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# Direct Solution of the Hill-Wheeler Equation for Alpha-Alpha Scattering*

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In the cluster model of Brink, Margenau, and Bloch, the motion of two clusters is described by an integral equation for the generator-coordinate amplitude. It is shown that a direct solution of this Hill-Wheeler equation provides a practical framework for the study of cluster-cluster scattering; however, the Coulomb potential is not yet included in the formalism. The case of $\alpha+\alpha$ scattering (with the Coulomb potential neglected) is studied in some detail and dineutron–dineutron scattering is also mentioned.

## I. INTRODUCTION

It is evidently desirable to have a theory which describes the elastic scattering of two light nuclei in terms of the nucleon-nucleon potential and with the Pauli principle properly taken into account. For a long time, the resonating-group method[1] was the only practical framework for such calculation and it has been extensively exploited.[2] However, it seems that extending this method to the scattering of clusters larger than an $\alpha$ particle is very difficult.

The generator-coordinate method of Margenau, Bloch, and Brink[3] is a more powerful theory that is not limited to small clusters. Its application to the scattering problem is very recent[4-6] and is still at a relatively primitive stage. The most effective approach to date is that of Giraud, Hocquenghem, and Lumbroso (GHL)[6] who transform the Hill-Wheeler equation for the generator-coordinate amplitude into a Schrödinger equation in momentum space for the true wave function of relative motion. Detailed calculations have been performed for dineutron scattering.[6]

In the present work, we propose an alternate formulation of the scattering problem in which the Hill-Wheeler equation of the generator-coordinate method is solved directly for the phase shifts. Only the simplest case of $\alpha$-$\alpha$ scattering is studied directly, and the Coulomb potential is neglected for the moment. The possibility of generalization to heavier clusters is indicated.

## II. FORMALISM: CLUSTER MODEL

Since the generator-coordinate method of Brink, Bloch, and Margenau has been described very clearly and in some detail in Ref. 3, we only summarize it here.

The intrinsic state $\Phi(\vec{r}_1, \ldots, \vec{r}_8; \vec{s})$ describes two $\alpha$ clusters located at $\pm\vec{s}$, respectively; and is constructed as a Slater determinant of single-particle orbitals $\phi_\pm$ centered on $\pm\vec{s}$:

$$\phi_{\pm\mu\nu}(\vec{r}) = (b^3\pi^{3/2})^{-1/2} \exp\left(-\frac{(\vec{r}\mp\vec{s})^2}{2b^2}\right)\chi_{\mu\nu},$$

where $\chi_{\mu\nu}$ is a spin-isospin state vector. The generator coordinate $\vec{s}$ determines only the mean positions of the two clusters. The basis states of good angular momentum are obtained from $\Phi(\vec{s})$ by projection

$$\Phi_l(\vec{r}_1, \ldots, \vec{r}_8; s) = \frac{2l+1}{2}\int_{-1}^{1} d\cos\beta\, P_l(\cos\beta) \times R(\beta)\Phi(\vec{r}_1, \ldots, \vec{r}_8; \vec{s}).$$

The complete wave function (including the intrinsic state of the clusters as well as their relative motion) is obtained by taking a linear combination of these basis states with all values of the cluster separation $2s$:

$$\Psi_l(\vec{r}_1, \ldots, \vec{r}_8) = \int_0^\infty f_l(s)\Phi_l(\vec{r}_1, \ldots, \vec{r}_8; s)s^2 ds\,, \tag{1}$$

where the generator-coordinate amplitude $f_l(s)$ is the solution of the Hill-Wheeler equation

$$\int_0^\infty [H_l(s', s) - EN_l(s', s)]f_l(s)s^2 ds = 0\,. \tag{2}$$

Here $H_l(s', s)$ is a matrix element of the many-body Hamiltonian taken between two states $\Phi_l(s')$ and $\Phi_l(s)$, and $N_l(s', s)$ is the overlap matrix element of the two states.

The extension of the method to heavier spherical clusters is straightforward, and only involves the introduction of $p$-shell (or higher) harmonic-oscillator orbitals about each cluster site in addition to the $s$-shell orbital $\phi_\pm$.

