Two electrons in an external oscillator potential: The hidden algebraic structure

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It is shown that the Coulomb correlation problem for a system of two electrons (two charged particles) in an external oscillator potential possesses a hidden sl_2-algebraic structure being one of recently discovered quasi-exactly-solvable problems. The origin of existing exact solutions to this problem, recently described by several authors, is explained. A degeneracy of energies in electron-electron and electron-positron correlation problems is found. It manifests the first appearance of a hidden sl_2-algebraic structure in atomic physics.

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The problem of the evaluation of effects of interelectronic interactions is one of the central problems in atomic physics. The main difficulty comes from the fact that this problem cannot be solved exactly even in particular cases, while numerical solutions are too complicated to gain a proper intuition. Therefore, it is quite important to find and elaborate situations where this problem can be modeled in some relevant way, admitting exact, analytic solutions. One such situation has been described recently in [1, 2]. A system of two electrons in an external harmonic-oscillator potential with an additional linear interaction in the relative coordinate studied defined by the Hamiltonian[1]

$$H = -\nabla_1^2 + \omega^2 r_1^2 - \nabla_2^2 + \omega^2 r_2^2 + \frac{2\beta}{|\mathbf{r}_1 - \mathbf{r}_2|} + \lambda|\mathbf{r}_1 - \mathbf{r}_2| \tag{1}$$

was studied, where $r_{1,2}$ are the coordinates of the electrons and $\beta = 1$. Atomic units $\hbar = m = e = 1$ are used throughout and an overall factor $\frac{1}{2}$ is omitted. It was found that for certain values of oscillator frequency ω and the parameter λ some eigenstate of (1) can be obtained analytically. The main purpose of this paper is to show that this feature is nothing but a consequence of the fact that (1) is one of recently discovered quasi-exactly-solvable Schrödinger operators [4, 5]. It implies an existence of a hidden algebraic structure [6]. Hereafter, we will focus on the case $\lambda = 0$.

Quasi-exactly-solvable problems are quantum-mechanical problems for which several eigenstates can be found explicitly. They occupy an intermediate place between exactly solvable (such as Coulomb potential, harmonic oscillator, etc.) and nonsolvable. The quasi-exactly-solvable Schrödinger equations appear in two forms: (i) the Hamiltonian with an infinite discrete spectrum with several eigenstates known algebraically and (ii) the Hamiltonian depending on a free parameter, say β, and a certain fixed magnitude of energy corresponds to the ith state of the Hamiltonian at ith value of parameter β (where $i = 0, 1, 2, \ldots, n$).[2] Those problems are named the first and the second type, respectively. Surprisingly, exactly solvable problems such as the Coulomb problem, the Morse oscillator, and the Pöschl-Teller potential have two equivalent representations, either as the first-type problems or as the second-type ones [4].[3]

The underlying idea behind quasi-exactly solvability is the existence of a hidden algebraic structure. Let us recall a general construction considering the one-dimensional Schrödinger equation as an example. Take the algebra sl_2 realized in the first-order differential operators

$$J_n^+ = r^2 d_r - nr,$$
$$J_n^0 = r d_r - \frac{n}{2}, \tag{2}$$
$$J_n^- = d_r ,$$

where $r \in \mathbb{R}$ and $d_r \equiv \frac{d}{dr}$. Those three generators obey sl_2-algebra commutation relations for any value of the

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[1] In [3] so-called pseudoatoms were introduced: a quantum system made from atomic ones in which all Coulomb interactions are replaced by oscillator ones, attractive or repulsive as the case may be. The system described by (1) can be treated as a modified two-electron pseudoatom: where Coulomb attractive interactions are replaced by oscillator ones, while Coulomb repulsion remains unchanged or modified by the linear interaction.

[2] Precisely speaking, this means that for the parameters $\beta_0, \beta_1, \ldots, \beta_n$, the ground-state energy at β_0 is equal to the energy of the first excited state at β_1, is equal to the energy of the second excited state at β_2, etc., is equal to the energy of the nth excited state at β_n.

[3] For the Coulomb the second-type representation is nothing but the well-known Sturm representation.

parameter n. If n is a nonnegative integer, the algebra (2) possesses $(n+1)$-dimensional irreducible representation

$$\mathcal{P}_{n+1}(r) = \langle 1, r, r^2, \ldots, r^n \rangle . \tag{3}$$

It is evident that taking any polynomial in the generators (2), we arrive at a differential operator having the space (3) as the finite-dimensional invariant subspace. In other words, almost any polynomial in the generators (2) possesses $(n+1)$ eigenfunctions in the form of a polynomial in r of degree n.

