228

96 228

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OSCILLATOR REPRESENTATION
AND GENERALIZED
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1   Introduction

There are many quantum mechanical systems that are described by axially symmetrical potentials. Such a system as atoms in a constant magnetic field, the Zeeman effect, was one of the earliest problems studied in quantum mechanics [1]. Although many numerical and analytical investigations of this system have been reported in the literature [2], there is still today considerable interest in its detailed properties, especially in strong magnetic fields. The main motivation comes from astrophysics [3], where very strong magnetic fields are needed to understand the physics of neutron star surfaces and white dwarf stars.

The energies and eigenfunctions of deformed nuclei [4] and the electronic shell structure effects in metallic clusters [5] are described by the Schrödinger equation with axially symmetrical potentials.

Most quantum systems described by the Schrödinger equation with an axially symmetrical potential cannot be solved analytically. Thus, the solution of the Schrödinger equation with sufficiently arbitrary potentials of this type represents the main mathematical problem. Many approximate analytical and numerical methods have been worked out. Great progress in the development of computer techniques and effective algorithms for a numerical solution of differential equations enables us to obtain numerical solutions for the energy spectrum and wave functions with quite a high accuracy although practical calculations are usually very laborious and require powerful computers. The main purpose of these investigations is in the majority the construction of highly accurate numerical solutions of the Schrödinger equation for the hydrogen atom in the uniform magnetic field as well as the energies and eigenfunctions of deformed nuclei and the electronic shell structure effects in metallic clusters.

Nevertheless, the development of analytical methods is very important because only analytical methods permit us to investigate qualitative features of quantum physical systems and indicate effective ways for improvement of numerical algorithms.

In this paper, the oscillator representation method(ORM) [6] will be formulated in the parabolic system of coordinates for the calculation of the energy spectrum of the hydrogen atom in external fields.

This paper is organized as follows. In section 2, the method of oscillator representation for the axially symmetric potential is formulated and used to consider the linear and quadratic Stark effect. In section 3, we considered the hydrogen atom perturbed and unperturbed by the van der Waals interactions with the conducting wall. In the Appendix some details of the calculations are given.

2   The oscillator representation method in the parabolic system of coordinates.

In the papers [6],[7] we formulated the ORM for the axial symmetric potential in the spherical system of coordinate. However, to determine an energy spectrum for some physical systems, it is convement to use the parabolic system of coordinates. In this section, we considere some physical examples for the demonstration of the oscillator representation method in the parabolic system of coordinates.
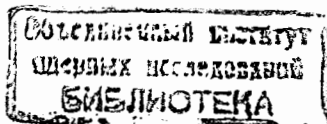
The Schrödinger equation in the parabolic system. We consider the Schrödinger equation for the Coulomb potential

$$\left[-\frac{1}{2}\Delta - \frac{1}{r} \right] \psi(\vec{r}) = E\psi(\vec{r}) . \tag{2.1}$$

Substituting the variables [1]

$$x = \sqrt{\xi\eta}\cos\phi , \qquad y = \sqrt{\xi\eta}\sin\phi , \qquad z = \frac{1}{2}(\xi - \eta) , \tag{2.2}$$

and taking into account the azimuthal symmetry of the problem, after some transformations, from (2.1) we get for the Schrödinger equation in the parabolic system

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial\xi^2} + \frac{1}{\xi}\cdot\frac{\partial}{\partial\xi} - \frac{m^2}{4\xi^2} \right) - \frac{E}{4} - \frac{\beta_1}{2\xi} \right] \psi_1(\xi) = 0 , \tag{2.3}$$

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial\eta^2} + \frac{1}{\eta}\cdot\frac{\partial}{\partial\eta} - \frac{m^2}{4\eta^2} \right) - \frac{E}{4} - \frac{\beta_2}{2\eta} \right] \psi_2(\eta) = 0 ,$$

where β_j are the separation parameters satisfying the identity

$$\beta_1 + \beta_2 = 1 . \tag{2.4}$$

The wave function initial system can be represented as

$$\psi(\vec{r}) = \frac{e^{im\phi}}{\sqrt{2\pi}}\cdot\psi_1(\xi)\cdot\psi_2(\eta) . \tag{2.5}$$

Our problem is formulated in the following way. Using the method of oscillator representation from (2.3) we determine the values of separate parameters β_j and the corresponding wave functions ψ_j. The desired energies E of the initial equations (2.1) are defined from (2.4). According to the ORM, we substitute (for details see ref.[6])

$$\xi = q^2 , \qquad \psi_1(\xi) = \psi_1(q^2) \rightarrow q^{|m|}\Phi_1(q^2) , \tag{2.6}$$

and after some transformation, from (2.3) we have

$$H\Phi_1(q^2) = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial q^2} + \frac{d-1}{q}\cdot\frac{\partial}{\partial q} \right) - Eq^2 - 2\beta_1 \right] \Phi_1(q^2) = 0 , \tag{2.7}$$

where $d = 2 + 2|m|$.

Now we can identify the operator

$$\Delta_d = \left(\frac{\partial^2}{\partial q^2} + \frac{d-1}{q}\cdot\frac{\partial}{\partial q} \right)$$

with the Laplacian in the auxiliary space R^d.

