Analytical number-projected BCS nuclear model

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(Received 1 December 1987)

Transforming both the overlap energy kernel and overlap functionals into polynomial forms, the well-known integral of the number-projected BCS theory is performed analytically. We then obtain the projected ground state BCS energy in the closed form.

Recently we reported[1] a result, in which a generalized Bardeen, Cooper, and Schriefer (BCS) neutron-proton wave function is projected in a state with definite isospin and number of particles, by transforming both energy kernel functional and overlap functional in simple polynomial forms. In that paper the complex treatment of the isospin projection obscures the simplicity of the analytic solution of the number projection. Therefore it is worth presenting the procedure used previously in a separated paper, solely about the treatment of number projection, since it can be more useful than the isospin projection. For the illustration of the importance of number projection in BCS theories, let us mention a recent paper of Grotz and Klapdor,[2] in which they used the projected BCS wave function in the well-known problem of neutrinoless beta decay.

The problem of nuclear number projection is almost as old as the BCS theory;[3] Ring and Schuck,[4] quote 16 papers that treat it. Here, we only quote those that are needed to show the achievement obtained in the present paper.

The first paper which established the problem of number projected BCS theory, in the mathematical sense, was made by Bayman[5] in the early sixties. He found the well-known Darwin-Fowler type integral, which he solved using the saddle-point approximation, but he only got the usual BCS approximation as a solution. This approach was improved later by Iwamoto and Onishi[6] for a large number of particles. Dietrich, Mang, and Pradal[7] (DMP) realized that the integrand of the already mentioned integral can be replaced by a Laurent series and the integration picks up only the components of the desired number of particles. However, in order to solve the energy kernel integral some recursion relation is needed which can be time consuming for realistic cases. Ma and Rasmussen[8] reported a different recurrence relation to overcome this difficulty. Finally, it is necessary to mention that the projection integral is also solved numerically,[9,10] in most cases associated with angular momentum projection.

In the present paper we look again at this almost 30 year old problem and exhibit a solution in which both the overlap and energy kernel are transformed into polynomials and the integrals are solved analytically without restrictions. Let us show, then, the procedure used to reach this goal.

Given u_j and v_j as the coefficients of the Bogoliubov-Valatin[11] transformation, it is shown in many places (see, for example, Ref. 4) that the ground state energy of a system of only one type of fermions in some mean field (ϵ_j) subjected to a pure pairing force (G) is given by

$$E=\frac{\frac{1}{2\pi}\int_0^{2\pi}e^{-i(N/2)\theta}h(\theta)d\theta}{\frac{1}{2\pi}\int_0^{2\pi}e^{-i(N/2)\theta}n(\theta)d\theta}\equiv\frac{I_E}{I_O}\ , \tag{1}$$

where N is the total number of active nucleons of the system. From now on we shall call I_E (I_O) the energy kernel (overlap) integral. The overlap function $n(\theta)$ is written as (see also Ref. 4)

$$n(\theta)=\prod_j(u_j^2+v_j^2e^{i\theta})^{\Omega_j}\ , \tag{2}$$

where $\Omega_j=j+\frac{1}{2}$, with j being the angular momentum of level. The integration of the above overlap function with weight $e^{-i(N/2)\theta}$, as in Eq. (1), is easily performed if we transform expression (2) into

$$n(\theta)=\sum_{l_{j_1}\cdots l_{j_m}}\left[\prod_{j=j_1}^{j_m}F_j\right]e^{il\theta}\ , \tag{3}$$

with

$$F_j=\begin{bmatrix}\Omega_j\\ l_j\end{bmatrix}(u_j^2)^{\Omega_j-l_j}(v_j^2)^{l_j}\ , \tag{4}$$

and $l=\sum l_j$, by use of repeated applications of Newton's binomial formula. Then finally, the integral of the denominator of expression (1) becomes

$$I_O=\sum_{l=N/2}\left[\prod_{j=j_1}^{j_m}F_j\right]. \tag{5}$$

The above expression (5) can also be obtained if we take $z=e^{i\theta}$ and transform the overlap integral form (1) in

$$I_O=\frac{1}{2\pi i}\oint\frac{\prod(u_j^2+zv_j^2)^{\Omega_j}}{z^{N/2+1}}dz\ , \tag{6}$$

and one solves[7] recognizing that the integrand can be replaced by a Laurent series (in the above case it is only a simple product of binomial series) and the integration just picks all the components with z^{-1}, or , in other words, all the members of the polynomial with component $l=N/2$. To solve the energy kernel integral is more problematic. DMP need some recurrence relation which make the solution a little more complicated, whereas in the present case the recurrence relation is not needed as we are going to see. In the present case, to transform the energy kernel functional into polynomial form is not as straightforward as (3) but it can be done very easily. Let us begin writing $h(\theta)$ as

