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Integrable system connected with the Coulomb three-body problem near two-particle thresholds

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Abstract. The problem of mixing of degenerated sublevels of a hydrogen-like system by a charged particle is reconsidered from the point of view of the theory of integrable systems on Lie algebras. The Lax representation is constructed both in classical and quantum mechanics. The corresponding dynamical system is a special limit case of a four-sites *XXX* magnet considered by Gaudin.

1. Introduction

We consider a quantum mechanical system of three particles with charges Z_a, Z_b, -1 and masses m_a, m_b, m_c interacting via pair Coulomb potentials. Suppose that the particles b and c are bound and that particle a is at a large distance from the pair. The Hamiltonian of the pair bc has a degenerated spectrum and this degeneracy is removed by the interaction of the pair with the charged particle a. In Jacobi coordinates $\boldsymbol{r} = \boldsymbol{r}_{ab}$, $\tilde{\boldsymbol{R}} = \boldsymbol{r}_{a,bc}$. When $\tilde{R} \to \infty$ one has the asymptotical Hamiltonian

$$H_{as} = \frac{p_R^2}{2\mu} + \frac{Z_a(Z_b-1)}{\tilde{R}} + h_{bc} + \frac{1}{2\mu\tilde{R}^2}\left(\boldsymbol{L}^2 + \frac{2\mu Z_a}{M_b}(M_b + Z_b - 1)\boldsymbol{rR}\right) + O(\tilde{R}^{-3}) \tag{1}$$

where $\mu = m_{a,bc}/m_{bc}$ and $\boldsymbol{R} = \tilde{\boldsymbol{R}}/\tilde{R}$. The operator multiplier of $\tilde{R}^{-2}$ connects the motions of $\boldsymbol{r}$ and $\boldsymbol{R}$. If we neglect the mixing of eigenstates of h_{bc} with different principal quantum numbers, the problem is drastically simplified. The physical idea can be formalised by the observation that the multiplier of $\tilde{R}^{-2}$ in (1) is a linear function of $\boldsymbol{r}$ and for a given shell with a fixed n there is an equivalence ($\hbar = 1$)

$$P_n \boldsymbol{r} P_n = -\tfrac{3}{2}\frac{n}{Z_b}\boldsymbol{a}. \tag{2}$$

Here P_n is a projector onto the subspace n and $\boldsymbol{a}$ is a normalised Runge-Lentz vector. The components of $\boldsymbol{a}$ and the angular momentum $\boldsymbol{l}$ of pair bc form an o(4) Lie algebra. Thus we arrive at the model Hamiltonian

$$H = \frac{p_R^2}{2\mu} + \frac{Z_a(Z_b-1)}{\tilde{R}} + h_{bc} + \frac{1}{2\mu\tilde{R}^2}\Lambda \tag{3}$$

$$\Lambda = \boldsymbol{L}^2 - \alpha\boldsymbol{aR} \qquad \alpha = \frac{3\mu Z_a n}{M_b Z_b}(M_b + Z_b - 1). \tag{4}$$

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The angular variables $\boldsymbol{R}$ obviously commute with $\tilde{R}$ and p_R, so the problem now is to find the spectrum Λ. This problem has a considerable literature (Nikitin and Ostrovsky 1981, Herrick 1983). In this paper the problem is reconsidered from the point of view of the theory of integrable systems on Lie algebras and the Lax representation for it is constructed.

2. The Lie algebra o(4)⊕e(3) and the spectrum

As mentioned before, $\boldsymbol{a}$ and $\boldsymbol{l}$ are the generators of the Lie algebra o(4) and also $\boldsymbol{R}$ and $\boldsymbol{L}$ form the Lie algebra e(3) of a Euclid Lie group, so we will study a dynamical system on the Lie algebra $g = \mathrm{o}(4)\oplus\mathrm{e}(3)$. Its Casimir operators are

$$\begin{aligned} &\boldsymbol{l}^2+\boldsymbol{a}^2=n^2-1 &\qquad \boldsymbol{RR}=1 \\ &\boldsymbol{al}=0 &\qquad \boldsymbol{RL}=0. \end{aligned} \tag{5}$$

The equality $\boldsymbol{RL}=0$ means that we restrict ourselves to spinless particles. If necessary this restriction can be removed.

