

Level shifts under the influence of a short-range potential

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Formulas are obtained for the shift of energy levels $E_n^{(0)} \ll r_c^{-2}$ in a field $V_f(\mathbf{r})$ under the influence of a short-range potential $U(r)$ of radius r_c in terms of low-energy scattering parameters (scattering length and effective range) corresponding to angular momentum l in this potential. For a nonresonant interaction between the particle and the center of force, this approach is equivalent to perturbation theory in the scattering length. The theory is generalized to systems with random degeneracy (V_f is the Coulomb potential). Formulas describing the quasicrossing of levels are obtained for the case of resonant interaction between a center of force and a partial wave with $l \neq 0$ when both U and V_f contain closely spaced levels. The properties of the level shift are indicated in the case where the corresponding binding energy is anomalously low and the wave function becomes delocalized as the binding energy is reduced to zero. The level shift when V_f is a potential well surrounded by a relatively impenetrable barrier is examined. Some applications of this theory to the problem of a particle in the field of two short-range potentials, or in the field of a short range and a Coulomb center, are discussed. Formulas are also obtained for the shifts and widths of Landau levels, and for a shallow level with arbitrary angular momentum that perturbs these levels.

1. INTRODUCTION

The solution of many problems in atomic and solid-state physics relies on a knowledge of the effect of various types of impurity center with short-range interaction on the energy spectrum of electronic states, where the interaction itself is not small and perturbation theory cannot be used. Such systems are described by the Hamiltonian

$$H = -\frac{1}{2}\Delta + V_f(\mathbf{r}) + U(r) \quad (1)$$

$\hbar = m = 1$, where $U(r)$ is the short-range central potential of radius r_c and $V_f(\mathbf{r})$ describes the external field or the interaction with other centers which themselves can bind a particle. Depending on the nature of the potentials U and V_f , we may have to consider the level shift in the potential U under the influence of an external field, or the effect of a center with a short-range interaction on levels in the potential V_f , including the rearrangement of the spectrum when the levels in both U and V_f are closely spaced.

Many such problems are discussed within the framework of the zero-range potential method in Refs. 1–5 on the assumption that the short-range potential affects only particles with zero angular momentum ($l = 0$). A generalization of this method to nonzero angular momenta and some of its applications are examined in Refs. 6 and 7.

In this paper, we develop an analytic theory of the shift of the energy levels of a particle under the influence of a short-range center of force. Simple formulas for the level shifts in terms of the parameters of low-energy scattering by the center U are obtained for levels $E_n^{(0)}$ satisfying the condition $E_n^{(0)} \ll r_c^{-2}$, in the potential $V_f(\mathbf{r})$. These formulas are valid in a wide range of values of these parameters, including the level crossing region. Some applications of these results to particular physical problems are discussed.

2. LEVEL SHIFTS PRODUCED BY A CENTER OF FORCE

Consider the influence of the short-range potential $U(r)$ on levels with energy $E = k^2/2 \ll r_c^{-2}$, in the field $V_f(\mathbf{r})$. The interaction V_f is assumed to be small ($V_f \ll r^{-2}$) for $r \ll L_f$, where $L_f \gg r_c$. Thus, for

$$r_c \ll r \ll \min\{L_f, k^{-1}\} \quad (2)$$

the particle may be looked upon as free with zero energy. There are no restrictions on V_f for $r \gg L_f$. Assumptions about the potential U will be formulated below in terms of the parameters of low-energy scattering with angular momentum l :

$$(2l-1)!!(2l+1)!!B_l(E) = k^{2l+1} \operatorname{ctg} \delta_l(k) = -\frac{1}{a_l} + r_l E + \dots, \quad (3)$$

where δ_l , a_l , r_l are the phase shift, scattering length, and effective range in the potential U , respectively. It will be convenient to have the values of these parameters for an impenetrable sphere of radius r_c :

$$B_l(E) \approx -r_c^{-2l-1} - \frac{2(2l+1)}{(2l-1)(2l+3)} r_c^{-2l+1} E.$$

We begin by deriving the formula for the shift of a discrete nondegenerate level $E_n^{(0)}$ in the potential V_f (random degeneracy is discussed in Section 4). The normalized wave function for this state at short distances $r \ll L_f$, k^{-1} has the form

$$\Psi_n^{(0)}(\mathbf{r}) = \sum_{l,m} R_n^{(lm)} [r^l Y_{lm}(\mathbf{n}) + \dots]. \quad (4)$$

The wave function for the level $E_n = E_n^{(0)} + \Delta E_n$ shifted by U can be represented by the following expansion⁸ that is valid in the overlap region (2):

$$\Psi_n(\mathbf{r}) = \sum_{l,m} \bar{R}_n^{(lm)} \{ [r^l Y_{lm}(\mathbf{n}) + \dots] + B_l^{-1} [r^{-l-1} Y_{lm}(\mathbf{n}) + \dots] \}. \quad (5)$$

Multiplying the Schrödinger equation

$$\left[-\frac{1}{2} \Delta + V_f - E_n^{(0)} \right] \Psi_n^{(0)} = 0,$$

$$\left[-\frac{1}{2} \Delta + V_f + U - E_n \right] \Psi_n = 0$$

by Ψ_n^* and $\Psi_n^{(0)*}$, respectively, and subtracting one from the other term by term, we obtain the following result after integration over all space with the exception of a sphere of radius d ($r_c \ll d \ll L_f, k^{-1}$) near the origin:

$$\Delta E_n \int_{r>d} \Psi_n^{(0)*} \Psi_n dv = \frac{1}{2} \int_{r=d} (\Psi_n^{(0)*} \nabla \Psi_n - \Psi_n^* \nabla \Psi_n^{(0)}) ds, \quad (6)$$

where the phases of the wave functions are chosen so that the ratio $\Psi_n^{(0)}/\Psi_n$ is real, so that the terms including $E_n^{(0)}$ and V_f cancel out. For

$$B_l^{-1}(E_n) \ll L_f^{2l+1}, \quad B_l^{-1}(E_n) \ll (-E_n)^{-l-1/2} \quad (7)$$

and for values of ΔE_n , much smaller than the separation between neighboring levels in V_f , we may put $\Psi_n \approx \Psi_n^{(0)}$, outside the overlap region, in which case $\bar{R}_n^{(lm)} \approx R_n^{(lm)}$. Replacing the integral on the left-hand side of (6) by unity, and transforming the right-hand side with allowance for (4), (5), and the orthogonality of the spherical harmonics, we obtain the explicit expression

$$E_n - E_n^{(0)} \approx -\frac{1}{2} \sum_{l,m} (2l+1) |R_n^{(lm)}|^2 B_l^{-1}(E_n^{(0)}) \quad (8)$$

for the level shift [see below about the replacement of E_n in $B_l(E_n)$ with $E_n^{(0)}$].

