Generator Coordinate Treatment of Composite Particle Reaction and Molecule-like Structures

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We propose a generator coordinate method as a numerically tractable alternative to the resonating group method for treating the composite particle reaction and for the study of the molecular model of nuclear structure. Adopting the wave function used by Margenau and Brink in their $\alpha$ particle model as a trial function the problem of the relative motion between composite particles is discussed. We give a method of transformation of the generator function to the wave function of the relative motion, and show that the solutions of the generator coordinate method include that of the resonating group method in the interaction region. To obtain the scattering amplitude we present the formulation which uses the boundary condition constraint method. As an example our procedure is applied to the phase shift calculation of the $\alpha-\alpha$ scattering case, and good agreement with experiment is obtained showing the utility of our method. We also discuss that the idea of the density localization in the molecular model can be adequately formulated in this method, using the fact that this method has a direct connection with the concept of intrinsic deformation. Some quantitative analyses are given of the $\alpha$ particle widths of $^8\text{Be}$ by our method of generator coordinates, providing the evidence of the molecule-like structure of this nucleus.

§ 1. Introduction

Various investigations of light nuclei in recent years have confirmed that the $\alpha$-like four-body correlation plays an important role and many experimental anomalies have been interpreted from this viewpoint.\(^1\),\(^2\),\(^3\) In particular the author and others have pointed out that in the self-conjugate $4n$-nuclei there are many states which show an enhanced effect of this correlation and are adequately termed to have the molecule-like structures.\(^4\),\(^5\) It is also pointed out that the appearances of these molecule-like structures show a systematic dependence on the excitation energy.\(^6\) One of the most important ways of understanding the mechanism of these phenomena is to obtain knowledge from the viewpoint of the relative motion between clusters which compose these structures.

On the other hand the experiments using heavy ions have become more and more popular and many interesting experimental data have been accumulated.\(^5\) Actually most of the states which we consider have the molecule-like structures are found as the resonances of the heavy ion reactions. In this region of scattering problem it is also urged to obtain a method to treat the relative motion between complex nuclei, and many attempts have been made for this purpose.\(^5\),\(^6\),\(^12\)

Microscopic theory to treat these phenomena, which uses the many-body Hamiltonian and takes into account the Pauli principle correctly, has been de-
The most crucial defect of this method is the increasing difficulty of calculation with the mass number, and beyond the $\alpha$-$\alpha$ system it is almost hopeless to treat by this method.

In this paper we show that the generator coordinate method can be applied as a powerful alternative to the resonating group method because it greatly reduces the computational difficulties. As a trial wave function we adopt the wave function used by Margenau and Brink\(^7\) in their $\alpha$ particle model calculations. We first investigate the structure of the wave function of the generator coordinate method and give the transformation formula of the weight function to the wave function of the relative motion. Thus the various quantities such as the effective potential between two clusters are easily obtained. Using this transformation formula we can prove that the solutions of the generator coordinate method include those of the resonating group method in the interaction region. We then consider the scattering problem between composite nuclei. The main point of our method is to use the generator coordinate wave function in the internal region, and in order to obtain the scattering amplitude we adopt the boundary condition constraints method developed by Tobocman and others.\(^8,9\) To test the utility of our method, application to the $\alpha$-$\alpha$ scattering case is made and it is shown that the calculated phase shifts fit fairly well with experiment. Finally, discussions of our method of generator coordinates are given from the viewpoint of the density localization which is the important idea of the molecular model. As a quantitative illustration of our discussions we give some analyses of the $\alpha$ particle widths of $^8\text{Be}$, providing a strong evidence of the molecule-like structure of this nucleus.

In § 2 we formulate in the case of two $^{16}\text{O}$ system the transformation of the generator function to the relative wave function. Then in § 3 we prove that the relative wave function obtained from the generator function satisfies the same equation as the resonating group method in the interaction region. In § 4 the boundary condition constraint method is adopted to treat the scattering problem and the application of our method is made in § 5 to the phase shift calculation of $\alpha$-$\alpha$ scattering. Finally in § 6 we discuss some distinctive features of our method from the viewpoint of the molecular model.

