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Partial Wave Expansion of Three-particle Continuum States in Hyperspherical Coordinates: Application to Ionisation Problems

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Abstract

A partial wave expansion of three-particle continuum states has been developed using hyperspherical coordinates. An approximate three-particle continuum state appears which may be useful in electron–hydrogen atom ionisation studies. Further improvement in the result is also possible. The analysis may be easily extended for application to other three-body ionisation problems.

1. Introduction

Correlation of the two electrons in the final channel is very important in the description of electron–hydrogen atom ionisation collisions. In most earlier calculations this correlation has not been properly handled. The calculation by Brauner *et al.* (1989) took into account the correlation effect quite satisfactorily. As a consequence, qualitatively, they produced very good cross section results. Recently Das and Seal (1993) have also taken into account the correlation in a piecewise manner. However, possibly the best way of taking this effect into account is to use hyperspherical coordinates, as suggested by analysis of H^- and He systems with two electrons in the excited states (see Fano 1983; Fano and Rau 1986). Hyperspherical coordinates have been used by Delves (1959, 1960), Peterkop (1960), Rudge and Seaton (1965) and others in ionisation calculations but possibly the usefulness of hyperspherical coordinates in studies of ionisation problems has not been fully appreciated. We believe its use will greatly simplify the ionisation calculation, if the problem is taken seriously. With this view we present here a partial wave analysis of the three-particle continuum states in this coordinate system. A simple three-particle continuum state also results in this analysis, which may be useful in ionisation studies of hydrogen atoms. More accurate wavefunctions may also be calculated in this framework. We present the analysis in a somewhat more general setting so that it may be useful or further generalised in other three-body ionisation problems.

2. Ionisation Calculation

The scattering amplitude for ionisation problems may be conveniently expressed in terms of the full three-particle continuum wavefunction in the final channel, so we begin with a discussion of the three-particle continuum wavefunction.

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(2a) Three-particle Continuum Wavefunction

First we consider three distinct nonrelativistic particles which interact by two-body spin-independent regular short-range forces. To be specific, we consider the collision of particle 2 with a bound system of particles 1 and 3. After the collision three free particles result. The initial unperturbed state is described by $\Phi_{\rm i}$ and the interaction in the initial channel is $V_{\rm i}$. If $\Psi_{\rm f}^{(-)}$ is the final three-particle continuum state with incoming wave boundary condition, then the (direct) ionisation amplitude is formally given by

$$f=-(2\pi)^2\langle\Psi_{\rm f}^{(-)}|V_{\rm i}|\Phi_{\rm i}\rangle\,. \tag{1}$$

The exchange amplitude may be similarly expressed.

Now the main problem here is to find a reliable and accurate result for $\Psi_{\rm f}^{(-)}$. For this we proceed to solve the corresponding Schrödinger equation:

$$(H-E)\Psi_{\rm f}^{(-)}=0\,. \tag{2}$$

Here we use hyperspherical coordinates and make a decomposition of the full wave $\Psi_{\rm f}^{(-)}$ in terms of angular eigenfunctions, as in the case of the two-body problem (Newton 1966), but with more complicated angular functions and with a more complicated result. Finally, the full wave has to be constructed from the partial waves determining fully the expansion coefficients.

(2b) Hyperspherical Coordinate System: Radial Wave Equations

With reference to a centre-of-mass coordinate frame, the coordinates and momenta of the three particles are $\boldsymbol{R}_1,\boldsymbol{R}_2,\boldsymbol{R}_3$ and $\boldsymbol{P}_1,\boldsymbol{P}_2,\boldsymbol{P}_3$ respectively. Considering the centre of mass to be at rest, we have

$$\boldsymbol{P}_1+\boldsymbol{P}_2+\boldsymbol{P}_3=0\,. \tag{3}$$

Then we have two independent coordinates and momenta. Let the masses of the three particles be m_1, m_2 and m_3, while μ is a representative mass, say that of an electron when we consider an ionisation problem in atomic physics, or that of a proton when we consider a problem in nuclear physics. We introduce the following independent coordinates and momenta:

