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Three-body Coulomb problem in the dipole approximation

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The doubly excited states of the two-electron atom (or ion) are considered in the case when one electron is excited much more than the other. The characteristic separation of the strongly excited electron from the atomic nucleus significantly exceeds that for the weakly excited electron. The electron-electron interaction can be approximated by the dipole term in its multipole expansion. The inner electron velocity is assumed to be much larger than that of the outer electron, which permits assigning a fixed principal quantum number for the inner electron. The same approach is extended to the general Coulomb three-body problem with the particles of arbitrary mass and charge. For the three-body states with symmetry S and P^e, the quantum problem reduces to the three-term recursion relations, which means that the system is effectively one dimensional. The slow evolution of the classical particle trajectories under the influence of interaction is described. It is shown that, depending on the parameters of the system, two types of librations or rotation can be realized. The semiclassical quantization rules (analogous to the well-known Bohr-Sommerfeld rules) are deduced. For S and P^e states they differ only by the substitution of a half-integer quantum number by an integer. Particularly simple results are obtained in the harmonic approximation, which is valid in the vicinity of the effective-potential curve extreme.

I. INTRODUCTION

The dipole approximation is applied to the description of the doubly excited states of the two-electron atom (or ion) when one electron is excited much more than the other[1-5] (the bibliography can be found in the cited papers and also in several reviews[6,7]). The electron-electron interaction is replaced by the dipole term of its expansion:

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}-\frac{1}{r_1}\approx\frac{\mathbf{N}_1\cdot\mathbf{r}_2}{r_1^2}\ ,\quad \mathbf{N}_1=\frac{\mathbf{r}_1}{r_1} \tag{1.1}$$

where the radius vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ define the electrons' position relative to the atomic nucleus. Atomic units are used throughout the paper: $m_e=\hbar=e=1$. The first (outer) electron is strongly excited, therefore its average distance from the nucleus exceeds that of the second (inner) electron: $r_1 \gg r_2$. Electron exchange can be neglected for the first stage of calculations because the electrons move mainly in different regions of space.

The same approximation can be applied to the general quantum three-body problem, when one considers the interaction of an arbitrary charged quantum particle (with the charge Z_B and the mass M_B) with the excited hydrogenlike system (with the "nucleus" charge Z_A and the mass M_A and the "electron" charge and mass used as the units of these magnitudes).

Let $\mathbf{r}$ be the radius vector of the outer (incident) particle relative to the center of masses of the atom. In the dipole approximation the related angular variables can be separated. The radial motion over r coordinate proceeds in the effective potential

$$V(r)=\frac{(Z_A-1)-Z_B}{r}+\frac{\lambda}{2\mu_r r^2}, \tag{1.2}$$

where λ is the eigenvalue of the dipole operator Λ[3]

$$\Lambda=\mathbf{l}_1^2-Gn_2\mathbf{N}_1\cdot\mathbf{A}_2\ , \tag{1.3}$$

$$G=3Z_B\mu_r g/\mu_{e\text{-nuc}}Z_A,\quad g=(M_A+Z_B)/(M_A+1)\ . \tag{1.4}$$

We assume also that the atomic electron has the definite principal quantum number n_2. This approximation along with (1.1) is justified by the large frequency of the electron motion as compared with the outer particle frequency. The other notations are as follows: $\mathbf{l}_1$ is the orbital momentum operator corresponding to the coordinate $\mathbf{r}$; $\mathbf{A}_2$ is the Runge-Lenz vector for the atomic electron (see, e.g., Refs. 1 and 4),

$$\mu_{e\text{-nuc}}=\frac{M_A}{M_A+1} \tag{1.5}$$

is the reduced mass of the electron-nucleus system, and

$$\mu_r=\frac{(M_A+1)M_B}{M_A+M_B+1} \tag{1.6}$$

is the reduced mass for the motion over coordinate $\mathbf{r}$. The operator Λ acts on the angular variables of the outer particle and the coordinates of the inner (atomic) electron. It is diagonal in the quantum number n_2. The total angular momentum of the whole system $\mathbf{L}=\mathbf{l}_1+\mathbf{l}_2$ (with $\mathbf{l}_2$ for the inner electron orbital momentum) is an exact integral of the motion (in the nonrelativistic case).

In the dipole approximation the three-body problem is reduced to the analysis of the spectrum of the dipole operator Λ (1.3). The radial equation with the potential (1.2) and the effective mass μ is readily solved analytically which gives the energy spectrum of the three-body system:

$$E_{n_1 n_2 \lambda} = -\frac{Z_A^2 \mu_r^4}{2n_2^2} - \frac{(Z_A-1)^2 Z_B^2 \mu_r^4}{2(n_{1r}+l_{\rm eff})^2}\ , \quad l_{\rm eff} = \sqrt{\lambda+\tfrac{1}{4}} - \tfrac{1}{2}\ , \tag{1.7}$$

where n_{1r} is the radial quantum number for the outer particle. [We assume here $(Z_A-1)Z_B<0$ so that the Coulomb term in (1.2) corresponds to the attraction.] It should be stressed that in this study we assume that the potential (1.2) is applicable at all r. This is not true for small values of r. Small values of r are classically inaccessible provided the centrifugal barrier is sufficiently large. Expression (1.7) is applicable for large L: $L \sim l_1 \gg n_2 - 1 \geq l_2$. The states considered here are generally unstable with respect to autoionization (deexcitation of the atomic electron with ejection of the outer particle). They are described by the complex values of the energy. The expression (1.7) gives the real part and describes the resonance position. The imaginary part of the energy (related with the resonance width) appears due to the mixing of the states with different n_2. Its calculation is beyond the scope of the present paper.