Using the same approach as Ref. 6, it can be shown that (apart from normalization factors)

$$\Psi_l(\vec{r}_1, \ldots, \vec{r}_8) = \psi_{\text{c.m.}}\mathcal{A}\{g_l(R)\psi_{\text{int}}\}\,, \tag{3}$$

where $g_l(R)$ is a true wave function of relative motion ($R$ is half the true cluster separation), $\psi_{\text{c.m.}}$ and $\psi_{\text{int}}$ are wave functions describing the internal motion within the clusters and the zero-point motion of the center of mass, respectively, and, finally, $\mathcal{A}$ is the antisymmetrization operator. The spurious center-of-mass motion arises, as in the shell model, because we use determinental basis states, but it does not cause any difficulties. The relationship between $g_l$ and $f_l$ is

$$g_l(R) = \int_0^\infty \Gamma_l(R, s)f_l(s)s^2 ds\,, \tag{4}$$

with

$$\Gamma_l(R, s) = i_l\left(\frac{8Rs}{b^2}\right)\exp\left(-4\frac{R^2+s^2}{b^2}\right). \tag{5}$$

In the present case, it is possible to carry out the angular momentum projections analytically. If we define

$$A_l(s', s) = 2(2l+1)\frac{1+(-)^l}{2}\exp\left(-\frac{2s^2+2s'^2}{b^2}\right),$$

then the overlap and kinetic energy functions are

$$N_l(s', s) = A_l(s', s)\left[i_l\left(\frac{4ss'}{b^2}\right) - 4i_l\left(\frac{2ss'}{b^2}\right) + 3\delta_{l,0}\right],$$

$$T_l(s', s) = \hbar\omega\left(6 - \frac{s^2+s'^2}{b^2}\right)N_l(s', s) + \frac{\hbar\omega}{2}A_l(s', s)\left[\frac{4ss'}{b^2}i_l'\left(\frac{4ss'}{b^2}\right) - \frac{8ss'}{b^2}i_l'\left(\frac{2ss'}{b^2}\right)\right],$$

where $i_l(x)$ is the regular spherical Bessel function of imaginary argument and $i_l'(x)$ is its derivative. If the nucleon-nucleon potential is central with a Gaussian shape,

$$V(\vec{r}_{12}) = V_0(W + MP_x)\exp(-r_{12}^2/a^2)\,,$$

then

$$V_l(s', s) = 2(X_D + X_E)N_l(s', s) + 4(X_D + X_E)\,(1 - e^{-s^2/\mu^2} - e^{-s'^2/\mu^2})A_l(s', s)\left[i_l\left(\frac{2ss'}{b^2}\right) - \delta_{l,0}\right]$$

$$+ A_l(s', s)e^{-(s^2+s^2)/\mu^2}\left[2X_D i_l\left(\frac{2ss'}{\sigma^2}\right) + 2X_E i_l\left(\frac{2ss'}{\tau^2}\right) + (2X_D - 4X_E)i_l\left(\frac{2ss'}{\mu^2}\right) + (2X_E - 4X_D)i_l\left(\frac{2ss'}{\nu^2}\right)\right],$$

where

$$X_D = (8W - 2M)(a/\mu)^3 V_0\,,$$
$$X_E = (8M - 2W)(a/\mu)^3 V_0\,,$$
$$\mu^2 = a^2 + 2b^2\,,$$
$$\nu^{-2} = b^{-2} - \mu^{-2}\,,$$
$$\sigma^{-2} = 2b^{-2} - \mu^{-2}\,,$$
$$\tau^{-2} = b^{-2} + \mu^{-2}\,.$$

If the two-body potential is a sum of Gaussians, then $V_l(s', s)$ is a sum of terms like the above. The Coulomb potential is omitted from this discussion, partially because we have been unable to carry out an analytic angular-momentum projection for this case. In all the calculations discussed below, the Brink and Boeker B1 potential[7] is used.

### III. FORMALISM: SCATTERING PROBLEM

In any scattering problem it is necessary to separate the coordinate space into an external region where the two clusters are moving freely, and an internal region where forces and exchange effects enter the picture. Although the Hill-Wheeler equation is an integral equation, such a separation is still possible because the kernel is strongly peaked about $s = s'$ with a spread of the order of $b$. Typically, the external region can be taken to begin at a value $s_0$ of the separation parameter which is a few times the value of $b$. The division between internal and external regions is not unambiguously sharp, but it is as clear as in the case of a Schrödinger equation with a potential that drops off exponentially with distance.