§ 2. Structure of the generator coordinate wave function

To explain our method of generator coordinates we treat the system of two $^{16}\text{O}$ nuclei as an example. As a trial wave function we construct a single Slater determinant

$$\phi(R) = \mathcal{A} \left\{ \phi \left( \frac{R}{2} ; r_1, \ldots, r_{16} \right) \phi \left( -\frac{R}{2} ; r_{17}, \ldots, r_{32} \right) \right\}, \quad (1)$$

where $\phi \left( \frac{R}{2} ; r_1, \ldots, r_{16} \right)$ and $\phi \left( -\frac{R}{2} ; r_{17}, \ldots, r_{32} \right)$ are the closed shell wave functions of two $^{16}\text{O}$ nuclei which have the mean positions of the centers of mass, $R/2$.
and $-R/2$, respectively, and $\mathcal{A}$ is the antisymmetrization operator. This kind of wave function was introduced by Margenau\cite{margenau1940} for the study of $^8\text{Be}$ and was developed by Bloch and Brink in their $\alpha$ particle model calculations.\cite{bloch1950} An approximate eigenfunction is generated by taking the linear combination of these determinants:

$$\psi = \int f(R) \phi(R) dR.$$  \hfill (2)

The weight function is determined by the Hill-Wheeler integral equation\cite{hill1953}

$$\langle \phi(R) | H | \phi(R) \rangle f(R) dR = E \langle \phi(R') | \phi(R) \rangle f(R) dR.$$  \hfill (3)

As is well known, energy and overlap kernels are easily calculated.

Now we suppose that we have obtained the function $f(R)$. Then we want to obtain the relative wave function of two $^{16}\text{O}$ nuclei from this $f(R)$. For this purpose we use the fact that the harmonic oscillator shell model functions $\phi(R/2; r_1, \ldots, r_{16})$ and $\phi(-R/2; r_{17}, \ldots, r_{32})$ can be written as\cite{jablonski1967}

$$\phi\left(\frac{R}{2}; r_1, \ldots, r_{16}\right) = e^{-\frac{16\nu(R_1+\cdots+R_{16})}{2}} \phi(16\text{O}_1),$$

$$\phi\left(-\frac{R}{2}; r_{17}, \ldots, r_{32}\right) = e^{-\frac{16\nu(R_2+\cdots+R_{32})}{2}} \phi(16\text{O}_2),$$  \hfill (4)

where $R_1 = \frac{1}{16}(r_1 + \cdots + r_{16})$, $R_2 = \frac{1}{16}(r_{17} + \cdots + r_{32})$ and $\phi(16\text{O}_1)$ and $\phi(16\text{O}_2)$ represent the internal wave function of two $^{16}\text{O}$ nuclei and $\nu$ is the oscillator constant of $^{16}\text{O}$ nucleus which is usually expressed as $M_\nu/2\hbar$. So that $\phi(R)$ takes the form

$$\phi(R) = \mathcal{A}\left\{ e^{-\frac{16\nu(R_1+R_2+\cdots+R_{16})}{2}} \phi(16\text{O}_1) \phi(16\text{O}_2) \right\}$$

$$= e^{-32\nu R_0^2} \mathcal{A}\left\{ e^{-8\nu(R_1+\cdots+R_{16})} \phi(16\text{O}_1) \phi(16\text{O}_2) \right\},$$  \hfill (5)

where $R_0 = \frac{1}{2}(R_1 + R_2)$ is the center-of-mass coordinate of the total system. Using this expression for $\phi(R)$, we can write the eigenfunction $\psi$ as

$$\psi = \int f(R) \phi(R) dR$$

$$= e^{-32\nu R_0^2} \mathcal{A}\left\{ \int f(R) e^{-8\nu(R_1+\cdots+R_{16})} dR \phi(16\text{O}_1) \phi(16\text{O}_2) \right\}.$$  \hfill (6)

