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SPHEROIDAL CORRECTIONS TO THE SPHERICAL AND PARABOLIC BASIS OF A HYDROGEN ATOM

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INTRODUCTION

The behaviour of a hydrogen atom in an external homogeneous electric field or in a field of an extra Coulomb center may be well described by a parabolic and a spheroidal basis rather than by a spherical basis [1]. Transformations between these bases were calculated by many authors directly, by using the explicit form of bases [2-3], and indirectly, with the use of extra integrals of motion [4-5]. To our knowledge, the latter method was never used for the expansion of the spheroidal basis over the parabolic one.

In this paper we shall make this expansion. In Sec. 1 we introduce the hydrogen-atomic bases, in Sec. 2 we obtain trinomial recurrence relations for the expansion of the spheroidal basis over the parabolic one, and in Sec. 3 we calculate spheroidal corrections to the spherical and parabolic basis.

1. BASES

By definition the spherical $\psi^{s}_{n\ell m}$ parabolic $\psi^{pr}_{n_1 n_2 m}$ and spheroidal ψ^{sp}_{nqm} bases in the discrete spectrum obey the following equations [1,6]:

a) the spherical basis

$$\hat{H}\psi^{s}_{n\ell m} = E_n \psi^{s}_{n\ell m}, \quad \hat{L}^2 \psi^{s}_{n\ell m} = \ell(\ell+1)\psi^{s}_{n\ell m}.$$

b) the parabolic basis

$$\hat{H}\psi^{pr}_{n_1 n_2 m} = E_n \psi^{pr}_{n_1 n_2 m}, \quad \hat{A}_z \psi^{pr}_{n_1 n_2 m} = (n_1 - n_2)\psi^{pr}_{n_1 n_2 m}.$$

c) the spheroidal basis

$$\hat{H}\psi^{sp}_{nqm} = E_n \psi^{sp}_{nqm}, \quad \hat{\Lambda}\psi^{sp}_{nqm} = \lambda_q \psi^{sp}_{nqm},$$

In the atomic units $(e = h = m = 1)$

$$E_n = -1/2n^2, \quad \hat{H} = \frac{1}{2}p^2 - \frac{1}{r}, \quad \hat{\Lambda} = -\hat{L}^2 - \frac{R}{n}\hat{A}_z, \quad \hat{\vec{A}} = n\{\frac{1}{2}\hat{\vec{L}}\times\vec{p} - \frac{1}{2}\vec{p}\times\hat{\vec{L}} - \frac{\vec{r}}{r}\}.$$

Here $\mathbf{R}$ is the parameter defining the spheroidal coordinates [1].

2. EXPANSION OF THE SPHEROIDAL BASIS OVER THE PARABOLIC ONE

Let us write the expansion we are interested in:

$$\psi^{sp}_{nqm} = \sum_{n_2=0}^{n-|m|-1} U^{n_2}_{nqm}\,\psi^{pr}_{n_1 n_2 m}.$$

Using the explicit form of operator $\hat\Lambda$ and definition of bases ψ^{sp}_{nqm} and $\psi^{pr}_{n_1 n_2 m}$ we have

$$\left[\frac{R}{n}(n-|m|-2n_2-1)+\lambda_q\right]U^{n_2}_{nqm} = -\sum_{n_2'=0}^{n-|m|-1} U^{n_2'}_{nqm}(\hat L^2)_{n_1 n_2'},$$

where

$$(\hat L^2)_{n_2 n_2'} = \int \psi^{*pr}_{n_1 n_2 m}\,\hat L^2\,\psi^{pr}_{n_1' n_2' m}\,dv.$$

If we expand, following /7/, the parabolic basis over the spherical one

$$\psi^{pr}_{n_1 n_2 m} = (-1)^{n_2+\frac{m+|m|}{2}} \sum_{\ell=|m|}^{n-1} (-1)^{\ell}\, C^{\ell,|m|}_{\frac{n-1}{2},\frac{n-1}{2}-n_2,\frac{n-1}{2},|m|+n_2-\frac{n-1}{2}}\,\psi^{s}_{n\ell m}$$

take account of trinomial recurrence relations for the Clebsch-Gordan coefficients /8/:

$$[(b-a+c)(a-b+c+1)]^{1/2}\,C^{c,\gamma}_{a,\alpha;b;\beta} = [(a-\alpha+1)(b-\beta)]^{1/2}\times$$

$$\times\, C^{c,\gamma}_{a+\frac{1}{2},\alpha-\frac{1}{2};b-\frac{1}{2},\beta+\frac{1}{2}} + [(a+\alpha+1)(b+\beta)]^{1/2}\,C^{c,\gamma}_{a+\frac{1}{2},\alpha+\frac{1}{2};b-\frac{1}{2},\beta-\frac{1}{2}}$$

and the orthogonality relation

$$\sum_{c=|\gamma|}^{|a+b|} C^{c,\gamma}_{a,\alpha;b,\beta}\,C^{c,\gamma}_{a,\alpha',b,\beta'} = \delta_{\alpha\alpha'}\,\delta_{\beta\beta'}$$

we obtain for the matrix elements of operator $\hat L^2$ over the parabolic basis the following formula