In the general case of arbitrary L the dipole operator also plays an important role. Its spectrum governs the boundary conditions in the formulation of three-body scattering problem employing a two-body adiabatic basis (see, e.g., Ref. 8). In simple terms this implies that the eigenvalues of Λ define the long-range asymptote for the interaction of the charged particle with the excited hydrogenlike atom. They play the key role in the description of the threshold behavior of partial cross sections for the excitation of the hydrogenlike atom by the charged particle[9] (see also Ref. 5, and references cited therein).

In the particular case of S states ($L=0$) one has $\mathbf{l}_1 = -\mathbf{l}_2$ which allows the representation of (1.3) as

$$\Lambda = l_2^2 - G n_2 \mathbf{N}_1 \cdot \mathbf{A}_2\ . \tag{1.8}$$

The operator Λ in fact acts only on the second electron coordinates, whereas the vector $\mathbf{N}_1$ can be treated as constant. The same operator arises in the one-electron two-center Coulomb problem when the Schrödinger equation for the hydrogen atom is considered in the spheroidal coordinates. Let R be the distance between the poles of the spheroidal coordinate system with the atomic nucleus placed into one of them. When the spheroidal variables are separated, the separation constant is the eigenvalue of the operator[10]

$$\tilde{\Lambda} = l_2^2 + \frac{R}{n_2} A_{2z} \tag{1.9}$$

where the index 2 is ascribed to the electron operators and the z axis is directed from the nucleus along the coordinate system axis. The operators (1.8) and (1.9) coincide provided their parameters are related: $G = R/n_2^2$. Since we assume that the principal quantum number n_2 is fixed, the diagonalization of the operator Λ generates the proper wave functions of the zero-order perturbation theory for the excited hydrogen atom perturbed by the point charge placed at distance R from the nucleus.

Thus the study of the dipole operator spectrum is important in the three-body problem as well as in other applications (see also the theory of very slow electron interaction with the dipole molecule[11]). Earlier the semiclassical asymptotic limit $L \sim l_1 \gg n_2 - 1 \geq l_2$ was analyzed[1,2] and the perturbation theory in small $(Gn_2)^{-1}$ was developed.[3]

The object of the present paper is to analyze the dipole operator spectrum for the cases $L=0$ and $L=1$. We consider both quantum (Sec. II) and semiclassical (Secs. IV and V) theory. Formally the latter is applicable for large n_2. In practice it gives an error of a few percent for $n_2=3$. The evolution of the classical electron trajectories also is described in Sec. III which gives qualitative insight into the character of the correlated particles motion.

II. EXACT QUANTUM FORMULATION OF THE PROBLEM

We consider the dipole operator Λ on the basis of states[1] $|l_1 l_2 LM\rangle$:

$$|l_1 l_2 LM\rangle = \sum_{m_1 m_2} C^{LM}_{l_1 m_1 l_2 m_2} Y_{l_1 m_1}(\mathbf{N}_1) \varphi_{n_2 l_2 m_2}(\mathbf{r}_2)\ , \tag{2.1}$$

where $\varphi_{n_2 l_2 m_2}$ is the hydrogenlike bound-state wave function for the nucleus charge Z_A, reduced mass $\mu_{e\text{-nuc}}$, and the principal quantum number n_2; Y_{lm} is the spherical harmonic, $C^{LM}_{l_1 m_1 l_2 m_2}$ are the Clebsch-Gordan coefficients; l_1, m_1, l_2, m_2 are the angular momentum quantum numbers for the first and the second electron, respectively, and M is the projection of the total orbital momentum $\mathbf{L}$ on the fixed axis.

The matrix elements of the operator Λ are straight forwardly calculated:

$$\begin{aligned}
&\langle l_1' l_2' LM|\Lambda|l_2 l_2 LM\rangle = l_1(l_1+1)\delta_{l_1 l_1'}\delta_{l_2 l_2'} + Gn_2 \langle l_1' \| N_1 \| l_1\rangle \langle n_2 l_2' \| A_2 \| n_2 l_2\rangle \begin{Bmatrix} L & l_2 & l_1' \\ 1 & l_1 & l_2' \end{Bmatrix} \\
&\langle l_1+1 \| N_1 \| l_1\rangle = \sqrt{l_1+1}\ , \\
&\langle n_2 l_2+1 \| A_2 \| n_2 l_2\rangle = \{(l_2+1)[n_2^2-(l_2+1)^2]\}^{1/2}\ .
\end{aligned} \tag{2.2}$$

They are nonzero only for $l_1' = l_1, l_1 \pm 1$; $l_2' = l_2, l_2 \pm 1$. The problem reduces to the three-term recurrence relations which are two dimensional (i.e., over the indexes l_1 and l_2). In general, the approximate methods in the theory of such three-term relations are not developed sufficiently well.