From this form of $\psi$ the relative wave function of two $^{16}\text{O}$ nuclei $\chi(r)$ is obtained as

$$\chi(r) \propto \int f(R) e^{-8\nu(R_1+\cdots+R_{16})} dR.$$  \hfill (7)

This is just the desired transformation formula from $f(R)$ to $\chi(r)$. As we now possess the relative wave function $\chi(r)$ we can calculate any quantities desired. For example the effective interaction between two $^{16}\text{O}$ nuclei is given by
\[ V_{\text{eff}}(r) = E + \frac{\hbar^2}{2\mu} \frac{\nabla^2 \chi(r)}{\chi(r)}, \]  

where \( \mu \) is the reduced mass of two \(^{16}\text{O} \) nuclei. This is because the effective potential should be defined by the Schrödinger equation

\[ -\frac{\hbar^2}{2\mu} \nabla^2 \chi(r) + V_{\text{eff}}(r) \chi(r) = E \chi(r). \]  

As is well known, however, the definition of \( \chi(r) \) is not unique because of the existence of solutions \( \chi^{(i)}(r) \) to the following equation,

\[ \mathcal{H} [\chi^{(i)}(R_1 - R_2) \phi(16\text{O}_1) \phi(16\text{O}_2)] = 0. \]  

This problem is discussed in detail in an excellent review article by Tamagaki.\(^{12}\) To obtain an unambiguous answer we must use the following redundancy free wave function \( \tilde{\chi}(r) \),

\[ \tilde{\chi}(r) = \chi(r) - \sum_i \langle \chi^{(i)} | \chi \rangle \chi^{(i)}(r). \]  

§ 3. Relation between generator coordinate method and resonating group method

In order to see the relation between the generator coordinate method and the resonating group method we must know what the Hill-Wheeler equation (3) means for the relative function (7). For this purpose we rewrite (3) using (2) as

\[ \langle \phi(R') | H | \Psi \rangle = E \langle \phi(R') | \Psi \rangle. \]  

To this equation we substitute the expressions (5) and (6) and then use the definition (7), obtaining

\[ \langle e^{-\psi \{(R_1 - R_2) - R'\}} \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} | H | e^{-\psi \{(R_1 - R_2) - R'\}} \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} \rangle \]

\[ \times \chi(R_1 - R_2) \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} = E \langle e^{-\psi \{(R_1 - R_2) - R'\}} \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} | e^{-\psi \{(R_1 - R_2) - R'\}} \chi(R_1 - R_2) \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} \rangle. \]  

If we adopt as the Hamiltonian operator \( H \) the form

\[ H = \sum_{i=1}^{2} T_i - T_0 + \frac{1}{2} \sum_{i,j=1}^{2} V_{ij}, \]  

where \( T_0 \) is the kinetic energy operator of the center of mass coordinate \( R_0 \), \( H \) has no dependence on \( R_0 \) and the integrations with \( R_0 \) on both sides of (13) give the same constants. Using the fact that we can drop one of the two antisymmetrization operators on each side of (13), we obtain

\[ \langle e^{-\psi \{(R_1 - R_2) - R'\}} \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} | H | \chi(R_1 - R_2) \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} \rangle \]

\[ = E \langle e^{-\psi \{(R_1 - R_2) - R'\}} \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} | \chi(R_1 - R_2) \phi^{(16\text{O}_1) \phi^{(16\text{O}_2)}} \rangle. \]  


Multiplying both sides of this equation by $e^{\mathbf{K} \mathbf{R}'}$ and integrating with respect to $\mathbf{R}'$, we can prove the following relation,

$$
\langle e^{\mathbf{K} (\mathbf{R}_1 - \mathbf{R}_2)} \phi^{(16\text{O}_1)} \phi^{(16\text{O}_2)} | H | \mathcal{A} \{ \mathcal{A} (\mathbf{R}_1 - \mathbf{R}_2) \phi^{(16\text{O}_1)} \phi^{(16\text{O}_2)} \} \rangle = E \langle e^{\mathbf{K} (\mathbf{R}_1 - \mathbf{R}_2)} \phi^{(16\text{O}_1)} \phi^{(16\text{O}_2)} | \mathcal{A} \{ \mathcal{A} (\mathbf{R}_1 - \mathbf{R}_2) \phi^{(16\text{O}_1)} \phi^{(16\text{O}_2)} \} \rangle.
$$

