Quantum Problem of Charged Particle Interacting with Conducting Sphere [1]

G.V.Zhuvikin, Yu.A.Nesvetaev

Physics Department, Saint Petersburg State University, Ulianovskaya 3, Saint Petersburg, 198504, Russia
Email: zhuvikin@niif.spb.su [2]

The quantum problem of the motion of the charged particle outside of the charged ideally conducting sphere is considered from the viewpoint of the dynamical symmetry of perturbed Coulomb potential. This problem is interesting for various applications. Some of them are mentioned in [1], where the case of the grounded conducting sphere has been considered. The other application is associated with droplet approximation in the physics of metal clusters [2]. This simple model satisfactory explaines the dependence of the ionization energy on the cluster size and is in good agreement with more complicated jellium models [2, 3]. In the present paper we use the model of charged conducting sphere to describe the spectrum of the cluster excited states below the energy of ionization.

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[2]Present e-mail: g.zhuvikin@spbu.ru

The interaction potential of the conducting sphere and the charged particle is determined by the electrostatic image method. The energy spectrum of the formulated problem can be derived from the analysis of the Schrödinger equation

$$[\mathbf{p}^2/2 - \frac{1}{r} - \frac{uR^3}{2r^2(r^2-R^2)} - E]\psi = 0, \qquad (1)$$

where $\mathbf{p}$ is the momentum of the particle, $u = q/Q$, Q and $-q$ are charges of the sphere and of the particle respectively, R is radius of the sphere, r is the separation of the particle and the center of the sphere. In this equation Bohr's units $r_0 = \hbar^2/mqQ$, $p_0 = mqQ/\hbar$, $E_0 = mq^2Q^2/\hbar^2$ are used.

Eq. (1) can be treated as the Schrödinger equation for perturbed hydrogen-like Coulomb system. It can be reduced to the form:

$$[(r^2 - R^2)(rp^2/2 - Er - 1) - \frac{uR^3}{2r}]\psi = 0 \qquad (2)$$

To make further progress we suggest to exploit the completely solved Coulomb quantum problem with d-papametrized centrifugal perturbation $U(r) = -1/r + d/r^2$, Lie algebra $SO(2,1)$ of which is given by generators [4]:

$$\begin{array}{l} N_3 = 1/2(rp^2 + r) + d/r, N_2 = \mathbf{rp} - i, \\ N_1 = 1/2(rp^2 - r) + d/r \end{array} \qquad (3)$$

The ladder operators of this algebra $N_+ = N_1 + iN_2$, $N_- = N_1 - iN_2$ are subjected to the commutation relations $[N_3, N_+] = N_+$, $[N_3, N_-] = -N_-$, $[N_+, N_-] = -2N_3$ and the invariant operator is $C_2 = N_3(N_3+1) - N_-N_+$.

The discrete representation of the algebra $SO(2,1)$ can be given by the set of joint eigenvectors of operators N_3 and C_2

$$\begin{aligned} C_2|\varphi, s\rangle &= \varphi(\varphi+1)|\varphi, s\rangle = [l(l+1)+2d]|\varphi, s\rangle, \\ N_3|\varphi, s\rangle &= (-\varphi+s)|\varphi, s\rangle \end{aligned} \tag{4}$$

Quantum number φ is coupled with the centrifugal parameter d and quantum number l of the angular momentum ($\varphi = -1/2 - \sqrt{(l+1/2)^2 + 2d}$) and number s is integer ($s = 0, 1, 2, ..., \infty$). In this, completely solvable case, the energy of the bound state is $E_{\varphi,s} = -1/2n^{*2}$, where $n^* = -\varphi + s$ is effective quantum number.

Making use of matrix elements of ladder operators given by

$$\begin{aligned} N_+|\varphi, s\rangle &= \sqrt{(-2\varphi+s)(s+1)}|\varphi, s+1\rangle, \\ N_-|\varphi, s\rangle &= \sqrt{(-2\varphi+s-1)s}|\varphi, s-1\rangle \end{aligned} \tag{5}$$

and imposing $d = uR/2$, eq.(2) can be presented in the form:

$$[(r^2-R^2)((N_3+N_1)/2-Er-1)-uRr/2]\psi = 0, r = N_3-N_1 \tag{6}$$

Thus, in the basis of vectors $|\varphi, s\rangle$ the original eq.(1) is reduced to 7-diagonal form given by eq.(6). By means of the tilt-trasformation [4] with parameter γ, defined by the equality $2+E\gamma^2=0$, this equation can be additionally reduced to 5-diagonal form. In the large distance approximation $r >> R$ it takes 3-diagonal form:

$$[N_-(u\gamma - N_3) + 2N_3^2 - 2u\gamma N_3 - R + N_+(u\gamma - N_3)]\tilde{\psi} = 0, \tag{7}$$

Highly excited Rydberg states correspond to the case of $n^* >> -\varphi$ and are characterized only by the diagonal term in eq.(7). In this approximation

$$E_{\varphi,s} = -1/2(n^* - uR/2n^*)^2. \tag{8}$$

The considered problem is not completely solvable, but with suggested substitution of centrifugal representation of the Lie algebra $SO(1,2)$ it was possible to transform the Schrödinger equation to 7- and 5-diagonal forms.

References

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