However, two cases exist where the problem is drastically simplified since it is reduced to the conventional one-dimensional recursion relation. One of them corresponds to zero value of the total orbital momentum L (S

states), where $l_1=l_2$. For P states the matrix elements of Λ are nonzero when $l_1=l_2\pm1$ or $l_1=l_2$. The basis states with $l_1=l_2\pm1$ are odd relative to inversion of all particles coordinates, whereas the states with $l_1=l_2$ are even. Since the state parity is an exact quantum number, the diagonalization problem is subdivided into two parts for given L. For P^e states one also obtains the one-dimensional three-term recurrence relations.

Consider first the S states. The dipole operator eigenfunction corresponding to some eigenvalue λ is expanded over the basis set (2.1)

$$|\Psi_\lambda\rangle=\sum_{l=0}^{n_2-1} C_l|ll00\rangle . \tag{2.3}$$

The equation $\Lambda|\Psi_\lambda\rangle=\lambda|\Psi_\lambda\rangle$ using expression (2.2) is directly given as a three-term recurrence relations for the coefficients C_l:

$$p_lC_{l-1}+(w_l-\lambda)C_l+p_{l+1}C_{l+1}=0 , \tag{2.4}$$

$$w_l=l(l+1),\quad p_l=Gn_2l\left[\frac{n_2^2-l^2}{4l^2-1}\right]^{1/2} . \tag{2.5}$$

In the case of P^e states the formula (2.3) is replaced by

$$|\Psi_\lambda\rangle=\sum_{l=1}^{n_2-1} C_l|ll1M\rangle . \tag{2.6}$$

The coefficients C_l satisfy the same recurrence relations (2.4) but with

$$p_l=Gn_2[(l^2-1)(n_2^2-l^2)/(4l^2-1)]^{1/2} . \tag{2.7}$$

III. TIME EVOLUTION OF THE CLASSICAL TRAJECTORIES

For large n_2 the system of Eqs. (2.4) can be solved in the semiclassical approximation. This approach makes it possible to obtain the analytic approximations to the eigenvalues and eigenfunctions. Probably the more important point is the qualitative insight into the nature of the system states. This can be achieved by analysis of the slow evolution of the classical particle trajectories under influence of the interaction.

In the semiclassical theory[12,13] of three-term recurrence relations (2.4) the following Hamiltonian function is introduced:

$$\begin{aligned}H&=w_l+2p_{l+1/2}\cos\varphi\\&\approx(l+\tfrac{1}{2})^2+Gn_2[n_2^2-(l+\tfrac{1}{2})^2]^{1/2}\cos\varphi .\end{aligned} \tag{3.1}$$

Here φ is the variable canonically conjugated with l. In the expressions for the matrix elements w_l and $p_{l+1/2}$ we retain the terms of the lowest and the next order in the semiclassical parameter n_2^{-1}. This is necessary when the WKB formalism is developed for approximate solution of the quantum problem. This is why we retain in the formulas the sum $(l+1/2)$ although l is large.

The Hamiltonian function (3.1) can also be obtained from the exact classical Hamiltonian when the latter is averaged over the fast elliptic orbit inner electron motion (the complete coincidence with expression (3.1) is achieved if (as is frequently assumed) the classical orbital moment is related with the sum $l+\frac{1}{2}$ instead of l). The position of the orbit perihelium is specified by the Runge-Lenz vector ($A_2=[n_2^2-(l+\frac{1}{2})^2]^{1/2}$) which varies slowly with time. φ is the angle between the vectors $\mathbf{N}_1$ and $\mathbf{A}_2$.

In the case $L=0$ the classical orbits are coplanar and the particles rotate along them in opposite directions. The evolution of the classical orbits is described as a slow variation of l and φ. In the present context it is convenient to assume that both of these variables can be positive or negative. For the variable l this implies that the motion of the inner electron over the ellipse proceeds clockwise or counterclockwise, respectively. Variation of l and φ in time is governed by the conventional Hamiltonian equations

$$\dot{l}=\frac{\partial H}{\partial\varphi},\quad \dot{\varphi}=-\frac{\partial H}{\partial l} , \tag{3.2}$$

which give

$$\dot{l}=-Gn_2[n_2^2-(l+\tfrac{1}{2})^2]^{1/2}\sin\varphi . \tag{3.3}$$

Bearing in mind that the function H is an integral of motion and denoting its numerical value as λ, one obtains from (3.1)

$$\cos\varphi=\frac{\lambda-(l+\frac{1}{2})^2}{Gn_2[n_2^2-(l+\frac{1}{2})^2]^{1/2}}\equiv B(\lambda,l) . \tag{3.4}$$