(16)

This is the Fourier transform of the equation

$$
\langle \phi^{(16\text{O}_1)} \phi^{(16\text{O}_2)} | H | \mathcal{A} \{ \mathcal{A} (\mathbf{R}_1 - \mathbf{R}_2) \phi^{(16\text{O}_1)} \phi^{(16\text{O}_2)} \} \rangle = E \langle \phi^{(16\text{O}_1)} \phi^{(16\text{O}_2)} | \mathcal{A} \{ \mathcal{A} (\mathbf{R}_1 - \mathbf{R}_2) \phi^{(16\text{O}_1)} \phi^{(16\text{O}_2)} \} \rangle.
$$

(17)

Equation (17) is just the same equation as that in the resonating group method. Thus it is proved that the relative wave function $\chi(r)$ obtained from the weight function $f(\mathbf{R})$ using the transformation formula (7) satisfies the same equation as the relative wave function in the resonating group method. But it must be noted that this does not mean the whole equivalence between the generator coordinate method and the resonating group method. In the latter method there is no restriction on the functional form of $\chi(r)$ in solving Eq. (17) but in the former method we seek the solution $\chi(r)$ of (17) within the restricted functional form, that is, $\chi(r)$ has a form:

$$
\chi(r) = \int F(\mathbf{R}) e^{-s_{r-r}^2} d\mathbf{R}.
$$

(18)

It may happen that while we have a solution $\chi(r)$ in the resonating group method calculation, we have no corresponding solution in the generator coordinate method just on account of the unfortunate fact that this $\chi(r)$ cannot be written in the form of (18). As a practical prescription to remedy this situation we restrict ourselves to using the generator coordinate wave function only in the interaction region. Then we can consider that the restriction on the functional form by Eq. (18) does no harm and two methods may be regarded as equivalent in solving the internal behaviour of the relative wave function.

Now we will try in a little more detail to compare the two methods. To this end we first notice the following fact. That is, in the interaction region it is important to take into account the effect that sizes of constituent clusters are different from that in the free states of the clusters. Adopting the size parameters as the generator coordinates besides the relative distance parameters we can treat in more natural way than the resonating group method this dynamical effect especially when it means the collective mode of motion. In this sense, we may say that the solutions of the generator coordinate method cover wider range than that of the resonating group method. On the other hand, as is clear from the discussions of this section, directly applicable cases of our procedure are limited to the systems which are composed of the clusters with the same value of oscillator constant. So we need appropriate approximations case by case when we treat the systems composed of different kinds of clusters.
This is the serious shortcoming of our device compared with the resonating group method.

So far in §§ 2 and 3 we have discussed two-cluster system, but it is easy to show that we can derive the same conclusions in the systems composed of more than two clusters.

§ 4. Calculation of scattering amplitude

As is discussed in the previous section, we use the generator coordinate method in the interaction region. So, in order to obtain the scattering wave function in the whole region of configuration space, it is necessary to connect this inside wave function with the outside wave function which is entirely determined by the asymptotic boundary conditions and the energetics of the situation. This sort of problem has been studied by many authors (9,10,11) and various methods are now available. In this paper we add nothing new to this kind of problems of reaction theories, but we instead utilize this $R$-matrix type of theories in order to show that our method of generator coordinates is a promising one in describing composite particle reactions.

Usually in these theories shell model wave functions are assumed to be used in the internal region. We therefore need only to replace the shell model wave functions by our wave functions of generator coordinates. In this section we practice this replacement adopting the boundary condition constraint method by Tobocman and Nagarajan (9) and in the next section we apply the formulae here obtained to the $aa$ scattering problem.

