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Raising and Lowering Operators for a Two-Dimensional Hydrogen Atom by an Ansatz Method

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Raising and lowering operators of a two-dimensional hydrogen atom are derived by an Ansatz method.

1. INTRODUCTION AND GENERAL DEFINITION OF RAISING AND LOWERING OPERATORS

Raising and lowering operators are important in quantum mechanics [1–6]. For a physical system described by an observable H, the eigenproblem $H|E\rangle = E|E\rangle$ can be solved exactly via its raising and lowering operators without dealing with the *Schrödinger equation*. In quantum mechanics, the factorization of H into raising and lowering operators for the discrete spectrum is a property of Hilbert space and is not restricted to any particular representation [7]. If H has a discrete spectrum, then it can be written as

$$H = \sum_n E_n |\psi_n\rangle\langle\psi_n| \tag{1}$$

where the $|\psi_n\rangle$ are the complete and orthonormal basis states of H. Thus one-way factorization

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$$\hat{\mathscr{L}}^{+}\hat{\mathscr{L}}^{-} = H - E_0$$

is provided by operators which have the following spectral decompositions:

$$\hat{\mathscr{L}}^{+} = \sum_n (E_{n+1} - E_0)^{1/2}|\psi_{n+1}\rangle\langle\psi_n|$$
$$\hat{\mathscr{L}}^{-} = \sum_n (E_{n+1} - E_0)^{1/2}|\psi_n\rangle\langle\psi_{n+1}| \tag{2}$$

These mutually adjoint operators perform the raising and lowering operations

$$\hat{\mathscr{L}}^{+}|\psi_n\rangle = (E_{n+1} - E_0)^{1/2}|\psi_{n+1}\rangle$$
$$\hat{\mathscr{L}}^{-}|\psi_n\rangle = (E_n - E_0)^{1/2}|\psi_{n-1}\rangle \tag{3}$$

From (1) and (2), one has

$$[H, \hat{\mathscr{L}}^{\pm}] = \hat{\mathscr{L}}^{\pm}F^{\pm} \tag{4}$$

where

$$F^{\pm} = \sum_n (E_{n\pm1} - E_n)|\psi_n\rangle\langle\psi_n| \tag{5}$$

is an adjacent energy interval operator, since $F^{\pm}|\psi_n\rangle = (E_{n\pm1} - E_n)|\psi_n\rangle$. [Here we have place $F^{\pm}$ to the right of $\hat{\mathscr{L}}^{\pm}$ in (4) to allow it to operate directly on the eigenfunction $|\psi_n\rangle$; this will simplify the calculations]. In particular, when $F^{\pm} = \pm\hbar\omega$, (4) corresponds to the usual one in a harmonic oscillator. When $F^{\pm}$ is a function of H, i.e., $F^{\pm} = f^{\pm}(H)$, (4) becomes

$$[H, \hat{\mathscr{L}}^{\pm}] = \hat{\mathscr{L}}^{\pm}f^{\pm}(H) \tag{6}$$

which is the case shown in ref. 1. Equation (4) or (6) is the general definition of raising and lowering operators expressed by a commutation relation. Note that the explicit forms of the raising and lowering operators $\hat{\mathscr{L}}^{\pm}$ for a specific Hamiltonian system need not be mutually adjoint [1].

The energy levels and wave functions of a two-dimensional (2D) hydrogen atom are well known. Raising and lowering operators for a two-dimensional hydrogen atom (especially for the radial part of the wave function) have been discussed by a factorization method [1, 8, 9]. The purpose of this paper is to derive them by an Ansatz method based on the general definition of raising and lowering operators [see equation (4)]. The plan of the paper is as follows. Since a 2D hydrogen atom can be connected to a 2D harmonic oscillator by the Kustaanheimo–Stiefel (KS) transformation [10–19] and the raising and lowering operators of a harmonic oscillator are already well known, in Section 2 we briefly review the physical background that we need. In Section 3, we establish the raising and lowering operators for a 2D hydrogen atom by an Ansatz method, and make some comments.

2. KS TRANSFORMATION AND DILATATION OPERATOR

We start with the time-independent Schrödinger equation for a 2D hydrogen atom,

$$H\psi = E\psi, \qquad H = \frac{\mathbf{p}^2}{2\mu} - \frac{\kappa}{r} \tag{7}$$

where μ is the reduced mass of the hydrogen atom, $\kappa = e^2$, $\mathbf{p}^2 = -\hbar^2 \sum_{i=1}^{2} (\partial^2/\partial x_i^2)$, the x_i being the Cartesian coordinates, and $r = (x_1^2 + x_2^2)^{1/2}$. We now transform the problem into a 2D harmonic oscillator via the KS transformation. With the variables u_1 and u_2 this transformation can be written

$$x_1 = u_1^2 - u_2^2, \qquad x_2 = 2u_1u_2 \tag{8}$$

Under the transformation we have $r = u^2 = u_1^2 + u_2^2$, and x_i and u_i are usually realized by

$$x_1 = r\cos\phi, \qquad x_2 = r\sin\phi \tag{9}$$

and

$$u_1 = \sqrt{r}\cos\frac{\phi}{2}, \qquad u_2 = \sqrt{r}\sin\frac{\phi}{2} \tag{10}$$

