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ORBITING AND RESONANCE STATES

I. LUKACH and Ya. A. SMORODINSKIĬ

Joint Institute for Nuclear Research

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A quantum-mechanical investigation of the features of elastic potential scattering is carried out for energies of the order of the effective barrier. In classical scattering theory this phenomenon is known as orbiting (spiral scattering). It is found that for energies of the incident particle equal to the height of the effective barrier, a resonance appears in the scattering cross section which corresponds to a quasi-stationary state. The height of the effective barrier is a function of the angular momentum of the incident particle; thus a resonance trajectory is obtained which determines a family of resonance energies for different angular momenta.

INTRODUCTION

It is known in the classical theory of scattering on a certain class of spherically-symmetric potentials that there exists the phenomenon of orbiting.[1-4] 1) The essence of this effect is that the scattered particle interacts with the scattering center in such a way that, in approaching this center, it makes a number of turns around it, after which it flies off to infinity under some observed scattering angle. Thus the particles are in interaction for a length of time, which must correspond to some resonance state with a definite lifetime.

In general, orbiting occurs when the effective potential energy

$$U_{eff}(r) = U(r) + M^2/2mr^2 \qquad (1)$$

[U(r) is the interaction potential, M is the angular momentum of the incident particle, and m is the reduced mass] has at least one maximum (barrier) and the energy of the incident particle is close to the height of this barrier.[3,4]

The condition for the existence of a maximum of the effective potential energy at the point r_B is

$$\left.\frac{dU_{eff}}{dr}\right|_{r=r_B} = 0, \quad \left.\frac{d^2U_{eff}}{dr^2}\right|_{r=r_B} < 0. \qquad (2)$$

If conditions (2) are satisfied, the effective potential energy can be expanded in powers of $r - r_B$ around the point r_B where the maximum E_B occurs. Keeping terms of second order, we have

$$U_{eff}(r) = E_B\left[1 - \frac{(r-r_B)^2}{\rho^2}\right], \quad \frac{1}{\rho^2} = -\frac{1}{2E_B}\left.\frac{d^2U_{eff}}{dr^2}\right|_{r=r_B} \qquad (3)$$

we investigate the phenomenon at energies close to the barrier height E_B with the approximation (3) for $U_{eff}(r)$.

First we convince ourselves that in the classical case a particle with energy $E \sim E_B$ revolves around the scattering center. According to the known formula of classical mechanics for the full polar angle

$$\theta_0 = 2\int_{r_{min}}^{\infty} \frac{M/r^2}{\sqrt{2m[E - U_{eff}(r)]}}\,dr$$

we find, using approximation (3),

$$\theta_0 = \frac{M\rho\,[3 + \mathrm{sign}(E - E_B)]}{2r_B^2\sqrt{2mE_B}} \ln\frac{E_B}{|E - E_B|} + \text{const.} \qquad (4)$$

It is seen from (4) that $\theta_0 \to \infty$ for $E \to E_B$, and the particle "sits on the barrier," where it revolves practically for an infinite time with the angular velocity

$$\omega = M/mr_B^2.$$

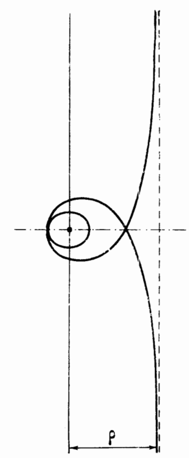

FIG. 1. Classical trajectory of the scattered particle in the potential $-\alpha/r^2$, which completes two revolutions around the scattering center and goes off at zero scattering angle.

For an illustration we show in Fig. 1 the form of the trajectory of a particle which completes two turns around the center and goes off under zero scattering angle.

Orbiting gives a contribution to the classical differential scattering cross section, which contains a sum over revolutions since particles completing different numbers of revolutions around the scattering center depending on their angular momentum can be scattered into one and the same angle.

