Asymptotic solution of the Schrödinger equation for three charged particles

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An analytic asymptotic solution is derived for the Schrödinger equation for three charged particles in a continuum, for the case in which two of the particles are separated only slightly in comparison with the distance to the third.

In order to calculate the cross sections for various processes in which there are three charged particles in the final state (ionization in atomic physics and disintegration in nuclear physics), one must know the asymptotic behavior of the three-particle Coulomb scattering wave function in the case in which two of the particles are separated by a distance which is small in comparison with the distance to the third particle. In the present letter we offer an exceptionally simple analytic expression for the asymptotic solution of the Schrödinger equation in this case. This expression has not previously been known, although it has been under discussion in the literature for years now.[1,2]

We consider a system of three unbound charged particles with masses m_α and charges e_α, where $\alpha=1,2,3$. To describe this system we use Jacobi variables: $\mathbf{r}_\alpha$, which is the radius vector between particles β and γ (this is pair α); $\mathbf{k}_\alpha$, which is their relative momentum; $\mu_\alpha=m_\beta m_\gamma/m_{\beta\gamma}$, $\vec{\rho}_\alpha$, which is the radius vector between particle α and the center of mass of pair α; $\mathbf{q}_\alpha$, which is the relative momentum which is the canonical conjugate of $\vec{\rho}_\alpha$; and $M_\alpha=m_\alpha m_{\beta\gamma}/M$, where $M=\Sigma_{\alpha=1}^3 m_\alpha$, $m_{\beta\gamma}=m_\beta+m_\gamma$.

The Schrödinger equation describing a system of three charged particles in a continuum is

$$(E-T\mathbf{r}_\alpha-T_{\vec{\rho}_\alpha}-V)\Psi^{(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)=0, \tag{1}$$

where $E=k_\alpha^2/2\mu_\alpha+q_\alpha^2/2M_\alpha$ $(\alpha=1,2,3)$ is the total energy of this system; and $V=\Sigma_{\alpha=1}^3 V_\alpha$, where V_α is the potential between the particles of pair α. For simplicity we assume for the time being that this is a purely Coulomb potential: $V_\alpha=V_\alpha^c$. We also have $T\mathbf{r}_\alpha=-(1/2\mu_\alpha)\Delta\mathbf{r}_\alpha$ and $T_{\vec{\rho}_\alpha}=-(1/2M_\alpha)\Delta_{\vec{\rho}_\alpha}$. We are using a system of units with $\hbar=c=1$.

We define some asymptotic regions: (1) Ω_0. In this region we have $r_\alpha\to\infty$, for all α $(\alpha=1,2,3)$, but in no case do we have a ratio $r_\alpha/\rho_\alpha\to 0$. In other words, all the particles are far apart. (2) Ω_α. In this region, the particles of pair α are separated only slightly; i.e., we have $r_\alpha/\rho_\alpha\to 0$ and $\rho_\alpha\to\infty$. The value of r_α may also go off toward ∞, but more slowly than ρ_α.

In leading order (within terms $\sim r_\alpha/\rho_\alpha^2$) we find an asymptotic equation in Ω_α from (1):

$$(E-T\mathbf{r}_\alpha-T_{\vec{\rho}_\alpha}-V_\alpha^C-v_\alpha^C)\Psi^{(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)=0, \tag{2}$$

where $v_\alpha^C(\rho_\alpha)=e_{\beta\gamma}e_\alpha/\rho_\alpha$ and $e_{\beta\gamma}=e_\beta+e_\gamma$. We cannot ignore v_α^C in (2), since in the limit $\rho_\alpha\to\infty$ it falls off too slowly, and it affects the asymptotic behavior in the wave function. By the "asymptotic solution" of Eq. (1) in Ω_α we mean a solution which satisfies (2) within terms $\sim 1/\rho_\alpha^2$, r_α/ρ_α^2 (for simplicity below we will write only $\sim 1/\rho_\alpha^2$) and which is simultaneously the leading term of the asymptotic behavior of the solution of Eq. (1), $\Psi^{(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)$, in region Ω_α. The latter is a very important circumstance, since the asymptotic solution of Eq. (2) is not single valued. For example, for (2) in separated-variables form, one of its solutions is

$$\Phi_0^{(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)=\psi_{C,\mathbf{k}_\alpha}^{(+)}(\mathbf{r}_\alpha)\bar{\psi}_{C,\mathbf{q}_\alpha}^{(+)}(\vec{\rho}_\alpha). \tag{4}$$