The Schrödinger equation (7) becomes

$$\left[-\frac{1}{8\mu}\frac{1}{u^2}\sum_{i=1}^{2}\frac{\partial^2}{\partial u_i^2} - \frac{\kappa}{r}\right]\psi = E\psi \tag{11}$$

After multiplying by r and taking $r = u^2$ into account, we find

$$\left[-\frac{1}{8\mu}\sum_{i=1}^{2}\frac{\partial^2}{\partial u_i^2} - Eu^2\right]\psi = \kappa\psi \tag{12}$$

This may be cast into the form of a Schrödinger equation for a 2D harmonic oscillator after first stipulating that $E < 0$ (for bound motions), and making the definitions

$$m = 4\mu, \qquad \omega = (-E/2\mu)^{1/2}, \qquad \epsilon = \kappa \tag{13}$$

We obtain

$$\left(-\frac{1}{2m}\sum_{i=1}^{2}\frac{\partial^2}{\partial u_i^2} + \frac{1}{2}m\omega^2u^2\right)\psi = \epsilon\psi \tag{14}$$

or $\mathcal{H}_0\psi = \epsilon\psi$, with

$$\mathcal{H}_0 = -\frac{1}{2m}\sum_{i=1}^{2}\frac{\partial^2}{\partial u_i^2} + \frac{1}{2}m\omega^2 u^2 \tag{15}$$

$\mathcal{H}_0$ and ϵ are the pseudo-Hamiltonian of a 2D harmonic oscillator and the pseudo-energy eigenvalue, respectively. In the usual way, we now introduce a set of two lowering and raising operators for the 2D harmonic oscillator,

$$b_j = \sqrt{\frac{m\omega}{2\hbar}}\,u_j + \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial u_j}, \tag{16}$$

$$b_j^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\,u_j - \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial u_j} \qquad (j = 1, 2)$$

where $[b_i, b_j^\dagger] = \delta_{ij}$, all other commutators being zero, and

$$[\mathcal{H}_0, b_j] = -\hbar\omega b_j, \qquad [\mathcal{H}_0, b_j^\dagger] = \hbar\omega b_j^\dagger \tag{17}$$

Thus (15) becomes

$$\mathcal{H}_0 = \hbar\omega\left(\sum_{j=1}^{2} b_j^\dagger b_j + 1\right) \tag{18}$$

Now writing $|\psi\rangle$ in the occupation number representation as $|\psi_n\rangle = |n_1 n_2\rangle = |n_1\rangle|n_2\rangle$, which can be obtained by $(b_1^\dagger)^{n_1}(b_j^\dagger)^{n_2}|0\rangle$, we immediately obtain from (14)

$$\epsilon = \kappa = (n_1 + n_2 + 1)\hbar\omega \qquad (n_1, n_2 = 0, 1, 2, \ldots) \tag{19}$$

Recalling $\omega = (-E/2\mu)^{1/2}$, we obtain the energy levels of a 2D hydrogen atom

$$E \equiv E_n = -\frac{\kappa}{2a}\frac{1}{(n - \frac{1}{2})^2} \qquad (n = 1, 2, \ldots) \tag{20}$$

where $a = \hbar^2/\mu\kappa$ is the Bohr radius.

The wave function $|\psi_n\rangle = |n_1 n_2\rangle$ can be expressed easily in polar coordinates as $\psi_{nl}(\mathbf{u}) = \langle \mathbf{u}|n_1 n_2\rangle = R_{nl}(u)\Phi_l(\phi)$, where $\Phi(\phi) = e^{il\phi}$ $(l = 0, \pm 1 \pm 2, \ldots)$, and $R_{nl}(u)$ is related to the confluent hypergeometric function. Essentially, $\psi_{nl}(\mathbf{u})$ is also the wave function of a 2D hydrogen atom under the KS transformation shown in (8). From the point of view of a 2D harmonic oscillator, the $b_j^\dagger$ and b_j are raising and lowering operators [see (17)], and they transform $|\psi_n\rangle$ into $|\psi_{n+1}\rangle$ and $|\psi_{n-1}\rangle$, respectively. Now a question arises naturally: With the known raising and lowering operators of a 2D harmonic oscillator, can one obtain some hints to establish those of a 2D hydrogen atom? The answer is yes. Let us focus on (16), and note that there is an operator $\omega = (-E/2\mu)^{1/2}$ in the $b_j^\dagger$ and b_j. After acting on $|\psi_n\rangle$, ω becomes

$$\omega_n = \sqrt{\frac{\kappa}{4a\mu}}\frac{1}{n - \frac{1}{2}}$$

In this sense, the $b_j^\dagger$ and b_j are n-dependent operators as follows:

