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OSCILLATOR REPRESENTATION METHOD
IN THE THEORY OF A HYDROGEN ATOM
IN AN EXTERNAL FIELD

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1 Introduction

One of the basic problems of nonrelativistic quantum mechanics is to find the energy spectrum and eigenfunctions of a microsystem described by the Schrödinger equation with an appropriate potential. Exact solutions of this equation have been found ([1]-[2]) for a quite limited class of potentials-like the harmonic oscillator, the Coulomb potential. However, most quantum systems are described by potentials for which the Schrödinger equation cannot be solved analytically. Thus, the solution of the Schrödinger equation with a sufficiently arbitrary potential represents the main mathematical task. For this aim, many approximate analytical and numerical methods were worked out. Great progress in the development of computer technique and effective algorithms of numerical solutions of differential equations permit one 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.

Approximate analytical methods imply a perturbative procedure when the Hamiltonian is divided into two parts $H = H_0 + H_I$, the solution of the zeroth approximation $H_0 \Psi^{(0)} = E^{(0)} \Psi^{(0)}$ is supposed to be obtained and perturbation corrections to the zeroth approximation $E^{(0)}$ and $\Psi^{(0)}$ can be calculated. The physical and mathematical top point is that the Hamiltonian H_0 in an appropriate representation of the Schrödinger equation should be chosen so as to catch the main dynamic properties of a quantum system and to give a possibility to analytically calculate all physical characteristics of the system under consideration. The interaction Hamiltonian H_I should give small corrections to the zeroth approximation and these corrections can be calculated.

Here we mention the standard perturbation Reley-Schrödinger theory ([1]-[2]), the quasiclassical or WKB method ([1]-[2]), $1/N$ -expansion([3],[4]). We will not go into details of these methods and refer readers to the numerous literature (see, for example, [1]-[4]).

In this paper, the oscillator representation method ([5],[6]) will be applied to Quantum Mechanics problems. The most remarkable difference between Quantum Field Theory and Quantum Mechanics is that quantized fields in QFT are sets of oscillators and any interactions of fields do not change the oscillator nature of these quantized fields. At the same time, in Quantum Mechanics, most of the potentials and therefore their corresponding wave functions are in behaviour quite different from the oscillator. The application of the oscillator representation method implies that a wave function, being a bound ground state of a quantum system with an attractive potential, is expanded over the oscillator basis in the representation, in which canonical variables (coordinate and momenta) are expressed through the creation and annihilation operators a^+ and a . However, in most cases the asymptotic behaviour of a true wave function (for example, the Coulomb wave functions) for large distances does not coincide with the Gaussian asymptotic behaviour of oscillator wave functions. This means that the expansion of these wave functions over the oscillator basis, although being mathematically correct, leads to a series converging not sufficiently fast for practical purposes.

Therefore, before applying the oscillator representation method we have to modify the variables in the starting Schrödinger equation to get a modified equation having solutions with the Gaussian asymptotic behaviour. In the Coulomb systems, such a modification

is performed by going over to the four-dimensional space where the wave function of the Coulomb system becomes an oscillator one.

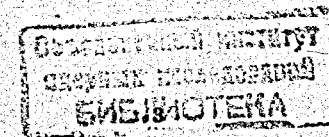
In an early paper [7], Schrödinger has noted the existence of such a transformation which transforms a three-dimensional Coulomb system into an oscillator one in the four-dimensional space. Kustaanheimo and Stiefel [8] gave the explicit form of this transformation and used it to solve the classical Kepler problem.

It should be taken into account that these transformations are not the canonical ones. It means that a quantum system after the Kustaanheimo-Stiefel transformation becomes another quantum system with another set of quantum numbers and corresponding wave functions. However, this new set contains a subset of wave functions which are wave functions of the initial system at the same time, and we are able to pick out necessary quantum numbers and wave functions. Therefore, these transformations should be considered as a successful mathematical technical method.

So, we get a modified Schrödinger equation the eigenfunctions of which have the oscillator Gaussian asymptotical behaviour. The next step is to write the Hamiltonian in terms of normal products over the creation and annihilation operators a^+ and a . Now one faces the question what is the optimal way to determine the frequency of this oscillator. In the language of the Hamilton formalism, the problem of calculation of the ground-state energy can be formulated in the following manner. Let the Hamiltonian of a system be given. Let us pick out the pure oscillator part with some unknown frequency ω and write this Hamiltonian in the form $H_0 = \omega a^+ a$. The rest of the Hamiltonian should be represented in terms of normal products over the operators a^+ and a . The requirement that this interaction Hamiltonian does not contain terms quadratic in the canonical variables leads to the equation which determines the oscillator frequency ω . This requirement is called the *oscillator representation condition* (ORC). As a result, the total Hamiltonian is written in the representation where the main quantum contributions to the ground state or vacuum of the system are taken into account.

The conception of normal product introduced into nonrelativistic quantum mechanics is actually not new (see, for example, [9]); however, the question is on which principles the realization of this idea should be based. All approaches which have used the formalism of creation and annihilation operators imply that the ground state wave function belongs to the oscillator basis although the true wave function can have a completely different asymptotic behaviour. Besides, the "free" Hamiltonians H_0 , for which the exact oscillator solutions exist, are usually chosen in the form which completely destroys the canonical quantum structure of the Hamiltonian (see, for example, [3]-[9]).

The paper is organized as follows: In sections 2 and 3, basic formulas of the oscillator representation method (ORM) for spherical axial symmetrical potentials are given. In sections 4 and 5, the method is applied to calculate the energy levels for the ground and orbital as well as radial excited states. The results of our calculations in the lowest approximation of the oscillator representation (OR) agree with the exact values very well.



2 The Oscillator Representation for spherical symmetric potentials

Our starting point is the radial Schrödinger equation in 3 dimensions:

$$\left[-\frac{1}{2r} \left(\frac{d}{dr} \right)^2 r + \frac{\ell(\ell+1)}{2r^2} + V(r) \right] \psi_{n\ell}(r) = E_{n\ell} \psi_{n\ell}(r). \quad (2.1)$$

We shall consider the potentials allowing a bound state.

Our aim is to calculate the energy spectrum $E_{n\ell}$ and to find the wave functions $\psi_{n\ell}(r)$ by using the oscillator representation method. This means that the wave functions $\psi_{n\ell}(r)$ should be expanded over the oscillator basis. This expansion can be carried out but it will not be effective for the simple reason that the asymptotic behaviours of the true and oscillator wave functions disagree for large, $r \rightarrow \infty$, and short, $r \rightarrow 0$, distances. Thus, we cannot apply the oscillator representation method directly but we have to transform the Schrödinger equation (2.1) so that the true wave function would acquire the necessary asymptotic behaviour for large and small distances. For this aim, we will use the well-known technique of changing the independent coordinate (see, for example, [10], [11]) which was applied to show the equivalence between solutions for different potentials in spaces of different dimensions. For example, there is equivalence between the Coulomb potential in 3 dimensions and the oscillator potential in 4 dimensions (see [8], [11]).

Our idea consists in the following. We want to change the variable $r = r(Q)$ and identify the transformed equation with the Schrödinger equation in a space with another dimension. The transition in the radial Schrödinger equation to higher dimensions from the general point of view has been considered earlier (see, for example, [12]). Thus, the calculation of the function $\psi_{0\ell}(r)$ is equivalent to the calculation of the ground state wave function of a modified Hamiltonian in another dimension. Moreover, the wave functions in this auxiliary space should have the oscillator Gaussian asymptotic behaviour. The radial excitation wave functions $\psi_{n\ell}(r) = |n_r\rangle$ will be equivalent to higher oscillator states.