Equation (37) of Tobocman and Nagarajan is their formula for the scattering matrix, and the information from the inside-region of configuration space is entirely contained in the Green function $G=1/(E-H)$. Now we give an explicit representation of this $G$ using the generator coordinate wave functions. We first construct the approximate eigenfunctions (19) by the Hill-Wheeler equation (20).

\[
\mathcal{W}_\lambda = \sum _\beta b_\lambda ^\beta \Phi (\beta),
\]

\[
\sum _\beta \langle \Phi (\beta') | H | \Phi (\beta) \rangle b_\lambda ^\beta = E_\lambda \sum _\beta \langle \Phi (\beta') | \Phi (\beta) \rangle b_\lambda ^\beta,
\]

where $\beta$ represents a set of generator coordinates. Instead of the integral combination like Eq. (2), here we have taken a finite linear combination of the trial wave functions for the sake of practical calculation. Then Green function is approximated as follows:

\[
G = \sum _\lambda \frac{|\mathcal{W}_\lambda \rangle \langle \mathcal{W}_\lambda |}{E - E_\lambda}
= \sum _\lambda \sum _\beta \sum _\beta' \langle \Phi (\beta') | \frac{b_\lambda ^\beta b_\lambda ^\beta}{E - E_\lambda} \langle \Phi (\beta) | \rangle
\]
where the vector \(\phi\) is defined as \(\phi(\beta)\) and the matrices \(\mathcal{H}\) and \(\mathcal{N}\) as \(\mathcal{H}_{\beta \beta'} = \langle \phi(\beta)| \mathcal{H} | \Phi(\beta') \rangle\) and \(\mathcal{N}_{\beta \beta'} = \langle \Phi(\beta)| \Phi(\beta') \rangle\). As an example we give formulae for the phase shift \(\delta\) and inside wave function \(\Psi\) in the single channel case of two spin zero particles rewriting Eqs. (37) and (30) of Tobocman and Nagarajan using the above formula (21).

\[
\delta = \tan^{-1} \frac{Z(E)F_L(ka) - kaF_L'(ka)}{kaG_L'(ka) - Z(E)G_L(ka)},
\]

\[
Z(E) = \frac{u \mathcal{G}(E)v - (2\mu/\hbar^2)a}{u \mathcal{G}(E)u},
\]

where

\[
\mathcal{G}(E) = \frac{1}{E \mathcal{N} - \mathcal{G}},
\]

\[
u_\beta = \langle \psi_L | \phi(\beta) \rangle_{r=a},
\]

\[
u_\beta = \left[ \frac{d}{dr} r \langle \psi_L | \phi(\beta) \rangle \right]_{r=a},
\]

\(\psi_L\): channel wave function with angular momentum \(L\) divided by \(r\),

\(r\): relative distance coordinate,

\(a\): channel radius,

\(\mu\): reduced mass,

\(F_L, G_L, F_L', G_L'\): regular and irregular Coulomb wave functions and their derivatives,

\(k\): wave number of relative motion.

The internal wave function is given by

\[
\Psi = \phi \mathcal{G}(E) \mathcal{d},
\]

where

\[
\mathcal{d} = Z(E)u - v.
\]

These formulae will be used in the next section.

\[\S\ 5.\ \text{Application to } \alpha-\alpha \text{ scattering}\]

In this section we deal with the \(\alpha-\alpha\) scattering problem\(^{19,14}\) to test our method described in the previous sections. Using the formulae (22) and (23),
we first calculate the phase shifts for \( L = 0, 2 \) and 4 waves in the laboratory energy range between 0\( \sim \)40 MeV. Then the relative wave functions are obtained using Eq. (24), and following the procedure of \( \S \) 2, at the laboratory energies 2 and 28.9 MeV to compare with the results of references 12). In the calculations we adopt only the relative distance parameter \( R \) as the generator coordinate and the oscillator constant \( \nu \) is fixed as the free \( \alpha \) particle value 0.287 fm\(^{-2}\). Then Eq. (19) for each partial wave takes the following form,

