Geometric interpretation of the adiabatic model for heavy-ion fusion

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The relation between the finite basis adiabatic model and the classical adiabatic model (corresponding to a complete set of degenerate states) is elucidated when the internal system is rotational or vibrational. It is shown that the finite basis results can be obtained from the classical model results using the Gaussian quadrature to evaluate the former and Hermite quadrature for the latter.

I. INTRODUCTION

The importance of nonelastic couplings on the fusion of heavy ions is well established.[1] It has been shown that the fusion cross sections are strongly influenced by deformation effects,[2] surface vibrations,[3] and transfer reactions.[4] The explicit inclusion of these couplings by means of coupled-channel calculations becomes prohibitively time consuming, particularly when heavy ions are involved in the collision. This has led to the introduction of several simplifying approximations to the coupled-channel calculations. The scattering of spherical projectiles by deformed nuclei has been studied by invoking the extreme adiabatic approximation by Chase, Wilets, and Edmonds.[5] This model assumes that the rotational motion of the axially symmetric target nucleus is very slow in comparison with the relative motion of the projectile and target nuclei. Thus, one can evaluate an orientation-dependent scattering amplitude, $f(\theta)$, for the scattering of the projectile by the target whose symmetry axis is oriented at angles θ with respect to the beam axis. The elastic and inelastic scattering amplitudes can be obtained by folding $f(\theta)$ with the distributions of orientation (D functions). This model essentially assumes that the complete set of states of the ground state rotational band are included and that the Coriolis term of the kinetic energy operator can be neglected. Within the context of the above model, the total fusion cross section is given by

$$\sigma_{\text{fusion}}^{\text{total}}=\int_0^{\pi/2}\sin\theta\,\sigma_{\text{fusion}}(\theta)d\theta\ , \tag{1.1}$$

where $\sigma_{\text{fusion}}(\theta)$ is the cross section of the fusion of the projectile and the target oriented at an angle θ with respect to the beam axis.

Similar adiabatic approximations have been made for the treatment of coupling to vibrational states. These have been studied for the case of a harmonic oscillator coupled linearly or quadratically to the translational motion.[3,6] The respective total fusion cross sections in these two cases are given in the extreme adiabatic limit as[6]

$$\sigma_{\text{fusion}}^{\text{total}}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dx\,e^{-x^2/2}\sigma_{\text{fusion}}[V(R)+x\alpha_0 f(R)] \tag{1.2}$$

and

$$\sigma_{\text{fusion}}^{\text{total}}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dx\,e^{-x^2/2}\sigma_{\text{fusion}}[V(R)+x^2\alpha_0 f(R)]\ , \tag{1.3}$$

respectively, where $V(R)$ is the monopole nuclear plus Coulomb potential, $f(R)$ is the coupling form factor, and α_0 is the amplitude of zero-point motion of the harmonic oscillator. Equations (1.2) and (1.3) can be interpreted as if the zero-point motion were very slow compared to the relative motion of the projectile and target, so that one evaluates the fusion cross section at different (frozen) points of the zero-point vibration and averages with the weight factors $e^{-x^2/2}$.

In contrast to these extreme adiabatic models, there exist more restricted adiabatic models, where a finite set of coupled-channel equations are simplified by making the adiabatic approximation (neglect of the internal excitation energies of the target) and ignoring the Coriolis term in the kinetic energy operator.[7] These models include a finite number of excited states of the target and, because of the separable nature of the coupling interaction, completely decouple the coupled equations. Thus, for both rotational and vibrational coupling, one obtains a simple expression for the total fusion cross section,[8]

$$\sigma_{\text{fusion}}^{\text{total}}=\sum_{\alpha=1}^{N}w_\alpha\sigma_{\text{fusion}}(\alpha)\ , \tag{1.4}$$

where $\sigma_{\text{fusion}}(\alpha)$ is the fusion cross section of the two heavy ions in the eigenchannel α where the real potential is $V_0(R)+\lambda_\alpha f(R)$, and the weight factors w_α satisfy the condition

$$\sum_{\alpha=1}^{N}w_\alpha=1\ . \tag{1.5}$$

In Eqs. (1.4) and (1.5), N refers to the number of target states included in the coupled-channel calculation. The parameters λ_α and w_α are dependent only upon the static properties of the target nucleus and independent of the dynamics of the collision.

In this article, we analyze the properties of the parameters λ_α and w_α for the cases of rotational and vibrational coupling and study how they tend to the classical limit [Eqs. (1.1)–(1.3)]. In Sec. II we discuss the scattering by an axially symmetric rotor and discuss the decoupling of the coupled equations. The properties of λ_α and w_α are discussed in this section for the rotational coupling. In Sec. III the decoupling of the coupled vibrator with both linear and quadratic coupling is discussed. The summary and conclusions are presented in Sec. IV.