The Schrödinger equation (2.1) can be written in the form:

$$\int d^3r \Psi(\mathbf{r}) \left[-\frac{1}{2} \Delta + V(r) - E \right] \Psi(\mathbf{r}) = 0.$$

If $\Psi(\mathbf{r}) = \psi_{n\ell}(r) Y_{n\ell}(\theta, \phi)$, then this equation for the wave function of the ℓ -th orbital excitation looks as

$$\int_0^\infty dr (r \psi_{n\ell}(r)) \left[-\frac{1}{2} \left(\frac{d}{dr} \right)^2 + \frac{\ell(\ell+1)}{2r^2} + (V(r) - E) \right] (r \psi_{n\ell}(r)) = 0.$$

The wave function $\psi_{n\ell}(r)$ depends only on one radial variable r . Usually, one can analytically find the asymptotic behaviour of the wave function $\psi_{n\ell}(r)$ for large $r \rightarrow \infty$. Let this asymptotic can be

$$\psi_{n\ell}(r) \rightarrow e^{-r^\alpha}.$$

In particular, for the Coulomb type potentials $\alpha = 1$. After the substitutions

$$r^\alpha = Q^2 \quad \text{and} \quad \psi_{n\ell}(r) = Q^{2\ell\rho} \Phi(Q), \quad (2.2)$$

where $\rho = 1/\alpha$, this equation becomes

$$\int_0^\infty dQ Q^{d-1} \Phi(Q) \left[-\frac{1}{2} \left(\frac{d}{dQ} \right)^2 + \frac{d-1}{Q} \cdot \frac{d}{dQ} \right] + W(Q^2, E) \Phi(Q) = 0, \quad (2.3)$$

with

$$W(Q^2, E) = 4\rho^2 Q^{4\rho-2} (V(Q^{2\rho}) - E), \\ d = 4\ell\rho + 2\rho + 2.$$

One can see that in the case when the function $\Phi(Q) = \Phi(Q)$ depends on Q^2 , only this equation can be identified with the equation in the space R^d with $d = 4\ell\rho + 2\rho + 2$ on a wave function $\Phi(Q)$ depending only on the radius Q . Equation (2.3) can be rewritten

$$\int d^d Q \Phi(Q) \left[-\frac{1}{2} \Delta_d + W(Q^2, E) - \varepsilon(E) \right] \Phi(Q) = 0,$$

where the function

$$\varepsilon(E) = \varepsilon(\ell, \rho, d; E)$$

should be considered as an eigenvalue of the Schrödinger equation in d -dimensions

$$\left[-\frac{1}{2} \Delta_d + W(Q^2, E) \right] \Phi(Q) = \varepsilon(E) \Phi(Q). \quad (2.4)$$

The desired energy E is defined by the equation

$$\varepsilon(E) = \varepsilon(\ell, \rho, d; E) = 0. \quad (2.5)$$

Formulation of the problem. We would like to stress that the energy E enters into the Schrödinger equation (2.4) as a parameter. Thus, our problem is formulated in the following way. The Hamiltonian H can be rewritten in the form

$$H = \frac{1}{2} (p^2 + \omega^2 Q^2) + (W(Q) - \frac{1}{2} \omega^2 Q^2), \quad (2.6)$$

where ω is an oscillator frequency. The oscillator canonical variables are

$$Q_j = \frac{1}{\sqrt{2\omega}} (A_j + A_j^\dagger) \quad (j = 1, \dots, d) \\ r_j = \frac{\sqrt{\omega}}{i\sqrt{2}} (A_j - A_j^\dagger), \quad [A_i, A_j^\dagger] = \delta_{ij}. \quad (2.7)$$

The ground or vacuum state $|0\rangle$ is supposed to exist and satisfy the conditions:

$$\langle 0|0\rangle = 1, \quad A_j|0\rangle = 0, \quad (j = 1, \dots, d).$$

Let us substitute the representation (2.7) into (2.6) and go to the normal product of the operators A_j^\dagger and A_j . One can get

$$\frac{1}{2}(p^2 + \omega^2 Q^2) = \omega \sum_j A_j^\dagger A_j + \frac{d}{2}\omega = \omega(A^\dagger A) + \frac{d}{2}\omega, \quad (2.8)$$

$$W(Q) - \frac{\omega^2}{2}Q^2 = \int \left(\frac{dk}{2\pi}\right)^d \widetilde{W}_d(k^2) \exp\left(-\frac{k^2}{4\omega}\right) : e^{i(kQ)} : - \frac{\omega^2}{2} \left(: Q^2 : + \frac{d}{2\omega} \right),$$

where $: * :$ is the symbol of the normal ordering and $(Qk) = \sum_j k_j Q_j$,

$$\widetilde{W}_d(k^2) = \int (d\rho)^d W(\rho) e^{i(k\rho)}$$

We require that the interaction part of the Hamiltonian should not contain the term with $: Q^2 :$ because this term is postulated to be included into the oscillator part completely. This requirement gives the equation for the frequency $\bar{\omega}$:

$$\omega^2 - \int \left(\frac{dk}{2\pi}\right)^d \widetilde{W}_d(k^2) \exp\left(-\frac{k^2}{4\omega}\right) \frac{k^2}{d} = 0. \quad (2.9)$$

Using these formulas we can rewrite the Hamiltonian (2.6) in the form:

$$H = H_0 + H_I + \varepsilon_0, \quad (2.10)$$

$$H_0 = \omega(A^\dagger A),$$

$$H_I = \int \left(\frac{dk}{2\pi}\right)^d \widetilde{W}_d(k^2) \exp\left(-\frac{k^2}{4\omega}\right) : e^{i(kQ)} - 1 + \frac{k^2 Q^2}{2d} : \\ = \int \left(\frac{d\rho}{\sqrt{\pi}}\right)^d e^{-\rho^2} W\left(\frac{\rho}{\sqrt{\omega}}\right) : \exp(-Q^2 + 2(\rho Q)) - 1 + Q^2 \left(1 - \frac{2\rho^2}{d}\right) :$$

$$\varepsilon_0 = \frac{d\omega}{4} + \int \left(\frac{dk}{2\pi}\right)^d \widetilde{W}_d(k^2) \exp\left(-\frac{k^2}{4\omega}\right).$$

Thus, the condition of the oscillator representation can be written as

$$\frac{\partial}{\partial \omega} \varepsilon_0(E; \omega, d) = 0. \quad (2.11)$$

This equation determines the parameter $\omega = \omega(E, d)$ as a function of the energy E , d and other parameters defining the potential $V(r)$ in (2.1).

The ground state energy $\varepsilon(E, d)$ of the Hamiltonian H in (2.10) will be calculated by the perturbation method over the interaction Hamiltonian H_I and in the N -th approximation it has the form:

$$\varepsilon_{(N)}(E, d) = \varepsilon_0(E, d) + \varepsilon_2(E, d) + \dots + \varepsilon_N(E, d).$$

According to (2.5) the ground state energy E of the initial problem in the N -th perturbation order of the oscillator representation method is defined by (2.11) and the equation

$$\varepsilon_{(N)}(E, d) = \varepsilon_0(E, d) + \varepsilon_2(E, d) + \dots + \varepsilon_N(E, d) = 0. \quad (2.12)$$

This equation determines the energy $E_{(N)}(d)$ in the N -th perturbation order as a function of d or ρ and other parameters defining the potential.

The accuracy of the oscillator representation can be evaluated as

$$\delta \sim \left| \frac{\varepsilon_2}{\varepsilon_0} \right|$$

The radial excitations. The radial excitations in the oscillator representation are defined in the form

$$|n_r\rangle = C_{n_r} (A_j^\dagger A_j^\dagger)^{n_r} |0\rangle, \quad C_{n_r}^{-2} = 2^{2n_r} n_r! \frac{\Gamma(d/2 + n_r)}{\Gamma(d/2)} \quad (2.13)$$

We shall apply the oscillator representation to the Hamiltonian in the form (2.10), and then we get the Schrödinger equation

$$H(E) \Phi^{[n_r]}(Q) = \varepsilon_{[n_r]}(E) \Phi^{[n_r]}(Q).$$

The desired energies E_{n_r} ($n_r = 0, 1, \dots$) of the initial equation (2.1) for the ground and radial excited states are defined by the equation

$$\varepsilon^{[n_r]}(E) = 0,$$

and therefore, we should find the functions $\varepsilon^{[n_r]}(E)$ for the ground and radial excited states. For the state $|n_r\rangle$ ($n_r = 1, 2, \dots$) the matrix element

$$\langle n_r | H_I | n_r \rangle = A^{[n_r]}(\omega, \alpha_j) - E_0 B^{[n_r]}(\omega, \alpha_j) \neq 0.$$

The energy $\varepsilon^{[n_r]}$ in the lowest approximation looks like

$$\varepsilon_1^{[n_r]}(E) = \langle n_r | H | n_r \rangle = \varepsilon_0(E) + 2n_r \omega + \langle n_r | H_I | n_r \rangle \\ = A_1^{[n_r]}(\omega, \alpha_j) - E B_1^{[n_r]}(\omega, \alpha_j), \quad (2.14)$$

where

$$A_1^{[n_r]}(\omega, \alpha_j) = A(\omega, \alpha_j) + 2n_r \omega + A^{[n_r]}(\omega, \alpha_j),$$

$$B_1^{[n_r]}(\omega, \alpha_j) = B(\omega, \alpha_j) + B^{[n_r]}(\omega, \alpha_j).$$

Two equations

$$\frac{\partial}{\partial \omega} A_1^{[n_r]}(\omega, \alpha_j) - E \frac{\partial}{\partial \omega} B_1^{[n_r]}(\omega, \alpha_j) = 0, \quad (2.15) \\ A_1^{[n_r]}(\omega, \alpha_j) - E B_1^{[n_r]}(\omega, \alpha_j) = 0,$$

determine the functions $\omega(\alpha_j)$ and $E(\alpha_j)$. The energy of the n_r -th excited state in the first approximation of the oscillator representation is determined as

$$E_1^{[n_r]} = \min_{\{\alpha_j\}} \frac{A_1^{[n_r]}(\omega(\alpha_j), \alpha_j)}{B_1^{[n_r]}(\omega(\alpha_j), \alpha_j)}$$