Here $\psi_{C,\mathbf{k}_\alpha}^{(+)}(\bar{\psi}_{C,\mathbf{q}_\alpha}^{(+)})$ is the two-particle Coulomb scattering wave function, which describes the relative motion of the particles of pair α [the particle α and the center of mass of (β,γ)] in the potential V_α^C (v_α^C). However, as can be seen simply in the example of a system with $V_\alpha^C=0$ and $m_\alpha=\infty$, for which an analytic solution is known, the leading term $\Phi_0^{(+)}$ in Ω_α is not the same as the leading term of the asymptotic form of the solution of (1) in Ω_α.

To find an asymptotic solution in Ω_α, we consider a Coulomb-distorted plane wave which is an asymptotic solution in Ω_0 (away from singular directions corresponding to $\hat{\mathbf{k}}_\nu\hat{\mathbf{r}}_\nu=1$, $\hat{\mathbf{p}}=\mathbf{p}/p$):[2-4]

$$\Psi_0^{(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)=e^{i\mathbf{k}_\alpha\mathbf{r}_\alpha}e^{i\mathbf{q}_\alpha\vec{\rho}_\alpha}\prod_{\nu=1}^{3}e^{i\eta_\nu\ln\zeta_\nu}, \tag{5}$$

where $\eta_\alpha=e_\beta e_\gamma\mu_\alpha/k_\alpha$ and $\zeta_\alpha=k_\alpha r_\alpha-\mathbf{k}_\alpha\mathbf{r}_\alpha$. It can be shown by direct substitution that with $V_\alpha^C=0$ the leading term of $\Psi_0^{(+)}$ in Ω_α,

$$\Psi_{0\alpha}^{as(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)=e^{i\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)\mathbf{r}_\alpha}\chi_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}^{as(+)}(\vec{\rho}_\alpha), \tag{6}$$

$$\chi_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}^{as(+)}(\vec{\rho}_\alpha)=e^{i\mathbf{q}_\alpha\vec{\rho}_\alpha}\prod_{\nu=\beta,\gamma}e^{i\eta_\nu\ln\zeta_\nu^{(\alpha)}}, \tag{7}$$

is the asymptotic solution of Eq. (1) in Ω_a and of asymptotic equation (2) in a nonsingular direction ($\hat{\mathbf{k}}_\nu\hat{\vec{\rho}}\neq 1$, $\nu=\beta,\gamma$). Here

$$\zeta_\nu^{(\alpha)}=k_\nu\rho_\alpha-\epsilon_{\alpha\nu}\mathbf{k}_\nu\vec{\rho}_\alpha,\quad \tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)=\mathbf{k}_\alpha+\mathbf{a}^{(\alpha)}(\hat{\vec{\rho}}_\alpha)/\rho_\alpha, \tag{8}$$

$$\mathbf{a}^{(\alpha)}(\hat{\vec{\rho}}_\alpha)=\sum_{\nu=\beta,\gamma}\mathbf{a}_\nu^{(\alpha)}(\hat{\vec{\rho}}_\alpha), \tag{9}$$

$$\mathbf{a}_\nu^{(\alpha)}(\hat{\vec{\rho}}_\alpha)=-\eta_\nu(m_\nu/m_{\beta\gamma})(\epsilon_{\alpha\nu}\hat{\vec{\rho}}-\hat{\mathbf{k}}_\nu)/(1-\epsilon_{\alpha\nu}\hat{\vec{\rho}}_\alpha\hat{\mathbf{k}}_\nu),\quad \nu=\beta,\gamma, \tag{10}$$