$$\boldsymbol{r}_1=\sqrt{\frac{\mu_1}{\mu}}(\boldsymbol{R}_1-\boldsymbol{R}_3)\,,\qquad \boldsymbol{r}_2=\sqrt{\frac{\mu_2}{\mu}}\left(\boldsymbol{R}_2-\frac{m_1\boldsymbol{R}_1+m_3\boldsymbol{R}_3}{m_1+m_3}\right) \tag{4a}$$

$$\boldsymbol{p}_1=\sqrt{\mu\mu_1}\,\frac{d\boldsymbol{r}_1}{dt}\,,\qquad \boldsymbol{p}_2=\sqrt{\mu\mu_2}\,\frac{d\boldsymbol{r}_2}{dt}\,, \tag{4b}$$

which are canonically conjugate and where

$$\mu_1=\frac{m_2(m_1+m_3)}{m_1+m_2+m_3}\,,\qquad \mu_2=\frac{m_1m_3}{m_1+m_3}\,.$$

The energy of the ionised system is then

$$E = \frac{p_1^2}{2\mu} + \frac{p_2^2}{2\mu}\,. \tag{5}$$

The corresponding three-particle Schrödinger equation is

$$\left(\frac{-\nabla_1^2}{2\mu} - \frac{\nabla_2^2}{2\mu} + V(\boldsymbol{r}_1, \boldsymbol{r}_2) - E\right)\Psi_{\mathrm{f}}^{(-)} = 0\,, \tag{6}$$

where V is the total interaction potential.

Next we introduce the hyperspherical coordinates $(R, \alpha, \hat{r}_1, \hat{r}_2)$, related to $(r_1, r_2, \hat{r}_1, \hat{r}_2)$ by $r_1 = R\cos\alpha$, $r_2 = R\sin\alpha$. In this coordinate system the Schrödinger equation takes the form (Morse and Feshbach 1953; Fano and Rau 1986, p. 313)

$$\left[-R^{-5/2}\left(\frac{\partial^2}{\partial R^2}\right)R^{5/2} + \frac{\Lambda^2 + \frac{15}{4}}{R^2} + 2\mu V - 2\mu E\right]\Psi_{\mathrm{f}}^{(-)} = 0\,, \tag{7a}$$

where

$$\Lambda^2 = -\frac{1}{\sin\alpha\cos\alpha}\left(\frac{\partial^2}{\partial\alpha^2}\right)\sin\alpha\cos\alpha + \frac{\boldsymbol{L}_1^2}{\cos^2\alpha} + \frac{\boldsymbol{L}_2^2}{\cos^2\alpha} - 4\,. \tag{7b}$$

Eigenstates of Λ^2 are $\phi_\lambda(\alpha, \hat{r}_1, \hat{r}_2) = P_n^{l_1 l_2}(\alpha)\,\mathcal{Y}_{l_1 l_2}^{lm}(\hat{r}_1, \hat{r}_2)$, with eigenvalues given by

$$\Lambda^2\phi_\lambda = \lambda(\lambda + 4)\phi_\lambda\,, \tag{8a}$$

where

$$\lambda = 2n + l_1 + l_2\,. \tag{8b}$$

Here $P_n^{l_1 l_2}$ is a (normalised) Jacobi polynomial given by

$$\begin{aligned} P_n^{l_1 l_2}(\alpha) = {} & \left(\frac{2\Gamma(n + l_2 + \frac{3}{2})\,\Gamma(n + l_1 + l_2 + 2)(2n + l_1 + l_2 + 2)}{\Gamma(n+1)\,\Gamma(n + l_1 + \frac{3}{2})[\Gamma(l_2 + \frac{3}{2})]^2}\right)^{\frac{1}{2}} \\ & \times \cos^{l_1}\alpha\,\sin^{l_2}\alpha\;{}_2F_1(-n, n + l_1 + l_2 + 2, l_2 + \tfrac{3}{2}, \sin^2\alpha)\,, \end{aligned} \tag{9a}$$

and

$$\mathcal{Y}_{l_2 l_2}^{lm}(\hat{r}_1, \hat{r}_2) = \sum_{m_1 m_2} C(l_1\, l_2\, l;\, m_1\, m_2\, m)\, Y_{l_1 m_1}(\hat{r}_1)\, Y_{l_2 m_2}(\hat{r}_2)\,. \tag{9b}$$