In the second approximation the energy is defined as

$$\epsilon_{(2)}^{[n_r]}(E) = \epsilon_0(E) + 2n_r\omega(E) + \langle n_r | H_I | n_r \rangle \quad (2.16)$$

$$- \langle n_r | (H_I - \langle n_r | H_I | n_r \rangle) \cdot \frac{1}{H_0 - 2n_r\omega(E)} \cdot (H_I - \langle n_r | H_I | n_r \rangle) | n_r \rangle.$$

The wave function in the second approximation is

$$\Phi_2^{[n_r]} = \left\{ 1 - \frac{1}{H_0 - 2n_r\omega(E)} \cdot (H_I - \langle n_r | H_I | n_r \rangle) \right\} | n_r \rangle.$$

The radial quantum number n_r does not enter into the Schrödinger equation (2.4) in the explicit form. The orbital quantum number ℓ enters into (2.4) but it is absorbed by the "dimension" parameter d . From the point of view of the space R^d the functions

$$\Phi_{n_r}(Q) = Q^{2\rho\ell} \psi_{n_r,\ell}(Q^{2\rho}) \quad \text{or} \quad \psi_{n_r,\ell}(r) = r^{\frac{d-2\rho-2}{4\rho}} \Phi_{n_r}(r^{1/2\rho})$$

for any n_r and for a fixed ℓ are eigenfunctions of the basic series of radial excitations in the space R^d with the radial quantum number n_r and zeroth orbital momenta.

Thus, the solution of the equation in 3 dimensions for the ℓ -th orbital excitation is equivalent to the solution of the Schrödinger equation in the space R^d for states with zeroth angular momenta.

As a result, the initial Schrödinger equation is represented in the form (2.4) in which the wave function of the ground state $\Phi(Q)$ has

- the Gaussian asymptotics for large distances $\Phi(Q) \sim \exp(-Q^2)$,
- a maximum at the point $Q = 0$.

The oscillator representation method consists in that we look for the solution of the Schrödinger equation (2.4) in the form

$$\Phi_{n_r}(Q) = \exp\left(-\frac{\omega}{2}Q^2\right) \sum_m c_{nm} P_m^{(d)}(Q^2\omega)$$

where $\{P_m^{(d)}(t)\}$ is the class of polynomials orthogonal on the interval $0 < t < \infty$ with the weight function

$$\rho_d(t) = t^{\frac{d}{2}-1} \exp(-t),$$

i.e.

$$\int_0^\infty dt t^{\frac{d}{2}-1} e^{-t} P_{n_r}^{(d)}(t) P_m^{(d)}(t) = \delta_{n_r,m},$$

These orthogonal polynomials can be constructed by using the formalism of creation and annihilation operators A_j and A_j^\dagger in the space R^d (see [6]). We have

$$|0\rangle \sim \exp\left(-\frac{\omega}{2}Q^2\right).$$

All radial excitations can be written in the form

$$\Phi_n \sim (A^+ A^+)^{n_r} |0\rangle \sim P_{n_r}^{(d)}(\omega Q^2) e^{-\frac{\omega}{2}Q^2} \sim P_{n_r}^{(d)}(\omega r^{1/\rho}) \exp\left(-\frac{\omega}{2}r^{1/\rho}\right) \quad (2.17)$$

where $P_{n_r}^{(d)}(t)$ is a polynomial of the n_r -th order. The parameter d in this representation can be considered as any positive number. These polynomials satisfy the orthogonality condition:

$$\begin{aligned} (\Psi_{n_r}, \Psi_m) &\sim \langle 0 | (AA)^{n_r} (A^+ A^+)^m | 0 \rangle \sim \int_0^\infty ds s^{d-1} \exp(-s^2) P_{n_r}^{(d)}(s^2) P_m^{(d)}(s^2) \\ &\sim \int_0^\infty dt t^{d/2-1} \exp(-t) P_{n_r}^{(d)}(t) P_m^{(d)}(t) \sim \delta_{n_r,m} \end{aligned}$$

This condition can be imposed on any positive d . Thus the algebra of creation and annihilation operators is nothing else than the mathematical method to perform any calculations connected with orthonormal polynomials.

3 The Oscillator Representation for the axially symmetrical potentials

There are many quantum mechanical systems described by axially symmetric potentials. Such a systems 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 [13], there is still today a considerable interest in its detailed properties, especially in strong magnetic fields. The main motivation comes from astrophysics [14], 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 [15] and the electronic shell structure effects in metallic clusters [16] are described by the Schrödinger equation with axially symmetric potentials.

Most quantum systems described by the Schrödinger equation with an axially symmetric potential cannot be solved analytically. Thus, the solution of the Schrödinger equation with sufficiently arbitrary potentials of this type represents the main mathematical problem.

Formulation of the problem. Let us consider the Hamiltonian with an axially symmetric potential

$$H = \frac{p^2}{2} + V(r, \cos \theta) \quad (3.1)$$

The Schrödinger equation looks like

$$\left[-\frac{1}{2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(r, \cos \theta) \right] \Psi(\vec{r}) = E \Psi(\vec{r}). \quad (3.2)$$

Taking into account the azimuthal symmetry of the problem we introduce the magnetic quantum number m so that the wave function can be represented as

$$\Psi(\vec{r}) = \frac{e^{im\phi}}{\sqrt{2\pi}} \Psi_m(r, \cos\theta) \quad (3.3)$$

Equation (3.2) acquires the form

$$\left\{ -\frac{1}{2} \left[\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left(\frac{\partial^2}{\partial \theta^2} + \cot\theta \frac{\partial}{\partial \theta} - \frac{m^2}{\sin^2\theta} \right) \right] + V(r, \cos\theta) \right\} \Psi_m(r, \cos\theta) = E_m \Psi_m(r, \cos\theta) \quad (3.4)$$

Our aim is to calculate the energy spectrum E_m and to find the wave functions $\Psi_m(r, \cos\theta)$ by using the oscillator representation method. The wave function $\Psi_m(r, \cos\theta)$ depends on two variables: the radius $r = \sqrt{r^2}$ and angle θ . The solutions of this equation are of the form

$$\Psi_m(r, \cos\theta) = \frac{P_\nu^m(\cos\theta)}{N_m(\nu)} \cdot \Phi_{m\nu}(r), \quad (3.5)$$

where $P_\nu^m(\cos\theta)$ satisfies the equation

$$\left[(1-x^2) \frac{d^2}{dx^2} - 2 \frac{d}{dx} - \frac{m^2}{1-x^2} - \nu(\nu+1) \right] P_\nu^m(x) = 0 \quad (3.6)$$

One can see that $P_\nu^m(x)$ is a solid spherical harmonic, $m = 0, \pm 1, \pm 2, \dots$ are azimuthal quantum numbers and ν is a parameter which can take any values. The normalization constant $N_m(\nu)$ is determined as

$$N_m(\nu) = \int_{-1}^1 dx P_\nu^m(x) P_\nu^m(x) \quad (3.7)$$

Let us introduce the functions

$$\mathcal{Y}_{\nu,m}(\theta, \phi) = (-1)^m \sqrt{\frac{(2\nu+1)}{4\pi} \frac{\Gamma(\nu-m+1)}{\Gamma(\nu+m+1)}} \cdot e^{im\phi} P_\nu^m(\cos\theta) \quad (3.8)$$

From (3.8) we see that when the parameter ν assumes only integers, then the functions $\mathcal{Y}_{\nu,m}(\theta, \phi)$ are spherical harmonics $Y_{\ell,m}(\theta, \phi)$. The action of the operators

$$\begin{aligned} \hat{l}_z &= -i \frac{\partial}{\partial \phi} \\ \hat{l}_\pm &= e^{\pm i\phi} \left(\pm \frac{\partial}{\partial \theta} + i \cot\theta \cdot \frac{\partial}{\partial \phi} \right) \\ \hat{l}^2 &= - \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right] \end{aligned} \quad (3.9)$$

on the functions represented in (3.8) is defined as

$$\begin{aligned} \hat{l}_z \mathcal{Y}_{\nu,m} &= m \mathcal{Y}_{\nu,m} \\ \hat{l}_\pm \mathcal{Y}_{\nu,m} &= -\sqrt{\nu(\nu+1) - m(m \pm 1)} \mathcal{Y}_{\nu, m \pm 1} \\ \hat{l}^2 \mathcal{Y}_{\nu,m} &= \nu(\nu+1) \mathcal{Y}_{\nu,m} \end{aligned} \quad (3.10)$$

We remark that the functions $\mathcal{Y}_{\nu,m}(\theta, \phi)$ and $P_\nu^m(\cos\theta)$ do not satisfy the orthogonality relations.