and $\epsilon_{\alpha\nu}=-\epsilon_{\nu\alpha}$, $\epsilon_{\alpha\alpha}=0$, and $\epsilon_{\alpha\nu}=1$ for all $(\alpha\nu)$ which are cyclic permutations of (1, 2, 3). In deriving (6) we used the expansion

$$\ln\zeta_\nu=\ln\zeta_\nu^{(\alpha)}+\frac{\mathbf{a}_\nu^{(\alpha)}(\hat{\vec{\rho}}_\alpha)\mathbf{r}_\alpha}{\rho_\alpha}+O\left(\frac{1}{\rho_\alpha{}^2}\right). \tag{11}$$

The phase factor $\exp[i\mathbf{a}^{(\alpha)}(\hat{\vec{\rho}}_{\alpha})\mathbf{r}_a/\rho_\alpha]$ must be retained in (6), since when (6) is substituted into (2), and the operator $T\mathbf{r}_a$ acts on $\exp[i\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)\mathbf{r}_\alpha]$, a term $\sim 1/\rho_\alpha$ arises. In other words, a term on the same order of magnitude as v_α^C arises. The effect of $T_{\vec{\rho}_\alpha}$ on $\exp[i\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)\mathbf{r}_\alpha]$, on the other hand, can be ignored, since we have $\vec{\nabla}_{\vec{\rho}_\alpha}\exp[i\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)\mathbf{r}_\alpha]\sim 1/\rho_\alpha^2$.

It is clear from (6) that in the case $V_\alpha^C\neq 0$ the asymptotic solution which we want should be sought in the form

$$\Psi_\alpha^{as(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)=\psi^{(\pm)}_{C,\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)\chi^{as(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\vec{\rho}_\alpha), \tag{12}$$

where $\psi_{C,\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)$ is some unknown function. Substituting (12) into (2), we find an equation for $\psi^{(\pm)}_{C,\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)$:

$$\left(\frac{\tilde{k}_\alpha^2(\vec{\rho}_\alpha)}{2\mu_\alpha}-T\mathbf{r}_\alpha-V_\alpha^C\right)\psi^{(\pm)}_{C,\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)=0\left(\frac{1}{\rho_\alpha^2}\right). \tag{13}$$

The solution of this equation is

$$\psi^{(\pm)}_{C,\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)=e^{i\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)\mathbf{r}_\alpha}\tilde{N}_\alpha(\vec{\rho}_\alpha)F[-i\tilde{\eta}_\alpha(\vec{\rho}_\alpha),1;\ i\tilde{\zeta}_\alpha(\vec{\rho}_\alpha)]+O\left(\frac{1}{\rho_\alpha^2}\right),$$

$$\tilde{\zeta}_\alpha(\vec{\rho}_\alpha)=\tilde{k}_\alpha(\vec{\rho}_\alpha)r_\alpha-\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)\mathbf{r}_\alpha,\tilde{\eta}_\alpha(\vec{\rho}_\alpha)=e_\beta e_\gamma\mu_\alpha/\tilde{k}_\alpha(\vec{\rho}_\alpha), \tag{14}$$

$$\tilde{N}_\alpha(\vec{\rho}_\alpha)=\exp[-\pi\tilde{\eta}_\alpha(\vec{\rho}_\alpha)/2]\Gamma[1+i\tilde{\eta}_\alpha(\vec{\rho}_\alpha)],$$

where $F(a,b;x)$ is the confluent hypergeometric function. Expression (12) with $\psi^{(\pm)}_{C,\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)$ and $\chi^{as(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\vec{\rho}_\alpha)$ given by (14) and (7) is thus the asymptotic solution of Eq. (2) in Ω_α which we have been seeking. It is simultaneously the leading term of the asymptotic form of the solution of (1) in Ω_α in a nonsingular direction $(\hat{\mathbf{k}}_\nu\hat{\vec{\rho}}_\alpha\neq 1$, $\nu=\beta,\gamma)$. We can draw some conclusions from (12).