We now assert that the solution of the Hill-Wheeler scattering equation in the external region is

$$f_l(s) = j_l(ks) + B_l n_l(ks)\,, \tag{6}$$

$$E = (6 - \tfrac{3}{4})\hbar\omega + 2(X_D + X_E) + \frac{\hbar^2 k^2}{16m}\,. \tag{7}$$

The first two terms in Eq. (7) represent the internal energy of the clusters (including the center-of-mass zero-point energy), while the third term is the kinetic energy of relative motion (recall that the cluster distance is $2s$). This can be proved by substituting the above expressions into the Hill-Wheeler integral and showing that this integral vanishes for all $s'$ in the external region. Although the integrals involving $j_l(ks)$ can all be done analytically (see Appendix), we have not been able to also do this for $n_l(ks)$. We have therefore carried out the integration numerically for a range of energies and angular momenta. A typical result is shown in Fig. 1. It can be seen that the Hill-Wheeler equation is accurately satisfied by the generator-coordinate function of Eq. (6) for $s' \gtrsim 4.5$ F, which implies that Eq. (6) is accurate for $s > 3f$.

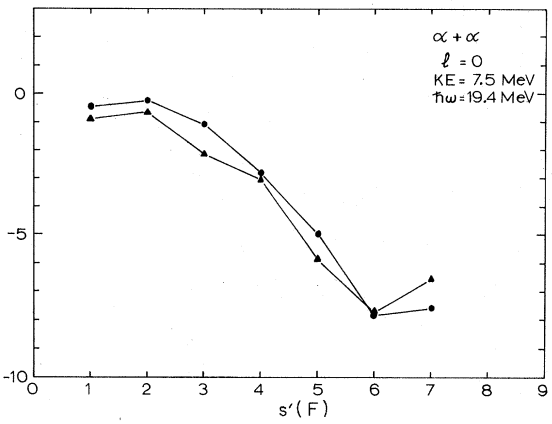


FIG. 1. The circles show the logarithm of the integral $|\int [H_l(s', s) - EN_l(s', s)] j_l(ks)\, s^2 ds|$ as a function of $s'$, for the Brink-Boeker B1 potential. A four-point Gaussian integration formula with a step size of 0.25 F is used. The triangles show the same integral but with $n_l(ks)$ replacing $j_l(ks)$. The slight rise in the curves near $s' = 7$ F is due to the nearness of the upper limit on the integral which was 11.0 F. The curves for different $l$ or different energies are very similar.

Noting that $\Gamma_l(R, S)$ is peaked about $R = s$, we can write, for $R \to \infty$, that

$$g_l(R) = \frac{b^2}{16Rk} \exp\left(\frac{4R^2}{b^2}\right) \int \exp\left(-\frac{4s^2}{b^2} + \frac{8Rs}{b^2}\right) \times [\sin(ks) + B_l \cos(ks)]\, ds$$

$$= \text{const} \times \frac{1}{kR} (\sin kR + B_l \cos kR)\,. \tag{8}$$

This immediately relates $B_l$ to the phase shift

$$B_l = \tan(\delta_l - \tfrac{1}{2} l\pi)\,.$$

The scattering equation now becomes a nonhomogeneous integral equation over a finite interval [$E$ and $k$ are related by Eq. (7)]:

$$\int_0^{s_0} [H_l(s', s) - EN_l(s', s)] f_l(s) s^2 ds = F_l(s'; E) + B_l G_l(s'; E)\,, \tag{9}$$

with

$$F_l(s'; E) = -\int_{s_0}^{\infty} [H_l(s', s) - EN_l(s', s)] j_l(ks) s^2 ds\,, \tag{10}$$

$$G_l(s'; E) = -\int_{s_0}^{\infty} [H_l(s', s) - EN_l(s', s)] n_l(ks) s^2 ds\,. \tag{11}$$

This equation is to be solved for $B_l$ and for the generator-coordinate amplitude $f_l(s)$.

