PERTURBATION OF A CONTINUOUS SPECTRUM BY A CLOSE-LYING LEVEL

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We consider the nature of the perturbation of the functions $\chi_k(r)$ of the continuous spectrum and the analytical properties of the S-matrix in the region as $k \to 0$ when there is a level close to zero. We obtain equations which express the parameters of the low-energy expansion of the S-matrix in terms of the wave-function $\chi_0(r)$ at the moment when the level first appears. We obtain an exact solution of the problem for a number of potentials.

1. INTRODUCTION

In a number of problems in nuclear physics or in solid state theory the situation arises when there is in a system of interacting particles a level with a small binding energy.[1-4] The elucidation of the problem of the nature of the perturbation of the functions $\chi_k(r)$ of the continuous spectrum as $k \to 0$ (k is the wave vector) when there is a close-lying level present (the level may be real, virtual, or quasi-stationary) is of interest.

The physical aspects of this problem were considered in detail in a paper by A. B. Migdal and the authors.[5] We showed there that there is for a wide range of r an approximate factorization of the wave-functions $\chi_k(r)$:

$$\chi_k(r) = \sqrt{\Delta(k)}\chi_0(r), \tag{1}$$

where $\Delta(k)$ is a factor which changes fast in the resonance region;[1)] for instance, for $l = 0$

$$\Delta(k) = \frac{8\varkappa^2k^2}{\pi[(k^2-k_0^2)^2+4\varkappa^2k^2]}. \tag{2}$$

Such a factorization is very convenient for the evaluation of matrix elements and for the solution of the integral equations in the scattering problem (see in this connection the papers by Galitsky and Cheltsov[6] and by Migdal[7]) since the integral equations can be reduced to algebraic ones, using the factorization. It turns out that the factorization (1) is, apparently, also useful for approximate solutions of solid state problems.

In the present paper, which is an extension of [5], we consider the problem of the factorization (1) in the framework of a simple, but rather general "narrow well" model. This model consists in replacing the attractive part of the potential by a boundary condition at the origin. Such an approximation retains correctly the qualitative peculiarities of the problem with a short-range potential and is often used in atomic and nuclear physics (for instance, in the problem of the ionization of atoms by an electric field,[8] in problems of collisions of a negative ion with a neutral atom,[9, 10] and so on).

We consider in Sec. 2 the analytical properties of the wave functions and of the S-matrix at low energies (for the case when there is a level with an energy close to zero). We obtain formulae for the parameters of the low-energy expansion of the S-matrix in terms of the wave-function $\chi_0(r)$ at the point when the level first appears. The case when the potential V(r) contains a rather wide barrier with a penetrability which is small for particles with small k is of particular interest. In this case the wave functions $\chi_k(r)$ are strongly perturbed when the bound level merges with the continuous spectrum; the perturbation consists in a steep amplification of the $\chi_k(r)$ under the barrier (for those values of the energy $\epsilon = k^2/2$ which lie close to the energy of the quasi-stationary state). This problem is considered in Secs. 2 and 4 and we obtain formulae which describe the perturbation of the functions $\chi_k(r)$ of the continuous spectrum.

These results are, apart from applications to nuclear physics, of considerable interest for the relativistic Coulomb problem for $Z > 137$ (see [11, 12]).

Section 3 is devoted to a consideration of a number of concrete examples where one is able to find explicit expressions for the S-matrix and to indicate the connection between the exact formulae and the resonance approximation.

ANALYTICAL PROPERTIES OF THE S-MATRIX AT LOW ENERGIES

Let V(r) be a potential which has a wide barrier (see Fig. 1). We assume that the attractive part of V(r) has a small radius. In that case it can be replaced by a boundary condition ($l = 0$) on the wave function $\chi(r)$:[2)]

$$\chi'(0)/\chi(0) = -\zeta \tag{3}$$

(if $V(r) \equiv 0$ for $r > 0$, condition (3) leads to the occur-

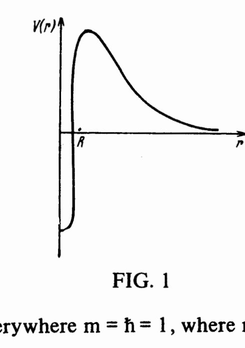

FIG. 1

[1)] Here κ is a quantity characterizing the penetrability of the barrier for an energy $\epsilon = 0$, k_0^2 is characteristic for the level position (vide infra Eq. (21)).

[2)] Henceforth everywhere $m = \hbar = 1$, where m is the particle mass.

rence of a single bound state with angular momenta $l = 0$ and energy $\epsilon = -\zeta^2/2$). In what follows we shall assume $V(r)$ for $r > 0$ to be fixed and the parameter ζ to change. The binding energy ϵ changes smoothly with ζ and for some $\zeta = \zeta_0$ it vanishes.