$$\frac{h(\theta)}{n(\theta)}=\sum_j \frac{2\Omega_j\epsilon_j v_j^2 e^{i\theta}}{(u_j^2+v_j^2e^{i\theta}}-G\sum_j \frac{\Omega_j v_j^4 e^{2i\theta}}{(u_j^2+v_j^2e^{i\theta})^2} -G\sum_{ij'}\frac{\Omega_j\Omega_{j'}u_jv_ju_{j'}v_{j'}e^{i\theta}}{(u_j^2+v_j^2e^{i\theta})(u_{j'}^2+v_{j'}^2e^{i\theta}}\ , \tag{7}$$

adding and subtracting a term

$$G\sum[\Omega_j(\Omega_j-1)u_j^2v_j^2e^{i\theta}]/(u_j^2+v_j^2e^{i\theta})^2$$

in the above expression (7), and after some algebraic manipulation we obtain

$$\frac{h(\theta)}{n(\theta)}=\sum_j \frac{\Omega_j(2\epsilon_j-G)v_j^2e^{i\theta}}{(u_j^2+v_j^2e^{i\theta})}-G\sum_j \frac{\Omega_j(\Omega_j-1)u_j^2v_j^2e^{2i\theta}}{(u_j^2+v_j^2e^{i\theta})^2} -G\sum_{j\neq j'}\frac{\Omega_j\Omega_{j'}u_jv_ju_{j'}v_{j'}e^{i\theta}}{(u_j^2+v_j^2e^{i\theta})(u_{j'}^2+v_{j'}^2e^{i\theta})}\ . \tag{8}$$

The above expression can also be expanded, as we mentioned before, into the polynomial form with the help of Newton's binomial, since the expression $n(\theta)=\prod(u_j^2+v_j^2e^{i\theta})^{\Omega_j}$ multiplies all the three terms of (8). Some doubts may appear in the second term because it is proportional to

$$\prod_{j'\neq j}(u_{j'}^2+v_{j'}^2e^{i\theta})^{\Omega_{j'}}(u_j^2+v_j^2e^{i\theta})^{\Omega_j-2}$$

and hence cannot be replaced by a polynomial form in the case of $\Omega_j=1$ and it is necessary to have a Laurent expansion in the term $(u_j^2+v_j^2e^{i\theta})^{-1}$. However, in our approach the factor $\Omega_j(\Omega_j-1)$ gets rid of this difficulty quite obviously.

Let us now use the procedure of repeated applications of Newton's binomial formula to the kernel energy functional $h(\theta)$ in order to get a polynomial expression in gauge angle $e^{i\theta}$. For this purpose let us call the three terms of Eq. (6) as $h(\theta)=h_1(\theta)+h_2(\theta)+h_3(\theta)$ and we will present only the method to obtain $h_1(\theta)$ in polynomial form, $h_2(\theta)$ and $h_3(\theta)$ can be derived in a similar way and hence it will not be done here.

The first step is to write $h_1(\theta)$ as

$$h_1(\theta)=\prod_{j'\neq j}(u_{j'}^2+v_{j'}^2e^{i\theta})^{\Omega_{j'}} \times\sum_{jl_j}\begin{bmatrix}\Omega_j-1\\ l_j\end{bmatrix}(u_j^2)^{\Omega_j-(l_j+1)}(v_j^2e^{i\theta})^{l_j+1} \times\Omega_j(2\epsilon_j-G)\ , \tag{9}$$

here $0\le l_j\le\Omega_j-1$. Then, using the following identity of binomial coefficients:

$$\begin{bmatrix}\Omega_j-1\\ l_j\end{bmatrix}=\begin{bmatrix}\Omega_j\\ l_j+1\end{bmatrix}\frac{(l_j+1)}{\Omega_j}\ , \tag{10}$$

and redefining $l_j=l_j-1$, $h_1(\theta)$ will vary from $l_j=1$ to $l_j=\Omega_j$. Since now we have $h_1(\theta)$ proportional to l_j due to the factor which appears in the above binomial identity (10), we can shift the initial value to $l_j=0$. Rewriting the expression (9) with the help of Newton's binomial as we did in (3) and collecting everything together we have simply

$$h_1(\theta)=\sum_{l_{j_1}\cdots l_{j_m}}\left[\prod_j F_j\right]\sum_j(2\epsilon_j-G)l_je^{il\theta}\ . \tag{11}$$