Let us take the quasi-exactly-solvable operator[4]

$$T_2 = -J_n^0 J_n^- + 2\omega_r J_n^+ - (n/2 + 2l + 2) J_n^- - \omega_r n . \tag{4}$$

Substituting (2) into (4), one gets the differential operator

$$T_2(r, d_r; n) = -r d_r^2 + 2(\omega_r r^2 - l - 1) d_r - 2\omega_r n r \tag{5}$$

for which one can define the spectral problem

$$T_2(r, d_r; n) p(r) = -\beta(n) p(r), \tag{6}$$

where $\beta(n)$ is a spectral parameter. It is clear that this problem possesses $(n+1)$ eigenfunctions, $p_0(r), p_1(r), p_2(r), \ldots, p_n(r)$ in the form of a polynomial of the nth power. Other eigenfunctions are nonpolynomial and in general, they cannot be found in closed analytic form. Now let us make a gauge transformation in (5),(6), introducing a new function,

$$u(r) = r^{l+1} p(r) \exp(-\omega_r r^2/2), \tag{7}$$

then make a replacement in the last term in (5),

$$2\omega_r n = \epsilon' - \omega_r(2l+3), \tag{8}$$

where ϵ' is a new parameter, and divide (6) over r. Finally, we obtain the equation

$$\left[-d_r^2 + \omega_r^2 r^2 + \frac{\beta^{(n)}}{r} + \frac{l(l+1)}{r^2} \right] u(r) = \epsilon' u(r). \tag{9}$$

Putting in (9) $\beta^{(n)} = 1$ and saying that now a spectral parameter is ϵ', we arrive at Eq. (9) of Ref. [2]. If $\omega_r = 2\omega$ and $2\epsilon' = \epsilon$ is the energy of the relative motion, this equation appears in [2] as a radial equation for the relative motion in (1) after separation of the c.m. motion.

Equation (9) is a particular case of the quasi-exactly-solvable Schrödinger equation of the second type (case VIII in the classification [5]).[5] From the physical viewpoint, the parameter β in (1) has a meaning of the constant of the interelectronic interaction. This parameter can be changed by replacing an electron by a charged particle with charge Z. In principle, keeping the frequency ω and the energy ϵ' fixed, for any n and l one can find $(n+1)$ systems of two particles with different charges in the oscillator potential related to each other via hidden sl_2-algebraic structure (see a discussion in footnote 2).

Now let us describe some features of the eigenvalue problem (6).

(i) It is clear that the operator T_2 is self-adjoint and hence its eigenvalues are real. The first $(n+1)$ eigenvalues coincide with the eigenvalues of the Jacobian matrix with vanishing diagonal matrix elements

$$\hat{H} = \begin{pmatrix} 0 & 2\omega_r & 0 & \cdots & 0 & 0 & \cdots \\ n(n+1+2l) & 0 & 4\omega_r & \cdots & 0 & 0 & \cdots \\ \vdots & \vdots & & \vdots & & \vdots & \vdots \\ 0 & \cdots & (i+1)(i+2+2l) & 0 & 2(n-i+1)\omega_r & \cdots & 0 \\ \vdots & \vdots & & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 0 & 2n\omega_r \\ 0 & 0 & \cdots & 0 & \cdots & 2(l+1) & 0 \end{pmatrix} . \tag{10}$$

One can show that the spectrum of (10) is symmetric,

$$S_{n+1}(\beta) = (-1)^n S_{n+1}(-\beta) , \quad S_{n+1}(\beta) \equiv \det || \hat{H} - \beta || \tag{11}$$

that follows from the fact that all odd powers of the matrix $\hat{H}$ are traceless, Tr $\hat{H}^{2j+1} = 0$, $j = 0, 1, \ldots$.[6] So, for any $\omega_r > 0$ there exist $[(n+1)/2]$ (footnote 7) positive eigenvalues and the same amount negative eigenvalues. This property leads to an important conclusion: for the fixed n, l, and ω_r there exist two eigenstates, one at $\beta > 0$ and another at $\beta < 0$, degenerate in energy [see (8)]. In particular, this may allow the electron-electron correla-

[4]It belongs to the case VIII in the classification [5].

[5]General case VIII corresponds to $\lambda \neq 0$. In [4] this problem was named the *generalized Coulomb problem.*

[6]I am grateful to P. Mello for a discussion of this point.

[7]$[a]$ means integer part of a.

tion energy to be to related to the electron-positron one in problem (1) (see discussion below).

(ii) Another important property of (6) is that all eigenvalues $\beta^{(n)} \propto \sqrt{\omega_r}$ and, hence, depend on ω_r monotonously. For instance,

$$\beta^{(1)}_{\pm} = \pm 2\sqrt{\omega_r(l+1)},$$

$$\beta^{(2)}_{\pm,0} = \{\pm 2\sqrt{\omega_r(4l+5)}\ ,\ 0\}.$$

Therefore, in order to find the eigenvalues of (6) it is enough to perform calculations in one point on the ω_r axis, e.g., at $\omega_r = 1$.

The situation becomes slightly more complicated if we want to keep the parameter β fixed in the formula (1), declaring that now we want to consider namely a two-electron (or electron-positron) system, which implies $\beta = 1$ (-1). The relevant formulation of the problem is the following.