We shall solve Eq. (2.7) by using the ORM. The oscillator canonical variables (p, q) can be written in the form

$$q_j = \frac{1}{\sqrt{2\omega}}\cdot\left(a_j^+ + a_j \right) , \qquad p_j = \sqrt{\frac{\omega}{2}}\cdot\frac{a_j - a_j^+}{i} , \quad j = 1, 2, \cdots d . \tag{2.8}$$

The operators a_j and a_j^+ are called annihilation and creation operators. The Hamiltonian (2.7) in the oscillator representation [6]-[8] looks like

$$H = H_0 + \varepsilon_0 + H_I \tag{2.9}$$

with

$$H_0 = \omega(a_j^+ a_j) , \qquad H_I = 0 ,$$
$$\varepsilon_0(\beta_1) = \frac{d\omega}{4}\cdot\frac{dE}{2\omega} - 2\beta_1 .$$

The condition of the oscillator representation [6] can be written as

$$\frac{\partial}{\partial\omega}\varepsilon_0(\beta_1) = 0 \tag{2.10}$$

and from this equation for the oscillator frequency we get

$$\omega = \sqrt{-2E} . \tag{2.11}$$

From (2.7) we see that the magnetic quantum number m is absorbed in the dimensions of the auxiliary space R^d. The parabolic quantum numbers n_1, and n_2 are defined as radial excitations, i.e.

$$|n_1\rangle = C_{n_1}\left(a_j^+ a_j^+ \right)^{n_1} |0\rangle , \qquad C_n^{-2} = 2^{2n}n!\frac{\Gamma(d/2 + n)}{\Gamma(d/2)} , \tag{2.12}$$

where $|0\rangle$ is the vacuum state i.e., $a_j|0\rangle = 0$ and $\langle 0|0\rangle = 1$.

The energy spectrum [6] with radial excitation in the lowest approximation of OR is defined as

$$\varepsilon_1^{[n_1]}(\beta_1) = \langle n_1|H|n_1\rangle = \left(\frac{d}{4} + 2n_1 \right)\omega - \frac{dE}{2\omega} - 2\beta_1 . \tag{2.13}$$

According to (2.7), the parameter β_1 with the radial excitation is defined by the equations

$$\varepsilon_1^{[n_1]}(\beta_1) = 0 . \tag{2.14}$$

Taking into account (2.11) and (2.13), from (2.14) we get (the second equation represented in (2.3) can be calculated analogously)

$$\beta_1 = \frac{1}{8}(2d + 8n_1)\cdot\sqrt{-2E} , \tag{2.15}$$

$$\beta_2 = \frac{1}{8}(2d + 8n_2)\cdot\sqrt{-2E} .$$

Taking into account (2.15) for the desired energies E_n of the initial equation (2.1) of the ground and radial excited states from (2.4) we have

$$E_n = -\frac{1}{2n^2} , \tag{2.16}$$

where $n = 1 + n_1 + n_2 + |m|$ is the principal quantum number.

The hydrogen atom in the uniform electric field. To describe low-order splitting of the hydrogen atom levels in the electric field is an earliest quantum-mechanical problem [1]. The Schrödinger equation for the hydrogen atom in the uniform electric[1] field has the form

$$\left[-\frac{1}{2}\Delta - \frac{1}{r} + w \cdot z \right] \psi(\vec{r}) = E\psi(\vec{r}) \,, \qquad (2.17)$$

where w is the electric field oriented along the z-axis. We consider the weak electric field limits, i.e., the asymptotic behaviour of the wave functions for the large distance are Coulomb functions. In this case, taking into account (2.6), after some transformation from (2.17) we have for the modified Schrödinger equations

$$H^{(1)}\Phi_1 = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial q^2} + \frac{d-1}{q} \cdot \frac{\partial}{\partial q} \right) - Eq^2 - 2\beta_1 + \frac{1}{2} \cdot wq^4 \right] \Phi_1(q^2) = 0 \qquad (2.18)$$

$$H^{(2)}\Phi_2 = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial Q^2} + \frac{d-1}{Q} \cdot \frac{\partial}{\partial Q} \right) - EQ^2 - 2\beta_2 - \frac{1}{2} \cdot wQ^4 \right] \Phi_2(Q^2) = 0 \,,$$

with $d = 2 + 2|m|$, and q_j, Q_j are vectors in the space R^d. Let us use the ORM and from (2.18) we determine the parameters β_j. According to (2.9), the Hamiltonian is represented in the form

$$H^{(1)} = H_0^{(1)} + H_I^{(1)} + \varepsilon_0^{(1)}(E, \beta_1) \,,$$

where

$$\varepsilon_0^{(1)}(E, \beta_1) = \frac{d}{4} \cdot \omega - 2\beta_1 - \frac{dE}{2\omega} + \frac{wd(d+2)}{8\omega^2} \,, \qquad (2.19)$$

and for the interaction Hamiltonian we have

$$H_I^{(1)} = \frac{1}{2} \cdot w : q^4 : \,, \qquad (2.20)$$

where $: * :$ is the symbol of the normal ordering. In this approximation limit, taking into account (2.19) and from the condition of the OR, i.e. (2.10) we get for the frequency ω

$$\omega = v + w \cdot \frac{d+2}{2v^2} - \frac{3}{8} \cdot \frac{(d+2)^2}{v^5} \cdot w^2 + O(w^3) \,, \qquad (2.21)$$