It is easy to see that the above term is in polynomial form since l_j is an integer and then the sum $l=\sum l_j$ is also an integer. The same procedure can be applied easily to $h_2(\theta)$ and $h_3(\theta)$ and therefore after some trivial algebraic manipulation we get

$$h(\theta)=\sum_{l_{j_1}\cdots l_{j_m}}\left[\prod_j F_j\right]\left\{\sum_j\left[(2\epsilon_j-G)l_je^{i\theta}-G\frac{u_j^2}{v_j^2}l_j(l_j-1)\right]-G\sum_{j\neq j'}l_jl_{j'}\frac{u_ju_{j'}}{v_jv_{j'}}\right\}e^{i(l-1)\theta}\ . \tag{12}$$

Let us now discuss whether all the terms above are expansions in the polynomial form or not. We have already discussed the first term in (11) and it is not worthwhile to repeat it here. The second term, as we see, is proportional to $l_j(l_j-1)e^{i(l-1)\theta}$; it will not be a polynomial unless $l=l_{j_1}+l_{j_2}+\cdots l_{j_m}=0$, but since all l_j's ≥ 0, then $l=0$ only when all l_j's are equal to zero, and, consequently, due to the factor $l_j(l_j-1)$ this term will not exist anymore. Consequently, the different values of the sum will form a polynomial in the gauge angle $e^{i\theta}$. The same reasoning is valid for the third term, where l_j and $l_{j'}$'s cannot be zero in order to provide a finite nonzero term.

Now, with the established polynomial, we can easily get the following form for the numerator of the expression (1) after performing the integration

$$I_E=\sum_{l=N/2}\left[\prod_j F_j\right]\sum_j(2\epsilon_j-G)l_j-G\sum_{l=N/2+1}\left[\prod_j F_j\right]\left[\sum_j \frac{u_j^2}{v_j^2}l_j(l_j-1)+\sum_{j\neq j'}l_jl_{j'}\frac{u_ju_{j'}}{v_jv_{j'}}\right]. \quad (13)$$

In order to illustrate the usefulness of the formulas (5) and (13) together with (1), let us apply it to the case of the degenerate model, where one can get easily from (5) the following formula for the overlap integral:

$$I_O=\begin{bmatrix}\Omega\\ \frac{N}{2}\end{bmatrix}(u^2)^{\Omega-N/2}(v^2)^{N/2} \quad (14)$$

and for the energy kernel solution (13) we obtain

$$I_E=\begin{bmatrix}\Omega\\ \frac{N}{2}\end{bmatrix}(u^2)^{\Omega-N/2}(v^2)^{N/2}(2\epsilon-G)\frac{N}{2}-G\begin{bmatrix}\Omega\\ N/2+1\end{bmatrix}(u^2)^{\Omega-N/2-1}(v^2)^{N/2+1}\frac{u^2}{v^2}(N/2+1)\frac{N}{2} \quad (15)$$

using (1), we simply get, assuming $\epsilon=0$

$$E=-\frac{G}{4}N(2\Omega-N+2)\ , \quad (16)$$

which is the well-known exact result for the degenerate model. Then, one notices that if the number symmetry is restored in the degenerate model, no place is provided for quasiparticle interaction and the exact result is recovered.

In conclusion we would like to mention that the present approach of transforming the kernel and the overlap functions into polynomials forms, from where the integration can be performed analytically, it is not limited to the present case of pure pairing force and gauge angle. As we mentioned already it was implemented in the case of isospin projection where additionally the integration in one Euler angle is needed in the case of axial symmetry. In the case of the nonconstant matrix element in (13) the generalization is quite straightforward but with general force and angular momentum projection, some courage is needed to tackle a somewhat big and tedious algebraic manipulation, but I guess it is feasible.

The author would like to thank Professor A. Faessler and Dr. K.W. Schmid for the hospitality extended to him. This work was partially supported by Conselho Nacional de Desenvolvimentio Científico e Technológico (CNPq).

[1] M. K. Kyotoku and H. T. Chen, Phys. Rev. C **36**, 1144 (1987).
[2] K. Grotz and H. Y. Klapdor, Nucl. Phys. **A460**, 395 (1986).
[3] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[4] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer-Verlag, New York, 1980).
[5] B. F. Bayman, Nucl. Phys. **15**, 33 (1960).
[6] F. Iwamoto and N. Onishi, Prog. Theor. Phys. **37**, 682 (1967).
[7] K. Dietrich, H. J. Mang, and J. H. Pradal, Phys. Rev. **135**, B22 (1964).
[8] C. W. Ma and J. O. Rasmussen, Phys. Rev. C **16**, 1179 (1977).
[9] R. A. Sorensen, Phys. Lett. **38B**, 376 (1972).
[10] K. W. Schmid, F. Gruemmer, and A. Faessler, Phys. Rev. C **29**, 308 (1984).
[11] N. N. Bogoliubov, Nuovo Cimento **7**, 794 (1958); J. G. Valatin, *ibid.* **7**, 843 (1958).