Let us fix n and l. This defines unambiguously the functional form of the pre-exponential factor in (7). Take a positive eigenvalue β in (6), which corresponds to repulsion of the particles in (1). It depends on the parameter ω_r monotonously, growing from zero up to infinity, which means that one can always find the value of ω_r for what $\beta = 1$ or any positive number. Since there exist $[(n+1)/2]$ positive eigenvalues of β (see above), each of them is equal to one for a certain value of ω_r. Correspondingly, the lowest eigenvalue [ground state, no nodes in $p(r)$ following the oscillation theorem] leads to the smallest value of ω_r, the next eigenvalue leads to bigger value of ω_r [one positive root in $p(r)$], etc. Finally, we arrive at $[(n+1)/2]$ values of the parameter ω_r, for each of them the problem (1) has the analytic solution of the form (7) with $p(r)$ as a polynomial of the nth degree with a number of positive roots varying from 0 up to $[(n+1)/2]$ (see Fig. 1, where the case $n = 3$ is described as an illustrative example).[8]

Taking the negative eigenvalues of β in (1) (that corresponds to attraction of the particles), one can repeat the above considerations with the only difference being that the number of positive roots varies from $[(n+1)/2]$ up to n. Following the property (i) for any eigenstate from the algebraized part of the spectra (see above) of the problem (1) with positive β one can find an eigenstate with negative β with the same energy. For example, for the fixed

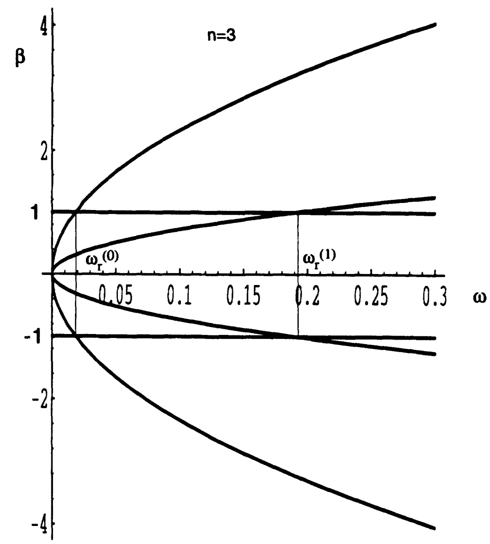

FIG. 1. Four eigenvalues of (6) at $n = 3$ having polynomial eigenfunctions as function of ω_r. Numbers in parentheses mean the amount of positive roots of the corresponding eigenfunctions.

n and the minimal ω_r: $\omega_r^{(0)}$, the ground-state energy at $\beta = 1$ [$p(r)$ has no positive roots] is equal to the energy of the nth excited state at $\beta = -1$ [$p(r)$ has n positive roots]. For $\omega_r^{(1)}$, the energy of the first excited state at $\beta = 1$ [$p(r)$ has one positive root] is equal to the energy of the $(n-1)$th excited state at $\beta = -1$ [$p(r)$has $(n-1)$ positive roots], etc. (see e.g., Fig. 1). This is reminiscent of the situation in one-dimensional supersymmetic quantum mechanics by Nicolai-Witten, where if the supersymmetry is unbroken, all states of the bosonic sector (except the lowest one) are degenerate with the states of the fermionic one.

It is worth noting that recently it was shown [6] that whenever some analytic solutions for eigenfunctions of a certain one-dimensional (or reduced to one-dimensional) Schrödinger equation occur, it signals the existence of the hidden algebra sl_2. Our present results manifest the appearance of quasi-exactly solvability in atomic physics. Developments of a hidden algebra method in quantum mechanics, solid-state physics, and quantum field theory, and also mathematical foundations can be found in Refs. [7].

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[8] It explains a systematics found in numerical calculation in [2].

[1] A. Samanta and S. Ghosh, Phys. Rev. A **42**, 1178 (1990).
[2] M. Taut, Phys. Rev. A **48**, 3561 (1993).
[3] M. Moshinsky, O. Novaro, and A. Calles, J. Phys. **31**, C4-125 (1970).
[4] A.V. Turbiner, Zh. Eksp. Teor. Fiz. **94**, 33 (1988) [Sov. Phys. JETP, **67**, 230 (1988)].
[5] A.V. Turbiner, Comm. Math. Phys. **118**, 467 (1988).
[6] A.V. Turbiner, J. Phys. A **25**, L1087 (1992).
[7] A.Yu. Morozov, A.M. Perelomov, A.A. Rosly, M.A. Shifman, and A.V. Turbiner, Int. J. Mod. Phys. **A5**, 803 (1990); V.V. Ulyanov and O.B. Zaslavsky, Phys. Rep. **216**, 179 (1992); P.B. Wiegmann and A.V. Zabrodin, Phys. Rev. Lett. **72**, 1890 (1994); Nucl. Phys. B **422**, 495 (1994); A.V. Turbiner, in *Contemporary Mathematics*, edited by N. Kamran and P. Olver (American Mathematical Society, Providence, 1994), Vol. 160, pp. 263-310.