where $v = \sqrt{-2E}$. In the second approximation [6] of the OR, the energy spectrum is defined as

$$\varepsilon_{(2)}^{[n_r]}(E, \beta_1) = \varepsilon_0^{(1)}(E, \beta_1) + 2n_1\omega(E, \beta_1) + \langle n_1|H_I^{(1)}|n_1 \rangle \qquad (2.22)$$

$$- \langle n_1| \left(H_I^{(1)} - \langle n_1|H_I^{(1)}|n_1 \rangle \right) \cdot \frac{1}{H_0^{(1)} - 2n_1\omega(E, \beta_1)} \cdot \left(H_I^{(1)} - \langle n_1|H_I^{(1)}|n_1 \rangle \right) |n_1 \rangle \,,$$

where n_1 is radial quantum number in the parabolic system. Taking into account (2.22), from (2.14) we obtaine for the parameter β_1

$$\beta_1 = \frac{d}{8} \cdot \omega - \frac{dE}{4\omega} + \frac{wd(d+2)}{16\omega^2} + n_1\omega(E, \beta_1) + \frac{1}{2}\langle n_1|H_I^{(1)}|n_1 \rangle \qquad (2.23)$$

$$- \frac{1}{2}\langle n_1| \left(H_I^{(1)} - \langle n_1|H_I^{(1)}|n_1 \rangle \right) \cdot \frac{1}{H_0^{(1)} - 2n_1\omega(E, \beta_1)} \cdot \left(H_I^{(1)} - \langle n_1|H_I^{(1)}|n_1 \rangle \right) |n_1 \rangle \,,$$

The calculation details of the matrix elements $\langle n_1|H_I^{(1)}|n_1 \rangle$ and the second corrections are given in the Appendix.

The parameter β_2 is determinedina similarly way. Finally we get

$$1 = \beta_1 + \beta_2 = nv + \frac{3(n_1 - n_2)n \cdot w}{2v^2} \qquad (2.24)$$

$$- \frac{w^2 \cdot n}{16 \cdot v^5} \cdot \left[17n^2 + 51(n_1 - n_2)^2 - 9m^2 + 19 \right] + O(w^3) \,,$$

where $n = 1 + n_1 + n_2 + |m|$. From (2.24) for the desired energies E_n of the initial system we have

$$E_n = -\frac{1}{2n^2} + \frac{3}{2}wn(n_1 - n_2) - \frac{w^2 n^4}{16} \left[17n^2 - 3(n_1 - n_2)^2 - 9m^2 + 19 \right] + O(w^3) \,. \quad (2.25)$$

So the dipole moment [1] in the normal state $(n_1 = n_2)$ looks like

$$d_z = -\frac{1}{w} \cdot \frac{\partial E}{\partial w} = \frac{n^4}{8} \cdot \left[17n^2 - 9m^2 + 19 \right] \,. \qquad (2.26)$$

Let us consider the Stark effect in the case of the strong electric field. The Schrödinger equation in the parabolic system coordinates can be written as

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial \xi^2} + \frac{1}{\xi} \cdot \frac{\partial}{\partial \xi} - \frac{m^2}{4\xi^2} \right) - \frac{E}{4} - \frac{\beta_1}{2\xi} + \xi^2 \cdot \frac{w}{8} \right] \psi_1(\xi) = 0 \qquad (2.27)$$

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial \eta^2} + \frac{1}{\eta} \cdot \frac{\partial}{\partial \eta} - \frac{m^2}{4\eta^2} \right) - \frac{E}{4} - \frac{\beta_2}{2\eta} - \eta^2 \cdot \frac{w}{8} \right] \psi_2(\eta) = 0 \,.$$

In the strong electric field case we assume that the asymptotic behaviour of the wave functions at large distances must define those terms of the potential which are proportional to w. From (2.27) we see that the asymptotic behaviour of the functions ψ_j at large distances are Gaussian. However, in this case transition to the modified Schrödinger equation from (2.27) is realized by the following substitutions

$$\xi = q \,, \qquad \psi_1(\xi) = \psi_1(q) \rightarrow q^{\frac{|m|}{2}}\phi_1(q^2) \qquad (2.28)$$

and the modified Schrödinger equation has the form

$$H^{(1)}\phi_1 = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial q^2} + \frac{d-1}{q} \cdot \frac{\partial}{\partial q} \right) - \frac{E}{4} - \frac{\beta_1}{2q} + q^2 \cdot \frac{w}{8} \right] \phi_1(q^2) = 0 \qquad (2.29)$$

$$H^{(2)}\phi_2 = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial Q^2} + \frac{d-1}{Q} \cdot \frac{\partial}{\partial Q} \right) - \frac{E}{4} - \frac{\beta_2}{2Q} - Q^2 \cdot \frac{w}{8} \right] \phi_2(Q^2) = 0 \,,$$

with $d = 2 + |m|$. We shall solve equation (2.29) by using the ORM. According to (2.9), the Hamiltonian $H^{(j)}$ can be represented in the form

$$H^{(1)} = H_0^{(1)} + \varepsilon_0^{(1)}(\beta_1) + H_I^{(1)} \,, \qquad (2.30)$$

with

$$H_0^{(1)} = \omega a_j^+ a_j \, , \qquad H_I^{(1)} = -\frac{\beta_1 \sqrt{\omega}}{2} \cdot h_I^{(1)} \, ,$$