The conditions given by (7) are the restrictions on the potential $U(r)$ and are definitely satisfied in the nonresonant situation when $\delta_l(E) \ll 1$ for all $E \ll r_c^{-2}$. We can then restrict our attention to the first term in the expansion (3) for B_l , and (8) assumes the form

$$E_n - E_n^{(0)} \approx \frac{1}{2} \sum_{l,m} [(2l+1)!!]^2 |R_n^{(lm)}|^2 a_l, \quad (9)$$

so that, since $a_l \lesssim r_c^{2l+1}$, only the $l=0$ term is in general important for an arbitrary interaction $V_f(r)$ in (9). We then have $|R_n^{(00)}|^2 = 4\pi |\Psi_n^{(0)}(0)|^2$, and (9) becomes identical with the usual result.^{9,10} When the Hamiltonian is axially symmetric, the leading term in the expression for the level shift with angular momentum component m is the term with $l = |m| \equiv \mu$:

$$E_{nm} - E_{nm}^{(0)} \approx (2\mu+1)! |Z_{nm}(0)|^2 a_\mu, \quad (10)$$

where $z_{nm}(0)$ is related to the wave function of the unperturbed level, whose form for $\rho \rightarrow 0$ is

$$\Psi_{nm}^{(0)} \approx \rho^\mu Z_{nm}(z) e^{im\phi} / (2\pi)^{1/2},$$

and ρ is the distance from the symmetry axis lying along the z

direction. If, on the other hand, the interaction is centrally symmetric, the sums in (4) and (9) reduce to a single term corresponding to the angular momentum l of the level, and neither the shift nor $R_n^{(lm)}$ will, of course, depend on m .

We note that the formula given by perturbation theory in the scattering length, i.e., (9), can be formally deduced with the aid of a device similar to that employed in Ref. 11 to find the ground-state energy of a degenerate and almost perfect gas. In particular, according to the usual perturbation theory in the potential,

$$\Delta E_n = \int U(r) |\Psi_n^{(0)}|^2 dv;$$

and, using the asymptotic behavior (4) to evaluate the integral, we can express the level shift in terms of the scattering length in the Born approximation:

$$a_l^{B=2} = 2[(2l+1)!!]^{-2} \int_0^\infty U(r) r^{2l+2} dr.$$

Replacement of these lengths with the exact scattering lengths in the short-range potential U results in (9). Subsequent substitution $a_l \rightarrow [a_l^{-1} - r_l E_n]^{-1}$ gives (8).

The conditions (7) can be violated only in the resonant case, when the potential U contains a shallow level with angular momentum l and energy $E_l^{(0)} \ll r_c^{-2}$. For $l=0$, the restrictions (7) signify that the potential U contains only s -levels with energy of the order of $E_n^{(0)}$. In the expression for B_l , we can then neglect the term for the effective range and the conditions (7) demand that $a_0 \ll L_f$, and $(-E^{(0)})^{-1/2}$. If, on the other hand, the short-range potential contains an s -level with energy of the order of $E_n^{(0)}$, the spectrum is modified. The particular feature of this modification is that, when U and V_f operate together, the spectrum may differ substantially from the spectra corresponding to these potentials taken separately.

A totally different situation prevails for angular momenta $l \geq 1$. In this case, conditions (7) can be violated only if the potential U contains a level $E_l^{(0)} \approx (a_l r_l)^{-1}$, anomalously close to $E_n^{(0)}$, so that

$$|r_l (E_l^{(0)} - E_n^{(0)})| \lesssim L_f^{-2l-1}, \quad (-E_n^{(0)})^{l+1/2}.$$

The spectrum in the field $V_f + U$ consists of slightly shifted levels obtained in the potentials V_f and U individually, and the modification of the spectrum reduces to the quasicrossing of levels. This is due to the presence of a relatively impenetrable centripetal barrier that ensures practically independent motion of a particle in the short- and long-range wells.

The replacement of E_n with $E_n^{(0)}$ in B_l in (8) relies on the assumption that the level shift is such that $|\Delta E_n| \ll |E_n^{(0)} - E_l^{(0)}|$. On the other hand, when this replacement is not introduced, (8) remains the equation for the level shift, the solution of which is

$$\Delta E_{nm}^{(\pm)} \approx 1/2 \{ \delta E_{nm}^{(0)} + \alpha_{\mu m} \pm [(\delta E_{nm}^{(0)} - \alpha_{\mu m})^2 + \beta_{Lm}]^{1/2} \} \quad (11)$$

and describes the quasicrossing of levels, where

$$\delta E_{nm}^{(0)} = E_l^{(0)} + V_f(0) - E_{nm}^{(0)},$$

$$\alpha_{\mu m} = 1/2 [(2\mu+1)!!]^2 |R_{nm}^{(\mu m)}|^2 a_\mu, \quad (12)$$

$$\beta_{Lm} = 2[(2L+1)!!]^2 |R_{nm}^{(Lm)}|^2 |r_L|^{-1}.$$

Equation (11) is written for the axially symmetric Hamiltonian. It includes the contribution of the two most important waves, namely, the nonresonant wave with the lowest possible angular momentum $l = \mu$ ($l = 0$ in the absence of symmetry) and the resonant wave with angular momentum $L > \mu$ (for central symmetry and for $L = \mu \geq 1$, we must put $\alpha_{\mu m} = 0$). The appearance of $V_f(0)$ in (12) corresponds to allowance for the action of the field $V_f(r)$ for $r \lesssim r_c$, which leads to the renormalization of the scattering length. When $V_f(r) \simeq V_f(0)$ for $r \lesssim r_c$, the renormalization is equivalent to the replacement

$$a_l^{-1} \rightarrow a_l^{-1} + r_l V_f(0), \quad (13)$$

which reflects the shift of the unperturbed level in U by $V_f(0)$:

$$E_l \approx E_l^{(0)} + V_f(0). \quad (14)$$

Equation (11) describes the quasicrossing of levels, and is valid for ΔE_{nm} , much smaller than the separation between levels in V_f . As the detuning from resonance increases, both this condition and (7) are violated for one of the roots: $\Delta E_{nm}^{(+)}$ for $\delta E_{nm}^{(0)} > 0$ or $\Delta E_{nm}^{(-)}$ for $\delta E_{nm}^{(0)} < 0$. However, the root that corresponds to the level in the short-range potential becomes identical with (14) well away from resonance. Under the same conditions, the other root describes the shift of the level $E_{nm}^{(0)}$ in the potential V_f under the influence of U , and reproduces (8) if we confine our attention in this expression to the partial waves indicated above, and introduce the level-shift correction $V_f(0)$.