$$(\hat L^2)_{n_2 n_2'} = [(n_2+1)(n-|m|-n_2-1)+(n-n_2)(n_2+|m|)\delta_{n_2' n_2} -$$

$$-[(n_2+1)(n-|m|-n_2-1)(n-n_2-1)(n_2+|m|+1)]^{1/2}\delta_{n_2',n_2+1} -$$

$$-[n_2(n-|m|-n_2)(n-n_2)(n_2+|m|)]^{1/2}\,\delta_{n_2',n_2-1}$$

and we may significantly simplify the above formula for coefficients $U^{n_2}_{nqm}$:

$$[\lambda_q+(n_2+1)(n-|m|-n_2-1)+(n-n_2)(n_2+|m|)+\frac{R}{n}(n-|m|-2n-1)]U^{n_2}_{nqm} =$$

$$= [(n_2+1)(n-|m|-n_2-1)(n-n_2-1)(n_2+|m|+1)]^{1/2}\,U^{n_2+1}_{nqm} +$$

$$+ [n_2(n-|m|-n_2)(n-n_2)(n_2+|m|)]^{1/2}\,U^{n_2-1}_{nqm}.$$

These trinomial recurrence relations for small n allow us to calculate eigenvalues of λ_q and coefficients $U^{n_2}_{nqm}$ analytically. An unambiguous choice of the coefficients requires also the normalization condition

$$\sum_{n_2=0}^{n-|m|-1} |U^{n_2}_{nqm}|^2 = 1.$$

In the general case the obtained recurrence relations can be disentangled only at the computer.

3. PERTURBATION THEORY

When R is small, the second term in operator $\hat\Lambda$ is a perturbation, and the spherical basis is a zero-order approximation. The equation for eigenvalues of operator $\hat\Lambda$ for large R upon dividing it by R/n is as follows:

$$(-A_z - \frac{n}{R}\hat L^2)\psi^{sp}_{nqm} = \frac{n}{R}\lambda_q\psi^{sp}_{nqm}.$$

As is seen, the pertirbation now is the term $n\hat L^2/R$. Then the corrections to λ_q and ψ^{sp}_{nqm} at small and large R can be calculated in a standard manner. It is only necessary, together with $(\hat L^2)_{n_2 n_2'}$, to know the explicit form of the matrix element of operator $\hat A_z$ over the spherical basis /9/:

$$(\hat A_z)_{\ell'\ell} = \int \psi^{*s}_{n\ell' m}\,\hat A_z\,\psi^{s}_{n\ell m}\,dv =$$

$$= -\left\{\frac{(\ell+|m|+1)(\ell-|m|+1)(n-\ell-1)(n+\ell-1)}{(2\ell+1)(2\ell+3)}\right\}^{1/2}\delta_{\ell',\ell+1} -$$

$$- \left\{\frac{(\ell+|m|)(\ell-|m|)(n-\ell)(n+\ell)}{(2\ell+1)(2\ell-1)}\right\}^{1/2}\delta_{\ell',\ell-1}.$$

We shall present the final result:

a) for small R:

$$\lambda_q(R) = -q(q+1) - \frac{R^2}{2n^2(2q+1)} \left\{ \frac{(q+|m|+1)(q-|m|+1)(n-q-1)(n+q+1)}{(q+1)(2q+3)} + \frac{(q+|m|)(q-|m|)(n-q)(n+q)}{q(2q-1)} \right\}$$

$$\psi^{sp}_{nqm} = \psi^{s}_{nqm} + \frac{R}{2n(q+1)} \left\{ \frac{(q+|m|+1)(q-|m|+1)(n-q-1)(n+q+1)}{(2q+1)(2q+3)} \right\}^{1/2} \psi^{s}_{n,q+1,m} + \frac{R}{2nq} \left\{ \frac{(q+|m|)(q-|m|)(n-q)(n+q)}{(2q-1)(2q+1)} \right\}^{1/2} \psi^{s}_{n,q-1,m} ,$$

b) for large R:

$$\lambda_q(R) = -\frac{R}{n}(n-|m|-2q-1) - (q+1)(n-|m|-q-1) - (n-q)(q+|m|)$$

$$\psi^{sp}_{nqm} = \psi^{pr}_{nqm} - \frac{2n}{R} \left[(q+1)(n-|m|-q-1)(n-q-1)(q+|m|+1) \right]^{1/2} \psi^{pr}_{n,q+1,m} + \frac{2n}{R} \left[q(n-q)(q+|m|)(n-|m|-q) \right]^{1/2} \psi^{pr}_{n,q-1,m} .$$

Higher-order corrections are calculated analogously.

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Сфероидальные поправки к сферическому и параболическому базисам атома водорода

Найдены рекуррентные соотношения, определяющие разложение сфероидального базиса атома водорода по его параболическому базису. Вычислены главные сфероидальные поправки к сферическому и параболическому базису методом теории возмущений.

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Spheroidal Corrections to the Spherical and Parabolic Basis of a Hydrogen Atom

Recurrence relations are found for the expansion of the spheroidal basis of a hydrogen atom over its parabolic basis. Spheroidal corrections to the spherical and parabolic basis are calculated by a perturbative method.

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

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