We find the form of the S-matrix for ζ close to ζ_0 and $k \to 0$. Let $f_\pm(k, r)$ be the solutions of the Schrödinger equation with potential $V(r)$ which change to $\exp(\pm ikr)$ as $r \to \infty$. One can express the wave function $\chi_k(r)$ of the continuous spectrum which as $r \to \infty$ behaves asymptotically

$$\chi_k(r) \approx \sqrt{\frac{2}{\pi}} \sin(kr + \delta),$$

in terms of them as follows:[3)]

$$\chi_k(r) = \frac{ie^{-i\delta}}{\sqrt{2\pi}} \{f_-(k, r) - S(k) f_+(k, r)\}, \tag{4}$$

where $S(k) = \exp[2i\delta(k)]$ is the required S-matrix. From the boundary condition (3) we get

$$S(k) = S_0(k) S_1(k), \tag{5}$$

$$S_0(k) = \frac{f_-(k)}{f_+(k)} \qquad S_1(k) = \frac{f_-'(k)/f_-(k) + \zeta}{f_+'(k)/f_+(k) + \zeta}$$

where $f_\pm(k) = f_\pm(k, 0)$ is a Jost function defined as in [13], while

$$f_\pm'(k) = \partial f_\pm(k, r) / \partial r|_{r=0}.$$

We note that $S_0(k) = \exp\{2i\delta_0(k)\}$ is the scattering matrix for the potential $V(r)$ (with the regular boundary condition $\chi(0) = 0$). As $\delta_0(k) \to 0$ as $k \to 0$ near resonance the phase $\delta_0(k)$ plays the role of the phase of the potential scattering and is unimportant for us. For a bound state $k = i\lambda$ ($\lambda > 0$) the equation that determines the dependence of the level energy $\epsilon = -\lambda^2/2$ on the coupling constant ζ follows from (5):

$$f_+'(i\lambda) / f_+(i\lambda) = -\zeta. \tag{6}$$

We change Eq. (5) for $S_1(k)$ in the physical region $k > 0$ to the form $S_1(k) = (a + ib)/(a - ib)$, where

$$a(k) = -\left\{\zeta + \mathrm{Re}\left[\frac{f_+'(k)}{f_+(k)}\right]\right\},$$
$$b(k) = \mathrm{Im}\left[\frac{f_+'(k)}{f_+(k)}\right] = \frac{k}{|f_+(k)|^2}. \tag{7}$$

The point $k = 0$ can, generally speaking, be a singular point for the functions $a(k)$ and $b(k)$. We assume that as $k \to 0$

$$a(k) = a_0 - a_1 k^2 + o(k^2) \qquad (a_0 = \zeta_0 - \zeta), \tag{8}$$

where we have dropped terms which are of higher order than k^2 (they may be non-analytical of the form $k^n \ln k$ with $n > 2$, and so on).

The expansion (8) is certainly valid in the following cases:

I) if $\lim \{r^5 V(r)\} = 0$ as $r \to \infty$—see [14];[4)]

II) if $V(r) \propto r^{-n}$ as $r \to \infty$ ($1 \le n < 2$) while $V(r) > 0$ for sufficiently large r (there is then as $r \to \infty$ a repulsive barrier of the Coulomb type). These two kinds of potentials will in what follows be denoted as I and II, respectively.

Putting $k_0^2 = a_0/a_1$ and $\gamma(k) = b(k)/a_1$ we are led to the following formula for the resonance part of the S-matrix:

$$S_1(k) = \frac{k_0^2 - k^2 + i\gamma(k)}{k_0^2 - k^2 - i\gamma(k)}. \tag{9}$$

We must still find the quantities k_0^2 and $\gamma(k)$. We note that when $\zeta > \zeta_0$ the function $S_1(k)$ has a pole for $k = i\lambda$, $\lambda > 0$ which determines the energy of the bound state: $\epsilon = -\lambda^2/2$. To reduce the problem to the problem considered in [5] we replace the boundary condition (3) by an additional potential $V_1(r)$ in the form of a deep and narrow potential well:

$$V_1(r) = \begin{cases} -K_1^2/2 & \text{when } 0 < r < R_1 \\ 0 & \text{when } r > R_1 \end{cases}$$

($R_1 \to 0$). The wave function $\chi_k(r)$ has then for $r < R_1$ the form

$$\chi_k(r) \approx \chi_k(R_1) \sin K_1 r,$$

and instead of (3) we have

$$K_1 \operatorname{ctg} K_1 R = -\zeta.$$

When $R_1 \to 0$ and $K_1 \to \infty$ (in such a way that $K_1 R \to \pi/2$) we find thence:

$$\delta\zeta = \zeta - \zeta_0 = \frac{\pi}{2}\delta K_1 = -\frac{\pi}{2}\frac{\delta V_1}{K_1} \tag{10}$$

On the other hand, we have from perturbation theory

$$\delta\varepsilon = -\lambda\delta\lambda = \int_0^\infty \delta V(r) \chi_\lambda^2(r) dr = \delta V \int_0^{R_1} \chi_\lambda^2(r) dr = \frac{\pi}{4}\frac{\delta V}{K_1}\chi_\lambda^2(R_1). \tag{11}$$

Comparing this with (10) we get[5)]

$$\delta\varepsilon = -\lambda\delta\lambda = -\tfrac{1}{2}\chi_\lambda^2(R_1)\delta\zeta. \tag{12}$$

This formula can be applied for any form of $V(r)$. However, the remaining argument (and the final formulae for the quantities k_0^2 and $\gamma(k)$ occurring in (9)) are somewhat different for the potentials of kinds I and II.