Equation (11) is thus seen to describe the spectrum for practically all the values of the parameters of the short-range potential. We note that the width of the region in which level quasicrossing occurs decreases rapidly with increasing angular momentum l , and for large detuning from resonance for which $\delta E_{nm}^{(0)} \sim E_{nm}^{(0)}$, the relative contribution to the level shift due to partial waves with $l = \mu$ and $l = L > \mu$ is of the order of $\alpha_{\mu m} \delta E_{nm}^{(0)} / \beta_{Lm} \propto r_c^{-2(L-\mu-1)}$, so that the contribution of the resonant wave is substantial only for $L = \mu + 1$.

In view of the foregoing, we must now introduce a remark about the relationship between binding energy in the initial level and its shift when it is the uppermost level and lies anomalously close to the continuous-spectrum limit. In this situation, the way in which the wave function decreases at large distances as the binding energy tends to zero is an important factor. If the wave function remains normalized at the edge of the continuum, the above result will also be valid for states with binding energy as small as desired. This is accomplished, for example, in a central potential $V_f(r)$ of finite range for states with angular momentum $l \geq 1$: $\Psi_{l,E=0}^{(0)} \propto r^{-1-l}$ as $r \rightarrow \infty$.

The case where the wave function is delocalized as the binding energy tends to zero (states with $n = 0$ in a central potential, Landau levels in a magnetic field, and so on) requires separate analysis. The relation $\Psi_n \approx \Psi_n^{(0)}$ used above outside the overlap region will definitely break down at large distances for a small change in the energy. However, if the function remains normalized at the edge of the continuum,

such distances become unimportant. For a delocalized wave function, large distances provide an important contribution to the normalizing integral, and we can no longer assume that $\Psi_n \approx \Psi_n^{(0)}$.

Let us generalize the above results to this case. We shall not assume that a shallow level in the field $V_f(r)$ is a true bound state (it may be a virtual or quasidiscrete state). Suppose that $\Psi_n(r, E_n)$ is the wave function of a true bound state with energy $E_n = E_n(B_l)$, normalized to unity and resulting from the combined action of E_f and U , whereas $\Psi_n(r, E_n + \delta E_n)$ is the wave function of this state for small change δU in the short-range potential for which $B_l^{-1} \rightarrow B_l^{-1} + \delta B_l^{-1}$. These functions have a form analogous to (5) in the region (2), whereas, in the essential part of the region in which the field acts, they have the same functional dependence on r as the function $\tilde{\Psi}^{(0)}(r, \tilde{E}_0)$ of a level in the potential $\tilde{V}_f = V_f + \delta V_f$ for zero binding energy:

$$\Psi_n(r, E_n) \approx N(E_n) \tilde{\Psi}_n^{(0)}(r, \tilde{E}_0),$$

where \tilde{E}_0 is the continuous-spectrum limit and the specific form of δV_f is unimportant. Writing down the Schrödinger equation for the functions Ψ_n , and proceeding as in the derivation of (6), we find that

$$\delta E_n \approx -\frac{1}{2} \sum_{l,m} (2l+1) |N(E_n) \tilde{R}_n^{(lm)}|^2 \delta B_l^{-1}. \quad (15)$$

The relationship between $\tilde{R}_n^{(lm)}$ and $\tilde{\Psi}_n^{(0)}$ is the same as between $R_n^{(lm)}$ and $\Psi_n^{(0)}$ in (4). We note that $|N(E_n) \tilde{R}_n^{(lm)}|^2$ does not depend on the normalization of $\Psi_n^{(0)}(r, \tilde{E}_0)$.

To use (15) to obtain the expression for the level shift, we must know the dependence of the normalizing factor $N(E)$ on the binding energy $\varepsilon = \tilde{E}_0 - E_n = \kappa^2/2$. In particular, when the function $\tilde{\Psi}_n^{(0)}$ with zero binding energy is normalizable, we have $N^2 \approx 1$ and integration of (15) leads to (8), which demonstrates its validity in a wider range: (8) is valid even for energies exceeding \tilde{E}_0 and describing quasidiscrete levels (the determination of their widths requires separate analysis). In particular, in the nonresonant case, it is clear from (10) that the initial real level becomes quasidiscrete at $(2\mu + 1)! |Z_{nm}(0)|^2 a_\mu \geq \tilde{E}_0 - E_{nm}^{(0)}$.

Delocalization of the function $\tilde{\Psi}_n^{(0)}$ means that $N(E)$ becomes strongly dependent on the binding energy: $N(E) \rightarrow 0$ as $\kappa \rightarrow 0$. Usually, $N(E_n) \approx N^{(0)} \kappa^{1/2}$, in which case integration of (15) yields

$$\kappa = \kappa_0 + \frac{1}{2} \sum_{l,m} (2l+1) |N^{(0)} \tilde{R}_n^{(lm)}|^2 B_l^{-1}. \quad (16)$$

For $\kappa_0 > 0$, the parameter κ_0 determines the binding energy $\varepsilon_0 = \kappa_0^2/2$ of the original real level in the field V_f . When $\kappa_0 < 0$, $(-\varepsilon_0)$ is the energy of the virtual level. Similarly, when the potential U is present, (16) gives the energy of a level that is real for $\kappa > 0$ and virtual for $\kappa < 0$. When the shift is much less than the binding energy, (16) becomes identical with (8), in which case, we must remember that $R_n^{(lm)} \approx N^{(0)} \kappa_0^{1/2} \tilde{R}_n^{(lm)}$. On the other hand, when the binding energy is low, these formulas describe different laws of variation of the position of the level under the influence of U , depend-

ing on the localization of the wave function at the continuum limit. This corresponds to the well-known laws whereby levels become depressed under the influence of a perturbation $\delta U \ll 0$: the variation in a central potential is quadratic for $l = 0$ and linear for $l \geq 1$.