Let us analogously represent the Schrödinger equation (3.2) for the spherical symmetrical case

$$\int d^3r \Psi(\mathbf{r}) \left[-\frac{1}{2} \Delta + V(r, \cos\theta) - E \right] \Psi(\mathbf{r}) = 0 \quad (3.11)$$

Taking into account Eqs. (3.7-3.10), substituting the representations (3.3) and (3.5) into (3.11) and after some transformations, one can get

$$\int_0^\infty dr (r \Phi_{\nu,m}(r)) \left[-\frac{1}{2} \left(\frac{d}{dr} \right)^2 + \frac{\nu(\nu+1)}{2r^2} + (\tilde{V}_m(r, \nu) - E_m) \right] (r \Phi_{\nu,m}(r)) = 0 \quad (3.12)$$

where

$$\tilde{V}_m(r, \nu) = \frac{1}{N_m(\nu)} \int_{-1}^1 dx P_\nu^m(x) V(r, x) P_\nu^m(x) \quad (3.13)$$

The new parameter ν is considered as a additional variational parameter.

The next step is to modify the variable r in radial equation (3.12) and the wave function $\Phi_{\nu,m}(r)$ so as to get a modified Schrödinger equation having the solution with the Gaussian asymptotic behaviour. These substitutions are

$$r = Q^{2\rho}, \quad \Phi_{\nu,m}(r) = Q^{2\rho\nu} \cdot \Phi_{\nu,m}(Q),$$

where the parameter ρ can be connected with the behaviour of the wave function at large distances to approximate the Gaussian asymptotics. The Schrödinger equation takes the form

$$\left[-\frac{1}{2} \left(\frac{\partial^2}{\partial Q^2} + \frac{d-1}{Q} \frac{\partial}{\partial Q} \right) + W(Q, \nu, E_m) \right] \Phi_{\nu,m}(Q) = 0, \quad (3.14)$$

where $d = 2 + 2\rho + 4\rho\nu$ and the potential $W(Q, \nu, E)$ equals

$$W(Q, \nu, E) = 4\rho^2 Q^{4\rho-2} \cdot [\tilde{V}_m(Q, \nu) - E_m] \quad (3.15)$$

The calculations details of the energy spectrum and wave functions of the system described by the Schrödinger equation represented in (3.14) are given in section 2.

Further steps should be done according to the rules formulated above.

4 The calculation energy spectrum spherical symmetrical potentials

Let us apply the above-formulated method to calculation of the energy spectrum of a wide class of potentials.

4.1 The molecular potentials

For the investigation of diatom molecules, Kratzer[17] and Morse[18] potentials are used. First of all we calculate the energy spectrum of the Kratzer potential

$$V(r) = -2D \cdot \left(\frac{a}{r} - \frac{1}{2} \cdot \frac{a^2}{r^2} \right) \quad (4.1)$$

The Schrödinger equation can be written in the form

$$\left[-\frac{1}{2} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial}{\partial r} - \frac{s(s+1)}{r^2} \right) - M \left(E + \frac{2Da}{r} \right) \right] \Psi_{nl} = 0, \quad (4.2)$$

with the notation

$$\begin{aligned} s(s+1) &= \ell(\ell+1) + 2Ma^2D, \\ s &= \frac{1}{2} \left(\sqrt{(2\ell+1)^2 + 4Ma^2D} - 1 \right). \end{aligned} \quad (4.3)$$

According to (2.2) we do the transformation

$$r = Q^2, \quad \Psi = Q^{2s} \Phi(Q^2)$$

and get the representation

$$\begin{aligned} H(E)\Phi(Q^2) &= \varepsilon(E)\Phi(Q^2), \\ H(E) &= \frac{1}{2}P_Q^2 + W(Q^2, E), \\ W(Q^2, E) &= -4MEQ^2 - 8DMa, \end{aligned}$$

where $Q_j \in R^d$ with $d = 4 + 4s$. Now we can apply the ORM. The Hamiltonian is

$$H(E) = \frac{1}{2}P_Q^2 + W(Q^2, E) = H_0 + \varepsilon_0,$$

where H_0 is given by (2.10) and ε_0 according to (2.13) equals

$$\varepsilon_0(E) = \frac{d\omega}{4} - \frac{2MEd}{\omega} - 8MDa.$$

From the oscillator representation conditions (2.11) we can get

$$\omega = \sqrt{-8ME}. \quad (4.4)$$

The energy in the lowest approximation with the radial excitation looks like

$$\varepsilon_1^{[nr]}(E) = \left(\frac{d}{4} + 2n_r \right) - \frac{2MEd}{\omega} - 8MDa. \quad (4.5)$$

According to (2.15) and taking into account (4.3) and (4.4) from (4.5) we have

$$E_{nl} = -\frac{4D\gamma^2}{(1 + 2n_r + \sqrt{(2\ell+1)^2 + 4\gamma^2})^2}, \quad (4.6)$$

where $\gamma^2 = 2MDa^2$ and for most molecules $\gamma \gg 1$. In the lowest order of the parameter $1/\gamma$ from (4.6) we get

$$E_{nl} = D \left[-1 + \frac{2(n_r + 1/2)}{\gamma} + \frac{(\ell + 1/2)^2}{\gamma^2} - \frac{3(n_r + 1/2)^2}{\gamma^2} - \frac{3(n_r + 1/2)(\ell + 1/2)}{\gamma^3} + O\left(\frac{1}{\gamma^4}\right) \right]. \quad (4.7)$$

The second and third terms of this expression describe the vibration and rotation energy levels, the fourth term is the correction to the vibration level and the fifth term characterizes the connection between vibration and rotation levels. The Kratzer potential played an important role in the early stage of the development of Quantum Mechanics. However, this potential is less physical than the Morse potential.

The Morse potential well describes the vibration character of diatom molecules and has the form[18]

$$V(r) = D \cdot [e^{-2x} - 2e^{-x}], \quad (4.8)$$

where $x = \alpha \cdot (r - r_0)/r_0$. The parameters of the this potential for some standard molecules are defined experimentally [19] and are represented in Table 1.

Table 1 The potential parameters.

molecules	$\frac{1}{2Mr_0^2} [cm^{-1}]$	D, $[cm^{-1}]$	α
H ₂	60.8296	38292	1.440
HCE	10.5930	37244	2.3801

After some transformation the Schrödinger equation looks like

$$\left\{ -\frac{1}{2} \left(\frac{\partial^2}{\partial Q^2} + \frac{d-1}{Q} \frac{\partial}{\partial Q} \right) - \frac{2\gamma^2 E}{D} + 2\gamma^2 Q^2 \left[e^{-2\alpha(Q^2-1)} - 2e^{-\alpha(Q^2-1)} \right] \right\} \Phi(Q^2) = 0, \quad (4.9)$$

where $d = 4 + 4\ell$ and $\gamma^2 = 2DMr_0^2$. The Hamiltonian can be represented in the form

$$H = H_0 + \varepsilon_0 + H_1,$$

where H_0 is given by (2.10) and

$$\varepsilon_0(E) = \frac{d\omega}{4} - \frac{dE\gamma^2}{D\omega} + \frac{d\gamma^2}{\omega} \cdot \left[\frac{e^{2\alpha}}{\left(1 + \frac{2\alpha}{\omega}\right)^{3+2\ell}} - \frac{2e^\alpha}{\left(\frac{\alpha}{\omega}\right)^{3+2\ell}} \right], \quad (4.10)$$

and for the interaction Hamiltonian we have

$$H_I = 2\gamma^2 \int \frac{d^d \eta}{\pi^{d/2}} \left[2e^\alpha \frac{\partial}{\partial \alpha} \frac{e^{-\eta^2(1/\alpha+1/\omega)}}{\alpha^{d/2}} - \frac{e^{2\alpha}}{2} \frac{\partial}{\partial \alpha} \frac{e^{-\eta^2(1/2\alpha+1/\omega)}}{(2\alpha)^{d/2}} \right] : e_2^{-2iQ\eta} : \quad (4.11)$$