II. SCATTERING BY AN AXIALLY SYMMETRIC ROTOR

Under the adiabatic approximation, the Hamiltonian of the system is

$$H=K+V_0+V_{\text{coupling}} , \tag{2.1}$$

where K is the kinetic energy operator of relative motion, V_0 is the sum of the monopole nuclear and Coulomb potential, and V_{coupling} is the projectile-target coupling interaction which we assume to have the form

$$V_{\text{coupling}}(\mathbf{R},\hat{\xi})=\beta_2 F(R)\sum_{\mu} Y_{2\mu}(\hat{\mathbf{R}})Y_{2\mu}^{*}(\hat{\xi}) , \tag{2.2}$$

where $\hat{\xi}$ represents the orientation of the symmetry axis of the rotor and $\mathbf{R}$ is the vector joining the centers of mass of the two colliding nuclei. We have assumed that the rotor has a deformation of a single multipolarity which we take to be quadrupole.

The wave function for a total angular momentum J and z component M can be expanded as

$$\Psi^{JM}(\mathbf{R},\hat{\xi})=\sum_{LI}\frac{U_{LI}^{J}(R)}{R}\phi_{LI}^{JM}(\hat{\mathbf{R}},\hat{\xi}) , \tag{2.3}$$

where

$$\phi_{LI}^{JM}(\hat{\mathbf{R}},\hat{\xi})=i^{L+I}\sum_{M_L M_I}\langle LM_L IM_I\,|\,JM\rangle Y_{LM_L}(\hat{\mathbf{R}})Y_{IM_I}(\hat{\xi}) . \tag{2.4}$$

In Eqs. (2.3) and (2.4), we have considered only the $K=0$ band of the rotor, and I is the spin of the state of the rotor, M is its projection on the space-fixed z axis, and L is the orbital angular momentum of the projectile-target relative motion. The radial functions $U_{IL}^{J}(R)$ satisfy the coupled equations

$$(K_L+V_0-E)U_{LI}^{J}(R)=-\beta_2 F(R)\sum_{L'I'}\Omega_{LI;L'I'}^{J}U_{L'I'}^{J}(R) , \tag{2.5}$$

where $\Omega_{LI;L'I'}^{J}$ is defined by

$$\Omega_{LI;L'I'}^{J}=\int d\hat{\mathbf{R}}\int d\hat{\xi}\,\phi_{LI}^{JM*}(\hat{\mathbf{R}},\hat{\xi})[Y_2(\hat{\mathbf{R}})\cdot Y_2(\hat{\xi})]\times\phi_{L'I'}^{JM}(\hat{\mathbf{R}}\hat{\xi}) . \tag{2.6}$$

If we now make the approximation of neglecting the Coriolis term in the kinetic energy operator, i.e., approximating L by J in

$$K_L=-\frac{\hbar^2}{2\mu}\left[\frac{d^2}{dR^2}-\frac{L(L+1)}{R^2}\right]\cong K_J , \tag{2.7}$$

the operator on the left-hand side of (2.5) becomes independent of L and I, and hence one can decouple the coupled equations by a unitary matrix whose elements are c numbers. This is a consequence of the assumption that the coupling form factor $F(R)$ is independent of L and I. It can be shown that a transformation matrix, $\Gamma_{\alpha LI}^{J}$, that diagonalizes the coupling interaction, is[9]

$$\Gamma_{\alpha LI}^{J}=i^{L+I-J}\left[\frac{2L+1}{2J+1}\right]^{1/2}\langle L0I0\,|\,J0\rangle\beta_{\alpha I} , \tag{2.8}$$

where $\beta_{\alpha I}$ satisfies the eigenvalue equation

$$\sum_{I'}\frac{[(2I+1)(2I'+1)]^{1/2}}{5}\langle I0I'0\,|\,20\rangle^2\beta_{\alpha I'}=\lambda_\alpha\beta_{\alpha I} . \tag{2.9}$$

