New type of resonances in elastic scattering

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A new type of quasistationary states, associated with bringing a classical particle into an unstable equilibrium state, is analyzed in the particular case of the problem of two Coulomb centers Z_1eZ_2.

In an exact numerical calculation of the S-matrix poles of the problem of two Coulomb centers Z_1eZ_2 $(e = -1)$,

$$\left[-\frac{\hbar^2}{2m_e}\Delta_r - \frac{Z_1}{|\mathbf{r}-\mathbf{R}/2|} - \frac{Z_2}{|\mathbf{r}+\mathbf{R}/2|}\right]\psi = E\,\psi\,, \qquad (1)$$

Ovchinnikov and Solov'ev[1] detected quasistationary states with a small width, whose origin was unclear since they could not be related to any features in the behavior of the effective quasiradial potential. We will show below that despite the exact separation of variables in the Schrödinger equation (1), the reason for the appearance of these narrow resonances cannot be explained in terms of exclusively the quasiradial one-dimensional problem and that the multidimensional nature of the system here plays the key role.

Schrödinger equation (1) admits a separation of variables in extended spheroidal coordinates $\xi\in[1,\infty)$, $\eta\in[-1,1]$, $\varphi\in[0,2\pi)$ and after substituting in this equation a wave function in the form $(m = 0, \pm 1, \pm 2,...)$

$$\varphi(\mathbf{r}) = [(\xi^2-1)(1-\eta^2)]^{-1/2}\,U(\xi)\,V(\eta)\,e^{im\varphi}$$

we can write it as a system of equations[2]

$$\frac{d^2U}{d\xi^2} + \left\{\frac{m_e}{\hbar^2}\left[c^2 + \frac{a\xi-\lambda}{\xi^2-1}\right] + \frac{1-m^2}{(\xi^2-1)^2}\right\}U = 0 \qquad (2)$$

$$\frac{d^2V}{d\eta^2} + \left\{\frac{m_e}{\hbar^2}\left[c^2 + \frac{b\eta+\lambda}{1-\eta^2}\right] + \frac{1-m^2}{(1-\eta^2)^2}\right\}V = 0, \qquad (3)$$

where $c^2 = ER^2/2$, $a = (Z_1+Z_2)R$, $B = (Z_2-Z_1)R$, and λ is a separation constant.

Since the quasistationary states of interest to us occur only at small values of m,[1] we will use to analyze them a semi-classical asymptotic expression with $m = 0$ [Eq. (1)], i.e., $\hbar m\to 0$. We note at once that the effective potential of quasi-radial equation (2) is the same in form as the radial potential of the hydrogen atom in which there are no known quasistationary states. We thus clearly see that we are dealing here with a non-standard case. On the other hand, a path on which a particle resides arbitrarily long near a scattering center corresponds, in the classical limit, to a narrow resonance. Such a path is not clearly seen in (2) because the quasiradial velocity depends on the momentum p_ξ in a nontrivial manner[3]:

$$\frac{d\xi}{dt} = \frac{4(\xi^2-1)}{m_e R^2(\xi^2-\eta^2)}\, p_\xi, \qquad p_\xi = \sqrt{m_e\left(c^2 + \frac{a\xi-\lambda}{(\xi^2-1)}\right)}. \tag{4}$$

The appearance of resonances indicates that the velocity near the point $\xi = 1$ behaves in a particular way when $a = \lambda$. The singularity of the momentum p_ξ in this case vanishes at the point $\xi = 1$ and $\dot{\xi} \sim (\xi - 1)$ near this point. As a result, the time tends logarithmically to infinity as $\xi \to 1$ and the path of a particle approaches the internuclear.axis asymptotically ($\xi = 1$) after an infinite number of oscillations in the quasiangular variable η (see Fig. 1). Such paths, which result in bringing the particle into an unstable equilibrium state on the internuclear axis, were discussed previously in celestial mechanics in the case of positive charges ($Z_1 > 0$, $Z_2 > 0$).[4] To calculate the position and width of the quasistationary states, we must evaluate the asymptotic behavior of $U(\xi)$ in the limit $\hbar \to 0$, $(a - \lambda) = 0(\hbar)$, and $a \sim \lambda \sim c = 0(1)$, which takes into account the singularity of the quasi-radial potential at the point $\xi = 1$. Since the appropriate variant of the standard-equation method is nearly the same as the method