Formally, the asymptotic solution can be written as a product of the wave functions $\psi^{(\pm)}_{C,\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)$ and $\chi^{as(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\vec{\rho}_\alpha)$, which may be thought of as wave functions corresponding to the relative motion of (a) the particles of pair α and (b) particle α and the center of mass of pair α, respectively. The reason is that the first of these wave functions satisfies Eq. (13), while the second satisfies

$$\left(\frac{q_\alpha^2}{2M_\alpha}-T_{\vec{\rho}_\alpha}-v_\alpha^C-\frac{\mathbf{a}^{(\alpha)}(\hat{\vec{\rho}}_\alpha)\mathbf{k}_\alpha}{\mu_\alpha}\frac{1}{\rho_\alpha}\right)\chi^{as(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\vec{\rho}_\alpha)=O\left(\frac{1}{\rho_2^\alpha}\right). \tag{15}$$

Each of the functions in (12), however, differs from (4) in that it is not a three-particle function; it instead incorporates three-particle effects. In the first function, this is seen in the appearance of an effective momentum $\tilde{\mathbf{k}}_\alpha(\vec{\rho}_\alpha)$ in place of $\mathbf{k}_\alpha$. This replacement is the result of the effect of particle α on the relative motion of the particles of pair α: The long-range Coulomb interaction of α with β and γ changes the momenta of the particles of pair α and therefore changes $\mathbf{k}_\alpha$. The wave function $\chi^{as(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\vec{\rho}_\alpha)$ depends on not only $\vec{\rho}_\alpha$ and $\mathbf{q}_\alpha$ but also $\mathbf{k}_\beta$ and $\mathbf{k}_\gamma$, separately, reflecting the fact that (β,γ) is an unbounded system. We have thus shown that the asymptotic solution in Ω_α for the case of an unbounded (β,γ) system is fundamentally different from the asymptotic solution Ω_α for a bound pair (β,γ) and for a particle α in a continuum.[2,4]

We can offer a generalization of asymptotic solution (12) which is valid in all the asymptotic regions Ω_α, $\alpha=0,1,2,3$, except in singular directions. Let us consider the wave function

$$\Psi^{as(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)=e^{i\mathbf{k}_\alpha\mathbf{r}_\alpha}e^{i\mathbf{q}_\alpha\vec{\rho}_\alpha}\prod_{\nu=1}^{3}\tilde{N}_\nu(R,\hat{\vec{\rho}}_\nu)F[-i\tilde{\eta}_\nu(R,\hat{\vec{\rho}}_\nu),1;\quad i\tilde{\zeta}_\nu(R,\hat{\vec{\rho}}_\nu)],$$

$$\tilde{\zeta}_\nu(R,\hat{\vec{\rho}}_\nu)=\tilde{k}_\nu(R,\hat{\vec{\rho}}_\nu)r_\nu-\tilde{\mathbf{k}}_\nu(R,\hat{\vec{\rho}}_\nu)\mathbf{r}_\nu, \tag{16}$$

$$\tilde{\mathbf{k}}_\nu(R,\hat{\vec{\rho}}_\nu)=\mathbf{k}_\nu+\frac{2\mathbf{a}^{(\nu)}(\hat{\vec{\rho}}_\nu)}{R},\quad R=\sum_{\nu=1}^{3}r_\nu,$$

$$\tilde{\eta}_\alpha(R,\hat{\vec{\rho}}_\alpha)=\frac{e_\beta e_\gamma\mu_\alpha}{\tilde{k}_\alpha(R,\hat{\vec{\rho}}_\alpha)},\quad \alpha=1,2,3,$$

$$N_\nu(R,\hat{\vec{\rho}}_\nu)=\exp[-\pi\tilde{\eta}_\nu(R,\hat{\vec{\rho}}_\nu)/2]\Gamma[1+i\tilde{\eta}_\nu(R,\hat{\vec{\rho}}_\nu)]. \tag{17}$$

The reason for choosing R instead of ρ_ν (the choice is ambiguous) is that there are directions in Ω_0 along which one of the distances ρ_ν remains finite as $r_\alpha\to\infty$ ($\alpha=1,2,3$). In any of the regions Ω_α ($\alpha=1,2,3$), the quantity $\tilde{\mathbf{k}}_\alpha(R,\hat{\vec{\rho}}_\alpha)$ is the same as $\mathbf{k}_\alpha(\vec{\rho}_\alpha)$ in the leading order [see (8)], while the leading term of the asymptotic function $\Psi^{as(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)$ in Ω_α is given by expression (12). In region Ω_0, the leading term of the asymptotic form of expression (16) is given by a distorted plane wave [expression (5)].