\[ \text{Fig. 1. Diagonal element of the energy kernel } \mathcal{K}(R,R). \]

\[ \text{Fig. 2. Non-diagonal element of the overlap kernel.} \]

\[ \text{Fig. 3. Three dimensional illustration of ratio of energy kernel to overlap kernel.} \]
Fig. 4. Energy dependence of the calculated phase shifts of $\alpha$-$\alpha$ scattering for three cases with channel radii $a=4.0$, 4.5 and 5.0 fm. The lowest eigenvalue of the Hill-Wheeler equation with $L=0$ is taken as the threshold energy. $E_{lab}$ means the laboratory energy.

Fig. 5. Redundancy free relative wave functions calculated for the channel radius $a=4.5$ fm at the laboratory energies 2.0 and 28.9 MeV. The definition of the relative wave functions of this figure and Fig. 6 is the radial part of $\tilde{z}(r)$ of Eq.(11) multiplied by $r$. Normalizations are arbitrary.

$$T_L = \sum_{E} b_{L}^{\lambda}(R) \int d \cos \theta d_{00}^{L}(\theta) e^{-i \theta_{R}} \Phi(R)$$

$$= \sum_{E} b_{L}^{\lambda}(R) \int d \cos \theta_{R} d_{00}^{L}(\theta_{R}) \Phi(R),$$

where the $z$ axis is chosen so as to connect the centers of the two $\alpha$ particles, $L_{z}$ is the $y$ component of the total orbital angular momentum operator, and $\theta_{R}$ is the polar angle of vector $R$. We note in this equation that the projection of the total angular momentum is equal to that of the angular momentum for
the relative motion, as is expected. Five trial wave functions are used in this
equation (25), the parameters \( R \) of which are 0.5, 1.5, 2.5, 3.5 and 4.5 fm. To
solve the inside behaviour of the wave function, we make use of the Volkov
interaction\(^{19}\) as the two-body force, and then the total Hamiltonian reads as
follows:

\[
H = \sum_{i=1}^{8} T_i - T_o + \frac{1}{2} \sum_{i,j=1}^{8} V_{ij} + \frac{1}{2 \cdot \tau_{ij}} \left( \frac{1 + \tau_{ij}}{2} \right) \cdot \frac{e^2}{r_{ij}},
\]

(26)

\[
V = (0.4 + 0.6P_e) (-60e^{-(r/4.80)f} + 60e^{-(r/4.81)f}).
\]

(27)

Figure 1 shows the diagonal element of the energy kernel \( \mathcal{H} \). Figures 2
and 3 give for the \( L=0 \) case some non-diagonal elements of the overlap kernel
\( \mathcal{I} \) and the ratio of the energy to the overlap kernel. Calculated phase shifts
are compared with the experimental ones in Fig. 4 for the three cases where
the channel radius \( a \) is chosen to be 4.0, 4.5 and 5.0 fm. We see from these
results that by choosing an appropriate channel radius, we can reproduce fairly
good experimental results and thus the utility of our method has been demon­
strated.

In Fig. 5 the relative wave functions for the channel radius \( a=4.5 \) fm are
shown at the laboratory energies 2.0 and 28.9 MeV. Comparing them with the
results of the resonating group method in references 12), we can see that our
wave functions exhibit almost the same inside region behaviour. Detailed com­
parison shows, however that the disagreement exists for \( L=2 \) and 4 waves of
laboratory energy 2.0 MeV at the point of the channel radius \( r=a \). The reason
why this disagreement does not affect the phase shifts lies in the fact that in
this low energy region between 0 \( \sim \) 4 MeV, the regular Coulomb functions with
\( L=2 \) and 4 are much smaller than the irregular ones and so the phase shifts
calculated by Eq. (22) are almost zero, irrespective of the values of the logarithmic
derivatives \( Z(E) \). Except this, the agreement with the resonating group method
is very good for all the energy ranges as is seen, for example, from the other
figures in Fig. 5.