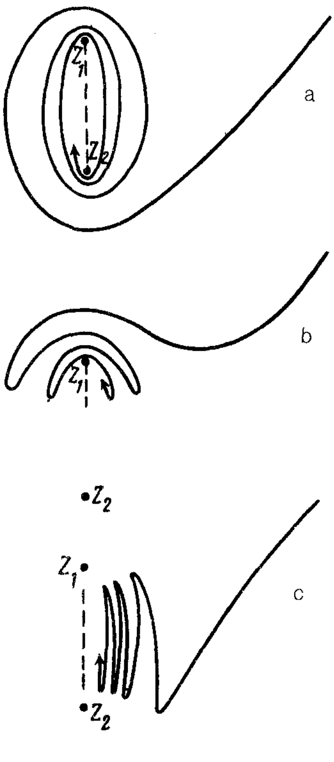

FIG. 1. Paths leading to the particle capture. a—$Z_1 > 0$, $Z_2 > 0$; b—$Z_1 > 0$, $Z_2 < 0$; c—$Z_1 < 0$, $Z_2 < 0$. Dashed line—limiting unstable periodic paths.

used by Solov'ev[5] in analyzing the highly excited states of the $Z_1 e Z_2$ problem, we will write immediately the final definitive expression, omitting the technical details,

$$U(\xi) = [\rho'(\xi)]^{-1/2} \rho^{(m+1)/2} \exp\left(-\frac{i}{\hbar}\kappa\rho\right) \Phi\left(\frac{m+1}{2} + i\frac{a-\lambda}{4\hbar\kappa},\ m+1,\ \frac{i}{\hbar} 2\kappa\rho\right),$$

$$\rho(\xi) = \frac{1}{\kappa}\int_1^{\xi} \sqrt{c^2 + \frac{a+\lambda}{2(\xi'+1)}}\, d\xi', \qquad \kappa = \sqrt{c^2 + \frac{a+\lambda}{4}}.$$

This wave function is the same, within an unessential term $[\rho']^{-1/2}$, as the hydrogen-like wave function in terms of the effective radial variable ρ, whose S-matrix poles are situated, as we know [see, for example, Eqs. (10) and (141) in Ref. 6], at a point where the following relation is valid:

$$a - \lambda = 2i\hbar\kappa(m + 2q + 1), \quad q = 0, 1, 2, \ldots \tag{5}$$

The separation constant λ appearing in (5) is determined from quasiangular equation (3). This constant generally cannot be evaluated explicitly. Analysis of the results of a numerical calculation shows, however, that the quasistationary states of interest to us are in the range where the expansion of the unified atom[2] can be used for λ:

$$\lambda = \lambda_0(R) - \frac{1}{4}ER^2, \quad \lambda_0(R) = \hbar^2\left(l + \frac{1}{2}\right)^2 - (Z_1 - Z_2)^2 R^2 / 8\hbar^2\left(l + \frac{1}{2}\right)^2. \tag{6}$$

where l is the orbital quantum number of the unified atom ($R = 0$). Substituting (6) into (5), we obtain a quadratic equation with respect to E. Hence the complex energy of the quasistationary state is

$$E_{qlm}(R) = 4R^{-2}\{\lambda_0(R) - (Z_1 + Z_2)R \pm i\hbar(m + 2q + 1)\sqrt{8\lambda_0(R) - 6(Z_1 + Z_2)R}\}. \tag{7}$$

Figure 2 shows, for comparison, the exact positions of the S-matrix poles in the $k = \sqrt{2E}$ plane and those calculated from Eq. (7). If more exact quasiclassical values of λ are used in Eq. (5), its solution will virtually coincide with the exact calculation on the scale of this figure.