According to (2.15), the equation

$$\frac{d+4n_r}{2} \omega + \frac{2d\gamma^2 \alpha(3+2\ell)}{\omega^2} \left[\frac{e^{2\alpha}}{(1+\frac{2\alpha}{\omega})^{4+3\ell}} - \frac{e^\alpha}{(1+\frac{\alpha}{\omega})^{4+2\ell}} \right] + \langle n_r | H_I | n_r \rangle = 0 \quad (4.12)$$

makes it possible to determine the parameter ω as a function of the vibration n_r and rotation ℓ quantum numbers. The energy levels in the first approximation of the oscillator representation are determined as

$$E_\ell^{[n_r]} = \frac{D\omega(d+8n_r)}{4d\gamma^2} + D \cdot \left[\frac{e^{2\alpha}}{(1+\frac{2\alpha}{\omega})^{4+3\ell}} - \frac{e^\alpha}{(1+\frac{\alpha}{\omega})^{4+2\ell}} \right] + \frac{D\omega}{d\gamma^2} \langle n_r | H_I | n_r \rangle, \quad (4.13)$$

where

$$\langle n_r | H_I | n_r \rangle = 2\gamma^2 \int \frac{d^d \eta}{\pi^{d/2}} \quad (4.14)$$

$$\left[2e^\alpha \frac{\partial}{\partial \alpha} \frac{e^{-\eta^2(1/\alpha+1/\omega)}}{\alpha^{d/2}} - \frac{1}{2} e^{2\alpha} \frac{\partial}{\partial \alpha} \frac{e^{-\eta^2(1/2\alpha+1/\omega)}}{(2\alpha)^{d/2}} \right] \langle n_r | : e_2^{-2iQ\eta} : | n_r \rangle,$$

$$\langle n_r | : e_2^{-2iQ\eta} : | n_r \rangle = \sum_{m=2}^{2n_r} C_m(n_r, d) \cdot \left(-\frac{\eta^2}{\omega} \right)^m,$$

$$C_m(n_r, d) = \frac{\Gamma(n_r+1) \cdot \Gamma(d/2)}{\Gamma(d/2+n_r) \cdot \Gamma(d/2+m)} \cdot \sum_p^{\lfloor \frac{m}{2} \rfloor} \frac{2^{m-2p} \Gamma(d/2+n_r+p)}{(n_r-m+p)!(m-2p)!(p!)^2}$$

$p = \max(0, m-n_r)$.

In particular $n_r = 1$ and $n_r = 2$ and for $C_m(n_r, d)$ we have

$$C_2(1, d) = \frac{2}{d}, \quad C_2(2, d) = \frac{4(d+8)}{d(d+2)}, \quad (4.15)$$

$$C_3(2, d) = \frac{16}{d(d+2)}, \quad C_4(2, d) = \frac{2}{d(d+2)}.$$

Our calculation results are given in Table 2.

The rotation energy of diatom molecules is considered as a perturbation correction [20] to the vibration energy and the expansion of the potential in the $(r-r_0)/r_0$ made. This approximation gives some possibility to determine the energy spectrum of diatom molecules with the vibration and rotation corrections. On the other hand, from (4.13) we see that our results make it possible to determine the vibration and rotation energy spectrum of diatom molecules exactly.

Table 2 The energy spectrum (in units $10^4 \cdot \text{cm}^{-1}$) of the diatom molecules.

		H_2		HCE	
		ω	E	ω	E
$n_r = 0$	$\ell = 1$	3.85565	-2.4149	2.50749	-0.7338
	$\ell = 2$	5.82656	-2.7780	4.48658	-1.3374
	$\ell = 3$	7.78429	-2.9914	6.47241	-1.7584
$n_r = 1$	$\ell = 1$	4.54585	-3.9834	2.83224	-1.8159
	$\ell = 2$	6.5111	-4.0530	4.84365	-2.5129
	$\ell = 3$	8.46430	-4.0659	6.84497	-2.8705
$n_r = 2$	$\ell = 1$	6.1540	-6.7576	4.96107	-14.7620
	$\ell = 2$	8.01054	-6.3432	6.68407	-11.285
	$\ell = 3$	9.8833	-5.9618	8.55037	-9.5162

From Table 2. we see that at fixed values of the vibrational quantum number the rotational energy can be considered as a perturbation correction, i.e., the dependence of the energy spectrum of diatom molecules on the rotational quantum number ℓ is weak. However, some fixed value, $n_r = 2$, by increasing the rotational quantum number ℓ , the module energy spectrum decreased. So, for given diatom molecules we find the values of rotational quantum number ℓ_c , for which the energy spectrum equal to zero, i.e. $E_{n_r \ell_c} = 0$.

4.2 The hydrogen atom with the spherical symmetrical van der Waals potentials

In papers [21, 22] the so-called generalized van der Waals Hamiltonian was introduced for investigation of different quantum mechanical systems. In this subsection we will apply the OR method to calculate the energy spectrum of the van der Waals potential.

The generalized van der Waals potential is [22]

$$V(\vec{r}) = \frac{1}{2} \gamma (x^2 + y^2 + \beta^2 z^2) - \frac{1}{r}, \quad (4.16)$$

where β and γ are dimensionless physical parameters. For $\beta = \sqrt{2}$ we recover the van der Waals potential [23]; for $\beta = 0$, the quadratic Zeeman effect (QZE) [24]. The case when γ is arbitrary and $\beta = 1$ represents the so-called spherical QZE [25]. It also represents the so-called charmonium potential existing between charmed quarks and antiquarks [26]. Moreover, it represents a special form of the so-called generalized Killingbeck potential applied in quantum mechanics [27].

Let us consider the hydrogen atom with the spherical symmetrical van der Waals potential. In this case from (4.16) the Hamiltonian can be written

$$H = \frac{1}{2} \vec{P}^2 - \frac{1}{r} + \frac{1}{2} \gamma \cdot r^2$$

After some calculations above the Schrödinger equation in the d-dimensional auxiliary space looks as

$$\left[\frac{1}{2} P_Q^2 - 4EQ^2 - 4 + 2\gamma Q^6 \right] \Phi_{nl} = 0. \quad (4.17)$$

According to (2.10) the Hamiltonian is represented in the form

$$H = H_0 + \varepsilon_0 + H_I,$$

where

$$\begin{aligned} \varepsilon_0(E) &= \frac{d\omega}{4} - \frac{2dE}{\omega} - 4 + \frac{\gamma}{\omega^3} \cdot \frac{d(d+2)(d+4)}{2}, \\ H_I &= \frac{6\gamma(d+4)}{\omega} : Q^4 : + 4\gamma : Q^6 :, \\ d &= 4 + 4\ell. \end{aligned} \quad (4.18)$$

We consider the case when $\gamma \ll 1$. In the lowest approximation from the condition of the oscillator representation (2.11) we determine

$$\omega = v + \frac{3\gamma(d+2)(d+4)}{v^3} + O(\gamma^2), \quad (4.19)$$

where we introduced the notation

$$v = \sqrt{-8E}.$$

The energy spectrum with orbital and radial excitation in the lowest approximation of OR is defined as

$$\varepsilon_1^{[n_r]} = \varepsilon_0(E) + 2n_r\omega + \langle n_r | H_I | n_r \rangle. \quad (4.20)$$

The calculation details of the matrix elements $\langle n_r | H_I | n_r \rangle$ are given in Appendix. Taking into account (4.18-4.19) and (A.5) from (4.20) we have for the energy spectrum

$$E_{nl} = -\frac{1}{2n^2} + \frac{\gamma n^2}{2} [5n^2 - 2\ell(\ell+1) + 1] + O(\gamma^2), \quad (4.21)$$

where $n = 1 + \ell + n_r$ is the principal quantum number.

4.3 Nonrelativistic quark potential

Let us consider the hadrons as bound states of quarks within nonrelativistic potential models. The basic problem is that nonrelativistic quark models describe the masses and static characteristic of hadrons. The Hamiltonian with the power law confining potential for the quark-antiquark pair can be represented as [28]

$$H = m_1 + m_2 + \frac{1}{2\mu} \vec{p}^2 + br^{2/3}, \quad (4.22)$$

where $\mu = m_1 m_2 / (m_1 + m_2)$ is the reduced mass of the two-particle system, b is the coupling constant. The Schrödinger equation can be written in the form

$$\left[\frac{1}{2} \vec{p}^2 + m_1 m_2 + \mu br^{2/3} - E\mu \right] \Psi_{nl} = 0. \quad (4.23)$$

After some transformations the modified equation looks like

$$\left[\frac{1}{2} P_Q^2 + 9\sqrt{Q} \cdot \left(b\mu + \frac{m_1 m_2 - E\mu}{Q} \right) \right] \Phi_{nl}(Q^2) = 0. \quad (4.24)$$

In this case according to (2.10) for the energy we have

$$\varepsilon_0(E) = \frac{\omega}{2} \left(\frac{3\ell}{2} + \frac{7}{4} \right) + \frac{9\omega^{1/4}}{\Gamma(\frac{3}{2}\ell + \frac{7}{4})} \left[(m_1 m_2 - \mu E) \Gamma(\frac{3}{2}\ell + \frac{3}{2}) + \frac{b\mu}{\sqrt{\omega}} \Gamma(\frac{3}{2}\ell + 2) \right]. \quad (4.25)$$

According to (2.11) the parameter ω is defined by

$$\frac{\partial}{\partial \omega} \varepsilon_0(E, \omega) = 0.$$

We consider the large orbital momentum case i.e. $\ell \rightarrow \infty$ and use the asymptotic representation of gamma functions

$$\lim_{x \rightarrow \infty} \Gamma(x) \cong \sqrt{2\pi} e^{-x} x^{x-1/2}.$$

From (4.25) we have

$$E \cong m_1 + m_2 + \left[\frac{128}{27} \cdot \frac{b^3}{\mu} \right]^{1/4} \cdot \sqrt{\ell}. \quad (4.26)$$

So, the corresponding squared masses of hadrons equal

$$M^2 \cong \beta \cdot \ell + const., \quad (4.27)$$

where

$$\beta = \sqrt{\frac{128 \cdot b^3}{27\mu}}.$$

On the other hand, we know that for large angular momenta the squared masses of hadrons are proportional to the angular momentum ℓ and are defined by (4.27) and the parameter β is the so-called *Regge slope*.