$$\varepsilon_0^{(1)}(\beta_1) = \frac{d\omega}{4} - \frac{E}{4} + \frac{wd}{16\omega} - \frac{\beta_1 \sqrt{\omega}}{2} \frac{\Gamma((d-1)/2)}{\Gamma(d/2)}$$

$$h_I^{(1)} = \int\limits_{-\infty}^{\infty} \frac{d\tau}{\sqrt{\pi}} \int \left(\frac{dt}{\sqrt{\pi}}\right)^d e^{-t^2(1+\tau^2)} : e_2^{-2i\tau\sqrt{\omega}(qt)} : \, ,$$

where $e_2^{-z} = e^{-z} - 1 - z - z^2/2$. From the condition of the oscillator representation, i.e. (2.10), we define the separation parameters

$$\beta_1 = \frac{2}{\sqrt{\omega}} \cdot \frac{\Gamma((d+2)/2)}{\Gamma((d-1)/2)} \cdot \left(\omega - \frac{w}{4\omega}\right) \, . \qquad (2.31)$$

According to (2.14), in the lowest approximation OR the equation for the oscillator frequency ω looks like

$$\left(\frac{d}{4} + 2n_1\right)\omega - \frac{E}{4} + \frac{wd}{16\omega} - \frac{\beta_1\sqrt{\omega}}{2}\left[\frac{\Gamma((d-1)/2)}{\Gamma(d/2)} + \langle n_1|h_I^{(1)}|n_1\rangle\right] = 0 \, . \qquad (2.32)$$

The second equation represented in (2.29) can be calculated analogously. The desired energy E of the initial system is determined from (2.4).

Now calculate the displacement of the frequency [9] $\Delta\nu$ for the component $(\pi 18)$ of the line H_γ of the hydrogen atom. In this case for the parameters β_j we have

$$\beta_1 = \frac{2}{\sqrt{\omega\pi}} \cdot \left(\omega - \frac{w}{4\omega}\right) \, , \qquad \beta_2 = \frac{2}{\sqrt{\Omega\pi}} \cdot \left(\Omega + \frac{w}{4\Omega}\right) \, . \qquad (2.33)$$

For the oscillator frequencies ω and Ω at the values of the parabolic quantum numbers $n_1 = 0$ and $n_2 = 1$ from (2.32) we get

$$\omega = \frac{\sqrt{E^2 + 12 \cdot w} - E}{4} \, , \qquad \Omega = \frac{\sqrt{E^2 + 27 \cdot w} + E}{6} \, . \qquad (2.34)$$

In the case $n_2 = 4$ for Ω we have

$$\Omega = \frac{\sqrt{E^2 + 32(3 + 2 \cdot S_4) \cdot w} + E}{32} \, , \qquad (2.35)$$

where $S_4 = 3.52789$ and the calculational details are given in Appendix. Taking into account (2.34) and (2.35) from (2.4) we determined the desired Energy E or the displacement of frequency [9] $\Delta\nu$ at the values of field strength $w = 10^6 v/cm$

$$\Delta\nu = 1052.69 \ cm^{-1} \, . \qquad (2.36)$$

From (2.36) we see that our results are in good agreement with the exact [9] values.

The correct choice the asymptotic behaviour of the wave functions at large distances gives a possibility to take into account the effect which is connected with the strong electric field. Our results are equivalent to the results of effectivel summing of the perturbation series.

3 The hydrogen atom with the van der Waals interactions

The problem of a hydrogen atom in the generalized van der Waals field [10]-[12]

$$\Delta V(x, y, z) = \frac{1}{2}\gamma\left(x^2 + y^2 + \beta^2 z^2\right) \qquad (3.1)$$

(where $\gamma > 0$ and β are constants) is of much interest in physics. A large number of recent publications deal with different aspects of the well-known particular case, $\beta = 0$, of the problem of quadratic Zeeman effect [1]. The case $\beta = \sqrt{2}$ corresponds to the instaneous van der Waals interaction between an atom and metal surfaces [13] and is a subject of extensive discussions so far [14].

The present section is devoted to solving the three-dimensional Schrödinger equation for the electron of the hydrogen atom in the external van der Waals field in a particular case, $\beta = 2$ and a general case of arbitrary values of this parameter. To solve a three-dimensional problem, we use the ORM suggested by us in earlier papers [6]-[8]. This approach has been applied to calculate the energy spectrum of the Schrödinger equation with the spherical symmetric potential [8].

Let us consider the three-dimensional Schrödinger equation for the hydrogen atom with the van der Waals interaction

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) - \frac{1}{r} + \frac{\gamma}{2}\left(x^2 + y^2 + \beta^2 z^2\right)\right]\Psi = E\Psi \, . \qquad (3.2)$$

After some transformation in the parabolic system of coordinates, from (3.2) we have

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial\xi^2} + \frac{1}{\xi} \cdot \frac{\partial}{\partial\xi} - \frac{m^2}{4\xi^2}\right) - \frac{E}{4} - \frac{\beta_1}{2\xi} + \xi^2 \cdot \frac{\gamma}{4}\right]\psi_1(\xi) = 0 \qquad (3.3)$$

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial\eta^2} + \frac{1}{\eta} \cdot \frac{\partial}{\partial\eta} - \frac{m^2}{4\eta^2}\right) - \frac{E}{4} - \frac{\beta_2}{2\eta} + \eta^2 \cdot \frac{\gamma}{4}\right]\psi_2(\eta) = 0 \, ,$$

where β_j is the separate parameter and satisfaction the equation (2.4). To determine the energy spectrum E of the initial system we first of all define the parameters β_j from (3.3).