The above dependence of the normalizing factor $N \propto \kappa^{1/2}$ for a wave function that becomes delocalized as $\kappa \rightarrow 0$ is usually preserved for values of κ satisfying the condition $\kappa r_f \ll 1$, where r_f is the range of the field V_f . This is so because contributions to the normalizing integral from the region in which the potential V_f is localized and from the "external" region are $\sim |\Psi(1)|^2 r_f^3$ and $\sim |\Psi(2)|^2 r_f^2 \kappa^{-1}$, respectively, where $\Psi(1,2)$ are the characteristic values of the function in the region of localization of the potential and just outside the region in which it operates. Generally speaking, $|\Psi(1)|^2 \sim |\Psi(2)|^2$. However, when V_f takes the form of a potential well surrounded by a relatively impenetrable barrier, we have $|\Psi(2)|^2 \sim D |\Psi(1)|^2$, where $D \ll 1$ is the barrier transmission. It then turns out that, even for small values of κ , the contribution to the normalizing integral due to the "external" region becomes unimportant, and $N(E)$ ceases to depend on the binding energy. Let us now consider the effect of the short-range center on the shift of a level with angular momentum $l = 0$ when $V_f = V(|\mathbf{r}-\mathbf{b}|)$ is the central potential. Suppose that the wave function

$$\tilde{\Psi}_n^{(0)} = (4\pi)^{-1/2} R_n^{(0)}(r)$$

with $l = 0$ and zero binding energy in the potential $V(r)$ is normalized by the condition $r R_n^{(0)}(r) \rightarrow 1$ as $r \rightarrow \infty$. We then have

$$N^2(E) \approx 2\kappa(1 - \rho_0 \kappa)^{-1}. \quad (17)$$

The effective range in the field V is then given by¹²

$$\rho_0 \approx L - L_0/2D, \quad D = \exp \left\{ -2 \int_{L_0}^L [2V(r)]^{1/2} dr \right\},$$

where L_0 and L define the walls of the barrier surrounding the well (see Ref. 12 for further details). For a barrier with a low transmission factor, the term $\rho_0 \kappa$ in (17) becomes important. Integrating (15) with $N^2(E)$ as given by (17), we obtain

$$\kappa - \frac{1}{2} \rho_0 \kappa^2 = \sum_l (2l+1) |\tilde{R}_n^{(l0)}|^2 B_l^{-1}, \quad (18)$$

which describes the change in the level energy in the potential V_f under the influence of the central potential U . When $\rho_0 \kappa \ll 1$, (18) becomes identical with (16) and, for $\rho_0 \kappa \gg 1$, with (8). It generalizes the results reported in Ref. 12 to the case of an arbitrary short-range potential. When $b = 0$, the right-hand side of (18) assumes the form $-|R_n^{(0)}(0)|^2 a_0$, in the non-resonant case, and the final result follows from Eqs. (12) and (13) of Ref. 12 if we use the above chain of replacements:

$$\int_0^\infty \delta U [R_n^{(0)}(r)]^2 r^2 dr \rightarrow \frac{1}{2} [R_n^{(0)}(0)]^2 a_0^3 \rightarrow \frac{1}{2} [R_n^{(0)}(0)]^2 a_0. \quad (19)$$

The coefficients $R_n^{(lm)}$ in (4), which appear in (8)–(11) and (16), can be found by direct differentiation of the wave func-

tion of the unperturbed level, using the formula

$$R_n^{(lm)} = \frac{4\pi}{(2l+1)!!} [Y_{lm} \cdot (\nabla) \Psi_n^{(0)}(\mathbf{r})]_{r=0} \quad (20)$$

(the coefficients $\tilde{R}_n^{(lm)}$ can be expressed in terms of $\tilde{\Psi}_n^{(0)}$ in a similar way). In these expressions, the differential operator $Y_{lm}(\nabla)$ is obtained by replacing n_i with $\partial/\partial x$ in the spherical harmonic

$$Y_{lm}(\mathbf{n}) = \varepsilon_{i_1 \dots i_l} (l, m) n_{i_1} \dots n_{i_l},$$

where $\varepsilon_{i_1 \dots i_l}$ is a tensor of rank l and zero trace, which is symmetric in any pair of indices. The derivation of (20) is based on

$$Y_{i_1 \dots i_l} \cdot (\nabla) r^l Y_{lm}(\mathbf{n}) = [(2l+1)!!/4\pi] \delta_{i_1 i_2} \dots \delta_{i_{l-1} i_l}. \quad (21)$$

On the other hand, when $V_f = V(|\mathbf{r}-\mathbf{b}|)$ is a central potential, the coefficients $R_n^{(lm)}$ corresponding to the leading partial waves can be expressed directly in terms of the radial wave functions of these states

$$\Psi_{nlm}^{(0)} = r^l R_n^{(0)}(r) Y_{lm}(\mathbf{n})$$

in the potential $V(r)$:

$$R_{nlm}^{(\mu m)} = i^{l-\mu} \left[\frac{2l+1}{(2\mu+1)!} \frac{(l+\mu)!}{(l-\mu)!} \right]^{1/2} b^{l-\mu} R_{nl}^{(0)}(b), \quad (22)$$

$$R_{nlm}^{(\mu+1, m)} = i(2\mu+3)^{-1/2} \frac{d}{db} R_{nlm}^{(\mu m)}.$$

In deriving these formulas, we used the relationship between the polar angles φ and ϑ at the point \mathbf{r} relative to the centers $r = 0$ and $\mathbf{r} = \mathbf{b}$, and the explicit form of the spherical harmonics.⁸

We must now consider some applications of the foregoing approach to specific physical problems.