We set $p_1 = P\cos\alpha_0$ and $p_2 = P\sin\alpha_0$; then the scattering state may be expanded as

$$\Psi_{\mathrm{f}}^{(-)}(R, \alpha, \hat{r}_1, \hat{r}_2) = \sum_\lambda A_\lambda\left(\frac{F_\lambda(PR)}{(PR)^{\frac{5}{2}}}\right)\phi_\lambda(\alpha, \hat{r}_1, \hat{r}_2)\,, \tag{10}$$

where A_λ are expansion coefficients and the radial wavefunctions F_λ satisfy the equation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}-1+\frac{\nu(\nu+1)}{\rho^2}\right)A_\lambda F_\lambda+2P^{-1}\sum_{\lambda'}\langle\lambda|2\mu V|\lambda'\rangle A_{\lambda'}F_{\lambda'}=0, \quad (11)$$

where $\nu=\lambda+\frac{3}{2}$. Equation (11) is a coupled system of equations for the radial waves which may be solved numerically, similar to those for close coupling calculations (see e.g. Burke and Seaton 1971).

For short-range regular potentials we have

$$\begin{aligned} F_\lambda(\rho) &\sim c_\lambda \rho^{\nu+1}, \quad \rho\to 0 \\ &\sim \sin(\rho-\nu\pi/2+\eta_\lambda), \quad \rho\to\infty. \end{aligned}$$

The A_λ are still unknown in equation (10). To determine these we next consider a partial wave decomposition of plane waves which results in the absence of any interaction.

(2c) Resolution of Three-particle Plane Waves in Partial Waves

Plane waves may be expanded as

$$\begin{aligned}(2\pi)^{-3}\exp(\mathrm{i}\boldsymbol{p}_1\cdot\boldsymbol{r}_1+\mathrm{i}\boldsymbol{p}_2\cdot\boldsymbol{r}_2)=\frac{2}{\pi}\sum_{l_1l_2m_1m_2}&(2l_1+1)(2l_2+1)\mathrm{i}^{l_1+l_2}j_{l_1}(p_1r_1)\,j_{l_2}(p_2r_2)\\ &\times Y^*_{l_1m_1}(\hat{p}_1)\,Y^*_{l_2m_2}(\hat{p}_2)\,Y_{l_1m_1}(\hat{r}_1)\,Y_{l_2m_2}(\hat{r}_2). \quad (12)\end{aligned}$$

Since we have

$$\begin{aligned} r_1&=R\cos\alpha, \qquad r_2=R\sin\alpha,\\ p_1&=P\cos\alpha_0, \qquad p_2=P\sin\alpha_0 \end{aligned} \quad (13)$$

the two spherical Bessel functions in equation (12) may be expressed in terms of a single such function in view of the identity

$$\begin{aligned} j_{l_1}(\rho\cos\alpha\cos\alpha_0)\,j_{l_2}(\rho\sin\alpha\sin\alpha_0)=\sqrt{\frac{\pi}{2}}\,\frac{1}{\rho^{3/2}}&\sum_{n=0}^{\infty}(-1)^n j_{2n+l_1+l_2+\frac{3}{2}}(\rho)\\ &\times P_n^{l_1l_2}(\alpha_0)\,P_n^{l_1l_2}(\alpha), \end{aligned} \quad (14)$$

which is easily derived from equation (8) of Erdélyi (1953).

Then equation (12) takes the form

$$\begin{aligned}(2\pi)^{-3}\exp(\mathrm{i}\boldsymbol{p}_1\cdot\boldsymbol{r}_1+\mathrm{i}\boldsymbol{p}_2\cdot\boldsymbol{r}_2)=\sqrt{\frac{2}{\pi}}\sum_{l_1l_2m_1m_2n}&\mathrm{i}^\lambda\frac{j_\nu(PR)}{(PR)^{3/2}}P_n^{l_1l_2}(\alpha_0)\,P_n^{l_1l_2}(\alpha)\\ &\times Y^*_{l_1m_1}(\hat{p}_1)\,Y^*_{l_2m_2}(\hat{p}_2)\,Y_{l_1m_1}(\hat{r}_1)\,Y_{l_2m_2}(\hat{r}_2).\end{aligned}$$