Obtaining the relative wave functions we can easily calculate the effective
potentials. But we do not give them in this paper because they will be the same
as the potentials of references 12) as a result of the agreement of the wave
functions.

§ 6. Discussion from the viewpoint of density localization

As mentioned in § 3, our method leads to almost the same results as the
resonating group method and so its application to both the bound-state and scat­
tering-state problems shares the same basic philosophy with the latter. Then,
one of the main purposes of our method is to serve as an alternative which enable
us to make practical calculations based on the viewpoints of the resonating group
method especially when we treat the heavy cluster systems. However, the merit of our method should not be restricted only to the feasibility of the calculations. It lies also in obtaining the deeper understanding of the system from the structural viewpoints. We are going to discuss this point in the case of $^{16}\text{O}$ system. As is well known, the low energy scattering of $\alpha$ particle on $^{16}\text{O}$ nucleus shows the marked negative parity resonances of angular momenta 1, 3, 5 and 7, and Davis\textsuperscript{16} proposed a model of the diatomic structure of $^{16}\text{O}$ and $\alpha$ to explain these resonances, and in particular the large $\alpha$ particle widths and the rotational band-like behaviour of the resonance energies. Ikeda and the present author\textsuperscript{17} have developed this idea and have proposed a model which treats both of these resonances and the positive parity rotational band built on the ground state of $^{20}\text{Ne}$\textsuperscript{18} on the same footing. In this model we consider that there exists the adiabatically stable diatomic molecule-like intrinsic structure of $^{16}\text{O}$ and $\alpha$. Projecting from this intrinsic structure, definite parity and angular momentum, we may find two rotational bands with $K=0^+$ and $0^-$ which correspond to the positive parity ground rotational band and negative parity resonance states, re-

| Table I. Lowest eigenvalue for each $L$ calculated by the five dimensional Hill-Wheeler equation which is described in §5. Energies are in MeV. |
|---|---|---|
| Excitation Energy | Calculated | Experimental |
| $L=0$ | 0.0 | 0.0 |
| $L=2$ | 3.18 | 2.90 |
| $L=4$ | 11.0 | 11.4 |

| Binding Energy |
|---|---|
| Calculated | Experimental |
| 53.6 | 56.4 |

Fig. 6. Redundancy free relative wave functions of the eigenwave functions belonging to the lowest eigenvalues of the Hill-Wheeler equations. The definition of the relative wave function is the same as that in Fig. 5. These eigenfunctions have their maximum overlap values 0.96, 0.96 and 0.93 for $L=0$, 2 and 4 respectively with the trial wave functions projected from the single Brink determinant with $R=3.5$ fm among the adopted five values of $R$, showing the availability of the adiabatic approximation.
spectively. When we treat this model, we can, of course, work using the resonating group method, but in view of the connection with the concept of the intrinsic structure or intrinsic deformation which plays an important role in this model as mentioned above, we are naturally led to the generator coordinate method in which we construct the wave function by superposition of the intrinsic wave functions with the parameter $R$ of the relative distance between $^4$O and $\alpha$. Just the same argument holds true also in the $\alpha-\alpha$ system, where we have the large $\alpha$ particle widths and rotational series of resonance energies. Therefore we should investigate further in quantitative fashion the above mentioned character of our method in this simple and representative $\alpha-\alpha$ system using the calculations in the previous section. The eigenfunctions belonging to the lowest eigenvalues of the Hill-Wheeler equation calculated in the previous section can be considered to represent the approximate resonance states. We present the lowest eigenvalues in Table I and the relative wave functions of their eigenfunctions in Fig. 6, where we see that the calculated eigenenergies fit well with experiment. What distinguishes our method from the usual deformed model such as the SU$_3$ model or Nilsson model is as follows. Compared with other deformed model our method takes into account the $\alpha$ particle correlation and the deformation means the dumbbell like density localization. This point is the most distinctive feature of the molecular model, and in the case of this $^9$Be nucleus, this has been emphasized and explicitly shown by Ikeda$^{20}$ in his Hartree-Fock calculation and by Kubodera and Ikeda$^{21}$ in their di-spherical potential model. One of the most important experimental checks of this idea of the density localization is obtained from the information of the particle widths. In Table II we give the reduced $\alpha$ particle widths of our wave functions of Fig. 6 and they are compared with the experimental values obtained by using the single level dispersion theory of Wigner and Eisenbud$^{22}$. The definition of the dimensionless reduced width amplitude $\theta$ in Table II is given by the following equation,$^{23}$

