Investigation of the Integral Equation of the Generator-Coordinate Method Applied to the Pairing Vibration*

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(Received 26 April 1973)

A method of solving the integral equation of the generator-coordinate method which makes use of the degenerate form of the overlap kernel is applied to three simple solvable problems. When a practical prescription to exclude numerical errors is used, good results are obtained for the lowest and the first excited states. Generator wave functions are presented explicitly as well as the modified generator wave functions by the broadening kernel defined by Griffin and Wheeler. The generator wave functions in the biorthogonal representation are also calculated. The generator wave function modified by using the broadening kernel rather than the original generator wave function is well behaved and seems to reflect the physical nature of the wave function. The numerical version of the Rayleigh-Ritz minimization method is discussed.

I. INTRODUCTION

The generator-coordinate method (GCM) has advantages over other methods to describe a variety of nuclear collective motion; it is not semiclassical as the cranking model but completely quantum mechanical, includes no redundant variables, and gives a visible image of the collective motion. Furthermore, no assumption of adiabaticity is necessary. The rotational states have been studied rather well by the angular momentum projection method which is a special application of the GCM. In this case the generator wave function is readily seen to be the $\mathfrak{D}$-function of the rotation group. The GCM is also applied to heavy-ion scattering, but has not yet been successfully applied to the description of collective motion of nuclei in the transitional region and fission processes which are supposed to be the most suitable cases. We believe the lack of successful application of the GCM to physically realistic and interesting problems is mainly due to the difficulty in solving the integral equation appearing in the GCM, as a result of which our knowledge of the generator wave function is very poor.

Some progress has been achieved in the case of heavy-ion scattering,[1,2] but very little research has been published on the integral equation in the case of collective motion. In the present paper we show that the integral equation can be solved to give accurate results at least in certain specific cases of the pairing vibration if a better method is used. The second purpose of the present work is to investigate numerically the nature of the solutions by using various representations. We hope this work will give an impetus and a basis for attacking more complicated problems.

The pairing vibration was treated previously in the framework of the GCM and the integral equation was solved by replacing it by an algebraic equation. This method, however, has some shortcomings. Before discussing this point, let us present the integral equation appearing in the GCM.

The trial wave function of the GCM is a linear combination of the generating wave function $\phi(x,\alpha)$, which is a many-body wave function containing dynamical variables $\{\vec{x}\}$ and depending on one or more generator coordinates α, weighted by the generator wave function $f(\alpha)$:

$$\Psi(\vec{x}) = \int \phi(\vec{x}, \alpha) f(\alpha)\, d\alpha\,. \tag{1}$$

The generator wave function is obtained by solving an integral equation derived through the variational principle

$$\int [\mathcal{H}(\alpha, \alpha') - E\mathcal{N}(\alpha, \alpha')] f(\alpha')\, d\alpha' = 0\,, \tag{2}$$

where the kernels $\mathcal{H}$ and $\mathcal{N}$ are called the energy-overlap and the overlap kernel, respectively, and given as

$$\mathcal{H}(\alpha, \alpha') = \int \phi^*(\vec{x}, \alpha)\langle \vec{x}|H|\vec{x}'\rangle \phi(\vec{x}', \alpha') d\vec{x} d\vec{x}'$$

and

$$\mathcal{N}(\alpha, \alpha') = \int \phi^*(\vec{x}, \alpha)\phi(\vec{x}, \alpha')d\vec{x}.$$

If we find the eigenfunctions of the overlap kernel

$$\int \mathcal{N}(\alpha, \alpha')g_i(\alpha')\,d\alpha' = \lambda_i g_i(\alpha), \tag{3}$$

then the generator wave functions can be expressed in terms of these eigenfunctions $g_i(\alpha)$. In the procedure used in Refs. 3 and 4, Eq. (3) is solved by replacing it approximately with an algebraic equation

$$\sum_{m=1}^{t} \mathcal{N}(\alpha_n, \alpha_m)g_i(\alpha_m) = \lambda_i g_i(\alpha_n), \text{ for } n = 1, \ldots, t. \tag{4}$$

In this procedure we get a secular equation in which the matrix elements are specified by the generator coordinates. Assume that the number of independent eigenfunctions of Eq. (3) is w. The problem of numerical accuracy is involved in two stages. The first is the approximation made from Eq. (3) to Eq. (4). At this stage better numerical accuracy is achieved by taking more points for α. The second stage is the numerical solution of Eq. (4). If the number of mesh points t is larger than w, there result $(t-w)$ redundant eigenfunctions, for which λ should be zero but in numerical calculations is not exactly zero. Besides these redundant eigenfunctions, there result other eigenfunctions which though not redundant may have very small eigenvalues and, therefore, suffer from serious numerical errors. When all of these eigenfunctions are used in the expansion of $f(\alpha)$, the lowest calculated energy often comes far below the exact lowest energy.[5] This situation has been noticed already in Ref. 4, where a relatively small number of mesh points are used to avoid the redundant and inaccurate eigenfunctions and numerical accuracy at the first stage is sacrificed to some extent. A dilemna is involved in which an effort to reach better numerical accuracy results in an increase in the relative number of unsatisfactory eigenfunctions, among which some are redundant and others though not redundant suffer from enormous numerical errors.

In this paper, we use an alternative method to solve Eq. (3), in which numerical accuracy can be much improved without introducing any redundant eigenfunctions. A brief outline of the method is given in the next section. In Sec. III the method is applied to the pairing vibration problem. The formulation developed in Sec. III is applied to three simple solvable problems in Sec. IV. The final section is devoted to a discussion and summary.