It can be shown that

$$\sum_{m_1 m_2} Y^*_{l_1 m_1}(\hat{p}_1)\, Y^*_{l_2 m_2}(\hat{p}_2)\, Y_{l_1 m_1}(\hat{r}_1)\, Y_{l_2 m_2}(\hat{r}_2) = \sum_{lm} \mathcal{Y}^{lm*}_{l_1 l_2}(\hat{p}_1,\hat{p}_2)\, \mathcal{Y}^{lm}_{l_1 l_2}(\hat{r}_1,\hat{r}_2)\,.$$

So we have finally

$$(2\pi)^{-3}\exp(\mathrm{i}\boldsymbol{p}_1\cdot\boldsymbol{r}_1+\mathrm{i}\boldsymbol{p}_2\cdot\boldsymbol{r}_2) = \sqrt{\frac{2}{\pi}}\sum_{l_1 l_2 lmn} \mathrm{i}^\lambda \frac{j_\nu(PR)}{(PR)^{3/2}} \times \phi^*_\lambda(\alpha_0,\hat{p}_1,\hat{p}_2)\,\phi_\lambda(\alpha,\hat{r}_1,\hat{r}_2)\,, \tag{15}$$

which appears to be an interesting result.

(2d) Three-particle Scattering State

Now after obtaining the partial wave expansion of plane waves, it is a relatively easy matter to write a formal expression for the full wave, which has only incoming converging waves and outgoing plane waves, as

$$\Psi_{\mathrm{f}}^{(-)}(R,\alpha,\hat{r}_1,\hat{r}_2) = \sqrt{\frac{2}{\pi}}\sum_{l_1 l_2 lmn} \mathrm{i}^\lambda\, \mathrm{e}^{-\mathrm{i}\eta_\lambda}\frac{F_\lambda(PR)}{(PR)^{5/2}}\,\phi_\lambda(\alpha_0,\hat{p}_1,\hat{p}_2)\,\phi_\lambda(\alpha,\hat{r}_1,\hat{r}_2) \tag{16}$$

Since $F_\lambda(\rho)\sim\sin(\rho-\nu\pi/2+\eta_\lambda)$ as $\rho\to\infty$, one may easily verify that in the asymptotic region the wave (16) has only incoming converging waves, the outgoing diverging waves combining into a plane wave because of the identity (15).

The result (16) may easily be extended to cases when the particles have spin, when two or more particles are identical and when the two-body forces are spin-dependent.

We next consider the case of ionisation of hydrogen atoms by electrons when long-range forces make the problem a little more complicated.

Electron–Hydrogen Atom Ionisation Collision

If the atomic nucleus is considered infinitely heavy, the centre-of-mass and laboratory frames coincide and $\boldsymbol{r}_1,\boldsymbol{r}_2$ become simply the coordinates of the atomic electron and the incident electron and $\boldsymbol{p}_1,\boldsymbol{p}_2$ become their canonical momenta. Then we have

$$V(\boldsymbol{r}_1,\boldsymbol{r}_2) = -\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{r_{12}} = \frac{1}{R}C(\alpha,\hat{r}_1,\hat{r}_2)\,, \tag{17a}$$

where

$$C(\alpha,\hat{r}_1,\hat{r}_2) = -\frac{1}{\cos\alpha}-\frac{1}{\sin\alpha}+\frac{1}{|\hat{r}_1\cos\alpha-\hat{r}_2\sin\alpha|}\,, \tag{17b}$$

and the equation for F_λ becomes

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}+1-\frac{\nu(\nu+1)}{\rho^2}\right)A_\lambda F_\lambda + \frac{2P^{-1}}{\rho}\sum_{\lambda'}\langle\lambda|C|\lambda'\rangle A_{\lambda'}F_{\lambda'} = 0\,. \tag{18}$$

