Eur. Phys. J. D **46**, 483–486 (2008)
DOI: 10.1140/epjd/e2007-00323-2

THE EUROPEAN
PHYSICAL JOURNAL D

A solution of the Coulomb three-body problem

S. Paul[a]

Theoretical Physics Division, Physical Research Laboratory, Navrangpura, Ahmedabad 380 009, India

Received 4 September 2007 / Received in final form 23 October 2007
Published online 28 November 2007 –

Abstract. In this work, a final state wave function is constructed which represents a solution of the three-body Schrödinger equation. The formulated wave function is superimposed of one basic analytical function with various parameters. The coefficients of these basic functions involved in final state wave function can be easily calculated from a set of linear equations. The coefficients depend only on incident energy of the system. The process can also be prolonged for application to the problems more than three bodies.

PACS. 34.80.Dp Atomic excitation and ionization by electron impact – 34.10.+x General theories and models of atomic and molecular collisions and interactions – 31.15.Ja Hyperspherical methods

1 Introduction

The combination of subtle correlation effects and the difficult boundary conditions required to describe two charged particles in the continuum have made 'three-body Coulomb problem' one of the outstanding challenges of atomic physics. Unfortunately, the Schrödinger equation that is fundamental to these problems, only possesses analytical solutions for two-body system, has no known analytical solution for three-body cases. It is a testament to the complexity of collision problems that proceeding from two-body collisions to a three-body system has taken almost a further century to formulate and solve numerically. The theories of Coulomb three-body problem can be classified into three groups. Firstly, those are based on 'Wannier theory' [1]. Secondly, there is a section of theories assuming approximate analytical expressions for the final state wave function in which the correlated motion of the three particles over all space is taken into account albeit in an approximate way. Thirdly, there are theories which abandon hope of an analytical or semi-analytical form, and work fully numerically with the aim of developing a method. At the commencement of collision theory, atomic physicists have used approximation techniques to find analytic and numerical solutions for Coulomb three-body problems, such as several Born approximation [2–4]. In 1960s, Peterkop [5], Rudge and Seaton [6,7] independently deduced the appropriate boundary conditions for electron-hydrogen-ionization but their boundary condition is extremely cumbersome to apply to numerical calculations. The leading term in the asymptotic expansion of the final state wave function, again for the case where all particles are well separated, was first obtained by Rosenberg [8]. In various close-coupling calculations [9–12], final state wave functions are expanded in terms of basis functions and ionization information are extracted from a solution of the unknown expansion functions. Kato and Watanabe [13,14] used hyperspherical coordinates and expanded the final state wave functions in terms of hyper-radius dependent angular functions. Matching with a wave function, which satisfies a roughly correct boundary condition, they obtained with remarkable success. Brauner et al. [15] and later Berakdar [16] and Berakdar et al. [17,18] made use of projection approach. They used the final state wave functions which are asymptotically correct (or nearly so) but are unlikely to be correct at finite distances. With the immense development of computational resources in the second half of the last century, there have been several very successful computational approaches to the three-body Coulomb problem like intermediate energy R-matrix method [19], R-matrix with pseudostates [12], time-dependent close-coupling [20], exterior complex scaling [21], convergent close-coupling [22], hyperspherical R-matrix method with semiclassical outgoing waves [23]. Another promising numerical approach for the electron-hydrogen atom ionization problem is the hyperspherical partial-wave approach [24–35], which is the base of the present work.

The goal of this investigation was threefold. Firstly, to construct a final state wave function for Coulomb three-body problem. Secondly, to construct a basis of state functions, these are generated final state wave function. Finally, study Coulomb N-body problems by using this approach. Here we prove that it is possible to generate a set of basis states to construct final state wave functions for Coulomb three-body problems, satisfy at the finite distances. The coefficients of the basis state functions are independent of any variable and can be obtained to solve a homogeneous system of linear equations.