II. OUTLINE OF THE METHOD

We start by expanding the generating wave functions $\phi(\vec{x}, \alpha)$ in terms of an appropriate orthonormal set of wave functions $\varphi_k(\vec{x})$ such as the shell-model wave functions,

$$\phi(\vec{x}, \alpha) = \sum_k Z_k(\alpha)\varphi_k(\vec{x}). \tag{5}$$

The overlap kernel, then, takes the following form of a sum of separable functions:

$$\mathcal{N}(\alpha, \alpha') = \sum_k Z_k^*(\alpha)Z_k(\alpha'). \tag{6}$$

Since the expansion (5) is always possible in principle, this form is a general property of the overlap kernel. Once the kernel is written in this form, Eq. (3) is easily solved. Defining

$$\xi_{ik} \equiv \int Z_k(\alpha)g_i(\alpha)d\alpha, \tag{7}$$

the eigenfunctions $g_i(\alpha)$ are expressed as a linear combination of $Z_k^*(\alpha)$ as follows:

$$g_i(\alpha) = \frac{1}{\lambda_i}\sum_k \xi_{ik}Z_k^*(\alpha). \tag{8}$$

Substituting Eq. (8) into Eq. (7), we obtain a secular equation for the $\xi_{ik'}$

$$\sum_{k'} U_{kk'}\xi_{ik'} = \lambda_i \xi_{ik}, \tag{9}$$

where

$$U_{kk'} = \int Z_k(\alpha)Z_{k'}^*(\alpha)d\alpha. \tag{10}$$

If we normalize the eigenvectors ξ as $\sum_k |\xi_{ik}|^2 = 1$, we get orthonormal wave functions

$$\psi_i(\vec{x}) = \int \phi(\vec{x}, \alpha)g_i(\alpha)d\alpha. \tag{11}$$

The coefficients ξ_{ik} are the amplitudes of φ_k contained in the wave function ψ_i,

$$\xi_{ik} = \int \varphi_k^*(\vec{x})\psi_i(\vec{x})\,|d\vec{x}. \tag{12}$$

The eigenfunctions $g_i(\alpha)$ satisfy the following orthogonality;

$$\int g_i^*(\alpha)g_j(\alpha)d\alpha = \lambda_i^{-1}\delta_{ij} \tag{13}$$

in accordance with orthonormality of ψ_i. Let the total number of independent wave functions φ_k and nonzero eigenvalues of Eq. (9) be equal to d and d', respectively. If $d = d'$, the GCM is completely equivalent to the diagonalization of the Hamiltonian in the space spanned by φ_k. The necessary and

sufficient condition for $d = d'$ is

$$\det U \neq 0 . \tag{14}$$

The above condition is satisifed if, and only if, all of the d functions $Z_k(\alpha)$ are linearly independent of each other.

Once the eigenfunctions $g_i(\alpha)$ are obtained, the GCM integral equation is easily solved by expressing $f(\alpha)$ in terms of $g_i(\alpha)$

$$f(\alpha) = \sum C_i g_i(\alpha) . \tag{15}$$

The amplitudes C_i are solutions of the eigenvalue problem

$$\sum_{j=1}^{d'} \langle \psi_i | H | \psi_j \rangle C_j = E C_i . \tag{16}$$

III. APPLICATION TO THE PAIRING VIBRATION

The problem to be treated consists of n pairs of nucleons moving in s single-particle orbits, each of which has single-particle energy ϵ_i and pair degeneracy Ω_i, interacting with each other via a two-body force. As a two-body force, we use a simple pairing force with constant matrix elements

$$H = \sum \epsilon_i c_i^\dagger c_i - \tfrac{1}{4} G \sum_{i,j} c_i^\dagger c_{\bar{i}}^\dagger c_{\bar{j}} c_j , \tag{17}$$

where $c_i^\dagger (c_i)$ is the creation (annihilation) operator, $\bar{i}$ is defined as the time-reversed orbit of i, and G is the matrix element of the pairing force. As in Ref. 3, we will formulate this problem by using number-projected BCS wave functions $\phi^n(\vec{x}, \Delta)$ as generating wave functions

$$\Psi(\vec{x}) = \int \phi^n(\vec{x}, \Delta) f(\Delta) d\Delta , \tag{18}$$

where the $\phi^n(\vec{x}, \Delta)$ are the normalized eigenstates of nucleon number $2n$ projected from a BCS wave function

$$\phi^n(\vec{x}, \Delta) = \frac{\int_0^{2\pi} e^{-in\theta} \phi(\vec{x};\, \Delta, \theta) d\theta}{\left[2\pi \int_0^{2\pi} e^{-in\theta} \langle \phi(\vec{x};\, \Delta, 0) | \phi(\vec{x};\, \Delta, \theta) \rangle d\theta\right]^{1/2}} , \tag{19}$$

where

$$\phi(\vec{x};\, \Delta, \theta) = \prod_i [u_i(\Delta) + e^{i\theta} v_i(\Delta) c_i^\dagger c_{\bar{i}}^\dagger] |0\rangle \tag{20}$$

and the u_i and v_i factors are given by Bardeen's equation. The integral equation takes the following form:

$$\int [\mathcal{H}(\Delta, \Delta') - E_v \mathcal{N}(\Delta, \Delta')] f_v(\Delta') d\Delta' = 0 , \tag{21}$$

where

$$\begin{bmatrix} \mathcal{H}(\Delta, \Delta') \\ \mathcal{N}(\Delta, \Delta') \end{bmatrix} = \langle \phi^n(\vec{x}, \Delta) | \begin{bmatrix} H \\ 1 \end{bmatrix} | \phi^n(\vec{x}, \Delta') \rangle ,$$

