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Reduction of coupled equations for heavy ion reactions

Osamu Tanimura

Fachbereich Physik, Universitaet Gesamthochschule Siegen, Siegen, West Germany (Received 30 July 1986)

The coupled channel method for heavy ion scattering is greatly simplified by suitable transformations of wave functions in the case of large reduced mass.

The coupled channel method is quite useful in treating collective excitations enhanced in nuclear scattering.¹ This method has succeeded remarkably in describing scattering with a small reduced mass such as nucleon-nucleus scattering 1,2 and scattering between light nuclei.²

For heavy ion scattering with large reduced mass, on the other hand, it is quite difficult to perform the coupled channel calculation using current computational codes. It is because low-lying collective states of high spin coupled to the scattering system generate a large number of subchannels of different orbital angular momenta, L. Then the total number of coupled channels can be very large.

Furthermore, at energies well below the Coulomb barrier, the coupled channel method is not feasible in the fusion calculation.³ Otherwise, one needs too high a numerical accuracy in solving the coupled equations. This difficulty is closely associated with the strong L dependence of the wave function at energies well below the barrier.

In this paper we present a feasible method of solving coupled equations for inelastic scattering under the assumption that the factor of L(L+1) in the centrifugal potential can be replaced by J(J+1), where J denotes the total angular momentum. We show that this method significantly resolves the difficulties noted above.

We start with coupled equations for inelastic scattering between two nuclei for the total J

$$\left[E - \left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu}\frac{L(L+1)}{r^2} + U(r) + \varepsilon_{I_1} + \varepsilon_{I_2}\right]\right]u_i^J$$
$$= \sum_j \langle i | V | j \rangle u_j^J , \quad (1)$$

with

$$i = [(I_1I_2)I, L] \text{ and } j = [(I'_1I'_2)I', L']$$
 (2)

The wave function $u_i^{J}(r)$ satisfies the following boundary

condition:

$$u_i^J(r \to \infty) \sim \left(\frac{2\mu}{\pi \hbar^2 k_i}\right)^{1/2} [F_L(k_i r) \delta_{i1} - \pi H_L(k_i r) T_{i1}] , \qquad (3)$$

where F_L and H_L are the regular and the outgoing Coulomb wave functions, and k_i denotes the wave number. The *T* matrix T_{ij} is defined by $S_{ij} = \delta_{ij} - 2\pi T_{ij}$. U(r)denotes the optical potential, $\varepsilon_{I_1(I_2)}$ the excitation energy of spin $I_1(I_2)$, and *I* the total spin. The interaction *V* is generally expanded by the spherical harmonics $Y_{\lambda V}$ as

$$V = \sum_{\lambda\nu} V_{\lambda}(r) Q_{\lambda\nu}^{\dagger}(1,2) Y_{\lambda\nu}(\hat{\mathbf{r}}) , \qquad (4)$$

where $Q_{\lambda\nu}(1,2)$ represents the operator of collective excitation for the total system. With the interaction (4) the matrix element $\langle i | V | j \rangle$ is reduced to the following form with the help of the Wigner-Eckart theorem:

$$\langle i | V | j \rangle = \frac{\hat{I}\hat{L}'}{\sqrt{4\pi}} \sum_{\lambda} (-)^{\lambda} \hat{\lambda} V_{\lambda} (L'0\lambda 0 | L0) W(JLI'\lambda; IL') \\ \times \langle (I_1 I_2) I | | Q_{\lambda} | | (I_1' I_2') I' \rangle , \qquad (5)$$

where $\hat{I} = \sqrt{2I+1}$. Here $W(JLI'\lambda;IL')$ and $\langle I | | Q_{\lambda} | | I' \rangle$ denote the Racah coefficient and the reduced matrix element, respectively.

Now we consider a heavy ion collision where the reduced mass is large enough that $\hbar^2 I^2 / (2\mu r^2)$ is neglected near the barrier distance r_b . Then we make a possible approximation:

$$\frac{\hbar^2}{2\mu} \frac{L(L+1)}{r^2} \approx \frac{\hbar^2}{2\mu} \frac{J(J+1)}{r^2} .$$
 (6)

The difference between right- and left-side values in Eq. (6) at $r = r_b$ amounts at most to $\hbar^2 I J / (\mu r_b^2)$. At energy below and near the Coulomb barrier (the grazing angular momentum ≈ 0), $\hbar^2 I J / (\mu r_b^2)$ becomes quite small. At

<u>35</u> 1600

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REDUCTION OF COUPLED EQUATIONS FOR HEAVY ION REACTIONS

energy well above the Coulomb barrier all the subchannels for а given $(I_1I_2)I_1$ i.e., $|I.L = J - I\rangle$. $|I, J - I + 2\rangle, \dots, |I, L + I\rangle$, may be more or less equally enhanced by the coupling interactions of roughly the same strengths. This may allow one to average the centrifugal potentials on L's, resulting roughly in $\hbar^2 J(J+1)/(2\mu r^2)$.