[a] e-mail: spaul@prl.res.in

2 Formulation of final state wave function

For precise information concerning Coulomb three-body problems, one may solve accurately the Schrödinger equation for the scattering states $\Psi_f^{(-)}$ (see Newton [36] for definition) given by

$$H\Psi_f^{(-)} = E\Psi_f^{(-)} \tag{1}$$

taking account of the appropriate boundary conditions. In the hyperspherical partial wave theory $\Psi_f^{(-)}$ is expanded in terms of hyperspherical harmonics, which are functions of five angular variables. The corresponding radial waves are functions of one radial variable, the hyper radius R only. The symmetrized wave $\Psi_{fs}^{(-)}$ may be expanded in terms of symmetrized hyperspherical harmonics ϕ_λ^s's as [24,29]

$$\Psi_{fs}^{(-)}(R,\omega) = 2\sqrt{\frac{2}{\pi}}\sum_\lambda \frac{F_\lambda^s(\rho)}{\rho^{\frac{5}{2}}}\,\phi_\lambda^s(\omega), \tag{2}$$

where F_λ^s satisfies an infinite coupled set of equations

$$\left[\frac{d^2}{d\rho^2} + 1 - \frac{\nu_\mu\,(\nu_\mu+1)}{\rho^2}\right] F_\lambda^s(\rho) + \sum_{\lambda'} \frac{2\,\alpha_{\lambda\lambda'}^s}{\rho}\, F_{\lambda'}^s(\rho) = 0, \tag{3}$$

for each symmetry s ($s = 0$ for singlet and $s = 1$ for triplet)and for each total angular momentum L (and its projection M, and so also for a definite parity π). In the above expression

$$\begin{aligned}
\alpha_{\lambda\lambda'}^s &= -\langle\phi_\lambda^s|C|\phi_{\lambda'}^s\rangle/P, \text{ and}\\
C &= -\frac{1}{\cos\alpha} - \frac{1}{\sin\alpha} + \frac{1}{|\hat{r_1}\cos\alpha - \hat{r_2}\sin\alpha|};\\
\phi_\lambda^s(\omega) &= \frac{1}{\sqrt{2}}\{P_{l_1l_2}^n(\alpha)\mathcal{Y}_{l_1l_2}^{LM}(\hat{r_1},\hat{r_2})\\
&\quad +(-1)^{l_1+l_2-L+S+n}P_{l_2l_1}^n(\alpha)\mathcal{Y}_{l_2l_1}^{LM}(\hat{r_1},\hat{r_2})\},\\
&\quad l_1 \neq l_2\\
&= \frac{1}{2}\{1+(-1)^{-L+S+n}\}P_{ll}^n(\alpha)\mathcal{Y}_{ll}^{LM}(\hat{r_1},\hat{r_2})\},\\
&\quad \text{for } l_1 = l_2 = l,
\end{aligned} \tag{4}$$

where $\nu_\mu = \mu + \frac{3}{2}$ and $\mu = l_1 + l_2 + 2n$ (here λ denotes the multiplet (l_1, l_2, n) depending on the context). Here $R = \sqrt{r_1^2 + r_2^2}$, $\alpha = \text{atan}(r_2/r_1)$, $\vec{r_1} = (r_1, \theta_1, \phi_1)$, $\vec{r_2} = (r_2, \theta_2, \phi_2)$. Similarly $P = \sqrt{p_a^2 + p_b^2}$, $\alpha_0 = \text{atan}(p_b/p_a)$, $\vec{p_a} = (p_a, \theta_a, \phi_a)$, $\vec{p_b} = (p_b, \theta_b, \phi_b)$, and $\rho = PR$, and $\omega_0 = (\alpha_0, \theta_a, \phi_a, \theta_b, \phi_b)$, and a corresponding expression for $\phi_\lambda^s(\omega_0)$ (similar expressions may be easily derived for product of more than two outgoing charged particles). Now we set

$$F_\lambda^s(\rho) = \rho\sum_k a_{\lambda k}^s j_k(\rho) + \rho\sum_l b_{\lambda l}^s j_{l+1/2}(\rho) \tag{5}$$

where all $a_{\lambda k}^s$ and $b_{\lambda l}^s$ are independent of ρ, for the above expression of F_λ^s equation (3) reduces to

$$\begin{aligned}
&\sum_{k=0}\left[\frac{1}{\rho}j_k(\rho)\left\{\left(k-\mu-\frac{3}{2}\right)\left(k+\mu+\frac{5}{2}\right)\right\}a_{\lambda k}^s\right.\\
&\left.\quad +2j_k(\rho)\sum_{\lambda'}\alpha_{\lambda\lambda'}^s a_{\lambda' k}^s\right] + \sum_{l=0}\left[\frac{1}{\rho}j_{l+1/2}(\rho)\{(l-\mu-1)\right.\\
&\left.\quad \times(l+\mu+3)\}b_{\lambda l}^s + 2j_{l+1/2}(\rho)\sum_{\lambda'}\alpha_{\lambda\lambda'}^s b_{\lambda' l}^s\right] = 0.
\end{aligned} \tag{6}$$