Let us consider an auxiliary dynamical system on the Lie algebra g with Hamiltonian Λ and let us introduce a time derivative according to the rule

$$\frac{\mathrm{d}}{\mathrm{d}t}=\frac{1}{\mathrm{i}}[\Lambda,\quad]. \tag{6}$$

A direct computation gives the equations of motion

$$\begin{aligned} &\dot{\boldsymbol{l}}=\alpha\boldsymbol{R}\wedge\boldsymbol{a} &\qquad \dot{\boldsymbol{a}}=\alpha\boldsymbol{R}\wedge\boldsymbol{l} \\ &\dot{\boldsymbol{L}}=-\alpha\boldsymbol{R}\wedge\boldsymbol{a} &\qquad \dot{\boldsymbol{R}}=2\boldsymbol{R}\wedge\boldsymbol{L} \end{aligned} \tag{7}$$

where the symbol $\wedge$ denotes the vector product. The rank of the algebra g is four. The system with the Hamiltonian Λ is integrable (and even degenerated), because the operators

$$B=\boldsymbol{aL}+\tfrac{1}{2}\alpha\boldsymbol{lR} \qquad \boldsymbol{J}=\boldsymbol{L}+\boldsymbol{l} \tag{8}$$

commute with Λ and the components of the total angular momentum J_i form the Lie algebra su(2) (Nikitin and Ostrovsky 1978). To find the common spectra of Λ, B, $\boldsymbol{J}^2$ and J_z, a few procedures based on the numerical diagonalisation of Λ in representation of the total angular momentum were presented. Both spherical and parabolic bases of the hydrogen atom were used (Vinitsky *et al* 1986).

Let us consider limiting cases of the problem for different values of J and α. For $J=0$ we arrive at diagonalisation of the operators

$$\Lambda_0=\boldsymbol{l}^2-\alpha\boldsymbol{aR} \tag{9a}$$

$$B_0=\tfrac{1}{2}\alpha\boldsymbol{lR} \tag{9b}$$

on the Lie algebra o(4). The solution is provided by the Coulomb spheroidal polynomials that are obtained after separation of variables in the hydrogen-like Hamiltonian h_{bc} in prolate spheroidal coordinates (Komarov *et al* 1976). Their symmetry axis is directed from the centre of mass of b and c, to the particle a and the focal distance is

$$d=\frac{\alpha n}{Z_{\mathrm{b}}}=\frac{3\mu Z_{\mathrm{a}}n^2}{M_{\mathrm{b}}Z_{\mathrm{b}}^2}(M_{\mathrm{b}}+Z_{\mathrm{b}}-1). \tag{10}$$

When $J \to \infty$, $\alpha = O(1)$, J becomes a classical vector directed along $\hat{\boldsymbol{J}} = \boldsymbol{J}/J$ and the integrals of motion are

$$[\Lambda - J(J+1)]/2J \to X = \hat{\boldsymbol{J}}\boldsymbol{l} \tag{11a}$$

$$B/J \to Y = \hat{\boldsymbol{J}}\boldsymbol{a}. \tag{11b}$$

The integrals X and Y correspond to a parabolic basis of the hydrogen-like atom bc with symmetry axis directed along $\boldsymbol{J}$, i.e. perpendicular to direction $\boldsymbol{R}$ on particle a.

The special limiting case when $J \to \infty$ and $\alpha \to \infty$ was considered by Nikitin and Ostrovsky (1978). Let us rearrange the algebra g by decomposing $o(4) = o(3) \oplus o(3)$

$$\begin{aligned} &\boldsymbol{S} = \tfrac{1}{2}(\boldsymbol{l} + \boldsymbol{a}) \qquad \boldsymbol{T} = \tfrac{1}{2}(\boldsymbol{l} - \boldsymbol{a}) \\ &\boldsymbol{S}^2 = \boldsymbol{T}^2 = j(j+1) \qquad j = \tfrac{1}{2}(n-1) \end{aligned} \tag{12}$$

and introducing the quantities

$$\boldsymbol{I}^{(+)} = \boldsymbol{J} + \tfrac{1}{2}\alpha\boldsymbol{R} \qquad \boldsymbol{I}^{(-)} = \boldsymbol{J} - \tfrac{1}{2}\alpha\boldsymbol{R}. \tag{13}$$

The operator Λ becomes

$$\Lambda = \boldsymbol{J}^2 + \boldsymbol{l}^2 - 2(\boldsymbol{I}^{(+)}\boldsymbol{S} + \boldsymbol{I}^{(-)}\boldsymbol{T}). \tag{14}$$