We make a transformation of u_i^J to $\psi_{(I_1I_2)I}^J$ under the as-

sumption (6):

$$\psi^{J}_{(I_{1}I_{2})} = \sum_{L} (J0I0 \mid L0) u^{J}_{i} .$$
⁽⁷⁾

This transformation assures the normalization property of the transformed wave function. Then the original coupled equation (1) is transformed as

$$(E - H_{I_1 I_2 I}^J) \psi_{(I_1 I_2) I}^J = \sum_{(I_1' I_2') I'} \frac{1}{\sqrt{4\pi}} \sum_{\lambda} (-)^{\lambda} \hat{\lambda} V_{\lambda} (I' 0 \lambda 0 | I 0) \langle (I_1 I_2) I | | Q_{\lambda} | | (I_1' I_2') I' \rangle \psi_{(I_1' I_2') I'}^J , \qquad (8)$$

with

$$H_{I_1I_2}^J = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{J(J+1)}{r^2} + U(r) + \varepsilon_{I_1} + \varepsilon_{I_2} . \quad (9)$$

In deriving Eq. (9) we have utilized the following relation:

$$\sum_{f} \hat{e}\hat{f}(b0d0|f0)(a0f0|c0)W(abcd;ef) = (a0b0|e0)(e0d0|c0), \quad (10)$$

where a, b, c, d, e, and f stand for angular momenta.

The wave function $\psi_{(I_1I_2)I}$ satisfies the following boundary condition:

$$\psi^{J}_{(I_{1}I_{2})I}(r \to \infty) \sim \left(\frac{2\mu}{\pi\hbar^{2}k_{l}}\right)^{1/2} [F_{J}(k_{l}r)\delta_{l1} - \pi H_{J}(k_{l}r)T_{l1}], \quad (11)$$

where the suffix *l* specifies the channel $(I_1I_2)I$.

In contrast to Eq. (1), the reduced coupled equation (8) does not depend on L, i.e., the subchannels. Consequently, the number of coupled equations in Eq. (8) is equal to that of the total combinations of $(I_1I_2)I$, while the original equations specified by index $[(I_1I_2)I_1,L]$ number I+1 for each I in the normal parity spins and thus can be very large in total.

In the conventional coupling interaction, which is usually given by the first order term in expansion on collective variable, the coupled equations are further reduced. The interaction is written as

$$V = \sum_{\lambda\nu} V_{\lambda}(r) Q_{\lambda\nu}^{\dagger}(1) Y_{\lambda\nu}(\hat{\mathbf{r}}) + \sum_{\lambda'\nu'} V_{\lambda'}(r) Q_{\lambda'\nu'}^{\dagger}(2) Y_{\lambda'\nu'}(-\hat{\mathbf{r}}) , \qquad (12)$$

where $Q_{\lambda\nu}[1(2)]$ denotes the collective operator of nucleus 1(2)

Here we make another transformation, which also assures the normalization property of the wave function:

$$\phi_{I_1 I_2}^J = \sum_{L,I} (I_1 0 I_2 0 | I0) (J0I0 | L0) u_i^J , \qquad (13)$$

which satisfies

$$\phi_{I_1I_2}^J(r \to \infty) \sim \left(\frac{2\mu}{\pi \hbar^2 k_n}\right)^{1/2} [F_J(k_n r) \delta_{n1} - \pi H_J(k_n r) T_{n1}] , \quad (14)$$

where the suffix *n* specifies the channel (I_1I_2) . Then we find

$$(E - H_{I_{1}I_{2}}^{J})\phi_{I_{1}I_{2}}^{J} = \frac{1}{\sqrt{4\pi}} \sum_{I_{1}'I_{2}'} \left[\sum_{\lambda} (-)^{\lambda} \hat{\lambda} V_{\lambda} (I_{1}'0\lambda 0 | I_{1}0) \langle I_{1} | | Q_{\lambda} | | I_{1}' \rangle \delta_{I_{2}I_{2}'} + \sum_{\lambda'} \hat{\lambda}' V_{\lambda'} (I_{2}'0\lambda' 0 | I_{2}0) \langle I_{2} | | Q_{\lambda'} | | I_{2}' \rangle \delta_{I_{1}I_{1}'} \right] \phi_{I_{1}'I_{2}'}^{J} .$$

$$(15)$$

This equation does not depend on I or L, so that the number of the coupled equations is equal to the combinations of spins I_1 and I_2 .

Let us consider, for example, a scattering between two different nuclei taking into account states of 0^+ , 2^+ , and 4⁺ for each nucleus. The number of coupled equations (1), (8), and (15) are, respectively, 117, 29, and 9 for even $J(J \ge 8)$. Therefore, we see that a coupled channel calculation using Eq. (1) is not practical for this system, but calculations using both Eqs. (8) and (15) are feasible.