The resulting decoupled equations are

$$[K_J+V_0(R)+\lambda_\alpha\beta_2F(R)-E]W_{\alpha J}(R)=0 , \tag{2.10}$$

where

$$W_{\alpha J}(R)=\sum_{LI}\Gamma_{\alpha LI}^{J}U_{LI}^{J}(R) . \tag{2.11}$$

The first term of the transformation coefficient,

$$\sum_{L}i^{L+I-J}\left[\frac{2L+1}{2J+1}\right]^{1/2}\langle L0I0\,|\,J0\rangle ,$$

can be immediately recognized as the coefficient of transformation from the laboratory to the intrinsic frame of reference.[10] (It should be noted, however, that we rotate the symmetry axis of the rotor toward the $\mathbf{R}$ vector.) The coefficient $\beta_{\alpha I}$ which is the eigenvalue of Eq. (2.9) is exactly the one that occurs in the sudden approximation to Coulomb excitation developed by Alder and Winther.[10] The resulting eigenvalues λ_α and eigenvectors $\beta_{\alpha I}$ have been listed by these authors for the cases of coupling of various rotational states with $I_{\max}=2$, 4, or 6. The adiabatic model then yields the total fusion cross section as[9]

$$\sigma_{\text{fusion}}^{\text{total}}=\sum_{\alpha=1}^{N}\beta_{\alpha 0}^{2}\sigma_{\text{fusion}}(\alpha) , \tag{2.12}$$

where $\sigma_{\text{fusion}}(\alpha)$ is the fusion cross section in the eigenchannel α with the effective spherical potential $V_0(R)+\lambda_\alpha\beta_2F(R)$. We expect that Eq. (2.12) should become identical to Eq. (1.1) in the limit that the number of states of the rotor, N, included in the coupled-channel calculations tends to infinity.

It is of interest to find a geometrical interpretation of the eigenvalue λ_α and the weight factors $\beta_{\alpha 0}^2$. An inspection of Eq. (2.9) shows that it is equivalent to the eigenvalue equation

$$\hat{P}_2(\cos\theta)f_\alpha(\theta)=\lambda_\alpha f_\alpha(\theta) , \tag{2.13}$$

where $f_\alpha(\theta)$ is an eigenstate of the operator $\hat{P}_2(\cos\theta)$ and λ_α is the corresponding eigenvalue. If $I_{\max}$ is the maximum spin to be included (all the spins are even), $f_\alpha(\theta)$ is of the form

$$f_\alpha(\theta)=\sum_{I=0}^{I_{\max}}\beta_{\alpha I}Y_{I0}(\theta,\phi)\ , \tag{2.14}$$

where $\beta_{\alpha I}$ satisfies Eq. (2.9). Thus, we find that λ_α is the eigenvalue of the operator $\hat{P}_2(\cos\theta)$ and if Eq. (2.13) has a solution for $f_\alpha(\theta)$ given by (2.14), we need $P_{I_{\max}+2}(\cos\theta)=0$. This is satisfied by the set of angles θ_α which are the zeros of $P_{I_{\max}+2}(\cos\theta)$, and the eigenvalues λ_α become equal to $P_2(\cos\theta_\alpha)$. Thus, we find that the λ_α are bounded, $-\frac{1}{2}\le\lambda_\alpha\le 1$. It follows that the equation for the eigenchannels, Eq. (2.10), can be rewritten as

$$[K_J+V_0(R)+\beta_2F(R)P_2(\cos\theta_\alpha)-E]W_{\alpha J}(R)=0\ . \tag{2.15}$$

The functions $W_{\alpha J}(R)$ are thus seen to describe the scattering of the projectile by the target nucleus at fixed orientations θ_α, where the θ_α's are the zeros of the Legendre function $P_{I_{\max}+2}$. If $I_{\max}=0$, θ_α corresponds to 54.74°, which corresponds to the zero of $P_2(\cos\theta_\alpha)$, so that the scattering contains only the spherical potential $V_0(R)$. For $I_{\max}=2$, we obtain two orientation angles corresponding to the zeros of $P_4(\cos\theta)$ in the range $0\le\theta\le\pi/2$. The corresponding weight factors β_0^2 are those corresponding to Gaussian integration,[11] i.e.,

$$\beta_{\alpha 0}^2=2/(1-X_\alpha^2)[P'_{I_{\max}+2}(X_\alpha)]^2\ , \tag{2.16}$$

where

$$X_\alpha=\cos\theta_\alpha \text{ and } P'_I(X_\alpha)=\frac{d}{dX_\alpha}P_I(X_\alpha)\ .$$