Substitution of $\sin\varphi=\pm(1-B^2)^{1/2}$ for the right-hand side (rhs) of Eq. (3.3) gives

$$\dot{l}=\pm\sqrt{[U^+(l)-\lambda][\lambda-U^-(l)]} , \tag{3.5}$$

where

$$\begin{aligned}U^\pm(l)&=w_l\pm2p_{l+1/2}\\&=(l+\tfrac{1}{2})^2\pm Gn_2[n_2^2-(l+\tfrac{1}{2})^2]^{1/2} .\end{aligned} \tag{3.6}$$

The differential equation (3.5) can be integrated easily for the function $l(t)$. Then $\varphi(t)$ is defined by the formula (3.4).

In the subsequent qualitative analysis an important role is played by the values of the orbital momentum l corresponding to the extreme of the function $\varphi(t)$. From Eq. (3.4) one sees that these values are l_0 and l_e:

$$l_0+\tfrac{1}{2}=0,\quad l_e+\tfrac{1}{2}=(2n_2^2-\lambda)^{1/2} \tag{3.7}$$

(the latter solution exists only in the case $\lambda>n_2^2$). The corresponding values of the angle φ are defined by the relations

$$\cos\varphi_0=\lambda/Gn_2^2,\quad \cos\varphi_e=2(\lambda-n_2^2)^{1/2}/Gn_2 \tag{3.8}$$

(note that $|\cos\varphi_0|>|\cos\varphi_e|$).

The derivative $\dot{l}$ is zero for those values l_t of the orbital momentum which are solutions of the equation $\lambda=U^+(l)$ or $\lambda=U^-(l)$ which follow from Eq. (3.5). These values of the orbital momentum l are named the turning points. The functions $U^\pm(l)$ in this sense are the potential curves for the motion over "coordinate" l. In contradistinction to the conventional case of a true coordinate, one deals here with double valued "potential function" with the branches $U^+(l)$ and $U^-(l)$ which match smoothly at the point $l+\frac{1}{2}=n$ where both curves have vertical tangents. In Fig. 1 three characteristic types of the potential curve are presented depending on the value of the parameter G (for the detailed discussion see below).

The condition $-1 \le \cos\varphi \le 1$ together with the formula (3.1) implies that the classical motion is possible provided the inequality $U^- \le \lambda \le U^+$ is satisfied. Thus the bounds for the allowed values of λ are

$$\lambda \ge \min U^+(l) = -Gn_2^2 \, ,$$
$$\lambda \le \max U^+(l) = \begin{cases} Gn_2^2, & G>2 \\ n_2^2(1+G^2/4) \equiv U_m, & G<2 \, . \end{cases} \tag{3.9}$$

If the turning point in l lies on the potential curve U^+ the corresponding value of the angle φ is equal to 0, whereas the curve U^- corresponds to $\varphi=\pi$. The variation of the angle φ corresponds to the oscillation in the vicinity of the point $\varphi=0$ (when both turning points lie on the curve U^-) or in the vicinity of the point $\varphi=\pi$ (when both turning points lie on the curve U^+). Just one other type of motion appears which is when one turning point lies on U^+ and the other lies on U^-. Here the variation of the angle φ corresponds to rotation. The type of motion in the particular case depends on the values of the parameters G and λ.

The classification of the possible situations is given below.

(a) The potential curve a (see Figs. 1 and 2) is realized for $G>2$. The orbital momentum $l(t)$ oscillates in the symmetric interval $[-l'_{t2}, l'_{t2}]$. The angle $\varphi(t)$ oscillates around the value $\varphi=0$ if $Gn_2^2 > \lambda > n_2^2$ or around the value $\varphi=\pi$ if $n_2^2 > \lambda > -Gn_2^2$. In the second case the oscillations proceed in the conventional way, namely, one extremum of the function $\varphi(t)$ lies within the half-period of oscillation. The oscillations look more unusual in the case $Gn_2^2 > \lambda > n_2^2$: within the half-period the function $\varphi(t)$ at first rises from zero to the value φ_e, then it decreases until the value φ_0 is reached, then it grows returning to the value φ_e and at last falls off to zero. Thus three extremes of the function $\varphi(t)$ are enclosed in one half-period.

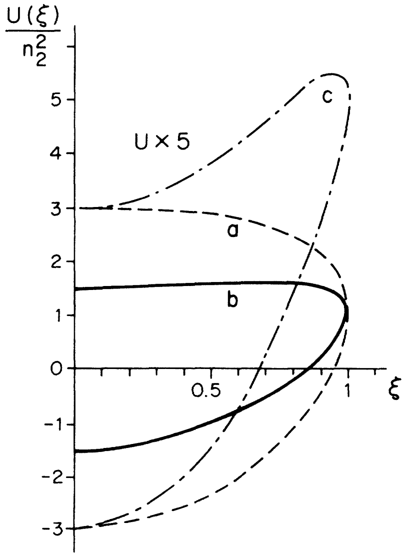

FIG. 1. The effective potential curve U/n_2^2 as a function of the reduced orbital momentum $\xi=(l+\frac{1}{2})/n_2$: (a) $G=3$ (which corresponds to the system H^*-e); (b) $G=1.5$ [the system $(\mathrm{He}^+)^*$-e]; (c) $G=0.6$ [the system $(\mathrm{B}^{4+})^*$-e]. The potential curves being an even function of ξ are shown only in the region $\xi>0$. In (c) the curve $5(U/n_2^2)$ is drawn.