the suffix v is used to denote the vth excited state, and $v = 0$ corresponds to the lowest state. First we find eigenfunctions of the overlap kernel

$$\int \mathcal{N}(\Delta, \Delta') g_i(\Delta') d\Delta' = \lambda_i g_i(\Delta) \tag{3'}$$

by means of the method of Sec. II. The expansion of $\phi^n(\vec{x}, \Delta)$ is conveniently accomplished by using shell-model wave functions $\varphi_k(\vec{x})$, where k is an abbreviation of $(k_1, \ldots, k_s)$, and k_i is the number of nucleon pairs coupled pairwise present in ith orbit. Under the conditions that $0 \leq k_i \leq \Omega_i$ and $\sum_i k_i = n$, this expression gives

$$\phi^n(\vec{x}, \Delta) = \sum_k Z_k(\Delta) \varphi_k(\vec{x}) ,$$

where

$$Z_k(\Delta) = z_k(\Delta) \Big/ \left[\sum_k z_k^2(\Delta)\right]^{1/2} \tag{22}$$

with

$$z_k(\Delta) = \prod_i \binom{\Omega_i}{k_i}^{1/2} u_i^{\Omega_i - k_i}(\Delta) v_i^{k_i}(\Delta) , \tag{23}$$

and $\binom{\Omega}{k}$ is the binomial coefficient. Equation (3') is solved in a straightforward manner by following the method of the preceding section. As seen from Eqs. (22) and (23), the $Z_k(\Delta)$ are real and the U matrix of Eq. (10) is a real symmetric matrix.

Since there exist relations between the u and v factors as pointed out by Justin, Mihailovic, and Rosina,[3]

$$\begin{aligned} p_i p_j [(\epsilon_j - \lambda) p_i - (\epsilon_i - \lambda) p_j][(\epsilon_l - \lambda) p_l - (\epsilon_k - \lambda) p_k] \\ = p_k p_l [(\epsilon_l - \lambda) p_k - (\epsilon_k - \lambda) p_l][(\epsilon_j - \lambda) p_j - (\epsilon_i - \lambda) p_i] , \end{aligned} \tag{24}$$

where

$$p_i = v_i / u_i ,$$

the condition given in Eq. (14) is not always satisfied. There are two examples in which Eq. (24) does not violate the linear independence between the Z's. One is a problem involving only two levels, each of which may have any large pair degeneracy. In this problem we have only u_1, v_1 and u_2, v_2, and the relation given in Eq. (24) turns out to be an identity. The other is a problem consisting of many doubly degenerate levels with no accidental degeneracy.

We must notice that the matrix element $U_{kk'}$ becomes infinite if the integration of Eq. (10) is performed from zero to infinity, because none of the $Z_k(\Delta)$'s tends to zero at infinity. This is easily understood if we think of the strong coupling limit ($\Delta \to \infty$) where $\phi^n(\vec{x}, \Delta)$ contains all the shell-model wave functions with appreciable amplitude. Therefore we have to terminate the integration at some value, $\Delta_{\max}$. This termination may bring about more linear dependence between the Z's. In such a case we would have to change the $\Delta_{\max}$ value. A more fundamental way to avoid this possibility would be the use of another parameter instead of Δ. For example, we could use the following parameter as a generator coordinate:

$$\bar{\Delta} = \left\langle \phi(\vec{x}, \Delta) \middle| \sum_i c_i^\dagger c_{\bar{i}}^\dagger \middle| \phi(\vec{x}, \Delta) \right\rangle = \Delta \sum_i \Omega_i / [(\epsilon_i - \lambda)^2 + \Delta^2]^{1/2},$$

when we see that $\bar{\Delta}$ is confined in the domain $[0, \sum_i \Omega_i]$ as Δ changes from 0 to ∞. It is easily seen that, if we reformulate the whole of this section by using the parameter $\bar{\Delta}$, the matrix corresponding to U remains finite without losing generality. In this paper, however, we will not use this method but follow the use of $\Delta_{\max}$ for simplicity.

We proceed now to two other representations. One of them is the biorthogonal representation[6] and the other is the one introduced by Griffin and Wheeler,[7] which we will call the GW representation.

We define a function D as follows:

$$D(\alpha, \alpha') = \sum_i g_i^*(\alpha) \lambda_i g_i(\alpha), \tag{25}$$

which becomes the Dirac δ function $\delta(\alpha - \alpha')$ if the set $\{g_i\}$ is a complete set. For any function $F(\alpha)$ that can be expanded in terms of $g_i(\alpha)$, the function D has the same property as the δ function, i.e.,

$$\int D(\alpha, \alpha') F(\alpha') d\alpha' = F(\alpha).$$

The biorthogonal wave function $\tilde{\phi}^n(\vec{x}, \Delta)$ is appropriately defined as

$$\langle \tilde{\phi}^n(\vec{x}, \Delta) | \tilde{\phi}^n(\vec{x}, \Delta') \rangle = D(\Delta, \Delta'). \tag{26}$$

Equation (26) is satisfied by the wave function

$$\tilde{\phi}^n(\vec{x}, \Delta) = \sum_i \left(\sum_k \xi_{ik} \varphi_k(\vec{x}) \right) g_i(\Delta). \tag{27}$$

The biorthogonal generator wave function is found to be

$$\tilde{f}_v(\Delta) = \sum_i C_i^v \lambda_i g_i(\Delta) \tag{28}$$

through the relation

$$|v\rangle = \int \tilde{f}_v(\Delta) \tilde{\phi}^n(\vec{x}, \Delta) d\Delta = \int f_v(\Delta) \phi^n(\vec{x}, \Delta) d\Delta. \tag{29}$$