In the limit $J \to \infty$, $\alpha \to \infty$, the vectors $\boldsymbol{I}^{(\pm)}$ can be considered as classical ones. Then the projection $\boldsymbol{S}$ onto the direction of $\boldsymbol{I}^{(+)}$ and the projection $\boldsymbol{T}$ onto the direction of $\boldsymbol{I}^{(-)}$ have values $n', n'' = -j, -j+1, \ldots, j-1, j$ and for the spectra of Λ and B one obtains

$$\Lambda = J(J+1) - 2\omega(n' + n'') \tag{15a}$$

$$B = \omega(n' - n'') \tag{15b}$$

where $\omega = [J(J+1) + \alpha^2/4]^{1/2}$. The solution can be interpreted in terms of the first-order perturbation theory for the hydrogen-like system bc in crossed electric and magnetic fields.

3. Lax representation in classical mechanics

The equations of motion (7) have a remarkable structure. On their right-hand sides there are products only of commuting pairs of generators of g and one of the multipliers of the vector products always coincides with R. This means that the equations are the same both in classical and in quantum mechanics. It also allows us to suppose the existence of a Lax representation. In other words, it is possible to construct matrices $\mathscr{L}(u, X)$ and $\mathscr{A}(u, X)$ depending on the set of generators $X = \{S_i, T_i, R_i, L_i\}$ of algebra g and an arbitrary complex parameter u in such a manner that the matrix equation

$$\dot{\mathscr{L}}(u, X) + [\mathscr{L}(u, X), \mathscr{A}(u, X)]_m = 0 \tag{16}$$

is equivalent to the system of equations (7). Here the symbol $[\ ,\ ]_m$ denotes a commutator of matrices $\mathscr{L}\mathscr{A} - \mathscr{A}\mathscr{L}$.

We will look for matrices $\mathscr{L}$ and $\mathscr{A}$ of the minimal dimension two. A universal classical integrable model with a two-dimensional auxiliary space is a magnetic model (Takhtajan and Faddeev 1987). Because of the conservation of an arbitrary component of the total angular momentum it is natural to use the XXX magnet having su(2) invariance. One can check that the Lax equation (16) with the matrices

$$\mathscr{L}(u)=\frac{1}{\mathrm{i}}\sigma_i\mathscr{L}_i(u) \qquad \mathscr{L}_i(u)=\frac{S_i}{u-\varkappa}+\frac{T_i}{u+\varkappa}+\frac{R_i}{u^2}+\frac{L_i}{u} \tag{17}$$

$$\mathscr{A}(u)=\frac{1}{\mathrm{i}}\boldsymbol{\sigma}\frac{\boldsymbol{R}}{u} \qquad \varkappa=2/\alpha \tag{18}$$

is equivalent to equations (7). The existence of the Lax representation allows us to use ideas and results of the spectral transform method (STM) (Takhtajan and Faddeev 1987). In classical mechanics $\det\mathscr{L}(u)$ is an integral of motion. It is a meromorphic function of the complex variable u with coefficients which are also integrals of motion

$$-\det\mathscr{L}(u)=\frac{I_1}{u^4}+\frac{I_2}{u^3}+\frac{I_3}{u^2}+\frac{I_4}{u}+\frac{I_5}{(u-\varkappa)^2}+\frac{I_6}{u-\varkappa}+\frac{I_7}{(u+\varkappa)^2}+\frac{I_8}{u+\varkappa}. \tag{19}$$

The coefficients of the highest degrees u^{-4}, u^{-3}, $(u\pm\varkappa)^{-2}$ are absent in the matrix $\mathscr{L}(u)$ and are determined by the Casimir operators of the algebra g

$$\begin{aligned} &I_1=R^2=1 && I_5=S^2=(n^2-1)/4 \\ &I_2=2RL=0 && I_7=T^2=(n^2-1)/4. \end{aligned} \tag{20}$$

The other coefficients are linearly connected with the constants of motion of the original problem introduced in (8):

$$\Lambda=I_3 \qquad B=-\tfrac{1}{2}\varkappa I_4 \qquad J^2=\varkappa(I_6-I_8)+I_3+I_5+I_7. \tag{21}$$

There is also the linear identity $I_4+I_6+I_8=0$ which reflects a possibility to choose an additional operator, depending on J_i and therefore commuting with J^2, Λ and B.