3. PARTICLE IN THE FIELD OF THE TWO SHORT-RANGE CENTERS $U(r)$ and $V_f(r) = V(|\mathbf{r}-\mathbf{b}|)$

The wave function of a bound state in the potential $V(r)$ with a finite range r_f has the following form outside the range of forces:

$$\Psi_{nlm}^{(0)}(\mathbf{r}) \approx 2\kappa_0 C_{\kappa l} (\pi r)^{-1/2} K_{l+1/2}(\kappa_0 r) Y_{lm}(\mathbf{n}), \quad (23)$$

where K_ν is a modified Bessel function of imaginary argument, $E_{nl}^{(0)} = -\kappa_0^2/2$ is the level energy, $C_{\kappa l}$ is the asymptotic coefficient which for weakly bound states is given by $[\kappa_0 r_f \ll 1; \rho_l$ is the effective range in the potential $V(r)]$

$$C_{\kappa l}^{-2} \approx -\rho_l \kappa_0^{1-2l} + (-1)^l (2l+1).$$

The approach described in the last section can be used as a basis for discussing various problems connected with the influence of the central field U on the spectrum in the field V_f for $b \gg r_c, r_f$. Here, we shall confine our attention to a few remarks.

The shift of a level with angular-momentum projection m is given according to (8), (22), and (23), when U is a non-resonant interaction for angular momenta $l' > \mu \equiv |m|$, by the following expression:

$$E_{nlm} - E_{nl}^{(0)} \approx \frac{(2l+1)(2\mu+1)!(l+\mu)!}{\pi 2^{2\mu-1}(\mu!)^2(l-\mu)!} \kappa_0^2 C_{\kappa_0}^2 \frac{K_{l+\frac{1}{2}}^2(\kappa_0 b)}{b^{2\mu+1}} \left[\frac{1}{a_\mu} - r_\mu E_{nl}^{(0)} \right]^{-1}. \quad (24)$$

This formula is valid for states with $m=0$ provided $a_0 \ll b$, κ_0^{-1} . When the latter conditions are satisfied, formula (24) becomes identical with formula (9) of perturbation theory in the scattering length. However, as noted above, for $l=0$ and anomalously low binding energies, for which the condition $\Delta E_s \ll \kappa_0^2$ is violated, the above formula is no longer valid. We then have $\kappa_0 b \ll 1$, and the level shift is given by (16): $\kappa = \kappa_0 - a_0 b^{-2}$.

When $m \neq 0$, and if the potential U does not contain shallow levels with angular momentum $l' = \mu$ and energy $E_\mu^{(0)} \ll r_c^{-2}$, the formula (24) again becomes identical with the formula obtained by perturbation theory in the scattering length. However, it is also valid even when such levels are present. We then have

$$1/a_\mu - r_\mu E_{nl}^{(0)} \approx r_\mu (E_\mu^{(0)} - E_{nl}^{(0)}),$$

and (24) with $r_\mu < 0$ leads to the following property of the level shift in the potential V_f under the influence of the center of force: the signs of the level shifts ΔE_{nlm} are uniquely determined by the relative disposition of unshifted levels $E_{nl}^{(0)}$ and $E_\mu^{(0)}$, so that $\Delta E_{nlm} > 0$ for $E_{nl}^{(0)} > E_\mu^{(0)}$, and vice versa.

As noted in Section 2, the presence of a level with energy $E_L^{(0)} \sim E_{nl}^{(0)}$ in the potential U has an important effect on the shift of a level not only with $|m|=L$, but also with $|m|=L-1$. In particular, using the above formulas and confining ourselves to the case $\kappa_0 b \ll 1$, we find that ($L = \mu + 1$)

$$E_{nlm} - E_{nl}^{(0)} = \frac{(2l)!(2l+1)!(2\mu+1)!(l+\mu)!}{2^{2l+2\mu}(l!)^2(\mu!)^2(l-\mu)!} \frac{C_{\kappa l}^2}{\kappa_0^{2l-1} b^{2l+2\mu+2}} \times \{a_\mu + (2\mu+3)(l+\mu+1)[r_L(E_L^{(0)} - E_{nl}^{(0)})b^2]^{-1}\}. \quad (25)$$

This indicates a limited validity of the zero-range approximation of the short-range center when it contains a shallow p -level (this restriction does not arise, generally speaking, for angular momenta $L \geq 2$).

In the region of the level crossing, the level shifts are determined by (11) and (12). In particular, when the initial level in the potential V corresponds to $l=0$, the coefficients α_{00} and β_{L0} in (12) are given by ($L \geq 1$)

$$\alpha_{00} = C_{\kappa_0}^2 \frac{\kappa_0 a_0}{b^2} e^{-2\kappa_0 b}, \quad \beta_{L0} = \frac{8}{\pi} (2L+1) C_{\kappa_0}^2 \frac{\kappa_0^{2L+2}}{|r_L| b} K_{L+\frac{1}{2}}^2(\kappa_0 b) \quad (26)$$

[to obtain β_{L0} from (4) and (12) we used the addition theorem for cylinder functions with index $\nu = 1/2$].

4. PARTICLE IN THE COULOMB $V_f(r) = V_C(|r-b|) = -\xi|r-b|^{-1}$ AND A SHORT-RANGE $U(r)$ CENTER

In the Coulomb problem $E_n^{(0)} \equiv -\kappa^2/2 = -\xi^2/2n^2$ and the condition $\kappa r_c \ll 1$ assumes the form $r_c \ll n a_B$, where $a_B = \xi^{-1}$ is the Bohr radius (when r_c is of the order of the

atomic dimensions, the above approach is valid only for highly excited states). We shall now confine our attention mostly to the case¹ where $b \gg r_c$. The condition $\xi |b| \ll r_c^{-2}$, is then definitely satisfied, i.e., we can neglect the Coulomb potential in the region of the $U(r)$ center.

The specific feature of this problem is random degeneracy in the Coulomb potential. For generality, let us consider the case where the potential $V_C(r)$ is distorted at short distances, so that the random degeneracy is lifted. We then have

$$E_n^{(0)} \rightarrow E_{nl}^{(0)} = E_n^{(0)} + \delta E_{nl},$$

and the Coulomb wave functions $\Psi_{nlm}^{(0)}(\mathbf{r}-\mathbf{b})$, remain the eigenfunctions in the zero-order approximation. The shifts ΔE_{nlm} of these levels under the influence of the short-range center can be determined directly from the formulas of Section 2 on the assumption that $\Delta E_{nlm} \ll \delta E_{nl}$.