It is easy to see that $\tilde{f}_v(\Delta)$ represents just the amplitude of $\phi^n(\vec{x}, \Delta)$ contained in the vth state

$$\langle v | \phi^n(\vec{x}, \Delta) \rangle = \tilde{f}_v(\Delta). \tag{30}$$

The transformation to the GW representation from the original one is done by the narrowing and broadening kernels. The narrowing kernel can be expressed in terms of the eigenvalues and eigenfunctions as

$$N(\eta, \Delta) = \sum_i g_i(\eta) \lambda_i^{1/2} g_i^*(\Delta) \tag{31}$$

and the broadening kernel as

$$B(\eta, \Delta) = \sum g_i(\eta) \lambda_i^{3/2} g_i^*(\Delta). \tag{32}$$

These kernels satisfy the following relation:

$$\int N(\alpha, \eta) B(\eta, \beta) d\eta = D(\alpha, \beta).$$

The original generator wave function is transformed by the broadening kernel into

$$f_v^{\mathrm{GW}}(\Delta) = \int B(\Delta, \Delta') f_v(\Delta') d\Delta' = \sum C_i^v \lambda_i^{1/2} g_i(\Delta). \tag{33}$$

This function is seen to be intermediate between $f_v(\Delta)$ and $\tilde{f}_v(\Delta)$. The associated wave function with $f_v^{\mathrm{GW}}(\Delta)$ is given by

$$\phi^{n,\mathrm{GW}}(\vec{x}, \Delta) = \int N(\Delta, \Delta') \phi^n(\vec{x}, \Delta') d\Delta' = \sum_i \lambda_i^{1/2} \left(\sum_k \xi_{ik} \varphi_k(\vec{x}) \right) g_i(\Delta). \tag{34}$$

The three representations are related to each other through the equations

$$\langle \phi^{n,\mathrm{GW}}(\vec{x}, \Delta) | \phi^n(\vec{x}, \Delta') \rangle = B(\Delta, \Delta'),$$

and

$$\langle \phi^{n,\mathrm{GW}}(\vec{x}, \Delta) | \tilde{\phi}^n(\vec{x}, \Delta') \rangle = N(\Delta, \Delta').$$

IV. NUMERICAL RESULTS

In this section the method developed in the preceding sections is applied to three solvable problems. In the first two $d = d'$, while in the last problem d' is smaller than d.

TABLE I. Overlap integrals calculated by double integration [Eq. (35)] of wave functions defined by Eq. (11) for the problem of Sec. IV A with $\Omega = 10$. Integration was performed by using parameters $d\Delta = 0.04$ MeV and $\Delta_{max} = 6$ MeV. Each wave function is specified by the eigenvalue λ_i to which the weight function $g_i(\Delta)$ belongs. It can be seen that only seven wave functions are orthonormal to each other.

λ	5.03529	0.66593	0.24799	0.04614	0.00441	0.00024	6.97×10^{-6}	9.58×10^{-8}	1.27×10^{-8}	9.78×10^{-10}	2.51×10^{-10}
5.03529	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.021	11.067	−1.142	−8.603
0.66593	0.000	1.000	0.000	0.000	0.000	0.000	−0.003	0.259	−0.008	−27.790	−93.968
0.24799	0.000	0.000	1.000	0.000	0.000	0.000	−0.002	0.090	0.019	57.466	−40.263
0.04614	0.000	0.000	0.000	1.000	0.000	0.000	−0.004	0.323	0.056	−33.234	-1.18×10^{2}
0.00441	0.000	0.000	0.000	0.000	1.000	0.000	0.016	1.140	−4.141	−24.996	-1.81×10^{2}
0.00024	0.000	0.000	0.000	0.000	0.000	1.000	−0.002	−0.043	0.082	58.982	5.11×10^{2}
6.97×10^{-6}	0.000	−0.003	−0.002	−0.004	0.016	−0.002	1.000	0.017	2.592	−57.569	-1.23×10^{2}
9.58×10^{-8}	0.021	0.259	0.090	0.323	1.140	−0.043	0.017	2.608	−1.470	36.376	-3.19×10^{2}
1.27×10^{-8}	11.067	−0.008	0.019	0.056	−4.141	0.082	2.569	−1.470	1.547×10^{2}	−36.695	3.89×10^{2}
9.78×10^{-10}	−1.142	−27.790	57.466	−33.234	−24.996	58.982	−57.569	−36.376	−36.695	1.26×10^{4}	2.50×10^{4}
2.51×10^{-10}	−8.603	−93.968	−40.263	-1.18×10^{2}	-1.81×10^{2}	5.11×10^{2}	-1.23×10^{2}	-3.19×10^{2}	3.89×10^{2}	2.50×10^{4}	4.94×10^{5}

A. Two-Level Problem with Multidegeneracy

This problem is characterized by the parameters $s = 2$, $\epsilon_1 = 0$, $\epsilon_2 = 1$ MeV, and

$$\Omega_1 = \Omega_2 = \Omega = n\,.$$

The shell-model states are specified by the number of nucleon pairs k present in the lower orbit, and the $z_k(\Delta)$ are given as

$$z_k(\Delta) = \binom{\Omega}{k} v_1^k(\Delta) u_1^{\Omega-k}(\Delta) v_2^{\Omega-k}(\Delta) u_2^k(\Delta)\,.$$