Thus, if we include $I=0$ and 2 of the rotor, we obtain the orientations 70.12° and 30.55° of the target with respect to the beam direction, and these contribute to the fusion cross sections with weight factors of 0.652 and 0.348, respectively. From Eq. (2.15), it can be noticed that, for prolate nuclei ($\beta_2>0$) and an attractive potential [$V_0(R)$ and $F(R)$ both negative], the barrier corresponding to 70.12° will be raised and that for 30.55° will be lowered relative to the case where the inelastic couplings were neglected. (It will be the reverse for oblate nuclei, $\beta_2<0$.) As we include more states with increasing $I_{\max}$, more orientation angles come into play, the largest of these tending toward 90° and the smallest approaching to 0°. Correspondingly, the weight factors for the largest orientation angle tend toward unity, while those for the smallest tend toward zero; the weight factors become proportional to $\sin\theta$. At energies much below the barrier, the lowest fusion barrier determines the fusion cross section, i.e.,

$$\sigma_{\text{fusion}}^{\text{total}}(E\ll V_B)\cong w_\alpha\sigma_{\text{fusion}}(\alpha)\ , \tag{2.17}$$

where $\sigma_{\text{fusion}}(\alpha)$ corresponds to the channel with the lowest fusion barrier. As we incorporate more states of the rotor, $\sigma_{\text{fusion}}(\alpha)$ keeps increasing, while at the same time w_α keeps decreasing. The product of these two very quickly reaches saturation, as has been clearly demonstrated by Lindsay and Rowley[8] in their analyses of the fusion of ^{16}O by samarium isotopes.

We have thus been able to show the correspondence between the extreme adiabatic limit, Eq. (1.4), and the corresponding expression when a finite number of rotor states are included, Eq. (2.12). This is merely the identity

$$\begin{aligned}\sigma_{\text{fusion}}^{\text{total}}&=\int_0^{\pi/2}\sin\theta\,\sigma_{\text{fusion}}(\theta)d\theta\\&=\sum w_\alpha\sigma_{\text{fusion}}(\alpha)\ ,\end{aligned} \tag{2.18}$$

where the abscissas, $\cos\theta_\alpha$, and weight factors, w_α, correspond to Gaussian integration.

III. HARMONIC OSCILLATIONS COUPLED TO TRANSLATIONAL MOTION

Now consider the case of a harmonic oscillator coupled to a translational coordinate either linearly or quadratically.[6] The oscillator Hamiltonian is

$$\hat{H}_0(q)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}+\frac{1}{2}m\omega_0^2q^2\ , \tag{3.1}$$

and the interaction term (considered separable) is of the form

$$\hat{H}_{\text{coupling}}^{\text{lin}}(q,R)=f(R)q\quad\text{(for linear coupling)} \tag{3.2}$$

and

$$\hat{H}_{\text{coupling}}^{\text{quad}}(q,R)=f(R)q^2\quad\text{(for quadratic coupling)}\ . \tag{3.3}$$

In terms of the creation and annihilation operators a and $a^\dagger$ for the harmonic oscillator, we have

$$\hat{H}_0=(a^\dagger a+\tfrac{1}{2})\hbar\omega_0\ , \tag{3.4}$$

$$\hat{H}_{\text{coupling}}^{\text{lin}}=\alpha_0 f(R)(a+a^\dagger)\ , \tag{3.5}$$

and

$$\hat{H}_{\text{coupling}}^{\text{quad}}=\alpha_0^2 f(R)(a^\dagger a^\dagger+aa+2a^\dagger a+1)\ . \tag{3.6}$$

The adiabatic (degenerate) limit is obtained by letting $\omega_0\to 0$ and at the same time keeping α_0 finite by allowing the mass parameter of the oscillator, m, to tend to infinity [cf. Eqs. (1.2) and (1.3)]. Let us now consider the cases of linear and quadratic coupling separately.

A. Linear coupling

This corresponds to the usual harmonic vibrational collective model of nuclei. Let us consider a finite number of oscillator quanta. The eigenvalue equation corresponds to

$$(a+a^\dagger)\sum_{n=0}^{N}\beta_n^{(\alpha)}|n\rangle=\lambda_\alpha\sum_{n=0}^{N}\beta_n^{(\alpha)}|n\rangle\ , \tag{3.7}$$

or

$$\hat{q}\sum_{n=0}^{N}\beta_n^{(\alpha)}h_n(q)=\lambda_\alpha\sum_{n=0}^{N}\beta_n^{(\alpha)}h_n(q)\ , \tag{3.8}$$

where $h_n(q)$ is the Hermite polynomial of rank n. The effect of the $\hat{q}$ operator on the left-hand side of the equation is to result in a superposition of Hermite polynomials up to the rank $N+1$. The polynomial $h_{N+1}(q)$ is absent on the right-hand side. Thus the discrete set of values q_α which allow for a solution of Eq. (3.8) correspond to the zeros of $h_{N+1}(q)$, and the total fusion cross section can be expressed as

$$\sigma_{\text{fusion}}^{\text{total}} = \sum_\alpha w_\alpha \sigma_{\text{fusion}}(\alpha) , \tag{3.9}$$