Along the nonsingular directions, the asymptotic behavior $\Psi^{as(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)$ in any of the asymptotic regions Ω_α ($\alpha=0,1,2,3$) is thus (in leading order) an asymptotic solution of Eq. (1) in this region. Expression (16) makes it possible to join the asymptotic solutions in the various regions Ω_α ($\alpha=0,1,2,3$).

We have another comment of practical importance. In the singular directions, where at least one of the $\mathbf{a}_\nu^{(\alpha)}(\hat{\vec{\rho}}_\alpha)$ becomes infinite, the expressions for the asymptotic solutions become singular. This singular nature creates a difficulty in the practical use of these expressions. We would like to suggest one possible way to overcome this difficulty. For this purpose we use a relation which is valid for $\rho_\alpha\to\infty$ and $\hat{\mathbf{k}}_\nu\hat{\vec{\rho}}_\alpha\neq1$:

$$\frac{\mathbf{a}_\nu^{(\alpha)}(\vec{\rho}_\alpha)}{\rho_\alpha}\approx ik_\nu\frac{m_\nu}{m_{\beta\gamma}}(\epsilon_{\alpha\nu}\hat{\vec{\rho}}_\alpha-\hat{\mathbf{k}}_\nu)\frac{d\ln F(-i\eta_\nu,1;\ i\zeta_\nu^{(\alpha)})}{d\zeta_\nu^{(\alpha)}} \tag{18}$$

$$=\eta_\nu k_\nu\frac{m_\nu}{m_{\beta\gamma}}(\epsilon_{\alpha\nu}\hat{\vec{\rho}}_\alpha-\mathbf{k}_\nu)\frac{F(1-i\eta_\nu,1;\ i\zeta_\nu^{(\alpha)})}{F(-i\eta_\nu,1;\ i\zeta_\nu^{(\alpha)})},\quad \nu=\beta,\gamma. \tag{19}$$

In a nonsingular direction, the right side of (19) is the same as $\mathbf{a}_\nu^{(\alpha)}(\hat{\vec{\rho}}_\alpha)/\rho_\alpha$, within terms $\sim1/\rho_\alpha^2$, and it is regular even in a singular direction. Consequently, if we replace

$\mathbf{a}_\nu^{(\alpha)}(\hat{\vec{\rho}})/\rho_\alpha$ by expression (19), the function $\Psi_\alpha^{as(+)}(\mathbf{r}_\alpha,\vec{\rho}_\alpha)$ modified in this manner is again an asymptotic solution of Eq. (1) in nonsingular directions of Ω_α, while it remains regular even in a singular direction ($\hat{\mathbf{k}}_\nu \hat{\vec{\rho}}_\alpha=1$, $\nu=\nu,\gamma$) [in which of course, $\Psi_\alpha^{as(+)}(\mathbf{r}_\alpha\vec{\rho}_\alpha)$ is no longer an asymptotic solution].

Up to this point we have been discussing the asymptotic solutions for the case $V_\alpha=V_\alpha^C$. If $V_\alpha=V_\alpha^N+V_\alpha^C$, where V_α^N is the potential of a nuclear interaction between particles β and γ, the function $\psi^{(+)}_{C,\mathbf{k}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)$ in (12) must be replaced by $\psi^{(+)}_{\mathbf{k}_\alpha(\vec{\rho}_\alpha)}(\mathbf{r}_\alpha)$, which is the solution of Eq. (13) with the potential V_α instead of V_α^C.

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