The numerical inaccuracy increases with decreasing energy below the Coulomb barrier when one solves the coupled equations given by Eq. (1). The strong L dependence of the magnitude of wave functions at the matching radius may lead to divergence of the S matrix in the iterative method.⁴ The present model resolves significantly this problem, since both Eqs. (8) and (15) do not depend on L,

i.e., assume L = J.

Let us make numerical comparisons between the exact and the reduced coupled channel methods. Since the reduced method contains only one partial wave L = J in each (I_1I_2) I channel, it is a critical test of the model to compare the inelastic angular distribution with the exact prediction, which contains the interference among different L's for each channel. To see the validity of the model with variation of energy, we compare the energy dependence of the fusion cross section.

We calculate the elastic, the inelastic, and the fusion cross sections for $^{232}Th + ^{16}O$. Since the system has a large reduced mass, the effect of spins of low-lying states on the centrifugal potential may be negligible. We, for simplicity, take into account only the ground state and the 2^+ (0.049 MeV) state in ²³²Th. The optical potential is assumed to be of the Woods-Saxon form with the parame-

1601



FIG. 1. Elastic and inelastic angular distributions for ${}^{16}\text{O} + {}^{232}\text{Th}$ at $E_{\text{lab}} = 80$ MeV. Solid and dashed curves show the reduced and exact coupled channel results, respectively. In the elastic cross sections the solid curve coincides with the dashed curve.

ters V = -100 MeV, W = -20 MeV, $r_0 = r_I = 1.3$ fm, and $a_0 = a_I = 0.5$ fm for elastic and inelastic scatterings. For the fusion calculation the range of absorption potential is determined so it will fit the cross section by the onechannel WKB method: $r_I = 1.15$ and $a_I = 0.25$ fm. We calculate fusion cross section by the usual prescription,

$$\sigma_F = \pi \lambda^2 \sum_J (2J+1) \left(1 - \sum_i |S_{i1}|^2 \right) , \qquad (16)$$

where $S_{i1} = \delta_{i1} - 2\pi i T_{i1}$.

The coupling interaction is assumed to be the one given by the left side of Eq. (15), i.e., the first order derivative of the optical potential on the deformation with the parameter $\beta_2 = 0.25$ (no Coulomb coupling and no reorientation effect).

In solving the coupled equation, we modified the Fox-Goodwin method⁵ to speed up the calculation: The subchannels are suitably rearranged so that the nonzero elements in the matrix of simultaneous equations come close to the diagonal elements. By this rearrangement the computing time is greatly reduced, which is proportional to N^2

³S. Landowne and S. C. Pieper, Phys. Rev. C 29, 1352 (1984).

TABLE I. Fusion cross sections for 232 Th + 16 O.		
E_{lab} (MeV)	Exact CC (mb)	Reduced CC (mb)
70	6.902×10^{-5}	6.940×10^{-5}
74	2.541×10^{-2}	2.556×10^{-2}
78	3.907	3.932
82	7.934×10^{1}	7.946×10^{1}
86	2.060×10^{2}	2.056×10^{2}
90	3.518×10^{2}	3.499×10^{2}
100	8.064×10^{2}	8.019×10^{2}
120	1.310×10^{3}	1.301×10^{3}

(N = the total number of coupled equations), while the time in the conventional Fox-Goodwin method is proportional to N^3 (as shown in Ref. 4).

Figure 1 shows the elastic and inelastic angular distributions at E_{lab} = 80 MeV, which corresponds to the Coulomb barrier height. The reduced method of Eq. (15) produces almost the same elastic angular distribution as the exact prediction (error < 1% in each angle). It also reproduces quite well the exact inelastic cross sections, except at backward angles. This indicates that the interference of the Tmatrix between different L's becomes effective at backward angles. However, this effect may not be important in the total inelastic cross section, since the backward cross section is relatively small. Indeed, the reduced method predicts the total inelastic cross section of 3240 mb, which is close to the exact vaue of 3244 mb. It was found that with decreasing and increasing energy the reduced method reproduces the exact inelastic angular distributions, respectively, worse and better than it does as seen in Fig. 1.

Table I shows the comparison of the fusion cross section at energies between well below and well above the Coulomb barrier. Obviously the reduced coupled channel method gives excellent agreement with the exact one given by Eq. (1). The error lies within 1%.

In conclusion, we have shown that in the scattering system of a large reduced mass the coupled equations are greatly reduced by the relevant transformation, especially in the coupling interaction of the first order expansion of the collective operator. We have also shown from the simple numerical comparisons that the reduced coupled channel method gives good approximations to the exact predictions in the elastic angular distributions, the fusion, and the total inelastic cross sections. The difference comes out in the backward cross sections in the inelastic scattering, although the magnitude is relatively small. It is interesting to investigate further the validity of the reduced coupled channel method in various systems.

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