In the numerous treatises on scattering, orbiting is mentioned very rarely, and the question of a quantum-mechanical treatment of orbiting is not posed at all. In the present paper we consider the behavior of the quantum-mechanical features of the scattering at energies of the order of the height of the effective barrier E_B. We shall find that for a sufficiently high and broad barrier a resonance appears at the incident energy $E = E_B$ which corresponds to a quasi-stationary state.

1) The most detailed analysis is that of Yakovlev [3] and Faingol'd. [4].

Using

$$E_B = U(r_B) + M^2/2mr_B^2, \quad (5)$$

where r_B is a function of the angular momentum M and the parameters of the potential, we have thus an equation for the trajectory of the resonances which determines a family of resonance energies $E_B^{(L)}$ for physical values of the angular momentum $M^2 = \hbar^2 L(L+1)$, $L = 0, 1, \ldots, L_{max}$.

Problems connected with the radiation from orbiting particles are also of interest.[5]

MODEL CALCULATION OF THE SCATTERING MATRIX

We find an expression for the S matrix in the case where the effective potential energy (1) has an effective barrier of height E_B at the point r_B inside of which there is a potential well of depth E_W at the point r_1. In order to obtain analytic formulas, we assume that this effective energy can be approximated by

$$U_{eff}(r) = \begin{cases} \dfrac{\hbar^2 L(L+1)}{2mr^2}, & r > r_2 \\ E_B\left[1 - \dfrac{(r-r_B)^2}{\rho^2}\right], & r_1 < r < r_2, \\ E_{\text{я}} + \dfrac{\hbar^2 L(L+1)}{2m}\left[\dfrac{1}{r^2} - \dfrac{1}{r_1^2}\right], & 0 < r < r_1 \end{cases} \quad (6)$$

as shown in Fig. 2.[2)]

The solution of the Schrödinger equation for the radial wave function (multiplied by r) having at infinity the form $\exp[i(kr - \pi L/2)]$, is

$$R_{kL}^{(+)}(r) = \begin{cases} f(r) & r > r_2 \\ \gamma g(z) + \delta h(z) & r_1 < r < r_2, \\ \alpha k(r) + \beta l(r) & 0 < r < r_1 \end{cases} \quad (7)$$

where α, β, γ, δ are constants which are determined from the matching conditions on the wave functions in the points r_1 and r_2,

$$f(r) = i(\pi kr/2)^{1/2} H_\lambda^{(1)}(kr),$$
$$g(z) = h^*(z) = \Gamma(3/4 - 1/4 i\varepsilon k_B\rho)\Psi(1/4 - 1/4 i\varepsilon k_B\rho, 1/2; iz),$$
$$k(r) = l^*(r) = i(\pi k_1 r/2)^{1/2} H_\lambda^{(1)}(k_1 r), \quad (8)$$

$H_\lambda^{(1)}(x)$ is the Hankel function, $\Gamma(x)$ is the Gamma function, and $\Psi(\alpha, \gamma; x)$ is the confluent hypergeometric function; we have further used the notation

$$E = \frac{\hbar^2 k^2}{2m}, \quad E_B = \frac{\hbar^2 k_B^2}{2m}, \quad E - E_{\text{я}} + \frac{\hbar^2 L(L+1)}{2mr_1^2} = \frac{\hbar^2 k_1^2}{2m},$$
$$\lambda = L + \frac{1}{2}, \quad \varepsilon = 1 - \frac{E}{E_B}, \quad z = \frac{k_B}{\rho}(r - r_B)^2. \quad (9)$$

The general solution $R_{kL}(r)$, having at infinity the form

$$R_{kL}(r)|_{r\to\infty} \sim \sin(kr - 1/2\pi L + \delta_L(k)),$$

is written as

$$R_{kL}(r) = [R_{kL}^{(-)}(r) - S_L(k) R_{kL}^{(+)}(r)], \quad (10)$$

where $R_{kL}^{(-)}(r) = [R_{kL}^{(+)}(r)]^*$. From the condition of regularity of the wave function $R_{kL}(r)$ in the origin we find that

$$S_L(k) = \exp[2i\delta_L(k)] = \frac{\alpha^* + \beta^*}{\alpha + \beta}. \quad (11)$$