Let us now consider the case $\Delta E_{nlm} \gtrsim \delta E_{nl}$. This gives rise to "mixing" of states with different l and the same n and m . The perturbation matrix has the form

$$\tilde{U}_{ll'}^{(nm)} = \delta E_{nl} \delta_{ll'} + U_{ll'}^{(nm)}, \quad (27)$$

where l and l' label the angular momentum and run through the values $l, l' = \mu, \mu+1, \dots, n-1; \mu \equiv |m|$. The first term in (27) represents the perturbation that lifts the random degeneracy in the absence of the center U , and $U_{ll'}^{(nm)}$ is the perturbation matrix associated with this short-range potential. The explicit form of $U_{ll'}^{(nm)}$ can readily be found by taking into account the short-range potential by the method noted above in connection with Eqs. (9) and (19) and based on considering the action of the potential as a perturbation, followed by the replacement of the Born phases with the exact phases:

$$U_{ll'}^{(nm)} = -\frac{1}{2} \sum_{j \geq \mu} (2j+1) R_{nlm}^{(jm)*} R_{nl'm}^{(jm)} B_j^{-1}, \quad (28)$$

where the quantities R are related to the Coulomb wave function by the expansion (4).

The level shifts are determined, as usual, by diagonalizing the perturbation matrix. If we neglect the first term in (27), and confine our attention in the sum (28) to the contribution of the first most significant two lowest partial waves, this diagonalization process yields

$$E_{nm}^{(\pm)} - E_n^{(0)} = \pm \frac{1}{2} (g_\mu^{(nm)} + g_{\mu+1}^{(nm)}) \pm \frac{1}{2} \{ (g_\mu^{(nm)} - g_{\mu+1}^{(nm)}) + (2\mu+1)(2\mu+3) |f_\mu^{(nm)}|^2 B_\mu^{-1} B_{\mu+1}^{-1} \}^{1/2}, \quad (29)$$

where

$$g_j^{(nm)} = -\left(j + \frac{1}{2}\right) B_j^{-1} \sum_{l=\mu}^{n-1} |R_{nlm}^{(jm)}|^2, \quad j = \mu, \quad \mu+1, \\ f_\mu^{(nm)} = \sum_{l=\mu}^{n-1} R_{nlm}^{(\mu m)*} R_{nlm}^{(\mu+1, m)},$$

and the quantities R are expressed directly in terms of the radial Coulomb wave functions $R_{nl}^{(0)}(b)$ in accordance with (22). According to (29), the random degeneracy is partially lifted: given n and m , only two states experience level shifts (one at $|m|=n-1$). The states that are unshifted under the

influence of U correspond to those combinations of the unperturbed functions $\Psi_{nlm}^{(0)}(\mathbf{r}-\mathbf{b})$ which, near $r=0$, do not contain partial waves with angular momenta $j=\mu$ and $j=\mu+1$. Thus, the initial n^2 -fold degenerate level splits into $2n$ components at $n \geq 3$, and three components at $n=2$ (further lifting of degeneracy occurs when higher-order partial waves are taken into account).

The expression (29) becomes much simpler when U does not contain a shallow level with angular momentum $j=\mu+1$: terms containing $B_{\mu+1}^{-1}$ can be discarded. If, in addition, there are no shallow levels with $j=\mu$, we can confine our attention to the term involving the scattering length a_μ in B_μ^{-1} . For states with $m=0$, we then obtain the well-known result of the perturbation theory in the scattering length.¹⁰

The approach to the analysis of level quasicrossing, presented in Section 2, can be generalized to the problem with random degeneracy. If we take into account only the interaction in the resonant wave with $L \neq 0$ (this is definitely valid for states with $|m|=L$), the level shifts in the region of quasicrossing of the Coulomb ($E_n^{(0)}$) and ionic $E_L^{(0)} - \zeta/b$ terms are given by

$$E_{nm}^{(\pm)} - E_n^{(0)} \approx \frac{1}{2} \left\{ E_L^{(0)} - \frac{\zeta}{b} - E_n^{(0)} \pm \left[\left(E_L^{(0)} - \frac{\zeta}{b} - E_n^{(0)} \right)^2 + 2|r_L|^{-1} [(2L+1)!!]^2 \sum_{l=|m|}^{n-1} |R_{nlm}^{(Lm)}|^2 \right]^{1/2} \right\}, \quad (30)$$

where $E_L^{(0)}$ is the level energy in the isolated potential U , and $-\zeta/b \equiv V_f(0)$ is its shift under the influence of $V_f(r)$. Quasicrossing regions correspond to $E_L^{(0)}$. We note that, in this particular approximation, the remaining $n - |m| - 1$ states with $|m| < L$ and the states with $|m| > L$ remain unshifted.

We now introduce a few remarks about the Coulomb problem with a short-range potential in connection with the theory of hadronic atoms.¹⁶⁻²⁰ In accordance with the general analysis given in Section 2, the spectrum of states with $l \geq 1$ in the potential $V_C(r) + U(r)$ consists of slightly distorted (on their own scale) levels in the nuclear and Coulomb potentials. Outside the narrow quasicrossing region, the shifts of the Coulomb nl -levels are given by the following expression in accordance with (8):

$$\Delta E_{nl} = \frac{2(n+l)! \zeta^{2l+3}}{(l!)^2 (n-l-1)! n^{2l+4}} \left[\frac{1}{a_l^{(cs)}} + \frac{\zeta^2}{2n^2} r_l^{(cs)} \right]^{-1}, \quad (31)$$

where a_l and r_l are replaced with the Coulomb-nuclear scattering length $a_l^{(cs)}$ and the effective range $r_l^{(cs)}$, respectively, which corresponds to the inclusion of the Coulomb interaction at short distances. The position of the shallow nuclear level can be found from the usual perturbation theory in the potential V_C :

$$E_l \approx \frac{1}{a_l r_l} - \zeta \int_0^\infty \chi_l^2 \frac{dr}{r} \equiv \frac{1}{a_l^{(cs)} r_l}, \quad l \geq 1, \quad (32)$$

where $\chi_l(r)$ is the radial wave function at the instant of appearance of the level in the strong potential (for the relation between a_l and $a_l^{(cs)}$, see Ref. 19).