We consider the case when the external field is weak i.e. $\gamma << 1$. In this limit, take into account (2.6) and after some simplification from (3.3) we have

$$H^{(1)}\phi_1 = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial q^2} + \frac{d-1}{q} \cdot \frac{\partial}{\partial q}\right) - Eq^2 - 2\beta_1 + \gamma \cdot q^6\right]\phi_1(q^2) = 0 \, , \qquad (3.4)$$

with $d = 2 + 2|m|$. According to (2.9) the Hamiltonian is represented in the form

$$H^{(1)} = H_0^{(1)} + \varepsilon_0^{(1)}(\beta_1) + H_I^{(1)} \, ,$$

where

$$\varepsilon(\beta_1) = \frac{d\omega}{4} - \frac{dE}{2\omega} - 2\beta_1 + \frac{\gamma d(d+2)(d+4)}{8\omega^3} + O(\gamma^2) \, , \qquad (3.5)$$

$$H_I = \frac{3\gamma(d+4)}{2\omega} : q^4 : + \gamma : q^6 : \, .$$

Taking into account (2.13), (2.14) and (3.5), from (2.4) we get for the energy spectrum initial system

$$E = -\frac{1}{2n^2} + \frac{\gamma n^2}{2}\left[5n^2 - 3m^2 + 7 + 15(n_1 - n_2)^2\right] + O(\gamma^2) , \qquad (3.6)$$

with $n = 1 + n_1 + n_2 + |m|$. In this case, the oscillator frequency equals

$$\omega = v + \gamma \cdot \frac{3(d+2)(d+4)}{4v^3} + O(\gamma^2) , \qquad (3.7)$$

where $v = \sqrt{-2E}$.

Now consider the non-perturbation behaviour of hydrogen atom in the van der Waals field. We assume that the external field is strong, i.e. $\gamma > 1$ and the asymptotic behaviour of the wave functions at large distances is Gaussian. Taking into account (2.28) and after some transformations, from (3.3) we have for the modified Schrödinger equation

$$H^{(1)}\phi_1 = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial q^2} + \frac{d-1}{q}\cdot\frac{\partial}{\partial q}\right) - \frac{E}{4} - \frac{\beta_1}{2q} + q^2\cdot\frac{\gamma}{4}\right]\phi_1(q^2) = 0 , \qquad (3.8)$$

$$H^{(2)}\phi_2 = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial Q^2} + \frac{d-1}{Q}\cdot\frac{\partial}{\partial Q}\right) - \frac{E}{4} - \frac{\beta_2}{2Q} + Q^2\cdot\frac{\gamma}{4}\right]\phi_2(Q^2) = 0 ,$$

with $d = 2 + |m|$. This system of equations is solved analogously to the system of equations represented in (2.29). According to (2.33) for the separate parameter we have

$$\beta_j = \frac{2}{\sqrt{\omega}}\cdot\left(\omega_j - \frac{\gamma}{2\omega_j}\right)\cdot\frac{\Gamma((d+2)/2)}{\Gamma((d-1)/2)} . \qquad (3.9)$$

In this approximation, the oscillator frequency looks like for the case $n_j = 0$

$$\omega_j = \frac{\sqrt{E^2 + 6d\gamma} - E}{2d} , \qquad (3.10)$$

and for the case $n_j > 0$

$$\omega_j = \frac{\sqrt{E^2 - 16\gamma D_j f_j} + E}{8D_j} , \qquad (3.11)$$

where

$$D_j = 2n_j - \frac{d}{4} - \frac{3d}{8}\cdot S_{n_j} , \qquad f_j = \frac{3d}{4}\left(2 + S_{n_j}\right) , \qquad j = 1 , 2 .$$

The calculational details of the parameter S_j are given in the Appendix. Taking into account (3.9), (3.10) and (3.11), from (2.4) we determine the energy spectrum and wave functions of the hydrogen atom in the strong van der Waals field.

Let us consider the hydrogen atom in the generalized van der Waals field. We assume that the external field is weak. Taking into account (2.2), (2.6) and (3.1) we have for the modified Schrödinger equation

$$\left\{-\frac{1}{2}\left(\frac{\partial^2}{\partial q^2} + \frac{d-1}{q}\cdot\frac{\partial}{\partial q}\right) - \frac{1}{2}\left(\frac{\partial^2}{\partial Q^2} + \frac{d-1}{Q}\cdot\frac{\partial}{\partial Q}\right) - 2 \qquad (3.12)\right.$$

$$\left. -E\cdot(q^2 + Q^2) + A\left(q^6 + Q^6\right) + Bq^2Q^2\left(q^2 + Q^2\right)\right\}\Phi(q^2, Q^2) = 0 ,$$

where $d = 2 + 2|m|$,

$$A = \frac{1}{4}\gamma\beta^2 , \qquad B = \gamma\cdot\left(1 - \frac{\beta^2}{4}\right) .$$