The classical motion is constrained by an algebraic curve $\mathscr{L}_i(u)\mathscr{L}_i(u)=c^2$. After reducing the common denominator we obtain that the parameters u and w belong to the hyperelliptic algebraic curve

$$P_6(u)+w^2=0 \tag{22}$$

where $P_6(u)$ is a polynomial of the sixth degree. The rank of the curve is two, therefore the equations of motion can be integrated in terms of Riemann θ functions, depending on two variables (Dubrovin *et al* 1976). The difference between the rank of the curve and the number of degrees of freedom reflects the su(2) invariance of the integrals of motion Λ and B under rotations of the system as a whole.

4. Lax representation in quantum mechanics and connections with magnetic models

In quantum mechanics we will work with the same matrix $\mathscr{L}(u)$ defined by (17). The quantum commutator of the components $\mathscr{L}_i(u)$ is

$$[\mathscr{L}_i(u),\mathscr{L}_k(u')]=\mathrm{i}\varepsilon_{ikl}\frac{1}{u'-u}(\mathscr{L}_l(u)-\mathscr{L}_l(u')) \tag{23}$$

thus an infinite-dimensional Lie algebra $\mathscr{C}$ appears. These commutational relations can be included in the scheme of the quantum spectral transform method (QSTM) (Kulish and Sklyanin 1982). Introducing 4×4 matrices $\overset{1}{\mathscr{L}}=\mathscr{L}\otimes\mathbb{1}$ and $\overset{2}{\mathscr{L}}=\mathbb{1}\otimes\mathscr{L}$ by a direct product with the 2×2 unit matrix $\mathbb{1}$ and introducing

$$r(u)=\frac{\mathrm{i}}{u}\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{pmatrix} \tag{24}$$

we rewrite (23) in the form

$$[\overset{1}{\mathscr{L}}(u),\overset{2}{\mathscr{L}}(u')]=[r(u-u'),\overset{1}{\mathscr{L}}(u)+\overset{2}{\mathscr{L}}(u')]. \tag{25}$$

For $\mathscr{L}^2(u)=-\mathscr{L}_i(u)\mathscr{L}_i(u)$ one has

$$[\mathscr{L}^2(u),\mathscr{L}^2(u')]=0. \tag{26}$$

The coefficients of the poles of $\mathscr{L}^2(u)$ as functions of u are in involution and correspond to integrals of motion of our problem according to (19)-(21).

Until now in the framework of QSTM there is no procedure for calculating the spectrum of $\mathscr{L}^2(u)$ for non-semisimple Lie algebras like $g=\mathrm{o}(4)\oplus\mathrm{e}(3)$, but for semisimple algebras the solution is known. Gaudin (1976) studied representations of algebra $\mathscr{C}$ for the N-site one-dimensional magnet on the semisimple Lie algebra $g_N=\bigoplus_{j=1}^N \mathrm{su}(2)$. For the components $S_i(u)$ of the matrix

$$S(u)=\frac{1}{\mathrm{i}}\sigma_i S_i(u) \qquad S_i(u)=\sum_{j=1}^{N}\frac{S_i^{(j)}}{u-\varepsilon_j} \tag{27}$$

the commutational relations (23) hold. Here the $S_i^{(j)}$ are the generators of su(2), the ε_j are given constants and u is an arbitrary complex variable. The operator $S^2(u)=-S_i(u)S_i(u)$ has an expansion

$$-S^2(u)=\sum_{j=1}^{N}\frac{\boldsymbol{S}^{(j)^2}}{(u-\varepsilon_j)^2}+2\sum_{j=1}^{N}\frac{1}{u-\varepsilon_j}\mathscr{H}_j \tag{28}$$

with $S^{(j)^2}=s_j(s_j+1)$ as Casimir operators of the sites j and $\mathscr{H}_j$ is a set of constants of motion

$$\mathscr{H}_j=\sum_{k=1}^{N}\frac{\boldsymbol{S}^{(j)}\boldsymbol{S}^{(k)}}{\varepsilon_j-\varepsilon_k}. \tag{29}$$

The $\mathscr{H}_j$ are linearly dependent, i.e. $\Sigma_{j=1}^N \mathscr{H}_j=0$. The dynamical system defined by $S^2(u)$ is, however, still integrable and moreover it is degenerated because of the relation

$$\boldsymbol{J}^2=\sum_{j=1}^{N}(\boldsymbol{S}^{(j)^2}+2\varepsilon_j\mathscr{H}_j) \tag{30}$$

that connects the Casimir operators of the sites $\boldsymbol{S}^{(j)^2}$ and the constants of motion $\mathscr{H}_j$ with the square of the total angular momentum $\boldsymbol{J}=\Sigma_{j=1}^N \boldsymbol{S}^{(j)}$. This relation compensates the lack of one integral of motion due to the linear dependence of the $\mathscr{H}_j$ and reflects the su(2) invariance of the system.