For convenience we again set,

$$\begin{aligned}
\left\{\left(k-\mu-\frac{3}{2}\right)\left(k+\mu+\frac{5}{2}\right)\right\}a_{\lambda k}^s &= A_{\lambda k}\\
2\sum_{\lambda'}\alpha_{\lambda\lambda'}^s a_{\lambda' k}^s &= \Gamma_{\lambda k}\\
\{(l-\mu-1)(l+\mu+3)\}b_{\lambda l}^s &= B_{\lambda l}\\
2\sum_{\lambda'}\alpha_{\lambda\lambda'}^s b_{\lambda' l}^s &= \Delta_{\lambda l}.
\end{aligned} \tag{7}$$

Then equation (6) reduces to

$$\begin{aligned}
&\sum_{k=0}\left[\frac{1}{\rho}j_k(\rho)A_{\lambda k} + j_k(\rho)\Gamma_{\lambda k}\right]\\
&\quad + \sum_{l=0}\left[\frac{1}{\rho}j_{l+1/2}(\rho)B_{\lambda l} + j_{l+1/2}(\rho)\Delta_{\lambda l}\right] = 0.
\end{aligned} \tag{8}$$

Using the expansions of spherical Bessel functions

$$j_k(\rho) = \sum_{n=0} C_{nk}\rho^{2n+k} \text{ and } j_{l+1/2}(\rho) = \sqrt{\rho}\sum_{n=0}\bar{C}_{nl}\rho^{2n+l}$$

equation (8) becomes

$$\begin{aligned}
&\sum_{n,k}\left[M_{nk}^\lambda\rho^{2n+k-1} + N_{nk}^\lambda\rho^{2n+k}\right]\\
&\quad + \sqrt{\rho}\sum_{m,l}\left[\bar{M}_{ml}^\lambda\rho^{2m+l-1} + \bar{N}_{ml}^\lambda\rho^{2m+l}\right] = 0
\end{aligned} \tag{9}$$

where

$$\begin{aligned}
M_{nk}^\lambda &= A_{\lambda k}C_{nk}, \quad N_{nk}^\lambda = \Gamma_{\lambda k}C_{nk},\\
\bar{M}_{ml}^\lambda &= B_{\lambda l}\bar{C}_{ml}, \quad \bar{N}_{ml}^\lambda = \Delta_{\lambda l}\bar{C}_{ml}.
\end{aligned}$$

After simplification we have

$$X(\rho) + \sqrt{\rho}Y(\rho) = 0 \tag{10}$$

where

$$\begin{aligned}
X(\rho) &= M_{0,0}^\lambda\frac{1}{\rho} + \sum_{k=0}\sum_{n=0}^{k}\left[M_{n,2k+1-2n}^\lambda + N_{n,2k-2n}^\lambda\right]\rho^{2k}\\
&\quad + \sum_{k=0}\left[\sum_{n=0}^{k+1}M_{n,2k+2-2n}^\lambda + \sum_{n=0}^{k}N_{n,2k+1-2n}^\lambda\right]\rho^{2k+1}
\end{aligned} \tag{11}$$

and

$$Y(\rho)=\bar{M}_{0,0}^{\lambda}\frac{1}{\rho}+\sum_{l=0}\sum_{m=0}^{l}\left[\bar{M}_{m,2l+1-2m}^{\lambda}+\bar{N}_{m,2l-2m}^{\lambda}\right]\rho^{2l}$$

$$+\sum_{l=0}\left[\sum_{m=0}^{l+1}\bar{M}_{m,2l+2-2m}^{\lambda}+\sum_{m=0}^{l}\bar{N}_{m,2l+1-2m}^{\lambda}\right]\rho^{2l+1}. \quad (12)$$

Equating the coefficients of like power of ρ in equation (10), we get two sets of recurrence relations for $a_{\lambda k}^{s}$ and $b_{\lambda l}^{s}$.