Calculations were made for $\Omega = 2, 3, 4, 10, 20$. Precisely the same results are obtained for $\Omega = 2$ and 3 as in the shell-model calculation. For $\Omega \geq 4$, however, the GCM calculation ceases to be complete. As an example, we describe the situation in detail for the case of $\Omega = 10$, for which $d = 11$. The critical value of the pairing strength, G_c, at which the energy gap of the Bardeen's equation vanishes, is 0.05 MeV. Integration was done from $\Delta = 0$ to $\Delta = 6$ MeV by Simpson's method. Various increments were tried, i.e., the integral domain was divided 10, 12, 18, 22, 50, 100, and 150 equidistant intervals. Inclusion of all the eigenfunctions coming from the diagonalization [Eq. (3′)] turned out to give very inaccurate results for any choice of $d\Delta$. This fact means that it is still difficult to resolve all the eigenfunctions of the overlap kernel numerically even with the present method, and that some of the eigenfunctions suffer from serious numerical errors. It is necessary then to identify eigenfunctions which suffer from enormous numerical errors from others which do not. For this purpose we adapt a practical prescription, which is to calculate scalar products of ψ_i by performing the double integration

$$\langle \psi_i | \psi_j \rangle = \int d\Delta \int d\Delta' g_i^*(\Delta') \langle \phi^n(\vec{x}, \Delta') | \phi^n(\vec{x}, \Delta) \rangle g_i(\Delta)\,, \tag{35}$$

which should give δ_{ij} if the $g_i(\Delta)$ are accurately obtained. We find that only 6 eigenfunctions are orthonormal to each other for 10 and 12 intervals, and 7 for 18 to 150 intervals. The calculation with 18 intervals gives essentially the same result as the one with 150 intervals. The scalar products of eigenfunctions calculated with the double integration are tabulated in Table I. This prescription turns out to give a rather clear-cut distinction. The calculated energies and wave functions are tabulated in Table II.

The generator wave functions in the original representation are illustrated in Figs. 1(a) and 1(b), and those in the biorthogonal and the GW representations are shown in Figs. 2(a) and 2(b).

TABLE II. Comparison of energies and wave functions of the exact calculation for the two-level problem with those of the present calculation of the GCM. The same parameters are used for integration as in Table I.

(a). Lowest states

G	0.0		0.03		0.06		0.09		0.12		0.15	
	Exact	GCM	Exact	GCM	Exact	GCM	Exact	GCM	Exact	GCM	Exact	GCM
$k=10$	1.0	1.000 00	0.977 88	0.977 88	0.741 82	0.741 82	0.238 67	0.238 66	0.091 05	0.091 05	0.047 59	0.047 59
9		0.000 02	0.205 76	0.205 75	0.571 76	0.571 74	0.515 68	0.515 66	0.318 68	0.318 67	0.214 41	0.214 42
8		−0.000 05	0.037 13	0.037 18	0.319 76	0.319 88	0.607 39	0.607 54	0.545 51	0.545 57	0.454 62	0.454 60
7		0.000 12	0.005 69	0.005 60	0.135 75	0.135 52	0.475 03	0.474 67	0.586 88	0.586 74	0.591 57	0.591 64
6		−0.000 21	0.000 73	0.000 85	0.044 48	0.044 72	0.264 42	0.264 84	0.433 74	0.433 91	0.519 92	0.519 82
5		0.000 25	0.000 08	−0.000 01	0.011 25	0.011 17	0.107 48	0.107 32	0.228 19	0.228 14	0.321 09	0.321 12
4		−0.000 18		0.000 01	0.008 11	0.002 04	0.031 93	0.031 69	0.086 04	0.085 90	0.140 66	0.140 72
3		−0.000 03		0.000 04	0.001 25	0.000 42	0.006 79	0.007 00	0.022 86	0.022 97	0.043 05	0.043 00
2		0.000 17		0.000 00	0.000 13	0.000 18	0.000 98	0.001 25	0.004 08	0.004 27	0.008 79	0.008 73
1		0.000 09		−0.000 01		0.000 06	0.000 09	0.000 19	0.000 44	0.000 52	0.001 08	0.001 06
0		0.000 02		0.000 00		0.000 01		0.000 02	0.000 02	0.000 03	0.000 06	0.000 06
Energy	0.0	0.000 00	−0.363 13	−0.363 13	−1.062 45	−1.062 45	−2.844 65	−2.844 64	−5.400 25	−5.400 25	−8.257 88	−8.257 88

(b). First excited states

G	0.00		0.03		0.06		0.09		0.12		0.15	
	Exact	GCM	Exact	GCM	Exact	GCM	Exact	GCM	Exact	GCM	Exact	GCM
$k=10$		−0.000 15	−0.206 46	−0.206 48	−0.628 32	−0.628 32	0.669 00	0.669 00	0.339 43	0.339 46	0.189 88	0.189 88
9	1.0	0.999 97	0.921 02	0.921 00	0.418 05	0.418 05	0.436 58	0.436 56	0.591 38	0.591 36	0.503 63	0.503 58
8		0.002 02	0.322 35	0.322 41	0.550 65	0.550 65	−0.110 98	−0.110 84	0.340 03	0.340 32	0.506 06	0.506 36
7		−0.002 72	0.071 11	0.071 04	0.329 19	0.329 20	−0.415 16	−0.415 49	−0.177 80	−0.178 67	0.069 10	0.068 20
6		0.003 80	0.011 70	0.011 81	0.131 69	0.131 66	−0.367 36	−0.366 95	−0.452 89	−0.451 73	−0.373 25	−0.372 01
5		−0.004 26	0.001 49	0.001 33	0.038 12	0.038 16	−0.193 14	−0.193 36	−0.378 86	−0.379 34	−0.460 85	−0.461 28
4		0.002 72	0.000 15	0.000 25	0.008 11	0.008 08	−0.068 07	−0.068 18	−0.188 09	−0.188 73	−0.290 22	−0.291 31
3		0.000 66	0.000 01	0.000 06	0.001 25	0.001 24	−0.016 39	−0.016 22	−0.060 43	−0.059 84	−0.112 83	−0.112 07
2		−0.002 39		−0.000 11	0.000 13	0.000 17	−0.002 61	−0.002 48	−0.012 44	−0.011 73	−0.027 45	−0.026 17
1		−0.001 36		−0.000 07		0.000 03	−0.000 25	−0.000 21	−0.001 50	−0.001 26	−0.003 86	−0.003 33
0		−0.000 22		−0.000 01			−0.000 01	−0.000 01	−0.000 08	−0.000 05	−0.000 24	−0.000 17
Energy	2.0	2.000 63	1.038 26	1.038 26	−0.200 79	−0.200 79	−1.487 32	−1.487 34	−3.290 71	−3.290 60	−5.478 56	−5.478 48