where $\sigma_{\text{fusion}}(\alpha)$ is the fusion cross section corresponding to the spherical potential $[V_0+\alpha_0 q_\alpha f(R)]$, where V_0 is a monopole (nuclear plus Coulomb) potential. It can be verified that w_α is the weight factor corresponding to the Hermite quadrature with $N+1$ points. In the limit $N\rightarrow\infty$, Eq. (3.9) becomes equal to Eq. (1.2). $\sigma_{\text{fusion}}[V_0+\alpha_0 q_\alpha f(R)]$ is the cross section for an oscillator frozen at a separation q_α. The zeros of $h_{N+1}(q)$ have both positive and negative values of q_α and, since $\lambda_\alpha = q_\alpha$, some of the fusion barriers will be lower and others higher than the barrier without the coupling. The saturation of subbarrier fusion in this case with the inclusion of a few oscillator quanta has been demonstrated in Ref. 12.

B. Quadratic coupling

A similar analysis can be carried out for quadratic coupling. Such couplings arise in models for nuclear fission.[13] In this case, the equation

$$\hat{q}^{\,2} \sum_{n=1}^{N} \beta_n^{(\alpha)} h_n(q) = \lambda_\alpha \sum_{n=1}^{N} \beta_n^{(\alpha)} h_n(q) \tag{3.10}$$

has solutions for values of q_α which are the zeros of $h_{N+2}(q)$. Unlike the case of linear coupling, the only basis states that appear in Eq. (3.10) correspond to an even number of oscillator quanta. Since $\lambda_\alpha = q_\alpha^2$, λ_α is always positive; this implies that the eigenchannel barriers are always higher [if $f(R)$ is positive] or lower [if $f(R)$ is negative] than the barrier with no coupling. This is a consequence of the fact that whereas there was no diagonal contribution in the case of linear coupling, the quadratic coupling leads to a diagonal contribution ("reorientation"). Once again, the total fusion cross section can be expressed as a weighted average of the eigenchannel fusion cross sections

$$\sigma_{\text{fusion}} = \sum_{\alpha=1}^{N} w'_\alpha \sigma_{\text{fusion}}(\alpha) , \tag{3.11}$$

where now the effective spherical potentials are $[V_0+\alpha_0 q_\alpha^2 F(R)]$ and where q_α are the zeros of $h_{N+2}(q)$ and w'_α are the appropriate weight factors. In the limit $N\rightarrow\infty$, this leads to Eq. (1.3).

IV. SUMMARY AND CONCLUSIONS

The relation between the finite basis adiabatic model and the classical adiabatic model (which includes a complete set of states assumed to be degenerate) was derived for the case of rotational and vibrational coupling. In the former case, it was shown that the finite basis results can be obtained from the classical model by means of a Gaussian quadrature. The weight factors and abscissas for an N state calculation can be deduced from the N point Gaussian integration formula and can be directly determined from published numerical tables. In the case of vibrational coupling, the corresponding quadrature is the Hermite quadrature. These results are useful if one wants to make a simple estimate of the number of states of the target needed for the saturation of the fusion cross section.

In the case of the rotational coupling, the weight factors w_α only determine the components, $\beta_{\alpha 0}$, of the eigenchannels in the ground state wave function. It is possible to show that one may calculate all the other components from the identity that

$$\beta_{\alpha I} = \sqrt{(2I+1)}\, P_I(\cos\theta_\alpha)\beta_{\alpha 0} . \tag{4.1}$$

Thus, once the weight factor is determined, all the components $\beta_{\alpha I}$ of Eq. (2.14) are known. Hence, all other adiabatic cross sections (elastic and inelastic) can be easily evaluated.

It should be noted that whereas the adiabatic model may be reasonable in the case of scattering by a strongly deformed nucleus in several cases, this is likely to be less favorable in the case of vibrational coupling, where the excitation energies involved are larger. Thus the adiabatic model will tend to overestimate the fusion probability.[12] However, its predictions can be used as a guideline before fuller coupled-channel calculations are undertaken.

As a final comment, the analysis of scattering by deformed nuclei with more than one multipole deformation (quadrupole and hexadecapole) becomes more difficult because the form factors $F_k(R)$ become dependent upon the multipolarity k of the coupling. Thus, one does not find it easy to totally decouple the coupled equations without making doubtful approximations of replacing the form factors with values at a predetermined radius. The same statement holds in the case of a superposition of linear and quadratic coupling in the case of a vibration. Thus, even though the extreme adiabatic limits are known,[6] one does not know how to extract the finite basis results from these.

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