Gaudin (1976) found the spectrum of $S^2(u)$ using the Bethe ansatz. The vacuum state is characterised by the maximum value of the component of the total angular momentum along the third axis. The eigenvector $|M\rangle$ of $S^2(u)$ is considered in the form

$$|M\rangle=S^-(u_1)\ldots S^-(u_M)|0\rangle \tag{31}$$

where $S^{-}(u)=S_1(u)-\mathrm{i}S_2(u)$ and M is the number of excitations. The rapidities u_α satisfy the M algebraic relations

$$\sum_{\beta=1}^{M}\frac{1}{u_\beta-u_\alpha}-\sum_{j=1}^{N}\frac{s_j}{\varepsilon_j-u_\alpha}=0 \qquad \alpha=1,\ldots,M \tag{32}$$

and determine the eigenvalues of $\mathscr{H}$ as

$$-\varepsilon_j\left(\sum_{k=1}^{N}\frac{s_k}{\varepsilon_k-\varepsilon_j}+\sum_{\alpha=1}^{M}\frac{1}{\varepsilon_j-u_\alpha}\right). \tag{33}$$

It was pointed out by Gaudin (1976) that the polynomials $P(u)=\Pi_{\alpha=1}^{M}(u-u_\alpha)$ satisfy the following equation of the Fuchs class:

$$P''(u)+\sum_{j=1}^{N}\frac{2s_j}{\varepsilon_j-u}P'(u)+\sum_{j=1}^{N}\frac{a_j}{\varepsilon_j-u}P(u)=0 \tag{34}$$

and they can be treated as a generalisation of Lamé polynomials.

The spectrum of $\mathscr{L}^2(u)$ can be obtained by a limiting transition from the spectrum of $S^2(u)$, where the matrix $S(u)$

$$S(u)=\frac{1}{\mathrm{i}}\sigma_i S_i(u) \qquad S_i(u)=\frac{S_i}{u-\varepsilon}+\frac{T_i}{u+\varepsilon}+\frac{P_i}{u-\gamma}+\frac{Q_i}{u+\gamma} \tag{35}$$

is defined on the Lie algebra $g_4=\bigoplus_{j=1}^{4}\mathrm{o}(3)$ with the Casimir operators $\boldsymbol{P}^2=\boldsymbol{Q}^2=(\tilde{N}^2-1)/4$ and γ is a parameter. (This matrix $S(u)$ can be of importance, for instance, in studying doubly excited states of helium-like atoms. The parameters ε and γ can be chosen by variational calculation.) Let us introduce the generators $\boldsymbol{L}=\boldsymbol{P}+\boldsymbol{Q}$, $\boldsymbol{A}=\boldsymbol{P}-\boldsymbol{Q}$ of the Lie algebra o(4) instead of $\boldsymbol{P}$ and $\boldsymbol{Q}$. In the limit $\gamma=1/\tilde{\boldsymbol{N}}\to 0$ and $\boldsymbol{A}\to\infty$ the components $R_i=\gamma^{-1}A_i=\mathrm{O}(1)$ and angular momentum L_i satisfy commutation relations of the Lie algebra e(3) with the Casimir operators $\boldsymbol{R}^2=1$, $\boldsymbol{LR}=0$. Thus we obtain a limit correspondence for $S(u)$ on g_4

$$\mathscr{L}(u)=\lim_{\gamma\to 0}S(u) \tag{36}$$

therefore the spectrum of $\mathscr{L}^2(u)$ can be obtained from those of $S^2(u)$ on g_4 (35) by a limiting transition.

5. Conclusion

Our results are important in studying peculiarities of scattering amplitude for the Coulomb three-body problem near two-particle thresholds (Kvitsinsky *et al* 1987).

This treatment demonstrates a new field of application of the spectrum transform method. Also further development of the QSTM needs to be done to provide various and efficient computational procedures.

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