Recurrence relations for $a_{\lambda k}^{s}$s are

$$A_{\lambda 0}C_{00}=0$$

$$\sum_{n=0}^{k}\left[A_{\lambda,2k+1-2n}C_{n,2k+1-2n}+\Gamma_{\lambda,2k-2n}C_{n,2k-2n}\right]=0$$

$$\sum_{n=0}^{k+1}A_{\lambda,2k+2-2n}C_{n,2k+2-2n}$$

$$+\sum_{n=0}^{k}\Gamma_{\lambda,2k+1-2n}C_{n,2k+1-2n}=0; \quad (13)$$

and recurrence relations for $b_{\lambda l}^{s}$s are

$$B_{\lambda 0}\bar{C}_{00}=0$$

$$\sum_{m=0}^{l}\left[B_{\lambda,2l+1-2m}\bar{C}_{m,2l+1-2m}+\Delta_{\lambda,2l-2m}\bar{C}_{m,2l-2m}\right]=0$$

$$\sum_{m=0}^{l+1}B_{\lambda,2l+2-2m}\bar{C}_{m,2l+2-2m}$$

$$+\sum_{m=0}^{l}\Delta_{\lambda,2l+1-2m}\bar{C}_{m,2l+1-2m}=0. \quad (14)$$

The recurrence relations for $a_{\lambda k}^{s}$ and $b_{\lambda l}^{s}$ imply that all the coefficients $a_{\lambda k}^{s}$ are equal to zero and the coefficients $b_{\lambda l}^{s}$ are nonzero for $l\geq\mu+1$. Finally, the symmetrized final state wave function can be written in terms of hyperspherical harmonics and spherical bessel functions as

$$\Psi_{fs}^{(-)}(\rho,\omega)=2\sqrt{\frac{2}{\pi}}\sum_{\lambda,l=\mu+1}\frac{b_{\lambda l}^{s}}{\rho^{\frac{3}{2}}}\,j_{l+1/2}(\rho)\phi_{\lambda}^{s}(\omega), \quad (15)$$

or one can write the unsymmetrized final state wave function as

$$\Psi_{f}^{(-)}(r_1,r_2;\hat{r}_1,\hat{r}_2)=\sqrt{\frac{2}{\pi}}\sum_{\lambda,l=\mu+1}b_{\lambda l}f_{\lambda l}(r_1,r_2)\mathcal{Y}_{l_1 l_2}^{LM}(\hat{r}_1,\hat{r}_2), \quad (16)$$

where the radial wave function for two charged particles is

$$f_{\lambda l}(r_1,r_2)=\frac{1}{(P\sqrt{r_1^2+r_2^2})^{3/2}}j_{l+1/2}\left(P\sqrt{r_1^2+r_2^2}\right)P_{l_1 l_2}^{n}(\mathrm{atan}(r_2/r_1)). \quad (17)$$

3 Calculation

In this section, as an illustration we calculated the coefficient of $b_{\lambda l}^{s}$ from the recurrence relations (14)

$$B_{\lambda 0}\bar{C}_{00}=0. \quad (18)$$

For $l=0$,

$$B_{\lambda 1}\bar{C}_{01}+\Delta_{\lambda 0}\bar{C}_{00}=0$$
$$B_{\lambda 2}\bar{C}_{02}+B_{\lambda 0}\bar{C}_{10}+\Delta_{\lambda 1}\bar{C}_{01}=0. \quad (19)$$

For $l=1$,

$$B_{\lambda 3}\bar{C}_{03}+\Delta_{\lambda 2}\bar{C}_{02}+B_{\lambda 1}\bar{C}_{11}+\Delta_{\lambda 0}\bar{C}_{10}=0$$
$$B_{\lambda 4}\bar{C}_{04}+B_{\lambda 2}\bar{C}_{12}+B_{\lambda 0}\bar{C}_{20}+\Delta_{\lambda 3}\bar{C}_{03}+\Delta_{\lambda 1}\bar{C}_{11}=0. \quad (20)$$

It follows from equation (7); if $i\neq\mu+1$ for $l=i$, $B_{\lambda i}=0$ implies $b_{\lambda i}^{s}=0$ and this value of $b_{\lambda i}^{s}$ corresponds to $\Delta_{\lambda i}=0$. Let us consider $\mu=1$, i.e., the first nonzero coefficient is $b_{\lambda 2}^{s}$.

From equation (18), we get $B_{\lambda 0}=0$ which corresponds to $b_{\lambda 0}^{s}=0$ and $\Delta_{\lambda 0}=0$.

It follows from equation (19a), $B_{\lambda 1}=0$ which implies $b_{\lambda 1}^{s}=0$ and $\Delta_{\lambda 1}=0$.

