Asymptotic Solutions for the Two-Centre Coulomb Continuum Problem.

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1 Introduction

The understanding and modeling of electrons moving in the fields of two fixed charges plays an important role in electron-molecule, slow meson-atom collisions and more generally in deflection experiments.

The Hamiltonian of the Coulomb two-centre problem separates in prolate spheroidal coordinates. [1,2]. A number of numerical methods for solving these equations both of discrete and continuum spectrum were developed. However, the solutions in spheroidal coordinates no contain any information about the momentum of the scattered electron. So, if we want to obtain a double differential cross sections for slow $M^- + A$ collisions, it is impossible to utilize these solutions to describe the electron in the final channel.

On the other hand, the three-body Coulomb problem with all three particles in the continuum has been studied extensively and in resent years some progress has been made. Using momentum dependent effective charges approximate solutions have been constructed by Tergiman [3] and Greenland *et al* [4] while Komarov *et al* [5] used an asymptotic Coulomb phase factor to describe the interaction between the particles, and Brauner Briggs and Klar (BBK) [6] represented this interaction by confluent hypergeometric functions. All of these solutions were constructed on the assumption that the distances between any two particles tends to infinity long after the collision.

It was recently shown by Alt and Mukhamedzhanov [7] that in the ca where all three distances tends to infinity while the ration between an two distances vanishes, the solutions by [3,4,6] fails to approach the corre asymptotic form. Describing the relative motion of the two closer particl by a momentum which depends on the position of the third particle. Alt an Mukhamedzhanov [7] obtained an asymptotically correct solution.

The wave function for an electron in the field of two fixed charges might a first be expected to correspond to the solution by Alt and Mukhamedzhano [7] in the limit of vanishing relative momentum between the two closer par ticles. This is however not the case since this momentum always depends o the position of the third particle.

It is the aim of this paper to study the wave function for a particle i the *fixed* two-centre field since this solution is not included in the state mentioned above.

2 The wave function for an electron in the field of two fixed charges

We consider a system of an incoming electron on two scattering centres The vector pointing from centre 1 to centre 2 is R. The vector pointing from centre i to the electron is written $\mathbf{r}_i$, while the vector pointing from the geometrical centre between the two centres to the electron is r. The momentum of the electron, that is the conjugated coordinate of r, is written as k.

The relation between $\mathbf{r}$,$\mathbf{r}_1$ and $\mathbf{r}_2$ are given by

$$\mathbf{r}_1 = \mathbf{R}/2 + \mathbf{r} \qquad \mathbf{r}_2 = \mathbf{r} - \mathbf{R}/2 \tag{1}$$

It is from eq. 1 readily seen that $\nabla_{\mathbf{r}} = \nabla_{\mathbf{r}_1} = \nabla_{\mathbf{r}_2}$. The Hamiltonian of the problem is given by

$$H = -\tfrac{1}{2}\nabla_{\mathbf{r}}^2 - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} =$$

$$= -\frac{1}{2}\nabla_{\mathbf{r}_1}^2 - \frac{1}{2}\nabla_{\mathbf{r}_2}^2 - \nabla_{\mathbf{r}_1}\nabla_{\mathbf{r}_2} - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} \tag{2}$$

Suppose the wave function can be written as a product wave function $\Psi_k^+(\mathbf{r}) = \psi(\mathbf{r}_1)\psi(\mathbf{r}_2)$, where $\psi(\mathbf{r}_i) = \exp(ikr_i/2)Q_i(\mathbf{r}_i)$. In this case the Schrödinger equation for 2 is written as follows:

$$Q_2\{\tfrac{1}{2}\Delta Q_1 + ik\nabla Q_1 + \tfrac{Z_1}{r_1}Q_1\} + Q_1\{\tfrac{1}{2}\Delta Q_2 + ik\nabla Q_2 + \tfrac{Z_2}{r_2}Q_2\} + (\nabla Q_1)(\nabla Q_2) = 0 \quad (3)$$

where the energy of the electron is given by $E = \frac{1}{2}k^2$.

2.1 The BBK Approximation

The Brauner, Brigss and Klar (BBK) approximation consists of neglecting the term $(\nabla Q_1)(\nabla Q_2)$ from eq. 3. This enables us to separate the $\mathbf{r}_1$ and $\mathbf{r}_2$ dependence and eq. 3 reduces to

$$\frac{1}{2}\Delta Q_i + ik\nabla Q_i + \frac{Z_i}{r_i}Q_i = 0 \quad (4)$$

for $i = 1, 2$. This equation may be solved exactly as the Confluent Hypergeometric Function

$$Q_i(\mathbf{r}_i) = N(\nu_i)\,{}_1F_1(-i\nu_i, 1, i(kr_i - \mathbf{k}\mathbf{r}_i)) \quad (5)$$

where $N(\nu) = \Gamma(1+\nu)\exp(-\nu\pi/2)$ is the standard Gammow factor, and $\nu_i = -\frac{Z_i}{k}$ is the Sommerfeld parameter. The total scattering function, $\Psi_k^{+CDW}(\mathbf{r})$, is now given by

$$\Psi_k^+(\mathbf{r}) = \exp(ik\mathbf{r})N(\nu_1)N(\nu_2)\,{}_1F_1(-i\nu_1, 1, i(kr_1 - \mathbf{k}\mathbf{r}_1))* \\ *\,{}_1F_1(-i\nu_2, 1, i(kr_2 - \mathbf{k}\mathbf{r}_2)) \quad (6)$$

A similar state has been used by a number of authors (see *ex* [6,8]) to describe the electronic wave function for ionization processes in ion-atom collisions. It is however to our knowledge the first time the state has been suggested to describe an electron in the field of two fixed charges.