For type I potentials the wave function is at the moment when the level first appears delocalized: $\chi_\lambda(r) \sim \sqrt{(2\lambda)} \exp -\lambda r$ and $\chi_\lambda^2(r)$ vanishes thus for fixed r and $\lambda \to 0$. At the moment when the level first appears the wave function $\chi_0(r)$ is not normalized in the usual sense: as $r \to \infty$ it reaches a constant value so that the integral

$$\int_0^\infty \chi_0^2(r) dr$$

diverges. On the other hand, $\chi_\lambda(r)$ is normalized to unity for any $\lambda > 0$. We therefore have as $\lambda \to 0$ and any finite r (such that $|V(r)| \gg \lambda^2$)

$$\chi_\lambda(r) \approx \sqrt{2\lambda}\chi_0(r), \tag{13}$$

where the normalization condition for $\chi_0(r)$ is taken in the form

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3) If $V(r) = \alpha/r$ as $r \to \infty$, the asymptotic behavior of $f_\pm(k, r)$ and of $\chi_k(r)$ is changed. It is well known that in that case

$$\chi_k(r) \approx \sqrt{\frac{2}{\pi}} \sin\left(kr - \frac{\alpha}{k}\ln 2kr + \sigma\right).$$

4) One can show that at the moment that the level first appears, i.e., when $\zeta = \zeta_0$, it is sufficient to require that $\lim \{r^3 V(r)\} = 0$ as $r \to \infty$.

5) We give another derivation of (12) in the Appendix.

$$\lim \chi_0(r) = 1. \tag{14}$$

Substituting (13) into (12) and dividing both sides by 2λ, we get[6)]

$$\lambda = \chi_0^2(0)(\zeta - \zeta_0), \quad \varepsilon = -\lambda^2/2. \tag{15}$$

The function $\gamma(k)$ has for small k the form $\gamma(k) = 2\kappa k$ and hence

$$S(k) = e^{2i\delta_0}\frac{k_0^2 - k^2 + 2i\kappa k}{k_0^2 - k^2 - 2i\kappa k} \tag{16}$$

The parameter k_0^2 changes together with ζ (viz., $k_0^2 < 0$ when $\zeta > \zeta_0$ when there is a real level while otherwise $k_0^2 > 0$). Close to the zero, the poles of the S-matrix are at the points

$$k_{1,2} = \pm(k_0^2 - \kappa^2)^{1/2} - i\kappa. \tag{17}$$

Hence it follows when $k_0^2 < 0$ and $|k_0^2| \ll \kappa^2$ that $k_1 = i\lambda_1 = -ik_0^2/2\kappa$; comparing this with (15) we are led to the equation

$$k_0^2 = -2\kappa\chi_0^2(0)(\zeta - \zeta_0). \tag{18}$$

We must still find the quantity κ. As the potential phase $\delta_0(k) = ck + 0(k^5)$ as $k \to 0$ the denominator in (16) takes the form

$$k_0^2 - (1 + c\kappa)k^2 - 2i\kappa\left(1 + \frac{ck_0^2}{2\kappa}\right).$$

As $k_0^2 = 0$ at the moment when the level first appears, comparison with the known expansion

$$k \operatorname{ctg}\delta(k) = -a^{-1} + {}^1/{}_2 r_0 k^2 \tag{19}$$

(here a is the scattering length and r_0 the effective radius) gives

$$r_0 = -(\kappa^{-1} + c). \tag{20}$$

In the case of a wide barrier κ is exponentially small and $c \sim 1$ so that

$$\kappa = -1/r_0, \quad k_0^2 = 2/r_0 a. \tag{21}$$

To find r_0 we can use a formula from [15]

$$r_0 = 2\int_0^\infty [1 - \chi_0^2(r)]\,dr. \tag{22}$$

The parameters k_0^2 and κ occurring in Eqs. (9) and (16) for the S-matrix near resonance are determined by Eqs. (18), (21), and (22) (we note that they are completely determined by the wave function χ_0).

Case II is the simplest one. As $\lambda \to 0$, $\chi_\lambda(r)$ changes here immediately into the normalized wave function $\chi_0(r)$ corresponding to a zero level energy. The function $\chi_0(r)$ decreases fast at infinity and the usual normalization of the discrete spectrum remains therefore valid:

$$\int_0^\infty \chi_0^2(r)\,dr = 1. \tag{23}$$

When $\zeta - \zeta_0 \ll \zeta_0$ we find from (12)

$$\varepsilon = {}^1/{}_2 k_0^2 = -{}^1/{}_2\chi_0^2(0)(\zeta - \zeta_0). \tag{24}$$

[6)]We usually in quantum mechanics have for the wave function the condition: $\chi(0) = 0$ (for regular potentials). In the case considered by us (boundary condition (3), i.e., a singular potential at the origin) this is no longer the case: $\chi_0(0) \neq 0$ (see, e.g., Eqs. (38) and (50) of the following section).