5 Calculation of the energy spectrum of axial symmetric potentials

In this section, the method of oscillator representation will be applied to calculate the energy values of ground and excited states of the hydrogen atom in a uniform magnetic field of arbitrary strength.

5.1 The hydrogen atom in a uniform magnetic field

The Hamiltonian of the hydrogen atom in an external magnetic field for spin-down states is [1] (in the Rydberg atomic units):

$$H = \frac{1}{2}(\vec{P} - \vec{A})^2 - \frac{1}{r} + (\vec{B}\vec{S}) = \frac{1}{2}\vec{P}^2 - \frac{1}{r} + \frac{1}{8}B^2(x^2 + y^2) + \frac{1}{2}B(L_z - 1), \quad (5.1)$$

where the vector potential $\vec{A} = \frac{1}{2}[\vec{B}, \vec{r}]$ and the magnetic field \vec{B} has been oriented along the z-axis; L_z is the z-component of the angular momentum operator and $S_z = 1/2$. The Schrödinger equation for the Hamiltonian (5.1) becomes

$$\left[\frac{1}{2}\vec{P}^2 - \frac{1}{r} + \frac{1}{2}r^2 \cdot \sin^2(\theta) \cdot \beta^2 + \beta(L_z - 1) \right] \Psi(\vec{r}) = E\Psi(\vec{r}), \quad (5.2)$$

where β is the strength parameter $\beta = \frac{1}{2}B$.

Our problem is to calculate the energy values E_m of the ground and excited states of the hydrogen atom in a uniform magnetic field for arbitrary strength parameters β .

Taking into account (3.4–3.15) and after some transformations the modified Hamiltonian has the form

$$H = \frac{1}{2}(P_Q^2 + \Omega^2 \cdot Q^2 - d\Omega) + \left[4\rho^2 Q^{4\rho-2} \cdot \left(U_m - \frac{1}{Q^{2\rho}} + \frac{\beta^2}{2} \cdot Q^{4\rho} \cdot A_m(\nu) \right) - \frac{\Omega^2}{2} \cdot Q^2 + \frac{d}{2}\Omega \right], \quad (5.3)$$

$$d = 2 + 2\rho(2\nu + 1),$$

where

$$A_m(\nu) = \frac{1}{N_m(\nu)} \int_{-1}^1 dx \left[\sqrt{1-x^2} \cdot P_\nu^m(x) \right]^2, \quad (5.4)$$

and $N_m(\nu)$ are defined by (3.7). The energy of the hydrogen atom is determined by

$$E_m = \beta(m-1) - U_m. \quad (5.5)$$

According to (2.10), for the calculation of the energy spectrum of the ground and excited state by using the oscillator representation method the Hamiltonian is represented in the form

$$H = H_0 + H_1 + \varepsilon_0(E),$$

where

$$\varepsilon_0(E) = \frac{d\omega}{4} - \frac{4\rho^2}{\omega^{\rho-1}} \cdot \frac{\Gamma(d/2 + \rho - 1)}{\Gamma(d/2)} + \frac{4U_m\rho^2}{\omega^{2\rho-1}} \cdot \frac{\Gamma(d/2 + 2\rho - 1)}{\Gamma(d/2)} + \frac{2\rho^2\beta^2}{\omega^{4\rho-1}} \cdot \frac{\Gamma(d/2 - 4\rho - 1)}{\Gamma(d/2)} \cdot A_m(\nu). \quad (5.6)$$

The interaction Hamiltonian looks as

$$H_I = 4\rho^2 \int_0^\infty dx \int \frac{d^d\eta}{\pi^{d/2}} \cdot e^{-\eta^2(1+\frac{x}{2})} : e_2^{-2iQ\eta\sqrt{x}} : \cdot \left[-U_m x^{-2\rho} \cdot \frac{2\rho-1}{\Gamma(2-2\rho)} + x^{-\rho} \cdot \frac{\rho-1}{\Gamma(2-\rho)} - x^{-4\rho} \cdot A_m(\nu) \cdot \frac{\beta^2}{2} \cdot \frac{4\rho-1}{\Gamma(2-4\rho)} \right]. \quad (5.7)$$

The energy levels with the radial excitations in the lowest approximations of the oscillator representations are determined as

$$\varepsilon_1^{[n_r]} = \varepsilon_0 + 2n_r\omega + (n_r | H_I | n_r), \quad (5.8)$$

where

$$(n_r | H_I | n_r) = 4\rho^2 \int_0^\infty dx \int \frac{d^d\eta}{\pi^{d/2}} \cdot e^{-\eta^2(1+\frac{x}{2})} (n_r | : e_2^{-2iQ\eta\sqrt{x}} : | n_r) \cdot \left[-U_m x^{-2\rho} \cdot \frac{2\rho-1}{\Gamma(2-2\rho)} + x^{-\rho} \cdot \frac{\rho-1}{\Gamma(2-\rho)} - x^{-4\rho} \cdot A_m(\nu) \cdot \frac{\beta^2}{2} \cdot \frac{4\rho-1}{\Gamma(2-4\rho)} \right]. \quad (5.9)$$

The matrix element $(n_r | : e_2^{-2iQ\eta\sqrt{x}} : | n_r)$ is defined by (4.14). In this section, we have obtained the numerical results only for the ground and low excited state, i.e. for (2s) with $m = 0$.

Table 2. Binding energy (in a.u.) of the hydrogen atom 2s ($m = 0$) state in a uniform magnetic field.

β	ν	$Z = \omega^\rho$	ρ	$U^{(0)}$	$E_0^{(0)}$	Rosner[29]
0.0	0.0	1.0	1.0	0.125	0.1250	.125
0.05	0.03	1.0	0.935	0.098	0.148	0.148089
0.5	0.316	1.0914	0.800	-0.3395	0.1605	0.160469
1.0	0.312	1.4231	0.798	-0.8263	0.1737	0.173944
1.5	0.313	1.689	0.796	-1.3170	0.1830	0.18259
2.5	0.313	2.116	0.7965	-2.3025	0.1975	
12.5	0.315	4.4962	0.7994	-12.2721	0.2279	
50.0	0.314	8.8149	0.801	-49.7457	0.2543	0.25619
100.0	0.3164	12.4155	0.802	-99.7294	0.2706	0.26897
1000.0	0.31656	38.9171	0.803	-999.70	0.300	0.30624

According to (2.15) for the energy parameter we obtain

$$U_0(\beta) = \max_{\{\rho, \nu\}} \left[Z \cdot \frac{B_1}{B_0} - Z^2 \cdot \frac{B_2}{B_0} - \frac{\beta^2}{Z^2} \cdot \frac{A_0(\nu)}{2} \cdot \frac{B_3}{B_0} \right] \quad (5.10)$$

where Z is defined by the equation

$$Z^4 - Z^3 \frac{D_1}{D_0} - \beta^2 A_0(\nu) \cdot \frac{D_2}{D_0} = 0$$

and we introduced the notations

$$D_0 = [2\rho - 1 + \rho^2(3 + 2\nu)] \Gamma(2\rho\nu + \rho + 1), \quad D_1 = 8\rho^4 \Gamma(2\rho\nu + 2\rho) \frac{2 - \rho + \nu}{1 + \rho + 2\rho\nu},$$

$$D_2 = 8\rho^4 \Gamma(2\rho\nu + 5\rho) \frac{3.5 - 4\rho + \nu}{1 + \rho + 2\rho\nu}, \quad B_0 = \Gamma(2\rho\nu + 3\rho) \left(1 + \frac{(2\rho - 2)(2\rho - 1)}{1 + \rho + 2\rho\nu} \rho \right),$$

$$B_1 = \Gamma(2\rho\nu + 2\rho) \left(1 + \frac{(\rho - 2)(\rho - 1)}{1 + \rho + 2\rho\nu} \rho \right), \quad B_2 = \frac{1}{2}(5 + \rho + 2\rho\nu) \Gamma(2\rho\nu + \rho + 5),$$

$$B_3 = \Gamma(2\rho\nu + 5\rho) \cdot \left(1 + \frac{(4\rho - 2)(4\rho - 1)}{1 + \rho + 2\rho\nu} \rho \right).$$

Equation (5.10) defines the energy parameter U_0 as a function of the strength parameters β .