### IV. METHOD OF SOLUTION

The integral equation for arbitrary $s'$ is changed into a set of algebraic equations for the values of $f_l$ over a discrete set of $N$ points $S_i$. We use a four-point Gauss-Legendre quadrature formula repeatedly applied over $\frac{1}{4}N$ intervals $\Delta S$. The $N+1$ simultaneous linear equations

$$\sum_{i=1}^{N} [H_l(s_j, s_i) - EN_l(s_j, s_i)] f_l(s_i) \omega_i s_i^2 = F_l(s_j) + B_l G_l(s_j) \quad (j = 1 \to N)$$

$$f_l(s_n) = j_l(ks_n) + B_l n_l(ks_n)$$

TABLE I. The parameter $B_0$ for $l=0$ $\alpha+\alpha$ scattering as a function of energy (c.m.). The integration parameters (see text) are ($S=0$, 2.4, 6.0, 12.0 F; $\Delta S=0.3$, 0.6, 0.3 F). The Brink-Boeker B1 potential is used, $\hbar\omega=19.4$, and the Coulomb potential is not included.

| $E$ (MeV) | $B_0$ Method 1 | $B_0$ Method 2 | $\delta_0$ |
|---|---|---|---|
| 0.5 | 1.7281 | 1.7246 | 1.046 |
| 1. | 0.7625 | 0.7615 | 0.651 |
| 2. | 0.1584 | 0.1586 | 0.157 |
| 4. | −0.5106 | −0.5102 | −0.472 |
| 6. | −1.2937 | −1.2946 | −0.913 |
| 8. | −3.1053 | −3.1090 | −1.259 |
| 10. | −42.270 | −42.016 | −1.547 |
| 12. | 4.3922 | 4.4016 | −1.794 |
| 14. | 2.1142 | 2.1159 | −2.012 |
| 16. | 1.3511 | 1.3507 | −2.207 |

are solved for the $N+1$ unknowns $f_l(s_i)$ and $B_l$. The $\omega_i$ are the weight factors associated with the quadrature formula, and $S_n$ is chosen near $S_0$. In practice it is preferable to solve for the values of $\tilde{f}_l(S_i)=[N_l(S_i,S_i)]^{1/2}f_l(S_i)$ after appropriate renormalization of $H_l$, $N_l$, $F_l$, and $G_l$ in order to avoid the strong zero of $H_l$ and $N_l$ that occurs at $s,s'\to 0$.

GHL[6] have noted that the Fourier transform of $f_l(s)$ diverges at high frequency. However, the Fourier transform of $H_l-EN_l$ converges more strongly, so that no fundamental difficulty exists provided that a high-frequency cutoff is introduced. This is done automatically by the finite step size used in the solution of Eq. (7). Nevertheless, the solution oscillates rapidly, the shortest wavelength ($\sim\frac{1}{2}\Delta S$) having the largest amplitude. Because of these oscillations, the $f_l(s_i)$ obtained using different step sizes cannot be compared; however, the phase shifts turn out to be completely stable.

TABLE II. The parameter $B_2$ for $l=2$ $\alpha+\alpha$ scattering as a function of energy (c.m.). The integration parameters are ($S=0$, 2.4, 6.0, 12.0 F; $\Delta S=0.3$, 0.6, 0.6 F). The Brink-Boeker B1 potential is used, $\hbar\omega=19.4$, and the Coulomb potential is not included.

| $E$ (MeV) | $B_2$ Method 1 | $B_2$ Method 2 | $\delta_2$ |
|---|---|---|---|
| 0.5 | 0.0158 | 0.0159 | 0.016 |
| 2.5 | 0.7624 | 0.7615 | 0.651 |
| 4.5 | 1.5453 | 1.5453 | 0.997 |
| 6.5 | 1.3134 | 1.3137 | 0.920 |
| 8.5 | 0.9661 | 0.9653 | 0.768 |
| 10.5 | 0.6968 | 0.6965 | 0.609 |
| 12.5 | 0.4904 | 0.4907 | 0.456 |
| 14.5 | 0.3239 | 0.3244 | 0.313 |

In the above method, the step size determines the accuracy of the integration and also serves as a short-wavelength cutoff. It is evidently desirable to divorce these two roles. This can be done by imposing a set of continuity conditions which relate the values of $f_l(s_i)$ at adjacent points. We have used a four-point Gaussian interpolation formula for this purpose. The $N+1$ unknowns $f_l(s_i)$ and $B_l$ are then overdetermined by the $N$ equations above and the (linear) continuity equations which can number up to $N-2$. This set of equations is solved by a linear least-squares fit.