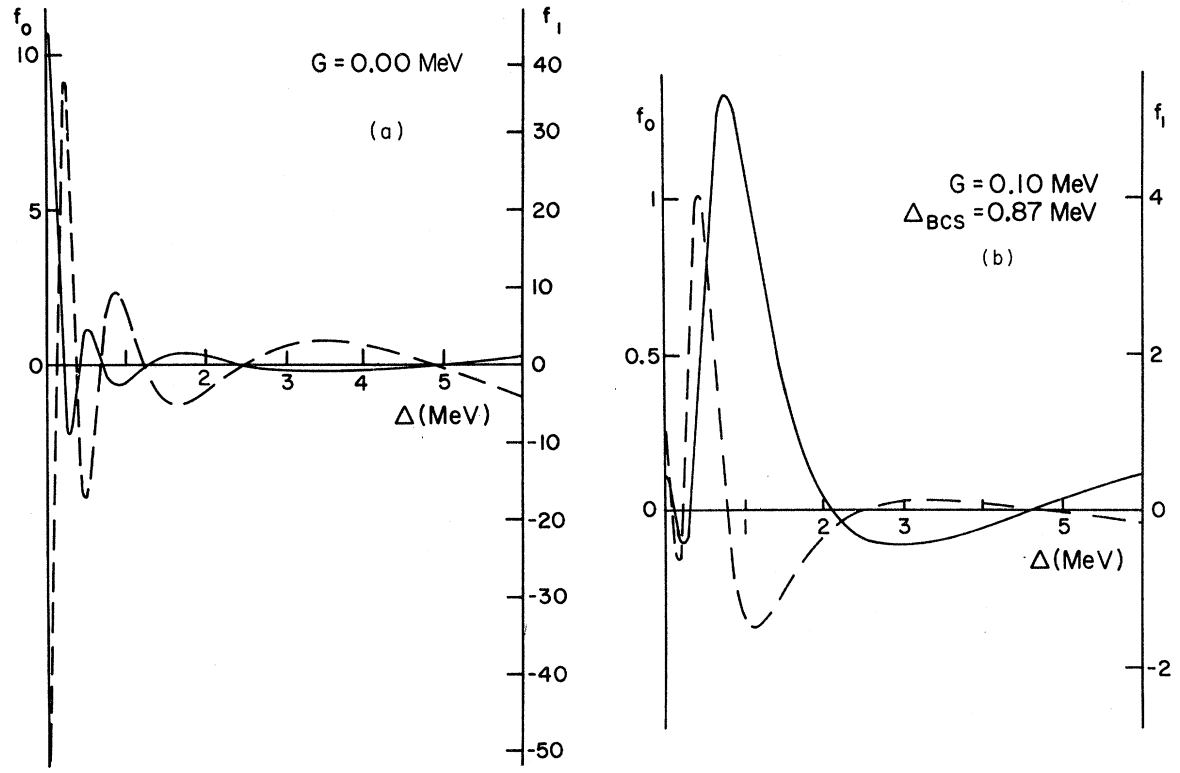

FIG. 1. Generator wave functions in the original representation for the two multidegenerate level problem. The solid and dashed curves are for the ground and first excited states, respectively.

B. Many Doubly Degenerate Levels

This problem consists of eight particles moving in eight doubly degenerate levels:

$$s=8, \quad n=4, \quad \Omega_i=1 \text{ for } i=1, \ldots, 8,$$

and

$$\epsilon_i=(-4.5+i) \text{ MeV}.$$

TABLE III. Comparison of energies of the exact calculation for many doubly degenerate levels with those of the present calculation of the GCM for the ground and the first excited states.

G	$E_{g.s.}$ (Exact)	$E_{g.s.}$ (GCM)	E_1 (Exact)	E_1 (GCM)
0.0	−16.000	−16.000	−14.000	−13.942
0.1	−16.428	−16.426	−14.424	−14.360
0.2	−16.927	−16.921	−14.895	−14.803
0.3	−17.521	−17.512	−15.410	−15.263
0.4	−18.242	−18.231	−15.956	−15.726
0.5	−19.111	−19.102	−16.519	−16.182
0.6	−20.136	−20.131	−17.091	−16.626
0.7	−21.309	−21.305	−17.674	−17.065
0.8	−22.610	−22.608	−18.275	−17.510
0.9	−24.018	−24.016	−18.903	−17.982
1.0	−25.513	−25.513	−19.565	−18.504
1.1	−27.081	−27.081	−20.263	−19.100

In this problem $d=70$ and $G_c=0.2983$ MeV. Integration was carried out with Simpson's method, varying the increments $d\Delta$, over the interval 0 to Δ_{max}: $d\Delta=0.05$, $\Delta_{max}=5$; $d\Delta=0.10$, $\Delta_{max}=10$; $d\Delta=0.12$, $\Delta_{max}=12$; $d\Delta=0.15$, $\Delta_{max}=18$.