The wave functions are defined by (3.5) and the parity with respect to the x-y plane is defined by the function $P_\nu^m(\cos(\theta))$ (see details in ref.[30]) The numerical results are shown in Table 2. In the paper [30] the energy spectrum for the states (1s) and (2p) of the hydrogen atom in a uniform magnetic field in the framework of ORM is calculated, too.

5.2 The hydrogen atom in a generalized van der Waals potential

Let us consider the hydrogen atom in a generalized van der Waals potential. In the this case from (4.16) the Hamiltonian can be rewritten in the form

$$H = \frac{1}{2} \tilde{P}^2 - \frac{1}{r} + \frac{\gamma}{2} r^2 \cdot [1 + (\beta^2 - 1) \cos \theta] \quad (5.11)$$

The term proportional to γ is considered as a perturbation correction, so that $\gamma \ll 1$. In this limit the transformation (2.2) can be rewritten as

$$r = Q^2, \quad \text{and} \quad \psi = Q^{2\nu} \Phi_{m\nu}(Q^2). \quad (5.12)$$

According to (3.14) after some transformations, the modified Schrödinger equation takes the form

$$\left[\frac{1}{2} P_Q^2 - 4 - 4EQ^2 + 2\gamma \cdot (\beta^2 + (1 - \beta^2) \cdot A_m(\nu)) Q^6 \right] \Phi_{m\nu}(Q^2) = 0, \quad (5.13)$$

where $A_m(\nu)$ is defined by (5.4). After some analogous calculations represented in (4.17-4.21) we get

$$H = H_0 + \varepsilon_0 + H_I,$$

where

$$\varepsilon_0(E) = \frac{d\omega}{4} - \frac{2dE}{\omega} - 4 + \frac{g}{\omega^3} \cdot \frac{d(d+2)(d+4)}{2},$$

$$H_I = \frac{6g(d+4)}{\omega} \cdot Q^4 + 4g \cdot Q^6, \quad (5.14)$$

$$d = 4 + 4\nu.$$

In the lowest approximation from the condition of the oscillator representation (2.11) we determine

$$\omega = \nu + \frac{3g(d+2)(d+4)}{\nu^3} + O(\gamma^2), \quad (5.15)$$

where we introduced the notation

$$\nu = \sqrt{-8E}, \quad g = \gamma \cdot (\beta^2 + (1 - \beta^2) \cdot A_m(\nu)).$$

The energy spectrum with orbital and radial excitation in the lowest approximation of OR is defined as

$$\varepsilon_1^{[n_r]} = \varepsilon_0(E) + 2n_r \omega + \langle n_r | H_I | n_r \rangle. \quad (5.16)$$

The calculation details of the matrix elements $\langle n_r | H_I | n_r \rangle$ are given in Appendix.

From (5.11) we see that if $\gamma(\beta - 1) = 0$, then the Hamiltonian is spherical symmetric and the parameter ν takes only integer values. If we take in to account only the terms proportional to γ in energy level corrections, then in the this approximation the parameter ν takes integer values. In this case, the expression (5.4) is calculated analytically. Taking into account (5.13-5.15) and (A.5) from (5.16) we have for the energy spectrum

$$E_{n\ell} = -\frac{1}{2n^2} + \frac{\gamma n^2}{2} [5n^2 - 3\ell(\ell+1) + 1] \quad (5.17)$$

$$\left[\beta^2 + (1 - \beta^2) \cdot \frac{1}{2\ell+1} \left(\frac{(\ell-m)(\ell-m-1)}{2\ell-1} + \frac{(\ell+m+1)(\ell+m+2)}{2\ell+3} \right) \right] + O(\gamma^2),$$

where $n = 1 + \ell + n_r$ is the principal quantum number. From (5.17) we see that the normalized energy shifts

$$\Delta E_{n\ell} = \frac{1}{n^4 \gamma} \left(E + \frac{1}{2n^2} \right)$$

are defined as a function of β . In the limit of large n and small m the boundary curves are given approximately by:

$$\text{a) } m = 0, \quad \ell = 0; \quad \Delta E \sim \frac{5}{6} \beta^2,$$

$$\text{b) } m = 0, \quad \ell \sim n; \quad \Delta E = \frac{1}{2} (1 + \beta^2).$$

The dipole transitions. Let us consider the dipole transitions from the ground state (1s) to excited states. Within the oscillator representation methods, the wave functions are defined in the d-dimensional auxiliary space. According to (2.2), $\Psi_{n\ell}$ are wave functions in the 3-dimensional space and Φ_{n_r} is those in the d-dimensional space. To establish relations between these functions, we consider the following equality in the 3-dimensional space

$$1 = C_{n\ell}^2 \int_0^\infty dr r^2 \Psi_{n\ell}(r) \Psi_{n\ell}(r), \quad (5.18)$$

where $C_{n\ell}$ is the normalization constant. According to (2.2), after changing variables from (5.18) we have

$$\begin{aligned} 1 &= 2C_{n\ell}^2 \int_0^\infty dQ Q^5 \Psi_{n\ell}(Q^2) \Psi_{n\ell}(Q^2) \\ &= 2C_{n\ell}^2 \int_0^\infty dQ Q^{3+4\ell} \Phi_{n_r}(Q^2) Q^2 \Phi_{n_r}(Q^2) = 2C_{n\ell}^2 \langle n_r | Q^2 | n_r \rangle. \end{aligned} \quad (5.19)$$

Taking into account (A.1), (A.4) and (5.19) for the wave function in the 3-dimensional space we get

$$\Psi_{n\ell}(r) \rightarrow \Psi_{n\ell}(Q^2) = \sqrt{\frac{\Omega}{4n}} \Phi_{n_r}(Q^2), \quad (5.20)$$

where $\Phi_{n_r} = |n_r\rangle$ and are defined by (2.13). One of the basic mathematical tasks of nonrelativistic quantum mechanics is to find the average of variables r^α . Taking into account (5.18) and (5.20) we have

$$\bar{r}^\alpha = \int_0^\infty dr r^2 (\Psi_{n\ell}(r) r^\alpha \Psi_{n\ell}(r)) = \frac{\Omega}{2n} \langle n_r | Q^{2+2\alpha} | n_r \rangle. \quad (5.21)$$

For the hydrogen atom, taking into account (A.1) and $\Omega = Z/n$, $d = 4 + 4\ell$ at $\alpha = \pm 1$ from (5.21) we get

$$\bar{r} = \frac{1}{2Z} (3n^2 - \ell(\ell+1)), \quad \text{and} \quad \bar{r}^{-1} = \frac{Z}{n^2}. \quad (5.22)$$

The matrix elements [31] of the dipole transitions from the ground state ($1s$) to the excited state ($n\ell$) can be written as

$$M_{1s}^{n\ell} = \int_0^\infty dr r^2 \Psi_{1s}(r) r \Psi_{n\ell}(r). \quad (5.23)$$

Taking into account (5.18-5.20) and after some transformation from (5.23) we have

$$\begin{aligned} M_{1s}^{n\ell} &= 2 \int_0^\infty dQ Q^7 \Psi_{1s}(Q^2) \Psi_{n\ell}(Q^2) \\ &= \frac{C_{n_r}}{2} \sqrt{\frac{\Omega_s \Omega_d}{n}} \cdot \frac{\sqrt{\Gamma(2+2\ell)}}{\Omega_d^{1+\ell}} \cdot \langle 0 | Q^{4-2\ell} e^{-bQ^2} (a_j^\dagger a_j^\dagger)^{n_r} | 0 \rangle, \end{aligned} \quad (5.24)$$

where C_{n_r} is the normalization constant determined by (2.13); Ω_s and Ω_d are oscillator frequencies in the 4- and d-dimensional space, respectively; $|0\rangle$ is the ground or vacuum state in the d-dimensional space, and we introduced the notation

$$b = \frac{\Omega_s - \Omega_d}{2}.$$

Let us separately calculate the matrix elements

$$T_{1n_r} = \langle 0 | Q^{4-2\ell} e^{-bQ^2} (a_j^\dagger a_j^\dagger)^{n_r} | 0 \rangle,$$

if $\ell = 2$, taking into account (A.2) we have

$$T_{2n_r} = \langle 0 | e^{-bQ^2} (a_j^\dagger a_j^\dagger)^{n_r} | 0 \rangle = \left(\frac{2}{\Omega_d} \right)^{n_r} \frac{b^{n_r}}{(1+b/\Omega_d)^{d/2+n_r}} \cdot \frac{\Gamma(d/2+n_r)}{\Gamma(d/2)} \quad (5.25)$$

and if $\ell = 1$, we get

$$T_{1n_r} = \langle 0 | Q^2 e^{-bQ^2} (a_j^\dagger a_j^\dagger)^{n_r} | 0 \rangle = \left(-\frac{d}{db} \right) T_{2n_r}. \quad (5.26)$$