Using the above values the set of equations (20) reduce to

$$B_{\lambda 3}\bar{C}_{03}+\Delta_{\lambda 2}\bar{C}_{02}=0$$
$$B_{\lambda 4}\bar{C}_{04}+\Delta_{\lambda 3}\bar{C}_{03}=0 \quad (21)$$

or, rewrite the values of $B_{\lambda 3}$, $B_{\lambda 4}$, $\Delta_{\lambda 2}$ and $\Delta_{\lambda 3}$ in the above equations we have

$$7\bar{C}_{03}b_{\lambda 3}^{s}+2\bar{C}_{02}\sum_{\lambda'}\alpha_{\lambda\lambda'}^{s}b_{\lambda' 2}^{s}=0$$
$$16\bar{C}_{04}b_{\lambda 4}^{s}+2\bar{C}_{03}\sum_{\lambda'}\alpha_{\lambda\lambda'}^{s}b_{\lambda' 2}^{s}=0. \quad (22)$$

So, ultimately we can calculate $b_{\lambda l}^{s}$ (for $l\geq 3$) in terms of $b_{\lambda 2}^{s}$ and the values of $b_{\lambda 2}^{s}$s depend on boundary condition.

4 Discussion

To construct the final state wave function, we produce a basis set of analytical functions $\{\rho^{-\frac{3}{2}}\,j_{l+1/2}(\rho)\,\phi_{\lambda}^{s}(\omega)\}$. The final wave function is a linear combination of the basic analytical functions and the coefficients $b_{\lambda l}^{s}$ can be calculated easily to solve the system of linear equations. From basic wave function with different sets of parameters we can analyze the processes precisely. The nature of the basic functions with different sets of parameters is very important to study any Coulomb three-body problems. The radial parts $f_{\lambda l}(r_1,r_2)$ (for various values of λ and l) of the unsymmetrized final state wave function for $P=1$ and $l=\mu+1$ are presented in Figure 1 for $l_1=1$, $l_2=1$ and $n=3$; in Figure 2 for $l_1=10$, $l_2=1$ and $n=3$; and in Figure 3 for $l_1=1$, $l_2=10$ and $n=3$.

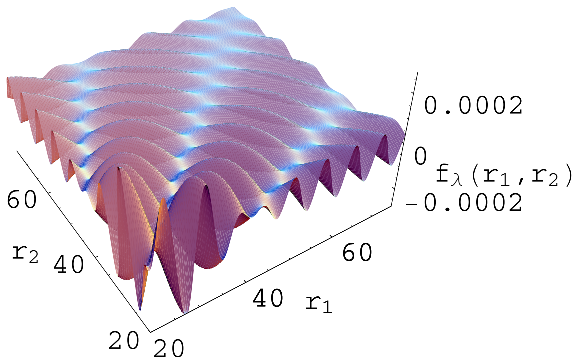

Fig. 1. (Color online) Radial part $f_{\lambda l}(r_1, r_2)$ of the unsymmetrized final state wave function for $l_1 = 1$, $l_2 = 1$, $n = 3$, $l = \mu + 1$ and $P = 1$.

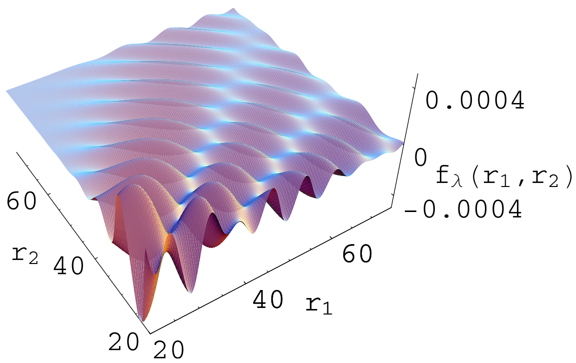

Fig. 2. (Color online) Radial part $f_{\lambda l}(r_1, r_2)$ of the unsymmetrized final state wave function for $l_1 = 10$, $l_2 = 1$, $n = 3$, $l = \mu + 1$ and $P = 1$.

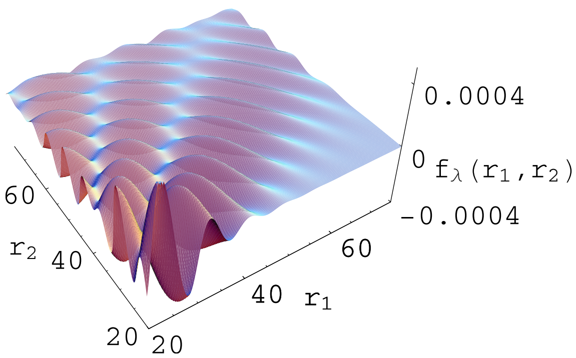

Fig. 3. (Color online) Radial part $f_{\lambda l}(r_1, r_2)$ of the unsymmetrized final state wave function for $l_1 = 1$, $l_2 = 10$, $n = 3$, $l = \mu + 1$ and $P = 1$.