In the hydrogen-like problem condition (5) leads to virtual states, whose conversion to quasistationary states in our case occurs by virtue of the energy dependence of λ, which reflects the multidimensionality of the original problem. As was shown by a numerical calculation, if any real value of λ is chosen in Eq. (2) (i.e., if it is treated as an isolated one-dimensional problem), then all the quasistationary states will again become virtual states. We see from (7) that in the limit $\hbar \to 0$ the width of the quasistationary states $\Gamma_{qlm} = 2\mathrm{Im}E_{qlm}$ approaches zero linearly in $\hbar$. In this limit the trajectories with $a = \lambda$, shown in Fig. 1 [see Eq. (5)], correspond to these states. The linear dependence of the width on $\hbar$ distinguishes these resonances from the tunneling resonances, whose width is exponentially small in $\hbar$, and from the above-the-barrier resonances, which have a finite width in the classical limit.

It is now clear that the quasistationary states of the type we are considering here

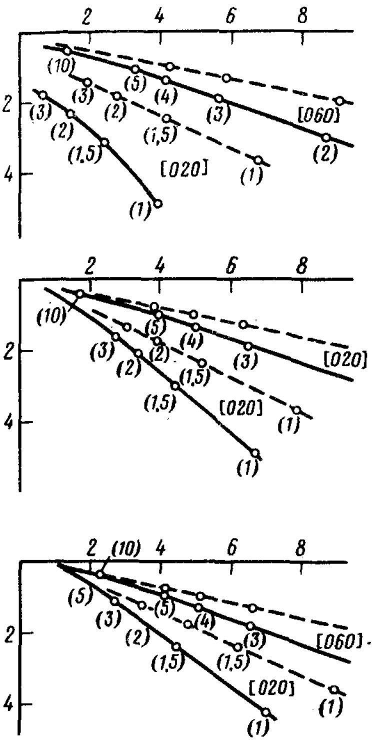

FIG. 2. Paths of the S-matrix poles in the complex plane of the wave number $k = (2E)^{1/2}$ resulting from the change in the nuclear spacing R. a—$Z_1 = 1$, $Z_2 = 1$; b—$Z_1 = 1$, $Z_2 = -1$; c—$Z_1 = -1$, $Z_2 = -1$. Solid curves—Result of an exact numerical calculation; dashed curve—calculation based on Eq. (7). The values of R are enclosed in parentheses and the quantum numbers of the $[q,l,m]$ states are enclosed in brackets.

are of considerable importance in various applications in physics. Only with their help, can the energy spectrum of free electrons produced in slow atomic collisions, for example, be explained and calculated in a number of cases.[1] The quasistationary states of the problem Z_1eZ_2, with $Z_1 < 0$ and $Z_2 < 0$ (Figs. 1c and 2c), were also used to explain the narrow peak in the differential cross section, with respect to the energy, for the production of positrons as a result of collision of superheavy nuclei.[7] The drawing of a particle into periodic unstable paths is apparently linked with quasi-Landau resonances[8] and resonances occurring at positive energies in the spectrum of hydrogen photoionization in a uniform electric field[9] F. The calculation technique developed above can be extended to the latter case virtually without any changes, since the Hamiltonian of this problem can be found from the Hamiltonian of the Z_1eZ_2 system by taking the limits $R \to \infty$, $Z_2 \to -\infty$, and $\lim Z_2R^{-2} = F(Z_1 = 1)$. Here the unstable equilibrium state is the motion along a line segment directed away from the nucleus Z_1 counter to the direction of the field **F** and the capture into this state is illustrated in Fig. 1b.

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