Using the explicit expressions for the coefficients α and β,

$$\alpha = \frac{W(f_2, h_2)W(j_1, g_1)}{W(g_2, h_2)W(k_1, l_1)}, \quad \beta = \frac{W(g_2, f_2)W(j_1, h_1)}{W(g_2, h_2)W(k_1, l_1)},$$

where $W(\xi, \eta) = \xi\partial\eta/\partial r = \eta\partial\xi/\partial r$ are the Wronskians of the corresponding functions in the corresponding points and

$$j(r) \equiv k(r) - l(r) = 2i(\pi k_1 r/2)^{1/2} J_\lambda(k_1 r),$$

we obtain[3)] for the S matrix

$$S_L(k) = \frac{W^*(f_2, h_2)W^*(j_1, g_1) - W^*(f_2, g_2)W^*(j_1, h_1)}{W(f_2, h_2)W(j_1, g_1) - W(f_2, g_2)W(j_1, h_1)}. \quad (12)$$

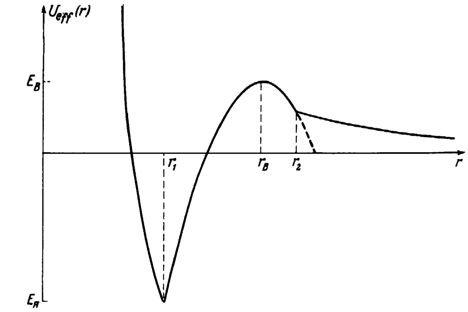

FIG. 2. Approximation for the effective potential energy.

RESONANCE STATES

The poles of the S matrix are determined by the zeros of the expression

$$F = W(f_2, h_2)W(j_1, g_1) - W(f_2, g_2)W(j_1, h_1)$$

or

$$F = f_2 j_1 k_B^2 \left\{\left(\frac{\partial \ln f_2}{k_B\partial r_2} - \frac{\partial}{k_B\partial r_2}\right)\left(\frac{\partial \ln j_1}{k_B\partial r_1} - \frac{\partial}{k_B\partial r_1}\right)\right\}(g_1h_2 - g_2h_1), \quad (13)$$

where the partial derivatives with respect to r_1 and r_2 act on the functions with index 1 and 2, respectively.

For the following we must write the function $g_1h_2 - g_2h_1$ in explicit form. Here we must take account of the fact that the point z = 0 is a branch point for the functions g and h, so that $g_1 \equiv g(z_1 e^{2\pi i}) = h_1^*$, where $\arg z_1 = 0$. It follows from the theory of confluent hypergeometric functions[7] that

$$\Gamma(\alpha - \gamma + 1)\Psi(\alpha, \gamma; ize^{2\pi i})$$
$$= [1 + e^{-2\pi i\gamma} - e^{2\pi i(\alpha-\gamma)}]\Gamma(\alpha - \gamma + 1)\Psi(\alpha, \gamma; iz)$$
$$+ e^{-2\pi i\gamma}[e^{2\pi i\alpha} - 1]\Gamma(1-\alpha)e^{iz}\Psi(\gamma - \alpha, \gamma; -iz). \quad (14)$$

Using (14), we find

$$g_1h_2 - g_2h_1 = h(z_1)h(z_2) - g(z_1)g(z_2)$$
$$- i\exp(1/2\pi k_B\rho\varepsilon)[g(z_1) - h(z_1)][g(z_2) - h(z_2)]. \quad (15)$$

We are interested in the value of (15) for energies E of the order of E_B, i.e., for small ϵ, and we therefore

[2)]This approximation for $U_{eff}(r)$ requires that the interaction potential U(r) have a finite range and its singularity in the origin be weaker than r^{-2}.