Now the off-diagonal elements $C_{\lambda\lambda'} = \langle\,\lambda|C|\lambda'\,\rangle$ $(\lambda \neq \lambda')$ are known (Lin 1974) to be generally small compared with the diagonal elements so, as a good approximation, one may choose F_λ to satisfy the equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + 1 - \frac{\nu(\nu+1)}{\rho^2} + \frac{2\alpha_\lambda}{\rho}\right) F_\lambda(\rho) = 0\,, \tag{19}$$

where $\alpha_\lambda = P^{-1}C_{\lambda\lambda}$. The solution $F_\lambda^{(0)}$ of (19) is nothing but a Coulomb wave with a variable charge $C_{\lambda\lambda}$. This appears to be an interesting and reasonable result, since different partial waves see different nuclear charges. The accuracy of the actual computed results remains to be seen. Even if the corresponding full wave

$$\Psi_{0\mathrm{f}}^{(-)}(R,\alpha,\hat{r}_1,\hat{r}_2) = \sqrt{\frac{2}{\pi}} \sum_{l_1 l_2 l m n} \mathrm{i}^\lambda\, \mathrm{e}^{-\mathrm{i}\eta_\lambda}\, \phi_\lambda^*(\alpha_0,\hat{p}_1,\hat{p}_2)\, \phi_\lambda(\alpha,\hat{r}_1,\hat{r}_2) \\ \times\, F_\lambda^{(0)}(PR)/(PR)^{5/2}\,, \tag{20a}$$

where

$$F_\lambda^{(0)}(PR) = \frac{\mathrm{e}^{\frac{1}{2}\pi\alpha_\lambda}|\Gamma(\nu+1+\mathrm{i}\alpha_\lambda)|}{\Gamma(2\nu+2)}\, 2^\nu (PR)^{\nu+1}\, \mathrm{e}^{-\mathrm{i}PR} \\ \times\, {}_1F_1(\mathrm{i}\alpha_\lambda + \nu + 1, 2\nu+2, 2\mathrm{i}PR)\,, \tag{20b}$$

with the asymptotic form

$$F_\lambda^{(0)}(PR) \sim \sin(PR - \nu\pi/2 + \alpha_\lambda \ln 2PR + \eta_\lambda)\,, \tag{20c}$$

fails to give satisfactory results for the scattering amplitude in conjunction with equation (1), one may adjust the α_λ suitably (a few of them) and proceed to represent the scattering amplitude analytically [consider in this connection the attempt by Bransden *et al.* (1978) with their distorted wave calculation].

The now symmetrised state corresponding to $\Psi_{0\mathrm{f}}^{(-)}$ is

$$\Psi_{0\mathrm{s}}^{(-)}(R,\alpha,\hat{r}_1,\hat{r}_2) = \sqrt{\tfrac{1}{2}}\{\Psi_{0\mathrm{f}}^{(-)}(R,\alpha,\hat{r}_1,\hat{r}_2) + (-1)^S \Psi_{0\mathrm{f}}^{(-)}(R,\pi/2-\alpha,\hat{r}_2,\hat{r}_1)\}\,, \tag{21}$$

where $S=0$ corresponds to the singlet and $S=1$ to the triplet state for ionisation of hydrogen atoms. The corresponding scattering amplitudes are given by

$$f^{(S)} = -(2\pi)^2\,\langle\,\Psi_{0\mathrm{s}}^{(-)}|V_\mathrm{i}|\Phi_\mathrm{i}\,\rangle\,. \tag{22}$$

The differential cross section for the unpolarised beam is then given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega_1\,\mathrm{d}\Omega_2\,\mathrm{d}E_1} = \frac{p_1 p_2}{p_\mathrm{i}}(\tfrac{3}{4}|f^{(1)}|^2 + \tfrac{1}{4}|f^{(0)}|^2)\,. \tag{23}$$

The result may possibly be further improved by solving a large number of the coupled equations in (18) numerically (see Burke and Seaton 1971) and then using the resultant radial waves in equation (16) to represent the final scattering state. A numerical study is now in progress and the results will be reported later.

3. Conclusions

We have succeeded in representing a three-particle continuum state in partial waves in hyperspherical coordinates. From the analysis it appears that hyperspherical coordinates are suitable for ionisation studies of three-body problems. Moreover, here we have a simple approximate result (equation 20) for the three-particle continuum state. How well it gives cross section results remains to be seen. Various extensions of the results are possible.

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