Comparison with (9) gives

$$a_1 = [\chi_0(0)]^{-2}, \quad \gamma(k) = k\chi_0^2(0)/|f_+(k)|^2. \tag{25}$$

As $k \to 0$ the Jost function $f_+(k) \to \infty$ exponentially (see Eq. (29) below) and for type II potentials the function $\gamma(k)$ therefore vanishes as $k \to 0$ faster than k^2. By virtue of this we get for the level energy: $\epsilon = -\lambda^2/2 = k_0^2/2$. Thereby are also for a type II potential the quantities k_0^2 and $\gamma(k)$ occurring in (9) determined.

We find the explicit form of $\gamma(k)$ for potentials with a power "tail":

$$V(r) \underset{(r\to\infty)}{\approx} \alpha r^{-n} \quad (\alpha > 0,\ 1 \leqslant n < 2). \tag{26}$$

One can in this case find the asymptotic behavior of $\chi_0(r)$ as $r \to \infty$ easily, for instance, from the quasi-classical formula:

$$\chi_0(r) \underset{r\to\infty}{\approx} C_0\frac{r^{n/4}}{(2\alpha)^{1/4}}\exp\left\{-\frac{\sqrt{8\alpha}}{2-n}r^{1-n/2}\right\} \tag{27}$$

(for a determination of the constant C_0 it is necessary to solve the Schrödinger equation in the whole range $0 < r < \infty$ and to use the normalization condition (23)). When $k_0^2 > 0$ the bound state changes into a Breit–Wigner pole to which corresponds a wave function with an asymptotic form of the kind of an outgoing wave:

$$\varphi_k(r) = \begin{cases} iAp^{-1/2}\exp\left\{i\left(\int_{r_0}^{r} p\,dr - \frac{\pi}{4}\right)\right\}, & r > r_0 \\ A|p|^{-1/2}\exp\left\{\int_r^{r_0}|p|\,dr\right\}, & r < r_0 \end{cases} \tag{28}$$

Here $p = (k^2 - 2\alpha r^{-n})^{1/2}$, $r_0 = (2\alpha/k^2)^{1/n}$ is the turning point (it goes to infinity as $k \to 0$), while the constant A determines the flux j of outgoing particles, i.e., the decay probability: $j = \gamma = |A|^2$.

When $r \ll r_0$ we have $\varphi_k(r) = \chi_0(r)$. In particular, in the range $R \ll r \ll r_0$ expressions (27) and (28) must be the same which enables us to connect the constants C_0 and A. We finally get

$$\gamma(k) = |C_0|^2\exp(-\beta k^{-\nu}) \text{ when } k \to 0, \tag{29}$$

where

$$\beta = \frac{\sqrt{\pi}\,\Gamma((2-n)/2n)}{\Gamma(1/n)}(2\alpha)^{1/n}, \quad \nu = \frac{2-n}{n}.$$

From this it is clear that $\gamma(k) \to 0$ as $k \to 0$ faster than k^n with an arbitrarily large n.

We note that there does not occur the orbital angular momentum l in these formulae (only the magnitude of the normalization constant C_0 can depend on l). This is explained by the fact that $V(r) \gg l(l+1)r^{-2}$ as $r \to \infty$.

We now consider the case when

$$V(r) \approx \alpha/2r^2 \text{ when } r \to \infty. \tag{30}$$

In that case we can express the solution of the Schrödinger equation in terms of Bessel functions. The wave function with zero energy has the asymptotic form

$$\chi_0(r) \underset{(r\to\infty)}{\approx} C_0 r^{-(\nu-1/2)}, \quad \nu = [(l + {}^1/{}_2)^2 + \alpha]^{1/2} \tag{31}$$

and is normalized in the sense of (23), provided $\nu > 1$. The k-dependence of $\gamma(k)$ is a power law:

$$\gamma(k) \underset{(k\to 0)}{\approx} \gamma_0 k^{2\nu}, \quad \gamma_0 = \frac{\pi |C_0|^2}{2^{2\nu-1}\Gamma^2(\nu)}. \tag{32}$$

For all type II potentials (and in the case (30) for $\nu > 1$) $\lim [\gamma(k)/k^2] = 0$ as $k \to 0$ and the poles k_1 and k_2 approach zero hugging the real axis. The poles meet in the point $k = 0$ after which one of them goes into the upper half-plane turning into a real level. In contrast to type I potentials with a finite barrier penetrability the S-matrix has here a singularity at $k = 0$ (generally speaking, a branch point, but in the Coulomb case an essential singularity with a condensation of an infinite number of poles). Because of this the picture in the lower half-plane ($\mathrm{Im}\, k < 0$) in the vicinity of the point $k = 0$ is complex; in particular, the number of poles on the first sheet can change (see example 3 in the next section).

3. SOME EXAMPLES

We illustrate the general formulae obtained above by a number of examples:

1) A barrier with a finite radius, 2) a barrier with a Coulomb tail as $r \to \infty$, 3) a centrifugal barrier. These cover practically all cases encountered in physics.