[3)]For more details cf. [6].

expand it in powers of ϵ, keeping terms of second order. Since we cannot write down an explicit expression for the derivative of the confluent hypergeometric function with respect to a parameter, we use the asymptotic expressions of these functions for large values of $k_B\rho$, since

$$z_1 = \frac{k_B}{\rho}(r_B - r_1)^2 \sim k_B\rho, \quad z_2 = \frac{k_B}{\rho}(r_B - r_2)^2 \sim k_B\rho.$$

Thus we are in fact expanding (15) under the condition

$$\varepsilon \ll 1/k_B\rho \ll 1. \tag{16}$$

Writing the functions g, h and their derivatives $\partial g/\partial\epsilon$, $\partial h/\partial\epsilon$ for large z in explicit form,

$$g|_{z\to\infty} = h^*|_{z\to\infty} = \Gamma(3/4 - 1/4 i\varepsilon k_B\rho) z^{-1/4} \exp[-i(1/8\pi + 1/2 z - 1/4\varepsilon k_B\rho \ln z) - 1/8\pi\varepsilon k_B\rho],$$
$$\partial g/\partial\varepsilon|_{z\to\infty} = \partial h^*/\partial\varepsilon|_{z\to\infty} = 1/4(k_B\rho)\Gamma(3/4 - 1/4 i\varepsilon k_B\rho) z^{-1/4} \cdot \times [1/2\pi - i(\ln z - \psi(3/4 - 1/4 i\varepsilon k_B\rho))] \exp[-i(1/8\pi + 1/2 z - 1/4\varepsilon k_B\rho \ln z) - 1/8\pi\varepsilon k_B\rho], \tag{17}$$

we find that

$$(g_1h_2 - g_2h_1)|_{k_B\rho\to\infty;\,\varepsilon\to0} = 1/2 i\Gamma^2(3/4)[G(z_1,z_2) - \varepsilon k_B\rho H(z_1,z_2)], \tag{18}$$

where $\psi(x)$ is the logarithmic derivative of the Gamma function and G and H are given by the following expressions:

$$G(z_1,z_2) = 4(z_1z_2)^{-1/4}\left[\cos\frac{z_1-z_2}{2} + \sqrt{2}\sin\frac{z_1+z_2}{2}\right],$$
$$H(z_1,z_2) = (z_1z_2)^{-1/4}\left\{\ln z_1\left[\sqrt{2}\cos\frac{z_1+z_2}{2} - \sin\frac{z_1-z_2}{2}\right] + \ln z_2\left[\sqrt{2}\cos\frac{z_1+z_2}{2} + \sin\frac{z_1-z_2}{2}\right] - \pi\cos\frac{z_1-z_2}{2} - [\psi(1/4) + \psi(3/4)]\sqrt{2}\cos\frac{z_1+z_2}{2}\right\}. \tag{19}$$

The action of the operator in (13) on the expression (18) leads to an equation for the determination of ϵ; from this we find that the scattering matrix has a pole at the energy

$$E = E_B - E_\varepsilon - 1/2 iE_\gamma, \tag{20}$$

where

$$E_\varepsilon = \frac{E_BG}{(k_B\rho)H}\left\{\left[\left(A - \frac{\partial\ln H}{k_B\partial r_1}\right)\left(B - \frac{\partial\ln H}{k_B\partial r_2}\right)\right]^2 + C^2\left(A - \frac{\partial\ln H}{k_B\partial r_1}\right)^2\right\}^{-1} \times\left\{\left[\left(A - \frac{\partial\ln H}{k_B\partial r_1}\right)\left(B - \frac{\partial\ln H}{k_B\partial r_2}\right) + \frac{\partial^2\ln H}{k_B^2\partial r_1\partial r_2}\right]\left[\left(A - \frac{\partial\ln G}{k_B\partial r_1}\right) \times\left(B - \frac{\partial\ln G}{k_B\partial r_2}\right) + \frac{\partial^2\ln G}{k_B^2\partial r_1\partial r_2}\right] + C^2\left(A - \frac{\partial\ln H}{k_B\partial r_1}\right)\left(A - \frac{\partial\ln G}{k_B\partial r_1}\right)\right\} \tag{21a}$$