By using the prescription described in Sec. IV A, we get seven trustworthy eigenfunctions for the last set of integration parameters, while we get only six for other sets. We used these seven eigenfunctions to solve the integral equation and tabulated the results in Table III. The generator wave functions for the lowest two states in the biorthogonal and the GW representations are shown in Fig. 3.

C. Three Levels with Equal Multidegeneracy

One of the problems in which $d=d'$ does not hold because of Eq. (25) is now treated. The parameters of the problem are as follows[1];

$$s=3, \quad n=6, \quad \Omega_1=\Omega_2=\Omega_3=6,$$

and

$$\epsilon_1=-1.5, \quad \epsilon_2=-1.2, \quad \epsilon_3=-1.0 \text{ MeV}.$$

In this problem $G_c=0.071\,45$ MeV and $d'=21$, while

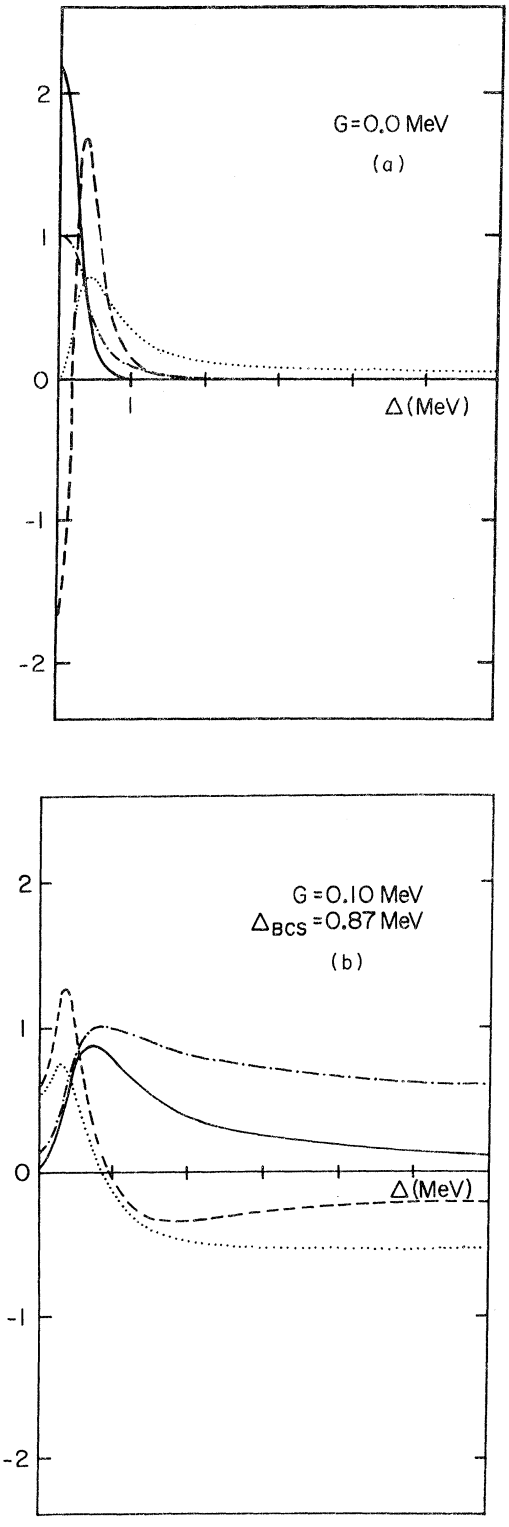

FIG. 2. Generator wave functions in the GW and biorthogonal representations for the same problem as in Fig. 1. The solid and dashed curves represent f_0^{GW} and f_1^{GW}, and the dash-dotted and dotted curves $\tilde{f}_0$ and $\tilde{f}_1$.

$d=28$. Integration was performed with Simpson's method to calculate the U matrix. Various values were tried for the increment $d\Delta$ and the interval $[0, \Delta_{max}]$: $d\Delta=0.025$, $\Delta_{max}=2.5$; $d\Delta=0.03$, $\Delta_{max}=4.5$; $d\Delta=0.04$, $\Delta_{max}=4.0$; $d\Delta=0.05$, $\Delta_{max}=2.5$, 4.0, 6.0; $d\Delta=0.10$, $\Delta_{max}=8.0$; $d\Delta=0.15$, $\Delta_{max}=18.0$; $d\Delta=0.10$, $\Delta_{max}=12.0$, 15.0. Eight trustworthy eigenfunctions of the overlap kernel are obtained for the last sets of the integration parameters and seven for other sets. The calculations were performed with these eight eigenfunctions. The calculated energies of the GCM for the lowest states agree with the exact ones up to five figures and the excitation energies of the first excited states are 10.7 to 3.5% off for $G=0.0$ to 0.10. The generator wave functions in the biorthogonal and the GW representations are illustrated in Fig. 4 for $G=0.10$

V. DISCUSSION AND SUMMARY

We have used in this paper a method to solve the integral equation which makes use of the degenerate form of the overlap kernel. The method has an advantage in that the integration over the generator coordinates is carried out very accurately. The accuracy is limited only by the accuracy of the computer and the numerical method of integration. In spite of these advantages, numerical calculations using this method show that some of the eigenfunctions of the overlap kernel suffer from serious numerical errors. This fact