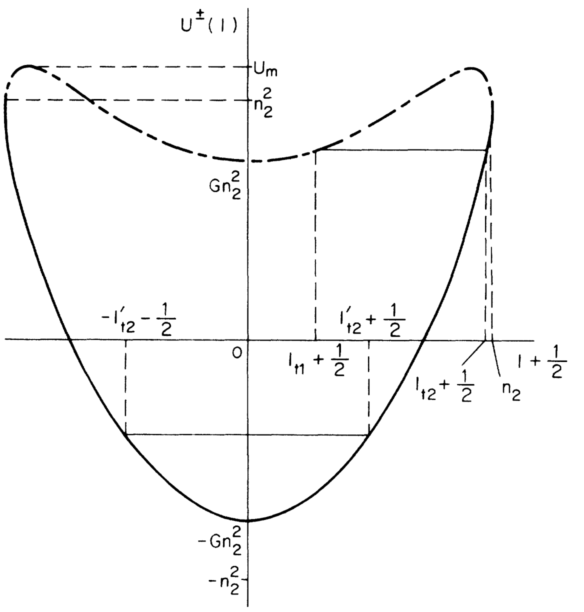

FIG. 2. The effective potential curve $U^{\pm}(l)$ for $G=0.75$ [which corresponds to the system $(\mathrm{Be}^{3+})^*$-e]. The solid curve is for the branch $U^-(l)$ and the dash-dotted line picture $U^+(l)$. The turning points are shown as follows: $l''_{t1}+\frac{1}{2}$, $l_{t2}=\frac{1}{2}$ in the case $\lambda > Gn_2^2$ and $-l'_{t2}-\frac{1}{2}$, $l'_{t2}+\frac{1}{2}$ in the case $\lambda < Gn_2^2$.

In case (a) the orbital momentum $l(t)$ passes through zero for all trajectories. At this moment the elliptic electron orbit is squeezed into the interval of the line. Before this moment and after it the electron rotation along the elliptic orbit proceeds in opposite directions.

(b) The potential curve b (see Fig. 1) is realized if $1<G<2$. The new region of the parameter λ variation $(U_m > \lambda > Gn_2)$ is added here to those described in case (a). The orbital momentum $l(t)$ oscillates in the interval $[l_{t1}, l_{t2}]$ with $\varphi=0$ at the turning points $l_{t1}, l_{t2} > 0$. Contrary to the motion described for case (a) the oribital momentum is always nonzero. The elliptic orbit of the inner electron never becomes a line. Only one extremum of the function $\varphi(t)$ lies on the oscillations half-period. The particular value $\lambda=U_m$ corresponds to the equilibrium and the variables φ and l are constant in time $(\varphi=0,\ l+\frac{1}{2}=n_2[1-G^2/4)^{1/2}]$.

(c) For $G<1$ the potential curve is c (see Fig. 1). In this case the regime of $\varphi(t)$ oscillations around the $\varphi=0$ is absent. Another characteristic region arises for $n_2^2>\lambda>Gn_2^2$. Here the angular momentum $l(t)$ varies in the interval $[l_{t1},l_{t2}]$ and never is zero. Onefold transition of this interval corresponds to variations of $\varphi(t)$ from 0 to π. The subsequent variation of the angle corresponds to rotation.

IV. SEMICLASSICAL APPROXIMATION FOR *S* STATES

If the canonical "momentum" φ is known as a function of the canonical coordinate l [see relation (3.4)], then the approximate semiclassical solutions of the three-term recurrence relation (2.4) can be constructed.[12,13] These solutions are inapplicable for l close to zero where the coefficient p_l is singular. It was shown above that for some values of parameters [$G<2$ and simultaneously $Gn_2^2<\lambda<n_2^2(1+G^2/4)$] the point $l=0$ is not reached on the classical trajectory, i.e., the singularity lies in the classically inaccessible region (under the effective potential barrier). Then the general quantization rule for the three-term recurrent relation[12] can be applied:

$$\int_{|B|\le 1}\frac{(l+\frac{1}{2})\dfrac{dB}{dl}dl}{(1-B^2)^{1/2}}=(N+\tfrac{1}{2})\pi,\quad B=\frac{\lambda-w_l}{2p_{l+1/2}}\ . \tag{4.1}$$

It defines the eigenvalues λ_N which are enumerated by the integer quantum number N.