We have used both these methods to study $\alpha+\alpha$ scattering in the energy range from 0 to 15 MeV for $l=0$ and 2 with a size parameter $\hbar\omega=19.4$ MeV and with the Brink-Boeker B1 interaction. The results are shown in Tables I and II. A typical set of points $S_i$ is obtained using a spacing $\Delta S=0.3$ F over $0\leq S\leq 2.4$ F and $\Delta S=0.6$ F over $2.4\leq S\leq 6.0$ F ($=S_0$), while the integral over the external region is done with a step size $\Delta S=0.6$ F over $6.0\leq S\leq 12.0$ F. We can abbreviate this into a more compact notation ($S=0$, 2.4, 6.0, 12.0 F; $\Delta S=0.3$, 0.6, 0.6 F). It should be mentioned again

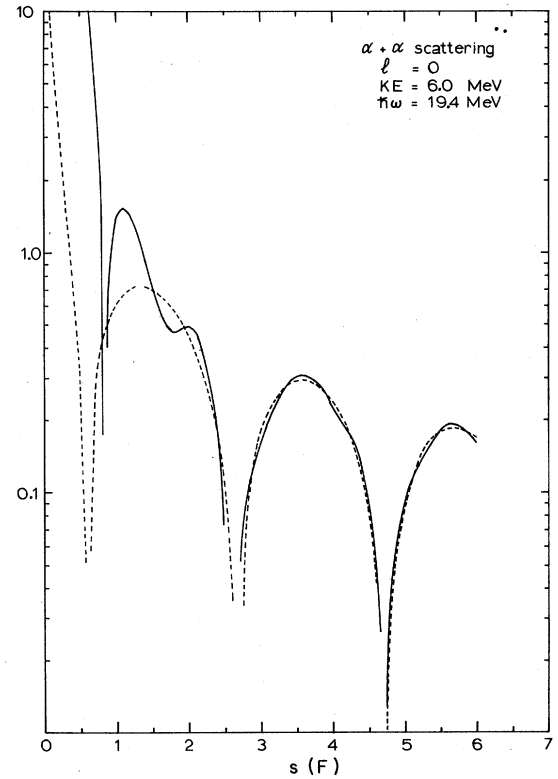


FIG. 2. The generator-coordinate amplitude $|f_0(s)|$ obtained by the second solution method (solid curve) is compared with $|j_0(ks)+B_0n_0(ks)|$ (dashed curve). The integration parameters (see text) are ($S=0$, 2.4, 6.0, 12.0 F; $\Delta S=0.3$, 0.6, 0.3 F).

that there are four points $s_i$ in each interval, their location being determined by the Gaussian integration formula.

It can be seen that the values of $B_l$ obtained by both methods and with different step sizes are all quite accurately the same, so that both methods may be said to work well. The qualitative behavior of the phase shifts is as expected, but a comparison with experiment is not meaningful, since the Coulomb potential has not been included.

Figure 2 compares the generator-coordinate amplitude $f_l(s_i)$ obtained by the second method with $j_l(ks)+B_l n_l(ks)$. As expected, the two functions coincide closely for $s>3$ F, and there still remains a small oscillation but of relatively long wavelength ($\sim 2\Delta S$) and small amplitude. The oscillations in $f_l(s_i)$ obtained by the first method are typically a few orders of magnitude greater in amplitude and have a wavelength $\sim\frac{1}{2}\Delta S$. The extent to which the oscillations are changed in the second method depends on the step size and also on the weight given to the continuity equations.

## V. DINEUTRON SCATTERING

The preceding calculations can easily be repeated for the scattering of two dineutrons. We have done this in order to compare our results to those of GHL.[6] We have used the parameters given in Ref. 6 and step sizes specified by ($S=0$, 2.4, 6.0, 12.0 F; $\Delta S=0.3$, 0.6, 0.3 F). The results are presented in Fig. 3 and show that both methods predict very much the same phase shifts. There is, however, a systematic difference between the two curves of a few percent. We have varied our step sizes by up to a factor of 2 without affecting the phase shifts by more than three parts in $10^4$, so the difference is not likely to come from this source.

## VI. CONCLUSIONS

We have shown that it is possible to solve the Hill-Wheeler equation for the scattering of two clusters by direct techniques. This direct method is simpler to use than the method of GHL[6] which is an important consideration if the scattering of heavier clusters is the ultimate aim of the project. However, a great deal of work must yet be done before heavier clusters can be treated: In particular, the Coulomb interaction must be properly included; the mathematical properties of $f_l(s)$ must be investigated more formally; and the possibility of including absorption in some approximation must be studied. It is therefore not yet clear whether a direct solution of the Hill-Wheeler equation will ultimately prove preferable to transforming it into a Schrödinger equation with a nonlocal potential.