1) We consider as a potential $V(r)$ with a finite penetrability as $k \to 0$ the rectangular barrier:

$$V(r) = \begin{cases} {}^1/_2 K^2 & \text{when } 0 < r < R \\ 0 & \text{when } r > R \end{cases} \tag{33}$$

Here

$$f_+(k, r) = e^{ikr} \quad \text{when } r > R, \tag{34a}$$

$$f_+(k, r) = \frac{e^{ikR}}{2\mu}[(\mu + ik)e^{\mu(r-R)} + (\mu - ik)e^{\mu(R-r)}] \quad \text{when } r < R; \tag{34b}$$

$\mu = \sqrt{K^2 - k^2}$. Hence we find the Jost function:

$$f_+(k) = e^{ikR}(\mathrm{ch}\, \mu R - ik\mu^{-1}\, \mathrm{sh}\, \mu R). \tag{35}$$

We find for the level energy $\epsilon = -\lambda^2/2$ from (6) and (35):

$$\mu \frac{\lambda + \mu\, \mathrm{th}\, \mu R}{\mu + \lambda\, \mathrm{th}\, \mu R} = \zeta, \tag{36}$$

where ζ is the "coupling constant" of the δ-potential (see (3)). At the moment when the level first appears $\epsilon = \lambda = 0$, the quantity $\zeta = \zeta_0$ where

$$\zeta_0 = K\, \mathrm{th}\, KR. \tag{37}$$

We give also the exact formula for the S-matrix

$$S(k) = e^{-2ikR}\{\mu[(\mu - \zeta) - (\mu + \zeta)e^{2\mu R}] + ik[(\mu - \zeta) + (\mu + \zeta)e^{-2\mu R}]\} \times \{\mu[(\mu - \zeta) - (\mu + \zeta)e^{-2\mu R}] - ik[(\mu - \zeta) + (\mu + \zeta)e^{-2\mu R}]\}^{-1} \tag{38}$$

The barrier parameters K and R are arbitrary in Eqs. (34) to (38); we have not yet used the assumption that the penetrability is small.[7)] We now impose this condition:

$$\xi = e^{-2KR} \ll 1.$$

Then $\zeta_0 = K(1 - 2\xi)$ and Eq. (38) takes the form (16) with

$$k_0^2 = 2K(\zeta_0 - \zeta), \quad \varkappa = 4K\xi, \tag{39}$$

[7)] In particular, we can put K = 0 which corresponds to the case of no barrier. Then $f_+(k) = 1$ and (38) gives $S(k) = (\zeta - ik)/(\zeta + ik)$.

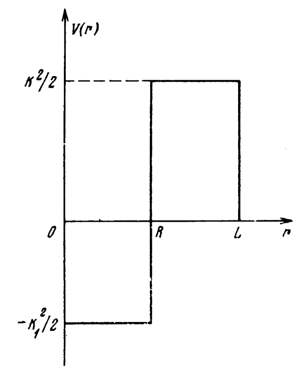

FIG. 2

while the potential scattering phase $\delta_0(k)$ is equal to

$$e^{2i\delta_0} = e^{-2ikR}(\mu + ik\, \mathrm{th}\, \mu R) \,/\, (\mu - ik\, \mathrm{th}\, \mu R),$$
$$\delta_0(k) = -(R - K^{-1})k + O(k^3). \tag{40}$$

The position of the poles $k_{1,2}$ is given by Eq. (17). We note that in this case it follows from an analysis of the exact Eq. (36) that there are no other poles of the S-matrix on the imaginary axis $k = i\lambda$.

We consider the motion of the real level with increasing ζ. Close to $\zeta = \zeta_0$ there is a narrow region in which the level deepens quadratically:

$$\varepsilon = -\frac{(\zeta - \zeta_0)^2}{32\xi^2} \quad \text{when} \quad 0 < \frac{\zeta - \zeta_0}{\zeta_0} \ll \xi^2, \tag{41}$$

and after that the dependence becomes a linear one:

$$\varepsilon = -K(\zeta - \zeta_0) \quad \text{when} \quad \xi^2 \ll \frac{\zeta - \zeta_0}{\zeta_0} \ll 1. \tag{42}$$

This dependence of the level energy ϵ on $\zeta - \zeta_0$ is characteristic of all type I potentials (provided the barrier is sufficiently wide). When $\zeta < \zeta_0$ there is a pair of virtual levels (if $0 > (\zeta - \zeta_0)/\zeta_0 > -8\xi^2$) or a pair of complex conjugate poles. The transition from the situation with Breit–Wigner poles to a bound state takes place not directly but through an intermediate region of ζ-values in which there are two virtual levels (see Fig. 2 in [5]). However, the width of this transition region is $\Delta\zeta \sim \xi^2 = \exp -4KR$, i.e., it is exponentially small even when compared with the width of the Breit–Wigner resonance (which is of the order of ξ according to (17) and (39).