According to (3.5) the Hamiltonian is represented in the correct form

$$H = H_0 + \varepsilon_0 + H_I , \qquad (3.13)$$

where

$$H_0 = \omega(a_j^+ a_j) + \Omega(A_j^+ A_j) ,$$

$$\varepsilon_0 = \frac{d\omega}{4} + \frac{d\Omega}{4} - 2 - \frac{dE}{2\omega} - \frac{dE}{2\Omega}$$

$$+A\cdot\frac{d(d+2)(d+4)}{8}\cdot\left(\frac{1}{\omega^3} + \frac{1}{\Omega^3}\right) + B\cdot\frac{d^2(d+2)}{8}\cdot\left(\frac{1}{\omega^3} + \frac{1}{\Omega^3}\right) + O(\gamma^2) ,$$

$$H_I = A\cdot\left[\frac{3(d+4)}{2}\left(\frac{1}{\omega}:q^4:+\frac{1}{\Omega}:Q^4:\right)+:q^6:+:Q^6:\right]$$

$$+B\cdot\left[\frac{2(d+2)}{\sqrt{\omega\Omega}}:q^2::Q^2:+\frac{d}{2\omega}:q^4::Q^2:+\frac{d}{2\Omega}:Q^4:+:Q^2::q^4:+:q^2::Q^4:\right] .$$

After some transformation, for the energy spectrum of the initial system we have

$$E = -\frac{1}{2n^2} + \frac{\gamma\beta^2 n^2}{8}\cdot\left[5n^2 - 3m^2 + 7 + 15(n_1 - n_2)^2\right] \qquad (3.14)$$

$$+\frac{1}{2}\gamma n^2\left(1 - \frac{\beta^2}{4}\right)\cdot\left[3n^2 - m^2 + 1 - 3(n_1 - n_2)^2\right] + O(\gamma^2) .$$

The oscillator frequency equals

$$\omega = v + \frac{3(d+2)(d+4)}{4v^3}\cdot A + \frac{3d(d+2)}{4v^3}\cdot B + O(\gamma^2) , \qquad (3.15)$$

where $v = \sqrt{-2E}$.

The dipole transitions. Let us consider the dipole transitions from the ground state (1s) to the excited state. In ORM the wave functions are defined in the d-dimensional auxiliary space and are Gaussian. To establish relations between 3- and d-dimensional wave functions, we consider the following equality:

$$1 = (\Psi\Psi) = N^2\int\limits_0^\infty\int d\eta d\xi\int\limits_0^{2\pi}d\phi\cdot\frac{1}{4}(\xi + \eta)\frac{e^{i\phi(m-m')}}{2\pi}\psi_m(\xi)\psi_{m'}(\xi)\phi_m(\eta)\phi_{m'}(\eta) , \qquad (3.16)$$

where N is the normalization constant. Taking into account (2.6) and after some transformations from (3.17) we get

$$
\begin{aligned}
1 &= N^2 \int\limits_0^\infty dq q^{d-1} \int\limits_0^\infty dQ Q^{d-1} \left(q^2 + Q^2\right) \psi_{n_1} \psi_{n_1}^* \phi_{n_2} \phi_{n_2}^* \\
&= N^2 \left[\langle n_1 | q^2 | n_1 \rangle + \langle n_2 | Q^2 | n_2 \rangle \right] ,
\end{aligned}
\tag{3.17}
$$

where $|n\rangle$ is the radial excitation in OR (2.12), and

$$
|0\rangle = \sqrt{2} \frac{\omega_n^{d/4}}{\Gamma(d/2)} \cdot e^{-\omega_n/2q^2}
$$

is the normalized vacuum state. The calculational details of the matrix elements $\langle n_1 | q^2 | n_1 \rangle$ are given in Ref. [8] and equal

$$
\langle n_1 | q^2 | n_1 \rangle = \frac{d}{2\omega} + \frac{2n_1}{\omega} .
$$

Thus, for the normalization constant we have

$$
N = \sqrt{\frac{\omega}{2n}} , \quad n = 1 + n_1 + n_2 + |m| .
\tag{3.18}
$$

The wave functions in the 3-dimensional space have the form

$$
\Psi_{n_1 n_2 m} = \frac{e^{im\phi}}{\sqrt{2\pi}} \cdot \sqrt{\frac{\omega_n}{2n}} \cdot \psi_{n_1}(\xi) \phi_{n_2}(\eta) .
\tag{3.19}
$$

The matrix element dipole transitions in the general case look like

$$
M_{n_1 n_2 m}^{n_1' n_2' m'} = \left(\Psi_{n_1 n_2 m} z \Psi_{n_1' n_2' m'}^* \right) = \delta_{mm'} \sqrt{\frac{\omega_n \omega_{n'}}{16 n n'}}
\tag{3.20}
$$

$$
\cdot \int\limits_0^\infty dq q^{d-1} \int\limits_0^\infty dQ Q^{d-1} \cdot \left(q^4 - Q^4\right) \psi_{n_1}(q^2) \psi_{n_1'}^*(q^2) \phi_{n_2}(Q^2) \phi_{n_2'}^*(Q^2) .
$$