It is readily seen that the state in eq. 2.1 asymptotically satisfies the Schrödinger equation $(E-H)\Psi_k^+ = 0$ to order $O(\frac{1}{r^2})$, which in turn shows that

the wave function itself is correct asymptotically to order $O(\frac{1}{r})$. However, in practical calculations of the scattering amplitude it is not the asymptotic form but rather the behavior of the wave function for small r_1 or r_2 that matters. Writing $\Psi_{\mathbf{k}}$ as a function of r_1:

$$\Psi_{\mathbf{k}}(\mathbf{r}_i) = \exp(i\mathbf{k}\mathbf{r}_1)N(\nu_1)_1F_1(-i\nu_1, 1, i(kr_1 - \mathbf{k}\mathbf{r}_1))$$
$$\exp(i\mathbf{k}\tfrac{\mathbf{R}}{2})N(\nu_2)_1F_1(-i\nu_2, 1, i(k|\mathbf{r}_1 - \mathbf{R}| - \mathbf{k}(\mathbf{r}_1 - \mathbf{R}))) =$$
$$\psi^+_{\mathbf{k}}(\mathbf{r}_1) \times \exp(i\mathbf{k}\tfrac{\mathbf{R}}{2})N(\nu_2)_1F_1(-i\nu_2, 1, i(k|\mathbf{r}_1 - \mathbf{R}| - \mathbf{k}(\mathbf{r}_1 - \mathbf{R}))) \quad (7)$$

(where $\psi^+_{\mathbf{k}}(\mathbf{r}_1)$ is a Coulomb state in the field of Z_1), we easily show that the state in eq. 2.1 approaches the intuitive result of a Coulomb distorted state in the closer centre. The distortion on the Coulomb state, $\psi^+_{\mathbf{k}}(\mathbf{r}_1)$, in eq. 7 is for not too small R well approximated by

$$(k|\mathbf{r}_1 - \mathbf{R}| - \mathbf{k}(\mathbf{r}_1 - \mathbf{R}))^{i\nu_2} \exp(i\mathbf{k}\frac{\mathbf{R}}{2}). \quad (8)$$

which is only a slowly varying phase factor. The same in true in the small r_2 region.

2.2 The Eikonal Approximation

Assuming that Q_i does not vary rapidly with r_i and neglecting the Laplasian in eq. 3 we find a solution corresponding to the eikonal approximation

$$\Psi^{+Eik}_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}\mathbf{r})\exp(-\frac{i}{v}\int_C \frac{-Z_1}{r_1} + \frac{-Z_2}{r_2}\, dr') \quad (9)$$

Here v is the velocity of the incoming electron and the integration path, C, is taken from long before the collision along and approximate (sometimes the classical) trajectory of the electron to the position r. When the energy of the electron is far greater than the potential in which the electron is moving, $1/2k^2 \gg V(r)$, it may be valid to approximated the integration path, C, by a straight line. When the charges at the two centres are of similar magnitude but different sign, $Z = Z_1 = -Z_2$, the combined potential falls of as $V(\mathbf{r}) \approx \frac{Z\mathbf{R}\hat{\mathbf{r}}}{r^2}$ for larger $\mathbf{r}$. In this case it is particular valid to use the straight line approximation. In this case the integral in eq. 9 is easily evaluated and we find

$$\Psi^{+Eik}_{\mathbf{k}}(\mathbf{R}, \mathbf{r}) = \exp(i\mathbf{k}\mathbf{r})(k|\mathbf{r} + \tfrac{\mathbf{R}}{2}| + \mathbf{k}\mathbf{r} + \tfrac{\mathbf{k}\mathbf{R}}{2})^{i\nu_1}$$
$$(k|\mathbf{r} - \tfrac{\mathbf{R}}{2}| + \mathbf{k}\mathbf{r} - \tfrac{\mathbf{k}\mathbf{R}}{2})^{i\nu_2} \quad (10)$$

=ere we have included the constant phase factor $k^{i(\nu_1+\nu_2)}$.

It is readily seen that the asymptotic form of $\Psi_{\mathbf{k}}^{+Eik}(\mathbf{R},\mathbf{r})$ is given by the ⊃duct of two single centre eikonal approximations

$$\lim_{r\to\infty} \Psi_{\mathbf{k}}^{+Eik}(\mathbf{r}) = \exp(i\mathbf{kr})(kr-\mathbf{kr})^{i\nu_1}(kr-\mathbf{kr})^{i\nu_2} \qquad (11)$$

ain to order $O(\frac{1}{r})$. This is the correct asymptotic form for an electron in e potentia. of the combined field from the two Coulomb centres. However, explained above the asymptotic form is not important in calculations the scattering amplitude - except for identifying the momentum of the ≥ctron long after the collision. It is our understanding that state in the ▮. 10 contains important two centre dynamics which is not present in the ymptotic state in eq. 11.

Conclusion

'e have derived two different approximations for the two Coulomb-centre roblem. Both approximations have a correct form for all charges in the ymptotic region but differs at smaller distances. The first approximation BBK type and the second one is an eikonal two centre approximation. oth of these approximations factories into a product wave function where ich factor only depends on one coordinate. Combined with a plan wave to escribe the inter-nuclear motion the first approximation has been used by number of authors in describing ionization in ion-atom collisions. Due to ie factorization of the wave function it is possible in theories of the CDW-IK type [9] to separate the resulting six dimensional T-matrix integration i two three dimensional integrations. This is also possible with the other pproximation obtained here and interesting two centre effect might appear.

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6 References

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