Let us consider also the parameter r_0 (usually called the "effective radius"). Substituting into (22) the quantity $\chi_0(r) = \cosh K(R - r)$ for $r < R$ we find

$$r_0 = -\frac{\mathrm{sh}\, 2KR - 2KR}{2K} = -\frac{1 + 2\xi \ln \xi - \xi^2}{4K\xi}. \tag{43}$$

For the potential (33) we have thus always $r_0 < 0$ so that the designation "effective radius" looks here somewhat arbitrary. For a wide barrier $\xi \ll 1$ so that we have $r_0 = -(4K\xi)^{-1}$. On the other hand, if there is no potential barrier, $r_0 > 0$. How r_0 changes sign can be seen from the example of the potential shown in Fig. 2. Here

$$r_0 = \frac{R}{2}\left[3 - \left(1 + \frac{K^2}{K_1^2}\right)\mathrm{ch}\, \beta - \frac{K}{K_1^2 R}\mathrm{sh}\, \beta - \frac{K^2}{K_1^2}\right] - \frac{\mathrm{sh}\, \beta - \beta}{2K} \tag{44}$$

($\beta = 2K(L - R)$; the rest of the notation is clear from Fig. 2). For a wide barrier we have

$$r_0 = -\frac{(KR+1)(K^2+K_1^2)}{4K_1^2K\xi} \quad (\xi = e^{-\beta} \ll 1),$$

i.e., r_0 is negative and exponentially large compared with the range of the forces.

2) As a second example which allows an exact solution we consider a potential with a Coulomb tail:

$$V(r) = \alpha / (r+R) \quad (0 < r < \infty). \quad (45)$$

Here $\alpha > 0$.

$$f_+(k, r) = \exp\left(\frac{\pi\alpha}{2k} - ikR\right) W_{-i\alpha/k, \frac{1}{2}}(-2i\rho), \quad (46)$$

where $\rho = k(r + R)$ and W is a Whittaker function. According to (6) and (46) the equation for the level energy has the form

$$xW'_{\mu,\frac{1}{2}}(x)/W_{\mu,\frac{1}{2}}(x) = -\zeta R \quad (\mu = -\alpha/\lambda, \quad x = 2\lambda R). \quad (47)$$

At the moment when the level first appears $\mu \to -\infty$, $x \to 0$. We use a method given in Appendix A of [11] and find that under those conditions

$$W_{\mu,\frac{1}{2}}(x) = \frac{z}{\Gamma(1-\mu)}\left\{K_1(z) - \frac{x^2}{6z}K_2(z) + \ldots\right\}, \quad (48)$$

where $K_\gamma(z)$ is a Macdonald function and $z = \sqrt{-\mu z} = \sqrt{8\alpha R}$.

Denoting by ζ_0 and $\chi_0(r)$ the value of the δ-potential coupling constant and the wave function at the moment when the level first arises, we have

$$zK_0(z) / 2K_1(z) = \zeta_0 R, \quad (49)$$

$$\chi_0(r) = C(r+R)^{\frac{1}{2}} K_1(\sqrt{8\alpha(r+R)}), \quad 0 < r < \infty. \quad (50)$$

if we normalize $\chi_0(r)$ using (23), we have[8)]

$$C = \frac{1}{R}\left[\frac{3}{K_2^2(z) - K_1^2(z)}\right]^{\frac{1}{2}} \quad (z = \sqrt{8\alpha R}).$$

When $\zeta > \zeta_0$ the level deepens linearly with $\zeta - \zeta_0$. The parameter k_0^2 from (9) is equal to (see Eq. (A-5))

$$k_0^2 = 2\varepsilon = \frac{3zK_0(z)K_1(z)}{2R^2[K_2^2(z) - K_1^2(z)]}\left(1 - \frac{\zeta}{\zeta_0}\right). \quad (51)$$

We now consider the function $\gamma(k)$. Using the asymptotic formula (48) we get from (46) and (25) when $k \ll \alpha$

$$|f_+(k)|^2 = \frac{k}{2\pi\alpha}[zK_1(z)]^2 e^{2\pi\alpha/k};$$

$$\gamma(k) = \gamma_0 e^{-2\pi\alpha/k}, \quad (52)$$

$$\gamma_0 = 3\pi / 4R^2[K_2^2(z) - K_1^2(z)]. \quad (53)$$

The function $\gamma(k)$ has in this case an essential singularity at $k = 0$.

Let us also consider the limiting case of a "weak Coulomb interaction" when $z \ll 1$. Then $C = 4\alpha\sqrt{3}$ and the calculation of the average radius gives $\bar{r} = 0.3/\alpha \gg R$. A particle with energy $\epsilon = 0$ "sits" thus mainly outside the well and the wave function depends weakly on the form of the potential inside the well (for $r < R$, see Fig. 1), i.e., the situation reminds us of the deuteron (however, the radius $\bar{r}$ is finite as $\epsilon \to 0$ which is explained by the Coulomb barrier). Equations (49) to (53) become

$$\zeta_0 = 2\alpha\Lambda, \quad k_0^2 = 12\alpha^2\Lambda(1 - \zeta / \zeta_0), \quad \gamma_0 = 12\pi\alpha^2 \quad (54)$$

($\Lambda = -\ln 8\alpha R$) and are independent of the form of the attractive potential in the interval $r < R$.