$$E_\gamma = -\frac{2CE_B}{k_B\rho}\left[\frac{\partial(H/G)}{k_B\partial r_2}\right]^{-1}\left\{\left[\left(A - \frac{\partial\ln H}{k_B\partial r_1}\right)\left(B - \frac{\partial\ln H}{k_B\partial r_2}\right) + C^2\left(A - \frac{\partial\ln H}{k_B\partial r_1}\right)^2\right\}^{-1}\left\{\left[A\frac{\partial\ln(H/G)}{k_B\partial r_2} - \frac{1}{2}\left(\frac{\partial\ln(H\cdot G)}{k_B\partial r_1}\frac{\partial\ln(H/G)}{k_B\partial r_2} + \frac{\partial^2\ln(H/G)}{k_B^2\partial r_1\partial r_2}\right)\right]^2 - \frac{1}{4}\left(\frac{G}{H}\right)^2\left[4\frac{\partial^2\ln G}{k_B^2\partial r_1\partial r_2}\frac{\partial(H/G)}{k_B\partial r_1}\frac{\partial(H/G)}{k_B\partial r_2} + \left(\frac{\partial^2(H/G)}{k_B^2\partial r_1\partial r_2}\right)^2\right]\right\} > 0 \tag{21b}$$

$$A(r_1) \equiv \frac{\partial\ln j_1}{k\partial r_1}\bigg|_{k=k_B} = -\frac{\lambda - 1/2}{k_Br_1} + \frac{\bar{k}_1}{k_B}\frac{J_{\lambda-1}(\bar{k}_1r_1)}{J_\lambda(\bar{k}_1r_1)},$$
$$\bar{k}_1^2 = \frac{2m}{\hbar^2}(E_B - E_R) + \frac{L(L+1)}{r_1^2},$$

$$B(r_2) \equiv \mathrm{Re}\frac{\partial\ln f_2}{k\partial r_2}\bigg|_{k=k_B} = -\frac{\lambda - 1/2}{k_Br_2} + \frac{J_\lambda(k_Br_2)J_{\lambda-1}(k_Br_2) - J_{-\lambda}(k_Br_2)J_{-\lambda+1}(k_Br_2)}{J_\lambda^2(k_Br_2) + J_{-\lambda}^2(k_Br_2)}, \tag{22}$$
$$C(r_2) \equiv \mathrm{Im}\frac{\partial\ln f_2}{k\partial r_2}\bigg|_{k=k_B} = \frac{2}{\pi k_Br_2}[J_\lambda^2(k_Br_2) + J_{-\lambda}^2(k_Br_2)]^{-1} > 0.$$

That $E_\gamma > 0$ can be seen by direct calculation of the derivatives of the functions G and H with respect to r_1 and r_2.

Thus we may conclude that for energies of the incident particle approximately equal to the height of the effective barrier, a quasi-stationary state ($E_\gamma > 0$) occurs. For sufficiently large $k_B\rho$, i.e., for a sufficiently high and broad barrier, $E_\epsilon \ll E_B$ and the quantity E_γ is sufficiently small so that we obtain a resonance at the energy $E = E_B$. Since the height of the effective barrier is a function of the angular momentum M of the incident particle, Eq. (5) determines, for a given interaction potential U(r), a family of resonance energies $E_B^{(L)}$ at physical values of the angular momentum $M^2 = \hbar^2 L(L+1)$, L = 0, 1, ..., L_{max}.