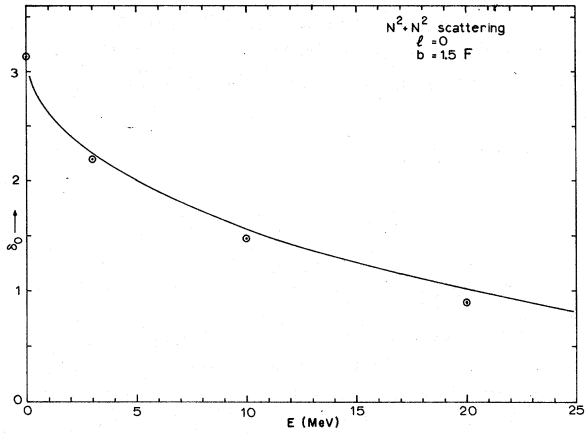


FIG. 3. The $l=0$ phase shifts for dineutron–dineutron scattering are shown as a function of energy (solid curve). The circled points are taken from Ref. 6. The integration parameters (see text) are ($S=0$, 2.4, 6.0, 12.0 F; $\Delta S=0.3$, 0.6, 0.3 F).

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## APPENDIX

If we omit from the usual overlap and energy functions all those terms which refer to either an interaction or an exchange between the clusters, then we obtain

$$N_l^f(s',s)=A_l(s',s)i_l\left(\frac{4ss'}{b^2}\right),$$

$$T_l^f(s',s)=\hbar\omega A_l(s',s)\times\left[\left(6-\frac{s^2+s'^2}{b^2}\right)i_l\left(\frac{4ss'}{b^2}\right)+\frac{2ss'}{b^2}i_l'\left(\frac{4ss'}{b^2}\right)\right],$$

$$V_l^f(s',s)=2(X_D+X_E)N_l^f(s',s).$$

The motion of two free clusters can then be described by the equation

$$\int_0^\infty [H_l^f(s',s)-EN_l^f(s',s)]f_l^f(s)s^2ds=0. \qquad \text{(A1)}$$

By direct evaluation of all the relevant integrals[8] it can be shown that the solution of the above equation is

$$f_l^f(s)=j_l(ks),$$

with the energy $E$ given by Eq. (7). Similarly a direct evaluation of the relevant integral [Eq. (4)] gives the expected result for the true wave function

$$g_l^f(R) = j_l(kR),$$

where all multiplicative constants have been omitted. This also establishes that $j_l(ks)$ is a solution of the full Eq. (2) for large $s'$, since it is not hard to show that $N_l(s', s) \to N_l^f(s', s)$ and $H_l(s', s) \to H_l^f(s', s)$ for large $s'$.

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# Nonschematic Random-Phase-Approximation Description of Gamma Vibrations in the Rare-Earth Nuclei

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$\gamma$-vibrational states in the rare-earth region are studied within the framework of the random-phase approximation (RPA), employing the surface $\delta$ interaction as the residual interaction. The calculations are performed without recourse to the schematic model. All terms in the interaction arising in the RPA matrix are taken into account. The results are compared with those obtained considering only the particle-hole term and with experiment. It is seen that previous schematic calculations overestimate the extent of the RPA correlations. Agreement with experiment, however, is not significantly improved.

## 1. INTRODUCTION

The quasiparticle random-phase approximation (QRPA)[1] has been employed by several authors with relation to the microscopic description of collective nonrotational states in deformed heavy nuclei. The method presents considerable numerical difficulties. Huge matrices must be diagonalized for every collective state, owing to the fact that in these nuclei the single-particle level density is very high.

The problem, however, can be easily overcome if one resorts to schematic separable forces. In this special case it suffices to look for the roots of a simple secular equation.[2] Thus, remarkable success has been achieved in the description of collective vibrational states in the rare-earth and transuranic regions,[3-7] using the pairing-plus-quadrupole or pairing-plus-octupole models (PQ or PO). More recently, similar calculations have been performed utilizing an even simpler (although more realistic) force, the surface $\delta$ interaction (SDI).[8-13]

The characteristic QRPA matrices are built with two types of interaction terms: particle-particle and particle-hole terms (and their corresponding