Now let the point $l+\frac{1}{2}=0$ be situated in the classically accessible region (the case $-Gn_2^2<\lambda<Gn_2^2$). The solution which is valid both for large and for small l is constructed in the Appendix with the help of the comparison equation method. It is shown that the quantization rule (4.1) is valid also for this case if the beginning of the integration interval is $l=-\frac{1}{2}$.

It is convenient to rewrite the quantization rule (4.1) in terms of reduced variables:

$$\int_{\xi_1}^{\xi_2}\frac{\xi^2(\lambda/n_2^2-2+\xi^2)d\xi}{(1-\xi^2)[G^2(1-\xi^2)-(\lambda/n_2^2-\xi^2)^2]^{1/2}}=\nu\ , \tag{4.2}$$

where ν is the reduced quantum number $[\nu=(N+\frac{1}{2})\pi/n_2]$ and $\xi=(l+\frac{1}{2})/n_2$. If the orbital momentum $l+1/2$ does not pass zero on the classical trajectory then ξ_1 and ξ_2 are defined as the roots of the expression under the radical in the left-hand side (lhs) of Eq. (4.2). These parameters are related to the turning points shown in Fig. 2: $\xi_i=(l_{ti}+\frac{1}{2})/n_2$. If l passes zero then one should put in (4.2) $\xi_1=0$; in this case $\xi_2=(l'_{t2}+\frac{1}{2})/n_2$, see Fig. 2.

The integral which enters Eq. (4.2) can be written as the elliptic integral of the third kind. It is a discontinuous function of λ consisting of two monotonic parts. The integral is positive for $\lambda>n_2^2$ and negative for $\lambda<n_2^2$, which means that the quantum number N can be a negative integer. At the point $\lambda/n_2^2=1$ the integral makes a jump equal to π. The dynamical interpretation of this behavior stems from the observation that the angle becomes undefined when the electron elliptic orbit turns into a circle. This occurs in the vicinity of the right turning point l_{t2} when $\lambda/n_2^2\to 1$: $\varphi(l_{t2})=0$ if $\lambda/n_2^2=1+0$ but $\varphi(l_{t2})=\pi$ if $\lambda/n_2^2=1-0$. This is the region of the jump in the integral (4.2) which in fact is essentially the action integral written in terms of the variables l,φ.

For the fixed value of the parameter G Eq. (4.2) generates a universal dependence (see Fig. 3) of the reduced eigenvalue λ/n_2^2 on the variable ν. The value of this function at the points $\nu=(N+\frac{1}{2})\pi/n_2$ defines the eigenvalue λ_N.

Particularly simple results for the spectrum of the dipole operator can be obtained in the vicinity of the extreme of the potential curve $U(l)$. Here the harmonic approximation is valid which leads to the equidistant sequence of the eigenvalues λ_N. Consider first the case $G<2$ where the harmonic approximation in the vicinity of the maximum of the branch $U^+(l)$ gives the following simple formula:

$$\lambda_{N'}=n_2^2(1+G^2/4)-(N'+\tfrac{1}{2})n_2(4-G^2)^{1/2}\ ,\qquad N'=0,1,2,\ldots\ . \tag{4.3}$$

For the vicinity of the minimum of the branch $U^-(l)$ the same approach gives

$$\lambda_{N''}=-Gn_2^2+(N''+\tfrac{1}{2})2n_2(G^2+2G)^{1/2}\ ,\qquad N''=0,1,2,\ldots\ . \tag{4.4}$$

The case $G<2$ is realized for the system $(\mathrm{He}^+)^*$-e. The upper "potential well" proves to be quite shallow here which seriously limits the applicability of the expression (4.3). For example, even in the case $n_2=10$ this formula gives a good approximation only for one eigenvalue (namely, for the highest one).

In the case $G>2$ the formula (4.3) is replaced by

$$\lambda_{N'}=Gn_2^2-(N'+\tfrac{1}{2})2n_2(G^2-2G)^{1,2}\ ,\qquad N'=0,1,2,\ldots\ , \tag{4.5}$$

whereas the formula (4.4) for the lowest eigenvalues is retained. As a typical example here one can refer to the

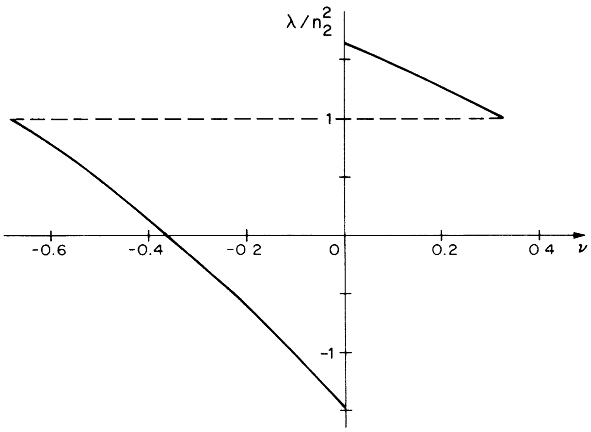

FIG. 3. The universal dependence of the reduced eigenvalue λ/n_2^2 on the reduced quantum number ν in the semiclassical approximation for $G=1.5$.