A similar result is obtained when a square barrier of height E_B is taken in the region $r_1 < r < r_2$. In this case we have the following solution in the region $r_1 < r < r_2$:

$$g = \exp(rk_B\sqrt{\varepsilon}), \quad h = \exp(-rk_B\sqrt{\varepsilon}) \tag{23}$$

and for G and H we obtain the simple expressions

$$G = a, \quad H = -1/6 a^3, \quad a = r_2 - r_1$$

correspondingly, we find for E_γ

$$E_\gamma = \frac{12CE_B}{(k_Ba)^3}\left[\left(A + \frac{3}{k_Ba}\right)^2 + \frac{3}{4(k_Ba)^2}\right] \times\left\{\left[B\left(A + \frac{3}{k_Ba}\right) - \frac{3}{k_Ba}\left(A + \frac{2}{k_Ba}\right)\right]^2 + C\left(A + \frac{3}{k_Ba}\right)^2\right\}^{-1},$$

where A, B, and C are given by (22).

SCATTERING CROSS SECTION

The elastic scattering cross section is given by

$$\sigma(E) = \frac{\pi\hbar^2}{2mE}\sum_{L=0}^{\infty}(2L+1)|1 - S_L(E)|^2. \tag{24}$$

The terms in (24) with angular momenta $0 \le L \le L_{max}$ have resonance character (there is a resonance for L = 0 when the potential energy has a barrier). Therefore (24) takes the form

$$\sigma(E) = \frac{\pi\hbar^2}{2mE}\sum_{L=0}^{L_{\kappa p}}(2L+1)\frac{(E_\gamma^{(L)})^2}{(E - E_B^{(L)})^2 + (E_\gamma^{(L)})^2}, \tag{25}$$

where $E_B^{(L)}$ is given by (5) and $E_\gamma^{(L)}$, by (21b), where the terms with $L > L_{max}$, which in the given case have no resonance character, are omitted. Formula (25) differs from the usual resonance formula in that all resonance energies $E_B^{(L)}$ lie on the same resonance trajectory determined by (5). This resonance trajectory is completely determined by the parameters of the interaction potential and is the analog of the Regge trajectory, although these two concepts do not coincide completely.

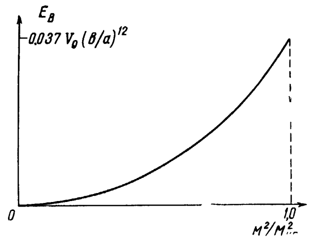

FIG. 3. Trajectory of the resonance energies for the potential (26).

Regge considered complex angular momenta as a function of complex energies, whereas our resonance trajectories are defined as poles of the S matrix for complex energies and real angular momenta.

EXAMPLE

For an illustration of our results we calculate the resonance trajectory for the potential

$$U(r)=V_0\left[\left(\frac{a}{r}\right)^6-\left(\frac{b}{r}\right)^4\right], \tag{26}$$

a special case of which (a = 0) is the known polarization potential. The effective potential energy for the potential (26) has a maximum at the point

$$r_B=\sqrt{\frac{3}{2}\frac{a^3}{b^2}}\left(\frac{2}{1-\xi}\right)^{1/2},$$

whose value is

$$E_B(M^2)=\frac{1}{27}V_0\left(\frac{b}{a}\right)^{12}(1-\xi)^2(1+2\xi), \tag{27}$$

where

$$0\leqslant\xi=\left(1-\frac{M^2}{M_{cr}^2}\right)^{1/2}\leqslant 1,\quad M_{cr}^2=\frac{2}{3}mV_0\frac{b^8}{a^6}.$$

For angular momenta $M > M_{max}$ there is no effective barrier. The resonance energies $E_B^{(L)}$ are obtained for values of the angular momentum $M^2 = \hbar^2L(L + 1)$ with $L = 1, 2, \ldots, L_{max}$, where

$$L_{\text{кр}}=\left[\sqrt{\frac{M_{cr}^2}{\hbar^2}+\frac{1}{4}}-\frac{1}{2}\right] \tag{28}$$

([x] is the integer part of x). The form of the curve $E_B = E_B(M^2)$ for the potential (26) is shown in Fig. 3.

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