We consider the dipole transition from the ground state to the excited one. After some transformations, from (3.20) we have

$$
\begin{aligned}
M_{00m}^{n_1 n_2 m} &= \frac{2^d}{\sqrt{n}} (\omega_1 \omega_n)^{(d+1)/2} \cdot \sqrt{\frac{\Gamma(n_1 + d/2)\Gamma(n_2 + d/2)}{n_1! n_2! \Gamma^2(d/2)}} \cdot \frac{(\omega_1 - \omega_n)^{n_1 + n_2}}{(\omega_1 + \omega_n)^{d + n_1 + n_2}} \\
&\left\{ \left[\frac{n_1(n_1 - 1)}{(\omega_1 - \omega_n)^2} - 2\frac{n_1}{(\omega_1 - \omega_n)} \cdot \frac{n_1 + d/2}{(\omega_1 + \omega_n)} + \frac{(n_1 + d/2)(n_1 + 1 + d/2)}{(\omega_1 + \omega_n)^2} \right] \right. \\
&\left. - \left[\frac{n_2(n_2 - 1)}{(\omega_1 - \omega_n)^2} - 2\frac{n_2}{(\omega_1 - \omega_n)} \cdot \frac{n_2 + d/2}{(\omega_1 + \omega_n)} + \frac{(n_2 + d/2)(n_2 + 1 + d/2)}{(\omega_1 + \omega_n)^2} \right] \right\} .
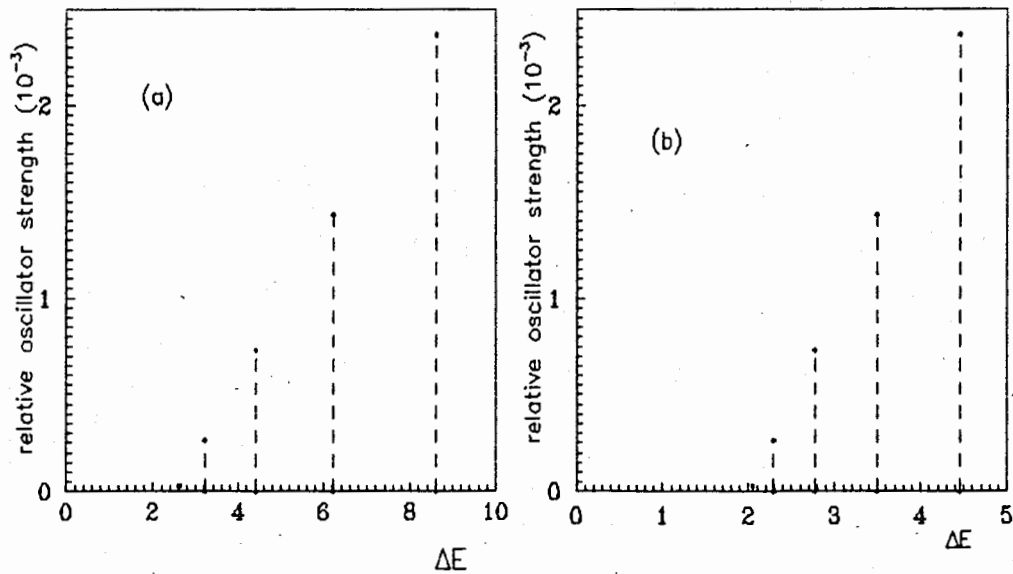\end{aligned}
\tag{3.21}
$$

Fig.1

Let us consider a particular case. For Coulomb interactions the oscillator frequency equals $\omega_n = 1/n$, and from (3.21) for the matrix element of dipole transitions we have standard results [9]

$$M_{00m}^{n_1 n_2 m} = -\frac{2^4 (n-1)^{n-3}}{(n+1)^{n+3}} \cdot n^3 (n_1 - n_2) . \tag{3.22}$$

In conclusion we would like to note that

i) The correctly chose asymptotic behaviour of the wave functions at large distances gives the possibility to investigate the problem of perturbative and non-perturbative behaviour of the system. This effect is most evidently developed for the energy spectrum of a hydrogen atom in the external uniform electric field and van der Waals field with $\beta = 2$.

ii) Our method gives the perturbation formulas (3.14) for the analytic spectrum of a hydrogen atom in the generalized van der Waals field, i.e.,arbitrary values of the parameter β in the entire region $0 \le \beta \le 2$.

iii) The relative oscillator strengths (dipole transition probabilities $W_{00m}^{n_1 n_2 m} = 3 |\Psi_{00m} Z \Psi_{n_1 n_2 m}|^2$) are given for $\beta = 2$ and $\beta = \sqrt{2}$, for γ from both perturbative and non-perturbative region. According to (3.15), (3.19) and (3.21), we can determine the dependence of oscillator strengths on ΔE for any values of quantum number n, m and the parameter β. Fig.1 represents the oscillator strengths for transitions from the ground state to the perturbed manifold $n = 10$, $m = 0$, a) the case $\beta = 2$ and b) the van der Waals case $\beta = \sqrt{2}$.

ACKNOWLEDGMENTS.