TABLE I. The eigenvalues λ of the dipole operator for the system $(\mathrm{He}^+)^* - e\,(G=1.5)$. The case of S states. λ_e, the exact values; λ_{WKB}, the semiclassical approximation (4.2); λ_h, the harmonic approximation [for each value of the principle quantum number n_2 the values λ_h given in the upper part of the column are obtained using formula (4.3) and those in the lower part are calculated with the help of expression (4.4)].

N	λ_e	λ_{WKB}	λ_h
		$n_2=4$	
0	22.08	22.70	22.35
−3	13.19	13.70	
−2	0.28	0.74	− 3.50
−1	−15.56	−15.13	−14.83
		$n_2=10$	
0	150.633 3	150.632 7	148.5
1	137.08	137.82	136.4
2	117.07	117.63	123.2
−7	92.04	92.55	
−6	63.03	63.51	
−5	30.57	31.04	
−4	− 4.97	− 4.51	
−3	− 43.33	− 42.89	− 35.43
−2	− 84.33	− 83.90	− 81.26
−1	−127.80	−127.37	−127.1

system H^*-e or to the interaction of heavy charged particles (e.g., bare atomic nuclei) with an excited hydrogenlike atoms.

As a numerical example we present in Table I the dipole operator eigenvalues calculated in various approximations for the system $(\mathrm{He}^+)^*$-e with $n_2=4$ and $n_2=10$.

V. SEMICLASSICAL APPROXIMATION FOR P^e STATES

For P^e states the coefficient p_l in the recursion relations (2.4) is given by the expression (2.7) which differs from (2.5) only by replacement of the factor l by $(l^2-1)^{1/2}$. This difference is negligible for large l where the semiclassical approximation is applicable. The semiclassical solutions of the recursion relations as well as the expression for the canonical momentum (3.4) can be employed in the same form as for S states. The recursion relations differ in the small l region which effectively produces different boundary conditions for the semiclassical solutions. Two cases should be considered here.

(i) Consider first the case $G<2$ and $Gn_2^2<\lambda<n_2^2(1+G^2/4)$. Here the orbital momentum l does not pass zero on the semiclassical trajectory. The solution C_l is appreciable only in the classically accessible domain where the recurrence relations practically coincide for S and P^e states. The eigenvalues λ_N differ little for S and P^e states the difference being of order of n_2^{-2} just like the error introduced by the semiclassical approximation (4.2) for the spectrum. The splitting of the eigenvalues can be obtained if one takes the difference of the Hamiltonians for P^e and S states and averages it over the wave function for S state. The semiclassical approximation gives

$$\lambda_N^P-\lambda_N^S \approx -\left[\int_{\xi_1}^{\xi_2}\frac{d\xi}{V(\xi)}\right]^{-1}\int_{\xi_1}^{\xi_2}\frac{d\xi}{V(\xi)}\,\frac{(\lambda_N^S/n_2^2-\xi^2)}{2\xi^2}\,, \tag{5.1}$$

$$V(\xi)=[G^2(1-\xi^2)-(\lambda_N^S/n_2^2-\xi^2)^2]^{1/2}\,.$$

(ii) For $-Gn_2^2<\lambda<Gn_2^2$ the semiclassical trajectory approaches small l; the difference between l and $(l^2-1)^{1/2}$ becomes appreciable. The matching of the solutions in the small l and large l regions is performed in the Appendix where the comparison equation method is used. It is shown that the quantization rule for the eigenvalues λ_N is of the same form (4.2) as before but with $\nu=N\pi/n_2$ in the rhs (N is an integer and the lower limit of integration ξ_1 is zero). This means that in the region of the spectrum considered the eigenvalues for P^e states lie halfway between the adjacent eigenvalues for S states.

Note that for P^e states in contrast to S states the quantization type is changed when λ passes from the interval $[Gn_2^2, n_2^2(1+G^2/4)]$ where $\nu\sim(N+\frac{1}{2})$ to the interval $[-Gn_2^2, Gn_2^2]$ where $\nu\sim N$. In the transition region $\lambda\approx\lambda_{\mathrm{crit}}=Gn_2^2$ the accuracy of the quantization rule is low. More accurate results can be obtained if one uses the uniform Bessel asymptote for the Legendre polynomial P_l^1 instead of simple trigonometric asymptote (A3). We shall not pursue this point further.

Our analytic results are illustrated by Table II where the eigenvalues for P^e states are presented for the same values of G and n_2 as for S states in the Table I. The exact quantum values are listed together with the semiclassical results obtained using the quantization rule (4.2) with $\nu=N\pi/n_2$ in the rhs. The accuracy of the semiclassical approximation is good for all eigenvalues except the highest one for $n_2=10$. The latter lies in the transition region (since $\lambda_{\mathrm{crit}}=150$ here). Comparison with Table I confirms that the eigenvalues of the symmetry P^e lie halfway between the adjacent eigenvalues of the symmetry S.

