Conservation of Particle Number in the BCS theory

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One of the drawbacks of the Bardeen Cooper and Schriffer (BCS) theory is that the ground state of the system is not eigenstate of the particle number operator. The conservation of the particle number is forced as constraint in the variational procedure as expectation value on the system ground state. This may be a good approximation for infinite systems, such as superconductor metals, but it is unsatisfactory when the system is composed by a relatively low number of fermions such as medium-light nuclei. A possible solution of the problem can be obtained by using the so-called *projection's techniques* [1].

The BCS ground state can be written as

$$
\begin{aligned}
|BCS\rangle &= \prod_{k>0}^{\infty} \left(u_k + v_k a_k^+ a_{-k}^+\right) |-\rangle \\
&= \left(u_1 + v_1 a_1^+ a_{-1}^+\right)\left(u_2 + v_2 a_2^+ a_{-2}^+\right) \ldots |-\rangle \\
&= \prod_{k>0}^{\infty} u_k \Bigg\{ 1 + \sum_{k>0} \frac{v_k}{u_k} a_k^+ a_{-k}^+ + \\
&\quad + \frac{1}{2} \sum_{kk'} \frac{v_k v_{k'}}{u_k u_{k'}} a_k^+ a_{-k}^+ a_{k'}^+ a_{-k'}^+ \ldots \Bigg\} |-\rangle \ , \qquad (1)
\end{aligned}
$$

where the combined action of the creation and annihilation operators $a_k^+ a_{-k}^+$ creates a pair of particles, characterized by zero angular momentum. In the above equation, we have indicated with u_k and v_k the variational parameters, normalized as

$$|u_k|^2 + |v_k|^2 = 1 \ . \qquad (2)$$

From this normalization one can attribute the physical interpretation that $|u_{\rm k}|^2$ represent the probability that the single particle level characterized by k is occupied, and $|v_{\rm k}|^2$ the probability that it is not occupied.

The idea of the projection is to select from the wave function (1), the components that preserve the correct number of particles. An expression of the projection operator is

$$\hat{P}^A = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \; exp \left[i\varphi \frac{\left(\hat{N} - A\right)}{2} \right] \qquad (3)$$

where we have indicated with $\hat{N}$ number operator and A is the total number of nucleons. When applied to the BCS ground state (1) the components with correct number of nucleons produce a zero to the exponent of the integrating function in Eq. (3), and in this case the integral has value 1. In case of exponent different from zero the periodicity of the integrated function produces a value of the integral equal to zero.

The expression (3) of the projection operator is difficult to use in actual calculations. For this purpose it is more convenient to express the projection operator in terms of integration in the complex plane [2]:

$$\hat{P}^A = \frac{1}{2\pi\imath} \oint dz \quad z^{-(n_0-1)} \ , \qquad (4)$$

where $n_0 = A/2$ is number of the fermion pairs in the system.

The above integral can be expressed in terms of special integrals of the residues defined as [3]:

$$
\begin{aligned}
R_n^m(k_1, k_2, ..., k_m) = \frac{1}{2\pi i} \oint dz \, z^{-(n_o - n) - 1} \\
\prod_{k \neq k_1, k_2, ..., k_m} \left(u_k^2 + z\, v_k^2\right) \ . \qquad (5)
\end{aligned}
$$

The ground state of the system having the correct number of nucleons can be expressed in terms of the BCS ground state as:

$$
\begin{aligned}
\hat{P}^A |BCS\rangle = \frac{1}{2\pi\imath} \oint dz \; z^{-(n_0-1)} \\
\prod_k \left(u_k + v_k\, a_k^+ \, a_{-k}^+\right) \ . \qquad (6)
\end{aligned}
$$

The energy of the system is obtained as expectation value of the Hamiltonian H

$$
\begin{aligned}
H &= \sum_{k_1 k_2} t_{k_1 k_2} a_{k_1}^+ a_{k_2} \\
&+ \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} \bar{v}_{k_1 k_2 k_3 k_4} a_{k_1}^+ a_{k_2}^+ a_{k_4} a_{k_3} \ , \qquad (7)
\end{aligned}
$$

on the number projected BCS state:

$$
\begin{aligned}
E^P &= \frac{\langle BCS|\hat{P}^+ H \hat{P}|BCS\rangle}{\langle BCS|\hat{P}^+ \hat{P}|BCS\rangle} \\
&= \frac{1}{R_0^0} \Bigg\{ \sum_k \; \varepsilon_k \; v_k^2 \;\; R_1^1(k) \qquad (8)
\end{aligned}
$$

$$+ \quad \frac{1}{2} \sum_{kk'} \bar{v}_{kk'\,kk'} \; v_k^2 \, v_{k'}^2 \, R_2^2(k,k^{'})$$

$$\left. + \quad \sum_{kk'>0} \bar{v}_{k-kk'-k'} \, u_k v_k u_{k'} v_{k'} \, R_1^2(k,k^{'}) \right\} \; , \quad (9)$$

where we used the R_n^m integrals defined in Eq. (5).

The values of the $u_{\rm k}$ and $v_{\rm k}$ parameters, linked by the normalization condition (2), are obtained by using the variational principle

$$\frac{\partial E^P}{\partial v_k} = \frac{\partial}{\partial v_k} \frac{\langle BCS|\hat{P}^+ H \hat{P}|BCS\rangle}{\langle BCS|\hat{P}^+ \hat{P}|BCS\rangle} = 0 \; . \qquad (10)$$

Developing equation (10), we obtain the following expression for the BCS equations:

$$(\tilde{\varepsilon}_k + \Gamma_k + \Lambda_k) \, u_k \, v_k + \Delta_k \left(u_k^2 - v_k^2 \right) = 0 \; . \qquad (11)$$

In this expression $\tilde{\varepsilon}_k$ represents the energy of the single particle level characterized by the quantum numbers k. The other terms, Γ_k, Λ_k and Δ_k are matrix elements of the interaction part of the hamiltonian (7). All these terms are functions of the R_n^m integrals.

The Γ_k and Δ_k are the mean-field and pairing interaction matrix elements that appear also in the expressions of the traditional BCS model. The term Λ_k has no counterpart in the traditional BCS theory, where a constant terms appears.

We have obtained the explicit expressions of Eq.(11) for spherically symmetrical systems. We are now writing a computer code to solve numerically the projected BCS equations.

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