3) Let now

$$V(r) = \frac{\alpha}{2(r+R)^2} \quad (0 < r < \infty) \quad (55)$$

(this case must be considered separately as the quasiclassical formulae (27) to (29) cannot be applied here). Here

$$f_+(k, r) = \sqrt{\frac{\pi\rho}{2}} \exp\left\{i\left[\frac{\pi}{2}\left(\nu + \frac{1}{2}\right) - kR\right]\right\} H_\nu^{(1)}(\rho), \quad (56)$$

where $\rho = k(r + R)$ and $\nu = \sqrt{\alpha + 1/4}$. We shall assume in what follows that $\alpha > 3/4$ (or $1 < \nu < \infty$) so that the integral (23) converges. The bound level occurs first when $\zeta = \zeta_0$ where

$$\zeta_0 = (\nu - 1/2) / R, \quad (57)$$

and Eq. (6) for the level energy can be changed to

$$yK_{\nu-1}(y) / K_\nu(y) = (\zeta - \zeta_0)R, \quad y = \lambda R. \quad (58)$$

For the S-matrix we get the expression $S = S_0 S_1$,

$$S_0(k) = \frac{H_\nu^{(2)}(kR)}{H_\nu^{(1)}(kR)} \exp\left\{i\left[2kR - \left(\nu + \frac{1}{2}\right)\pi\right]\right\},$$

$$S_1(k) = \frac{q_\nu^{(2)}(kR) + (\zeta - \zeta_0)R}{q_\nu^{(1)}(kR) + (\zeta - \zeta_0)R}, \quad (59)$$

where, by definition, $q_\nu^{(i)}(z) = zH_{\nu-1}^{(i)}(z)/H_\nu^{(i)}(z)$ while the $H_\nu^{(i)}(z)$ are Hankel functions. The functions $q_\nu(z)$ and with them also S(k) have a branch point at $k = 0$ (except for half-odd-integer values $\nu = n + 1/2$). If, however, $\nu = n + 1/2$, then $q_\nu(z)$ is a meromorphic function of z. For instance,

$$q_{3/2}^{(1)}(z) = \frac{z^2}{1 - iz}, \quad q_{5/2}^{(1)}(z) = \frac{z^2(1 - iz)}{3(1 - iz) - z^2}. \quad (60)$$

We determine now the position of the S-matrix poles close to the point $k = 0$. Using the expansion

$$q_\nu^{(1,2)}(x) = \frac{x^2}{2(\nu - 1)} \pm i\frac{\pi x^{2\nu}}{2^{2\nu-1}\Gamma^2(\nu)} \quad (x \to +0, \ \nu > 1),$$

we find (for $\zeta < \zeta_0$)

$$k_{1,2}R = c_1(\pm p^{\frac{1}{2}} - ip^{\nu-\frac{1}{2}}), \quad E = \varepsilon_0 - ic_2\varepsilon_0^{\nu}. \quad (61)$$

Here $p = c_3(\zeta_0 - \zeta)R$, $\epsilon_0(\nu - 1)(\zeta_0 - \zeta)/R$; c_1, c_2, and c_3 are numerical coefficients which depend on ν. The poles k_1 and k_2 approach the point $k = 0$ along the real axis, which corresponds to the case of a Breit–Wigner resonance. The poles strictly coincide in the point $k = 0$. When $\zeta > \zeta_0$ the pole occurs for $k = i\lambda$ (real level, determined by Eq. (58)) and there is also a pair of complex poles close to the imaginary axis in the lower k-half-plane, i.e., there are always three poles close to $k = 0$ on the first sheet of the k-plane. The change in the number of poles ($2 \to 3$) can be explained by the fact that for $\zeta = \zeta_0$ in general an infinite number of poles on different sheets meet in the point $k = 0$ (see [13], p. 360).

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8)To evaluate the normalizing constant C we use the value of the integral

$$\int_z^\infty K_1^2(x)x^3\,dx = \frac{z^4}{6}[K_2^2(z) - K_1^2(z)],$$

the validity of which can be most simply checked by direct differentiation (see also [16]).

In the particular case $\nu = n + ^1\!/_2$ the point $k = 0$ is not a branch point for the S-matrix and the pair of poles k_1 and k_2 turns into a real and a virtual level. This is particularly clearly evident for $\nu = ^3\!/_2$ when by virtue of (60) the equation for the position of the pole can easily be solved exactly:

$$k_{1,2}R = 2(\pm\sqrt{p - p^2} - ip), \qquad p = {}^1\!/_4(\zeta_0 - \zeta)R. \qquad (62)$$

4. FACTORIZATION OF THE FUNCTIONS $\chi_k(r)$ IN THE RESONANCE REGION

Let $\chi_k(r)$ be the wave function of the continuous spectrum normalized to $\delta(k - k')$:

$$\chi_k(r) \underset{(r\to\infty)}{\approx} \sqrt{\frac{2}{\pi}}\sin(kr + \delta(k)). \qquad (63)$$

As $k \to 0$ we have for a wide range of r-values $|V(r)| \gg k^2$. Near the resonance (i.e., when $|\zeta - \zeta_0| \ll \zeta_0$) the r-dependence of χ_k is the same as for $k = 0$, i.e., the factorization (1) is valid.