If we suppose that $E_l \gg \zeta^2/n^2$, we have from (31) and (32)

the following simple formula for the energy of the nuclear level in terms of the shift of the Coulomb level:

$$E_l \approx \frac{2(n+l)! \zeta^{2l+3}}{(l!)^2 (n-l-1)! n^{2l+4}} (r_l \Delta E_{nl})^{-1}, \quad l \geq 1. \quad (33)$$

In particular, for kaonic helium $K^- {}^4\text{He}$, assuming that $\Delta E_{2p} = 43$ eV, $\Gamma_{2p} = 0$, $r_1 = 47.5$, $\zeta = 1.53$ fm⁻¹ ($E_C = \zeta^2 = 92.8$ keV), we find from (33) that the binding energy of the nuclear state is $\varepsilon_p \approx 0.79$ MeV. This result agrees with the value $\varepsilon_p = 0.74$ MeV to within the limits of precision of the theory developed in Refs. 18 and 19. The latter result was obtained by numerical methods in Ref. 20.

We note that if $E_l \sim (r_c/a_B)^{2l} \zeta^2$, i.e., the nuclear level is anomalously close (on the Coulomb scale) to the continuum limit, Eq. (31) ceases to be valid for highly-excited Coulomb states. These states experience a rearrangement similar to the rearrangement of s -states in the case where the nuclear level energy is of the order of the Coulomb energy.

5. ELECTRON IN A UNIFORM MAGNETIC FIELD IN THE PRESENCE OF A CENTER OF FORCE

We can now use (16) to determine the shift of Landau levels

$$E_N^{(0)} = (N+1/2)\omega_H, \quad N=0, 1, \dots; \quad \omega_H = 2\omega = |e|H/c,$$

which are virtual levels with zero binding energy $\kappa_0 = 0$ (against the background of the continuous spectrum for $N > 0$) and correspond to the limit of the continuum \tilde{E}_0 . The function $\tilde{\Psi}_n^{(0)}(\mathbf{r}, \tilde{E}_0)$ must be understood as the wave function for transverse motion⁸

$$\tilde{\Psi}_{Nm}^{(0)}(\mathbf{r}) = \frac{1}{\mu!} \left[\frac{(\mu+n)! \omega}{2^\mu n! \pi} \right]^{1/2} \rho^\mu e^{-\rho^2/4 + i m \varphi} {}_1F_1 \left(-n, \mu+1, \frac{\rho^2}{2} \right),$$

where $\mu = |m|$, $n = N - (\mu + m)/2$ is the radial quantum number ($n = 0, 1, \dots$), $\rho = (2\omega)^{1/2} r \sin\vartheta$, and the function $\Psi_n(\mathbf{r}, E_n)$ corresponds to

$$\Psi_{Nm}(\mathbf{r}, E_{Nm}) \approx \kappa^{1/2} e^{-\kappa|z|} \tilde{\Psi}_{Nm}^{(0)}(\mathbf{r}), \quad r \gg r_c,$$

so that $N^{(0)} = 1$. When $r_c \ll L_f = \omega^{-1/2}$ and $N \ll (\omega r_c^2)^{-1}$, the formula given by (16) yields

$$\kappa_{Nm} \equiv [2(E_N^{(0)} - E_{Nm})]^{1/2} \approx -\frac{1}{2} \sum_{l=\mu}^{\infty} [(2l+1)!!]^2 |\tilde{R}_{Nm}^{(lm)}|^2 \left[\frac{1}{a_l} - r_l (E_N^{(0)} - m\omega) \right]^{-1}. \quad (34)$$

In the expression for $B_l(E)$, we have introduced the replacement $E \rightarrow E - m\omega$, corresponding to the inclusion of the term ωl_z in the Hamiltonian at short distances $r \lesssim r_c$ (formally, this is a renormalization of the scattering length in the first order in \mathbf{H} ; the relative size of the second-order effects is $\sim \omega r_c^2$). In accordance with (4), the coefficients $\tilde{R}_{Nm}^{(lm)}$ are determined by the expansion of $\tilde{\Psi}_{Nm}^{(0)}$ for $r \ll \omega^{-1/2}$. They are nonzero only for values of l with the same parity, $l = \mu + 2k$, $k = 0, 1, 2, \dots$. In particular,

$$|\tilde{R}_{Nm}^{(\mu m)}|^2 = 2^{2\mu+2} \frac{(\mu+n)!}{(2\mu+1)! n!} \omega^{\mu+1}, \quad (35)$$

$$|\tilde{R}_{Nm}^{(\mu+1, m)}|^2 = \frac{1}{(\mu+1)(2\mu+5)} \left(\frac{\mu+2n+1}{2\mu+3} \right)^2 |\tilde{R}_{Nm}^{(\mu m)}|^2 \omega^2.$$

We now supplement the results reported in Refs. 21-25 and 6 with a number of remarks about the spectrum of weakly-bound states in the above problem. The Landau level shifts are described, in general, by the simple expression

$$\Delta E_{Nm} \approx -2 \left\{ \frac{(2\mu+1)!(\mu+n)!}{(\mu!)^2 n!} \times \left[\frac{1}{a_\mu} - (E_N^{(0)} - m\omega) r_\mu \right]^{-1} \omega^{\mu+1} \right\}^2. \quad (36)$$

For $\kappa_{Nm} > 0$ and $n \geq 1$, their widths associated with transitions to Landau levels with lower values of n are

$$\Gamma_{Nm} = \sum_{k=0}^{n-1} \frac{n!(\mu+k)!}{k!(\mu+n)!} (n-k)^{-1/2} \kappa_{Nm}^2 \omega^{-1/2}, \quad (37)$$

and are calculated from the imaginary part of the level shift in second-order perturbation theory, using the transition matrix element

$$U_{Nm\kappa}^{N'm\kappa} = -(\mu+1/2) (\kappa/2\pi)^{1/2} \tilde{R}_{Nm}^{(\mu m)*} \tilde{R}_{Nm}^{(\mu m)} B_\mu^{-1} \quad (38)$$

[see the discussion in connection with (28)].

