothing happens, because the eigenvectors are the same. But at some point both eigenvalues of the A matrix become positive (and those of the B matrix both negative). This switches the second quasiparticle operator from the B matrix eigenvector to the second eigenvector of the A matrix; I will call it α'_A. It is given by the orthogonal linear combination of $a_1^\dagger$ and $a_2^\dagger$, namely

$$\alpha'_A = -u a_2^\dagger + v a_1. \tag{11}$$

For the α'_A operator to annihilate the state $|wxz\rangle$, the conditions are $x = 0$ (again) and $(w, z) \sim (-v, u)$. The last is incompatible with the condition on (w, z) from α_A. Then the only possibility for the quasiparticle vacuum is, up to a factor,

$$|HFB\rangle = a_2^\dagger|\rangle. \tag{12}$$

We thus end up with an odd number of particles in our vacuum.

Summarizing what we have learned: the HFB procedure has the capability to produce an odd-particle system as the ground state. It is easy to recognize when this happens in the canonical representation. We only require that both eigenvectors of some 2×2 subblock have positive eigenvalues.

II. A DISCUSSION POINT

Can we determine when we have an odd-particle solution without going to the canonical representation to examine the HFB matrix? Of course we don't need to construct the matrix explicitly. It would be enough to have t-odd operators such as $a_1^\dagger a_1 - a_2^\dagger a_2$ at our disposal. Its expectation value is ± 1 in an odd-particle HFB vacuum and is zero in the normal vacuum. More generally, we would like some operator that behaves this way but is more independent of the representation. If j_z is conserved, the operator $j_z/|j_z|$ would serve the purpose.

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[1] P. Ring, P. Schuck, The Nuclear Many-Body Problem, Springer-Verlag, New York (1980) eq. 7.2.