5 Conclusion

Using this approach, one can easily calculate final state wave function for Coulomb three-body problems without taking any approximation. Here we considered Coulomb three-body problems only, it should be noted that the method can be extended for Coulomb N-body problems. Our future plan is to study the system of linear equations: its necessary order, convergent condition, essential triplets, generalized the process for N-body system, i.e., calculate the corresponding hyperspherical harmonics for N-body system.

References

1. J.M. Feagin, J. Phys. B **28**, 1495 (1995)
2. H.S.W. Massey, C.O.B. Mohr, Proc. R. Soc. A **146**, 880 (1934)
3. N.F. Mott, H.S.W. Massey, *Theory of Atomic Collisions*, 2nd edn. (Clarendon Press, Oxford, 1949)
4. K. Omidvar, Phys. Rev. A **140**, 26 (1965)
5. R.K. Peterkop, Opt. Spectrosc. **13**, 87 (1962)
6. M.R.H. Rudge, M.J. Seaton, Proc. R. Phys. Soc. **283**, 262 (1965)
7. M.R.H. Rudge, Rev. Mod. Phys. **40**, 564 (1968)
8. L. Rosenberg, Phys. Rev. D **8**, 1833 (1973)
9. E.P. Curran, H.R.J. Walters, J. Phys. B **20**, 337 (1987)
10. E.P. Curran, C.T. Whelan, H.R.J. Walters, J. Phys. B **24**, L19 (1991)
11. K. Bartchat et al., J. Phys. B **29**, 115 (1996)
12. K. Bartschat, I. Bray, J. Phys. B **29**, L577 (1996)
13. D. Kato, S. Watanabe, Phys. Rev. Lett. **74**, 2443 (1995)
14. D. Kato, S. Watanabe, Phys. Rev. A **56**, 3687 (1997)
15. M. Brauner, J.S. Briggs, H. Klar, J. Phys. B **22**, 2265 (1989)
16. J. Berakdar, Phys. Rev. A **53**, 2314 (1996)
17. J. Berakdar, J. Röder, J.S. Briggs, H. Ehrhardt, J. Phys. B **29**, 6203 (1996)
18. J. Berakdar, J.S. Briggs, I. Bray, D.V. Fursa, J. Phys. B **32**, 895 (1999)
19. T.T. Scholz, H.R.J. Walters, M.P. Scott, P.G. Burke, J. Phys. B **24**, 2097 (1991)
20. J. Colgan et al., Phys. Rev. A **65**, 042721 (2002)
21. T.N. Rescigno, M. Baertschy, W.A. Isaacs, C.W. McCurdy, Science **286**, 2474 (1999)
22. I. Bray, A.T. Stelbovics, Phys. Rev. A **46**, 6995 (1992)
23. L. Malegat, P. Selles, A.K. Kazansky, Phys. Rev. Lett. **85**, 4450 (2000)
24. J.N. Das, Pramana-J. Phys. **50**, 53 (1998)
25. J.N. Das, K. Chakrabarti, Pramana-J. Phys. **47**, 249 (1996)
26. J.N. Das, K. Chakrabarti, Phys. Rev. A **56**, 365 (1997)
27. J.N. Das, Phys. Rev. A **64**, 054703 (2001)
28. J.N. Das, J. Phys. B **35**, 1165 (2002)
29. J.N. Das, S. Paul, K. Chakrabarti, Phys. Rev. A **67**, 042717 (2003)
30. J.N. Das, S. Paul, K. Chakrabarti, AIP-Conf. Proc. **697**, 82 (2003)
31. J.N. Das, K. Chakrabarti, S. Paul, J. Phys. B **36**, 2707 (2003)
32. J.N. Das, K. Chakrabarti, S. Paul, Phys. Lett. A **316**, 400 (2003)
33. J.N. Das, K. Chakrabarti, S. Paul, Phys. Rev. A **69**, 044702 (2004)
34. J.N. Das, S. Paul, K. Chakrabarti, Phys. Rev. A **72**, 022725 (2005)
35. J.N. Das, S. Paul, K. Chakrabarti, Eur. Phys. J. D **39**, 223 (2006)
36. R.G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966)
37. A. Erdelyi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. II
38. J.N. Das, Aust. J. Phys. **47**, 743 (1994)