From (36) and (37), we have

$$\Delta E_{Nm} = \Delta E_{N-m, -m}, \quad \Gamma_{Nm} = \Gamma_{N-m, -m},$$

which reflects the general property of the energy spectrum $E_m - m\omega = E_{-m} + m\omega$ in an arbitrary axially symmetric potential $U(\rho, z)$ in the presence of a uniform magnetic field, directed along the z axis, for states with opposite values of the projections of the angular momentum onto this axis.

When the potential U does not contain a shallow level with $l = \mu$, we can discard the term containing the range in (36) and (37), and the resulting expression obtained from perturbation theory in the scattering length is found to agree with that given in Refs. 6 and 25. Equation (34) enables us to take into account the effect of the higher-order partial waves on the level shift. Confining our attention to the case $m = 0$, and using (34) and (35), we obtain

$$E_{N,0} - E_N^{(0)} = -2\omega^2 \{a_0 + 5(2N+1)\omega^2 [a_2^{-1} - r_2(2N+1)\omega]^{-1}\}^2. \quad (39)$$

Let us now examine the case where the potential U contains a shallow level. If its angular momentum is $l = 0$ and $r_c \ll -a_0 \ll \omega^{-1/2}$, the shifts and widths of the low-lying levels with $N \ll E_0/\omega$ in the presence of this virtual state are, as before, described by the perturbation theory formulas (36) and (37) for $\mu = 0$, and the effect of the center on the higher-lying Landau levels requires separate examination. If the energy of the level (virtual or real) is $E_0 \sim \omega$, a substantial rearrangement of the spectrum, investigated in Refs. 22 and 24, takes place: the level shifts and widths are comparable with the widths of the Landau bands. If, on the other hand, the level in the potential U is real and $|E_0| \gg \omega$, it is well-known that the level will be slightly shifted by the magnetic field²² and the Landau levels will become low-energy virtual levels.

A totally different situation arises in the spectrum when the level angular momentum l is nonzero. We note the particular features of the spectrum of states with given angular momentum projection m .

1. The unperturbed level $E^{(0)}$ corresponds to "well"

states (i.e., states localized in the region $r \lesssim r_c$), and the change in the energy of these states under the influence of the magnetic field is largely determined by the paramagnetic shift:

$$E_{lm} \approx E_l^{(0)} + m\omega, \quad |m| \leq l.$$

The change in the width of these levels as compared with the width $\Gamma_{lm} \approx 2[2E_{lm}]^{l+1/2}/|r_l|$ of the particle state with energy $E_{lm} > 0$ in the potential U under the influence of the magnetic field will be more substantial. When $E_{lm} < (m + |m| + 1)\omega$, such states are truly bound (if the initial level is real, all the "well" states with different m remain bound; if, on the other hand, the initial level is quasistationary, application of the magnetic field may result in stabilization of the states, beginning with a certain value of $|m|$). The expression for the width of the "well" state with $m = \pm l$ is

$$\Gamma_{l,\pm l} \approx 2^{3/2} \frac{(2l+1)!}{(l!)^2} \frac{\omega^{l+1}}{|r_l|} \sum_n \frac{(n+l)!}{n!} (E_{l,\pm l} - E_N^{(0)})^{-1/2}, \quad (40)$$

where the sum is evaluated over all the n for which $E_N^{(0)} < E_{l,\pm l}$ (when the magnetic field is turned off, i.e., $\omega \rightarrow 0$, this expression becomes identical with the expression for the width of the unperturbed level).

2) The presence of a shallow level with $l \neq 0$ in the potential U has an important effect only on the Landau levels with $|m| = l$. These levels now correspond to bound states (or, more precisely, quasibound states for $n \geq 1$) only for values of N for which $E_N^{(0)} < E_{lm}$. Their shifts and widths are then described by (36) and (37), as before. Higher-lying Landau levels with $E_N^{(0)} > E_{lm}$ become virtual levels [in (34) for $\kappa_{Nm} < 0$]. In particular, when an isolated level $E_l^{(0)} < 0$ is real, all Landau levels with $|m| = l$ become virtual.

As far as Landau levels with $|m| \neq l$ are concerned, they are almost insensitive to the presence of a shallow level with angular momentum l , and their shift is largely determined by the scattering length a_μ .

The picture described above must be modified somewhat when E_{lm} is anomalously close to the energy $E_N^{(0)}$ of the unperturbed Landau level. We then have a quasicrossing of the Landau and "well" levels, which can be investigated with the aid of (34) if we neglect transitions to lower-lying Landau levels. Proceeding as in the derivation of (11), we obtain, for example, for $m = \pm l$

$$(\Delta E_{\pm l})^{1/2} [\delta E_{\pm l}^{(0)} - \Delta E_{\pm l}] = i \frac{2^{1/2} (2l+1)! (l+n)!}{(l!)^2 n! |r_l|} \omega^{l+1}, \quad (41)$$

where

$$\Delta E_{\pm l} = E_{\pm l} - E_N^{(0)}, \quad \delta E_{\pm l}^{(0)} = E_l^{(0)} \pm l\omega - E_N^{(0)}.$$

It is clear from (41) that quasicrossing regions correspond to the following detuning from resonance:

$$|\delta E_{\pm l}^{(0)}| \leq \omega (\omega r_c^2)^{(2l-1)/3} \equiv \gamma.$$

When $\gamma \ll |\delta E_{\pm l}^{(0)}| \ll \omega$ and $\delta E_{\pm l}^{(0)} > 0$, one of the roots $E_{\pm l}$ leads to the results for the shift and width of the "well" level mentioned above, while the other gives the shift of the quasibound Landau level (in the approximation under consideration, this level does not have a width). When $\delta E_{\pm l}^{(0)} < 0$, one of the roots of (41) corresponds to a virtual Landau level and

the other to a “well” level (for $|m| \neq l$, the character of the Landau level—whether quasibound or virtual—does not change as a result of quasicrossing). It is clear from (40) and (41) that the width of the “well” state under the conditions of quasicrossing is very sensitive to the detuning from resonance.

We note that, in the case of a very weak magnetic field, the Landau levels lying within the width of the “well” state $\Gamma_{lm} \gtrsim \omega$ undergo a substantial rearrangement.

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¹¹The opposite limiting case, $b \rightarrow 0$, for which the Coulomb potential becomes highly distorted at short distances, has frequently been examined in the literature.^{13–20}

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