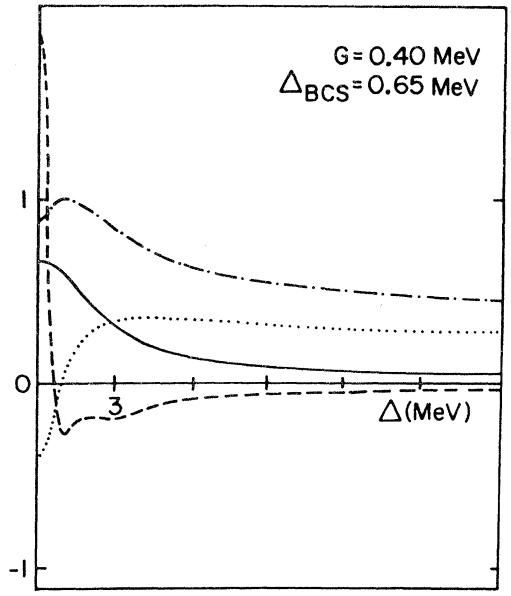

FIG. 3. The same as Figs. 2 for the eight doubly degenerate level problem.

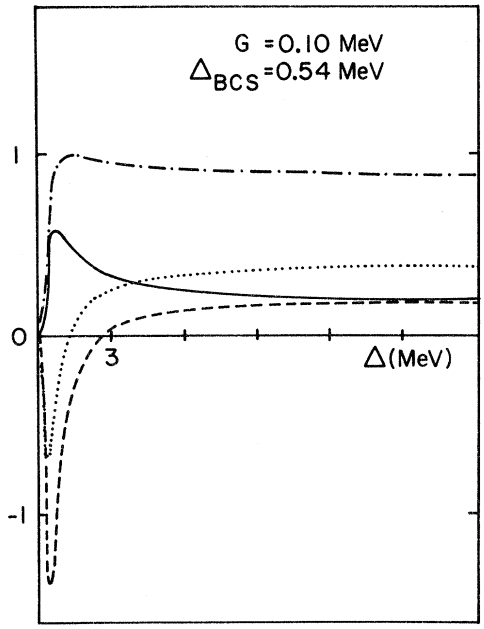

FIG. 4. The same as Fig. 2 for the three multidegenerate level problem.

means that the original generating wave function is too complicated for all the eigenfunctions to be resolved numerically. We have seen, however, that those eigenfunctions of the overlap kernel which are obtained without appreciable numerical errors span a subspace in which the lowest and the first excited states are described well from the normal to the superconducting phase for both the $d = d'$ and $d > d'$ cases. The problem is how to distinguish the accurate eigenfunctions from the inaccurate. We proposed a practical prescription in Sec. IV A which gave a rather clear criterion for the distinction. It should be noted that the prescription can be used in the conventional method mentioned in Sec. I.

We want to point out a dangerous aspect of the numerical version of the Rayleigh-Ritz minimization method. This method is described in detail in Ref. 8, and used safely to solve the Schrödinger equation of the Bohr Hamiltonian. Although this method may be conveniently used, for example, for a large dimensional shell-model calculation in which we do not need all the states solved but only a few low-lying states, it may be dangerous if used for the GCM calculation. As we have seen, there are many eigenfunctions of the overlap kernel which belong to very small eigenvalues and have large numerical errors. Those eigenfunctions should have been excluded in the calculation. If we do not exclude them as in the Rayleigh-Ritz minimization method, the resultant wave functions have many unsatisfactory components and therefore cannot be trusted. One of the reasons why Siegal and Sorensen[4] got good results by using this method may be that they utilized relatively few points for the generator coordinate to carry out the summation, so that the determinant of the overlap kernel is not vanishingly small. If we use more mesh points than the number of the independent eigenfunctions of the overlap kernel in this procedure, the resultant wave functions contain redundant components. If the number of mesh points is reduced, inaccurate calculation is inevitable for the energy-overlap kernel because it is calculated by using those rough mesh points. This is a shortcoming of this numerical method.

The problem treated in Sec. IV B has been solved by Siegal and Sorensen. They used the 2-λ method, in which λ is treated as another generator coordinate. This method results in improvement of Z_k's behavior, though the meaning of Δ becomes vague. The 2-λ method can be used to make the GCM theory mathematically equivalent to the exact shell-model theory for some of the problems to which the present one-parametric GCM theory gives d' smaller than d. An example of this kind of problem is the one treated in Sec. IV C.

The expressions have been given for the generator wave functions in the three different representations in terms of the eigenvalues and eigenvectors of the overlap kernel. All the present calculations show that the generator wave functions in the original representation oscillate rapidly. One of the reasons for this oscillation may be found in the fact that the generating wave function $\phi^n(\vec{x}, \Delta)$ changes its nature slowly with the generator coordinate, which is reflected in the wide width of the overlap kernel. Oscillation of the biorthogonal generator wave functions $\tilde{f}_v(\Delta)$ is seen to be most slow. This is because the biorthogonal wave function $\tilde{\phi}^n(\vec{x}, \Delta)$ changes its nature very rapidly with Δ. For $G > G_c$ the functions $f_0(\Delta)$ and $\tilde{f}_0(\Delta)$ have a peak around the optimum value of the generator coordinate Δ_{BCS} which is the solution of Bardeen's equation with pairing strength G. The GW representation is intermediate between these two. The functions $f_0^{GW}(\Delta)$ also have a peak around Δ_{BCS} and no node, and damp at distances far from Δ_{BCS}. The functions for the first excited states, $f_1^{GW}(\Delta)$ have a node and damp similarly as $f_0^{GW}(\Delta)$.

ACKNOWLEDGMENT

The authors express their sincere gratitude to Dr. N. Onishi for stimulating discussions. They are grateful to Professor J. J. Griffin for a reading of the manuscript.

*Work supported by the U. S. Atomic Energy Commission.
†Work supported in part by the National Science Foundation.

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