In the case of $\ell > 2$ the matrix element can be rewritten in the form

$$\begin{aligned} T_{\ell n_r} &= \langle 0 | Q^{4-2\ell} e^{-bQ^2} (a_j^\dagger a_j^\dagger)^{n_r} | 0 \rangle = (-2)^{n_r} \frac{\Omega_d^{d/2}}{\Gamma(d/2)} \\ &\sum_{j=0}^{n_r} \frac{n_r!}{j!(n_r-j)!} \cdot \frac{\Gamma(2\ell+j-4)}{\Gamma(2\ell-4)} \cdot \frac{b^{n_r-j} \Gamma(6+n_r-j)}{(b+\Omega_d)^{6+n_r-j}}. \end{aligned} \quad (5.27)$$

Substituting (5.25), (5.26) and (5.27) into (5.24) and after some simplifications, we get for the dipole transitions at $\ell = 1, 2$, and $\ell > 2$

$$\begin{aligned} M_{1s}^{n2} &= (-1)^{n-1} 16 \Omega_s \Omega_d^2 \sqrt{\frac{\Omega_s \Omega_d}{n}} \sqrt{\frac{(n+1)! (\Omega_s - \Omega_d)^{n-2}}{(n-2)! (\Omega_s + \Omega_d)^{n+2}}} \left[\frac{n+2}{\Omega_s + \Omega_d} - \frac{n-2}{\Omega_s - \Omega_d} \right]; \\ M_{1s}^{n\ell} &= (-1)^{n-1} 32 \Omega_s \Omega_d^3 \sqrt{\frac{\Omega_s \Omega_d}{n}} \sqrt{\frac{(n+2)! (\Omega_s - \Omega_d)^{n-3}}{(n-3)! (\Omega_s + \Omega_d)^{n+3}}}; \\ M_{1s}^{n\ell} &= (-1)^{n-\ell-1} 32 \Omega_s \Omega_d^{1+\ell} \sqrt{\frac{\Omega_s \Omega_d}{n}} \sqrt{\frac{(n-\ell-1)!}{(n+1)!}} \sum_{j=0}^{n-\ell-1} \frac{\Gamma(5+n-\ell-j)}{\Gamma(j+1)\Gamma(n-\ell-j)} \\ &\quad \cdot \frac{\Gamma(2\ell+j-4)}{\Gamma(2\ell-4)} \cdot \frac{(\Omega_s - \Omega_d)^{n-\ell-j-1}}{(\Omega_s + \Omega_d)^{n+5-\ell-j}}. \end{aligned} \quad (5.28)$$

The square of these matrix elements defines [31] the oscillator strengths for transitions from the ground state ($1s$) to the manifold ($n\ell$). In our approximation the oscillator frequency Ω is defined as a function of the potential parameters. So that every potential corresponds to any oscillator frequency. In the case of generalized van der Waals potentials for the oscillator frequency from (5.15) and (5.17) we have

$$\Omega_{n\ell} = \frac{2}{n} \cdot \left[1 - \gamma n^6 \Delta E \left(1 - \frac{3(3+2\ell)(2+\ell)}{5n^2 - 3\ell(\ell+1) + 1} \right) \right] + O(\gamma^2). \quad (5.29)$$

According to (5.17) ΔE is defined as

$$\begin{aligned} \Delta E &= \frac{1}{2n^2} [5n^2 - 3\ell(\ell+1) + 1] \\ &\cdot \left[\beta^2 + (1-\beta^2) \cdot \frac{1}{2\ell+1} \left(\frac{(\ell-m)(\ell-m-1)}{2\ell-1} + \frac{(\ell+m+1)(\ell+m+2)}{2\ell+3} \right) \right]. \end{aligned} \quad (5.30)$$

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Appendix

Let us give some calculation details of the matrices $\langle n_r | H_I | n_r \rangle$. First of all, the variables $Q^{2\tau}$, where τ is arbitrary, represented in the normal form. Let $\tau = 1, 2, 3, \dots$, then taking in to account (2.7) and (2.8), we have

$$\begin{aligned} Q^2 &= \frac{d}{2\Omega} + : Q^2 : , & (A.1) \\ Q^4 &= \frac{d(d+2)}{4\Omega^2} + \frac{d+2}{\Omega} : Q^2 : + Q^4 , \\ Q^6 &= \frac{d(d+2)(d+4)}{8\Omega^3} + \frac{3(d+2)(d+4)}{4\Omega^2} : Q^2 : + \frac{3(d+4)}{2\Omega} : Q^4 : + : Q^6 : . \end{aligned}$$

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

$$\frac{1}{Q^{2\tau}} = \int_0^\infty \frac{d\alpha}{\Gamma(\tau)} \alpha^{\tau-1} e^{-Q^2\alpha} = \int_0^\infty \frac{d\alpha}{\Gamma(\tau)} \alpha^{\tau-1} \cdot \int \left(\frac{d\eta}{\sqrt{\pi}} \right)^d \cdot \frac{e^{-\eta^2(\frac{1}{\alpha} + \frac{1}{\hbar})}}{\alpha^{d/2}} : e^{-2iQ\eta} : \quad (A.2)$$

Now consider

$$\langle n_r | Q^{-2\tau} | n_r \rangle = \int_0^\infty \frac{d\alpha}{\Gamma(\tau)} \alpha^{\tau-1} \cdot \int \left(\frac{d\eta}{\sqrt{\pi}} \right)^d \cdot \frac{e^{-\eta^2(\frac{1}{\alpha} + \frac{1}{\hbar})}}{\alpha^{d/2}} \langle n_r | : e^{-2iQ\eta} : | n_r \rangle , \quad (A.3)$$

where $|n_r\rangle$ and the matrix $\langle n_r | : e^{-2iQ\eta} : | n_r \rangle$ are defined by (2.13) and (4.14), respectively. For the calculation of the matrix elements of the variables represented in (A.1) we used the following relations

$$\begin{aligned} \langle n_r | : Q^2 : | n_r \rangle &= \frac{2n_r}{\Omega} & (A.4) \\ \langle n_r | : Q^4 : | n_r \rangle &= \frac{n_r}{\Omega^2} [d + 6n_r - 4] , \\ \langle n_r | : Q^6 : | n_r \rangle &= \frac{2n_r(n_r - 1)}{\Omega^3} [3d + 10n_r - 8] . \end{aligned}$$

Taking into account (A.1) and (A.4) for the matrix $\langle n_r | H_I | n_r \rangle$ we have

$$\langle n_r | H_I | n_r \rangle = \frac{\gamma n_r}{\Omega^3} \cdot [3d^2 - 12d + 30n_r d + 40n_r^2 - 16] , \quad (A.5)$$

where H_I is defined by (4.18).

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Атом водорода во внешнем поле
в рамках метода осцилляторного представления

Энергетический спектр сферически-симметричного и аксиально-симметричного потенциалов, допускающих связанные состояния, вычислен методом осцилляторного представления в рамках нерелятивистского уравнения Шредингера. В частности, метод применен к вычислению энергетического спектра $2s$ -состояния атома водорода во внешнем постоянном магнитном поле с произвольной напряженностью. В приближении теории возмущений по внешнему полю вычислен энергетический спектр атома водорода в случае квадратичной и сферически-квадратичной задачи Зеемана и обобщенного потенциала ван дер Ваальса. Результаты нулевого приближения метода осцилляторного представления хорошо согласуются с точными значениями.

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Oscillator Representation Method
in the Theory of a Hydrogen Atom in an External Field

The Wick-ordering method called the Oscillator Representation in the non-relativistic Schrödinger equation is proposed to calculate the energy spectrum for spherically symmetric and axially symmetric potentials allowing the existence of a bound state. In particular, the method is applied to calculate the energy spectrum of $(2s)$ -states of a hydrogen atom in a uniform magnetic field of an arbitrary strength. In the perturbation (external field) approximation, the energy spectrum of the so-called quadratic and spherical quadratic Zeeman problem and the problem of a hydrogen atom in a generalized van der Waals potential is calculated analytically. The results of the zeroth approximation of oscillator representation are in good agreement with the exact values.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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