$$\theta_L = a\sqrt{a/2} \cdot \left(\frac{8}{a}\right)^{1/2} \cdot \int \phi_a(\xi_1) \phi_a(\xi_2) Y_L(\Omega) \mathcal{F}_L(\xi_1, \xi_2, \Omega, r = a) d\xi_1 d\xi_2 d\Omega,$$  \hspace{1cm} (28)

where $\phi_a(\xi_i) \propto \exp\left[-\nu \sum_{i=1}^4 (r_i - (r_1 + r_2 + r_3 + r_4)/4)^2\right]$ is the internal wave function of the $\alpha$ particle, and $\Omega$ is the angle of the relative coordinate between the two $\alpha$ particles. The agreement of the calculated widths with experiment turns

<table>
<thead>
<tr>
<th>$L$</th>
<th>$\theta_{\text{cal}}$</th>
<th>$\theta_{\text{exp}}$</th>
<th>channel radius $a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.16</td>
<td>0.23</td>
<td>$a=5.7$ fm</td>
</tr>
<tr>
<td>2</td>
<td>0.67</td>
<td>1.0</td>
<td>$a=5.0$ fm</td>
</tr>
<tr>
<td>4</td>
<td>1.2</td>
<td>1.5</td>
<td>$a=4.5$ fm</td>
</tr>
</tbody>
</table>
Fig. 7. Channel radius dependence of the dimensionless reduced width amplitude of the \( \langle 40 \rangle \) SU\(_3\) wave function with \( L=0 \) whose \( \nu \) is 0.242 fm\(^{-2}\).

out to be good, showing the strong evidence in favour of the molecular structure for this nucleus. This agreement can be regarded as a natural consequence, considering the facts that Eq. (23) which reproduces the experimental phase shifts correctly near the resonances has almost the same form\(^8\) as the \( R \)-matrix theory, and that the lowest eigenvalues of the Hill-Wheeler equations are separated from other eigenvalues more than 20 MeV in the laboratory energy resulting in the single level form of Eq. (23) near the resonances. To ascertain our analyses, we give in Fig. 7 the channel radius dependence of the reduced width amplitude of the \( SU_3 \) wave function of which representation is \( \langle 40 \rangle \), \( L \) is 0 and \( \nu \) is 0.242 fm\(^{-2}\). This figure can also be regarded as the relative wave function of the \( \alpha \) particles when this is divided by \( \sqrt{\nu} \). We see from this figure that the reduced width amplitude of this \( SU_3 \) wave function is more than ten times smaller than the experimental one and so it is almost hopeless to remedy this discrepancy even if we rectify the well-known deficiencies of this wave function such as the Gaussian behaviour of the tail and normalization in the internal region, etc. The characteristic feature of the density localization of our wave functions can be seen explicitly from the viewpoint of the molecular orbits and the reader may refer to reference 21) where the Brink wave function is also investigated from this point. To obtain a more unambiguous conclusion, we need to perform the calculation which takes correct account of the resonance boundary condition at the channel radius, and shall report elsewhere.

From the foregoing discussions, we may say that the most suitable application of our method of the generator coordinates is to the system whose dominant feature is determined by the collective modes of motion of the constituent clusters such as rotation, vibration, volume oscillation and so on. In the heavy ion reaction case this collective feature in the reaction process has been emphasized by Morinaga\(^{20}\) in his “collective model theory of nuclear reactions”, and by Michaud and Vogt\(^{25}\) for the \(^{12}\)C-\(^{12}\)C reaction process. We can expect that our method will be useful to formulate these collective features of the heavy ion reaction.

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