Using for $\chi_k(r)$ Eq. (4) and substituting Eq. (5) for $S_1(k)$ in it we get

$$\chi_k(0) = \sqrt{\frac{2}{\pi}}e^{-i\delta}\frac{f_-(k)\gamma(k)}{k_0^2 - k^2 - i\gamma(k)} = \sqrt{\frac{2}{\pi}}\frac{|f_-(k)|\gamma(k)}{[(k^2 - k_0^2)^2 + \gamma^2(k)]^{1/2}} \qquad (64)$$

For the case I (barrier with a finite penetrability and $l = 0$) $\chi_0(r) = f_+(0, r)$ if $\chi_0(r)$ is normalized according to (14). Hence $\chi_0(0) = f_+(0)$, $\gamma(k) = 2\kappa k$ and for $\Delta(k)$ we have Eq. (2).

On the other hand, in case II (i.e., for levels with $l \geq 1$ or for $l = 0$ and zero barrier penetrability) we have, using (25), for $\Delta(k)$

$$\Delta(k) = \left|\frac{\chi_k(0)}{\chi_0(0)}\right|^2 = \frac{2}{\pi}\frac{k\gamma(k)}{(k^2 - k_0^2)^2 + \gamma^2(k)}. \qquad (65)$$

We discussed above the behavior of $\gamma(k)$ as $k \to 0$. In particular, $\gamma(k) = \gamma_0(kR)\exp 2l + 1$ for a level with angular momentum l in a short-range potential of radius R.

To estimate the range of the applicability of the factorization (1) we consider a potential with the rectangular barrier (33). In that case ($\xi = \exp -2KR \ll 1$)

$$\frac{\chi_0(R)}{\chi_0(0)} = \frac{1}{\operatorname{ch} KR} \approx 2\xi^{-1/2},$$

$$\frac{\chi_k(R)}{\chi_k(0)} = \operatorname{ch}\mu R - \frac{\zeta}{\mu}\operatorname{sh}\mu R \approx 2\xi^{-1/2}\left(1 + \frac{k_0^2 - k^2}{2K\varkappa}\right).$$

From this it follows that the factorization (1) is valid everywhere under the barrier, provided $|k_0^2 - k^2| \ll 2K\kappa$. One can easily change this condition to a more lucid form:

$$|\varepsilon - \varepsilon_0| / \gamma \ll {}^1\!/_2\sqrt{V/\varepsilon_0}, \qquad (66)$$

where $V = K^2/2$ is the barrier height. Since $V \gg \epsilon_0$ the factorization of $\chi_k(r)$ occurs in the range of energies ϵ which appreciably exceed the resonance width γ.

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APPENDIX

We derive Eqs. (15) and (18) of the paper.

Let a bound state first occur for $\zeta = \zeta_0$. There is then for $0 < \zeta - \zeta_0 \ll \zeta_0$ a level with a small binding energy $|\epsilon| = \lambda^2/2$ and a wave function $\chi_\lambda(r)$ where

$$\chi_\lambda'' - 2V\chi_\lambda = \lambda^2\chi_\lambda. \qquad (A.1)$$

We give the parameter ζ a small increment $\delta\zeta$. Then $\chi_\lambda(r) \to \chi_\lambda(r) + \delta\chi_\lambda(r)$ where

$$\delta\chi_\lambda'' - 2V\delta\chi_\lambda = 2\lambda\delta\lambda\chi_\lambda(r). \qquad (A.2)$$

Multiplying (A.1) by $\delta\chi_\lambda$, (A.2) by χ_λ, subtracting the one from the other and integrating over r from 0 to ∞ we find

$$2\lambda\delta\lambda = [\chi_\lambda'\delta\chi_\lambda - \chi_\lambda\delta\chi_\lambda']_{r=0}. \qquad (A.3)$$

The expression on the right-hand side can easily be expressed in terms of a variation of the logarithmic derivative $\chi_\lambda'/\chi_\lambda$ at $r = 0$:

$$2\lambda\delta\lambda = \chi_\lambda^2(0)\delta\zeta. \qquad (A.4)$$

The remaining calculations are slightly different for type I and type II potentials (i.e., potentials with a finite and with a zero penetrability at $k = 0$, see section 2). In the simplest case II the function $\chi_\lambda(r)$ changes as $\lambda \to 0$ to the normalized wave function $\chi_0(r)$ corresponding to a zero level energy. Therefore, (A.4) gives directly the equation determining the level energy for $\zeta - \zeta_0 \ll \zeta_0$:

$$\varepsilon = -{}^1\!/_2\lambda^2 = -{}^1\!/_2\chi_0^2(0)(\zeta - \zeta_0). \qquad (A.5)$$

For type I potentials the function $\chi_0(r)$ cannot be normalized. On the other hand, $\chi_\lambda(r)$ for any $\lambda > 0$ is normalized to unity. The functions $\chi_\lambda(r)$ and $\chi_0(r)$ are thus as $\lambda \to 0$ and for any finite r connected through Eq. (13). Substituting it into (A.4) and dividing both sides by 2λ we find

$$\lambda = \chi_0^2(0)(\zeta - \zeta_0), \qquad \varepsilon = -\lambda^2/2. \qquad (A.6)$$

With increasing ζ the level which appears deepens thus linearly with $\zeta - \zeta_0$ for the case of type II potentials and quadratically in the case of type I.

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