Appendix

Let us give some calculational details for the matrices $\langle n_r | H_I | n_r \rangle$. First of all, the variables $q^{2\tau}$, where τ is arbitrary, is represented in the normal form. Let $\tau = 1$, 2, 3, ...; then taking into account (2.8) we have

$$q^2 = \frac{d}{2\omega} + : q^2 : , \tag{A.1}$$

$$q^4 = \frac{d(d+2)}{4\omega^2} + \frac{d+2}{\omega} : q^2 : + q^4 : ,$$

$$q^6 = \frac{d(d+2)(d+4)}{8\omega^3} + \frac{3(d+2)(d+4)}{4\omega^2} : q^2 : + \frac{3(d+4)}{2\omega} : q^4 : + : q^6 : .$$

If $\tau < 0$, we use the following representation:

$$\frac{1}{q^{2\tau}} = \int_0^\infty \frac{d\alpha}{\Gamma(\tau)} \alpha^{\tau-1} e^{-q^2 \alpha} = \int_0^\infty \frac{d\alpha}{\Gamma(\tau)} \alpha^{\tau-1} \cdot \int \left(\frac{d\eta}{\sqrt{\pi}}\right)^d \cdot \frac{e^{-\eta^2(\frac{1}{\alpha}+\frac{1}{\Omega})}}{\alpha^{d/2}} : e^{-2iq\eta} : . \tag{A.2}$$

For the calculation matrices $\langle n_r | H_I | n_r \rangle$ we used thefollowing relations:

$$e^{i\vec{k}\vec{a}} e^{i\vec{p}\vec{a}^+} = e^{i\vec{p}\vec{a}^+} e^{i\vec{k}\vec{a}} e^{-(\vec{k}\vec{p})} , \tag{A.3}$$

$$e^{i\vec{k}\vec{a}} \vec{a}^+ e^{i\vec{k}\vec{a}} = \vec{a}^+ + i\vec{k} ,$$

$$e^{\alpha \vec{a}^+\vec{a}} \vec{a} e^{-\alpha \vec{a}^+\vec{a}} = \vec{a} e^{-\alpha} .$$

Taking into account (2.12) and (A.3) we have

$$\langle n_r | : q^2 : | n_r \rangle = \frac{2n_r}{\omega} \tag{A.4}$$

$$\langle n_r | : q^4 : | n_r \rangle = \frac{n_r}{\omega^2} [d + 6n_r - 4] ,$$

$$\langle n_r | : q^6 : | n_r \rangle = \frac{2n_r(n_r - 1)}{\omega^3} [3d + 10n_r - 8] .$$

According to (2.30) for the matrix $\langle n_1 | h_I^{(1)} | n_1 \rangle$ we have

$$\langle n_1 | h_I^{(1)} | n_1 \rangle = \int_{-\infty}^\infty \frac{d\tau}{\sqrt{\pi}} \int \left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2(1+\tau^2)} \langle n_1 | : e_2^{-2i\tau\sqrt{\omega}(q\eta)} : | n_1 \rangle . \tag{A.5}$$

Taking into account (A.3) and after some transformation we get

$$\langle n | : e_2^{-iB(a^+ \eta) - iB(a\eta)} : | n \rangle = C_n^2 \frac{\partial^{2n}}{\partial \alpha^n \partial \beta^n} \cdot \sum_{j=2}^{2n} \frac{(B^2\eta^2)^j}{j!} \cdot \frac{(\alpha + \beta - 4\alpha\beta)^j}{(1 - 4\alpha\beta)^{j+d/2}} \bigg|_{\alpha,\beta=0}$$

so, that from (A.5) we have

$$\langle n_j | h_I^{(j)} | n_j \rangle = \frac{3}{4} \cdot \frac{\Gamma(d/2 - 1/2)}{\Gamma(d/2)} \cdot S_{n_j} , \tag{A.6}$$

where

$$S_n = \frac{4\Gamma(1+n)}{3\sqrt{\pi}} \cdot \sum_{k=2}^{2n} \frac{(-1)^k \Gamma(k+1/2)}{\Gamma(k+d/2)} \cdot N_k(n,d) ,$$

and

$$N_k(n,d) = \sum_{p=0}^n \frac{2^{2p-k}\Gamma(k+n-p+d/2)}{(n-p)!(2p-k)!((k-p)!)^2} .$$

In a particular case, $n = 1$, and $n = 2$ for S_n we have

$$S_1 = \frac{2}{d} , \qquad S_2 = \frac{4}{d(d+2)} \cdot \left[d + \frac{19}{8}\right] .$$

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14

Динейхан М.   E4-96-228

Осцилляторное представление
и обобщенный гамильтониан ван дер Ваальса

Метод осцилляторного представления сформулирован в параболической системе координат и использован для вычисления энергетического спектра систем связанных состояний, описываемых аксиально-симметричным потенциалом. В частности, метод применен для нахождения энергий основного и возбужденного состояний атома водорода в постоянном электрическом поле и в поле сил ван дер Ваальса. Получено аналитическое выражение для энергетического спектра атома водорода в обобщенном поле ван дер Ваальса в приближении теории возмущений. Определена сила осциллятора для перехода из основного состояния в возбужденное с $n = 10, m = 0$.

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Oscillator Representation
and Generalized van der Waals Hamiltonians

The method called the oscillator representation is extended to calculate the energy spectrum of bound state described by axially symmetrical potentials in the parabolic system coordinates. In particular, the method is applied to calculate the energy of the ground and excited states of the hydrogen atom in the uniform electric field and van der Waals field. The method gives the perturbation formulas for the analytic spectrum of the hydrogen atom in the generalized van der Waals field and defined oscillator strengths for transitions from the ground state to the perturbed manifold $n = 10, m = 0$.