TABLE II. The same as in Table I but for P^e states.

N	λ_e	λ_{WKB}
	$n_2=4$	
1	19.12	18.82
−2	7.71	7.63
−1	−6.83	−6.85
	$n_2=10$	
1	147.03	145.51
2	128.79	128.42
3	105.82	105.63
−6	78.61	78.50
−5	47.76	47.69
−4	13.68	13.63
−3	−23.32	−23.36
−2	−63.05	−63.07
−1	−105.32	−105.32

VI. CONCLUSION

The physical essence of the problem considered in the present paper is the interaction of a charged particle with the dipole momentum which generally bears a hydrogen atom in the excited state. This dipole can be named dynamical since both its direction and magnitude vary in time being described by the canonically conjugated variables. The system is characterized by the parameter G which varies in wide range for the cases of interest in the atomic physics.

In the domain of applicability of the dipole approximation the three-body problem for the states of S and P^e symmetry is effectively one dimensional. It is reduced to the three-term recursion relations over single index. The semiclassical approach makes it possible to obtain here good quantitative results and also to describe the slow evolution of the classical trajectories. It is interesting that several types of motion can be realized: the rotations, the simple librations, and the quite unusual type of librations with three extrema of the angle $\varphi(t)$ situated on a half-period. In the rotation regime the orbital momentum never becomes small for the electron as well as for the outer particle. For purely dynamical reasons the outer particle does not approach the atomic nucleus what extends the applicability region for the dipole approximation.

In conclusion, we should like to stress that the motion of the particles is highly correlated in the situation considered in the present paper. Strong electron correlations are typical in the doubly excited states of the atom. They were the subject of extensive studies in recent years (see, e.g., review by Berry[14]). We find that the electron correlations are strong not only for the intrashell states but also in the case where one electron is excited much more than the other. Correlation is strong both in the case of large[1,2] and small (present paper) values of the total angular momentum.

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APPENDIX

Due to the singularity of the coefficient p_l in the small l region the recursion relation (2.4) should be treated by a method different from the semiclassical approximation. The comparison recursion relation is obtained by omitting the term w_l which is negligible for small l. The coefficient p_l is approximated by the following expression:

$$p_l = G n_2^2 \left[\frac{l^2 - m^2}{4l^2 - 1} \right]^{1/2} , \tag{A1}$$

which is applicable for $l^2 \ll n_2^2$. The additional parameter m is introduced here so that for $m = 0$ one obtains the recursion relations describing S states and for $m = 1$ the relations for P^e states.

We need the solution of the comparison recursion relation which is regular for $l = m$. It is expressed in terms of the adjoint Legendre polynomials:

$$C_l^{(m)} = \frac{1}{2} \left[\pi (2l+1) \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_l^m(\epsilon), \quad \epsilon = \frac{\lambda}{G n_2^2} , \tag{A2}$$

where the constant factor is chosen so that the subsequent formulas are simpler. For $l \gg m$ the asymptote of the Legendre polynomials can be used:

$$C_l^{(m)} = (1-\epsilon^2)^{-1/4} \cos \left[(l + \tfrac{1}{2}) \arccos\epsilon + \frac{m\pi}{2} - \frac{\pi}{4} \right] . \tag{A3}$$

On the other hand, in the semiclassical limit $l^2 \gg m^2$ (but in the region where $n_2^2 \gg l^2$) the comparison recurrent relation takes the form

$$\tfrac{1}{2}(C_{l-1} + C_{l+1}) - \epsilon C_l = 0 . \tag{A4}$$

The general semiclassical solution of the three-term recurrence relation[12,13]

$$C_l = (1-\epsilon^2)^{-1/4} \cos \left[\int_{-1/2}^{l} \arccos B \, dl + \theta \right] \tag{A5}$$

in the latter case is presented as

$$C_l = (1-\epsilon^2)^{-1/4} \cos[(l + \tfrac{1}{2}) \arccos\epsilon + \theta] , \tag{A6}$$

where we take into account that $B = \epsilon$ is independent of l. The lower limit of integration $l = -\frac{1}{2}$ in the expression (A5) is chosen for convenience reasons. The arbitrary constant θ should be chosen from the condition that the expression (A3) matches smoothly with (A6). This gives $\theta = -\pi/4 + m\pi/2$.

Thus in the case $m = 0$ (S states) the phase θ in the WKB solution is the same ($\theta = -\pi/4$) as for the simple turning point lying at $l = -\frac{1}{2}$. For $m = 1$ (P states) the phase is $\theta = \pi/4$. It is implied here that in all WKB formulas the coefficient $p_{l+1/2}$ is replaced by its semiclassical asymptote $\frac{1}{2} G n_2 [n_2^2 - (l + 1/2)^2]^{1/2}$ which leads to the expression (3.4) for $B(\lambda, l)$.

A similar approach was applied earlier in the analysis of the Stark effect on Rydberg states of nonhydrogenic atoms.[15]

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