$$\begin{aligned} b_{j(n)} &= \sqrt{\frac{m\omega_n}{2\hbar}}\, u_j + \sqrt{\frac{\hbar}{2m\omega_n}}\frac{\partial}{\partial u_j}, \\ b_{j(n)}^\dagger &= \sqrt{\frac{m\omega_n}{2\hbar}}\, u_j - \sqrt{\frac{\hbar}{2m\omega_n}}\frac{\partial}{\partial u_j} \qquad (j = 1, 2) \end{aligned} \tag{21}$$

so when referring to $b_{j(n)}^\dagger$ and $b_{j(n)}$, they always act on $|\psi_n\rangle$. Combining (21) with (10), one notes that $b_{j(n+1)}^\dagger$ (which will act on $|\psi_{n+1}\rangle$) can be obtained from $b_{j(n)}^\dagger$ through replacing ω_n by ω_{n+1}, or equivalently, through replacing r by ρr with $\rho = (n - 1/2)/(n + 1/2)$. Hence, the raising operators of a 2D hydrogen atom must contain a kind of operator which can transform r into ρr; as we know from the literature [1], this kind of operator is just the dilatation operator as follows (for 2D):

$$D_n^\pm = \exp\left[\left(\frac{i}{\hbar}\mathbf{r}\cdot\mathbf{p} + 1\right)\ln\rho^\pm\right], \qquad \rho^\pm = \frac{n - 1/2}{n \pm 1 - 1/2}$$

$$D_n^\pm f(x_j) = f(\rho^\pm x_j), \qquad D_n^\pm f(p_j) = f(p_j/\rho^\pm) \qquad (j = 1, 2) \tag{22}$$

Note that $(D_n^+)^\dagger = D_n^-$, and D_n^- is not defined for $n = 1$. In the next section, we derive raising and lowering operators of a 2D hydrogen atom by an Ansatz method using the dilatation operator.

3. DERIVATION USING AN ANSATZ METHOD

We now write (7) in polar coordinates as

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right) + \frac{1}{2\mu}\frac{L_3^2}{r^2} - \frac{\kappa}{r}\right]R(r)\Phi(\phi) = ER(r)\Phi(\phi) \tag{23}$$

where the angular part of the wave function $\Phi(\phi)$ is the eigenfunction of the angular momentum along the third direction $L_3 = -i\hbar\partial/\partial\phi$. Since $[L_3, \hat{\mathbf{r}}^\pm] = \pm\hbar\hat{\mathbf{r}}^\pm$, where $\hat{\mathbf{r}}^\pm = (x_1 \pm ix_2)/r$, from (4) we know that $\hat{\mathbf{r}}^\pm$ are raising and lowering operators of L_3 and they shift $\Phi_l(\phi) = e^{il\phi}$ to $\Phi_{l\pm 1}(\phi)$, respectively. Hence the raising and lowering operators for the angular part of the wave function of a 2D hydrogen atom are clear. In the following we establish those of the radial part of the wave functions based on the definition (4).

Denote by Q_n^+ the raising operator of a 2D hydrogen atom; it should commute with L_3, otherwise it will change the angular part of the wave function when it acts on $\psi(r, \phi) = R(r)\Phi(\phi)$. Guided by the observation

$$[L_3, D_n^{\pm}] = [L_3, r] = [L_3, \mathbf{r}\cdot\mathbf{p}] = 0 \tag{24}$$

we make the Ansatz

$$Q_n^+ = T_n^+ D_n^+, \qquad T_n^+ = \frac{i}{\hbar}\,\mathbf{r}\cdot\mathbf{p} - \alpha_n \frac{r}{a} + \beta_n \tag{25}$$

where α_n and β_n are some unknown n-dependent coefficients that need to be determined later.

Due to

$$[\mathbf{p}^2, r] = -\frac{2\hbar^2}{r}\left(\frac{i}{\hbar}\,\mathbf{r}\cdot\mathbf{p} + \frac{1}{2}\right), \qquad \mathbf{r}\cdot\mathbf{p} - \mathbf{p}\cdot\mathbf{r} = 2i\hbar$$

$$\left[\mathbf{r}\cdot\mathbf{p}, \frac{1}{r}\right] = i\hbar\,\frac{1}{r}, \qquad [p^2, \mathbf{r}\cdot\mathbf{p}] = -2i\hbar p^2 \tag{26}$$

$$D_n^{\pm}\,\frac{r}{n - 1/2} = \frac{r}{n \pm 1 - 1/2}\,D_n^{\pm}, \qquad D_n^{\pm}(n - 1/2)^2 p^2 = (n \pm 1 - 1/2)^2 p^2 D_n^{\pm}$$

we obtain

$$HT_n^+ = T_n^+ H + 2H + \frac{\kappa}{r} + \alpha_n \frac{\kappa}{r}\left(\frac{i}{\hbar}\,\mathbf{r}\cdot\mathbf{p} + \frac{1}{2}\right)$$

$$HD_n^+ = D_n^+ \frac{(n - 1/2)^2}{(n + 1/2)^2}\left[H + \left(1 - \frac{n + 1/2}{n - 1/2}\right)\frac{\kappa}{r}\right] \tag{27}$$

thus

$$\begin{aligned}
[H, T_n^+ D_n^+] = {} & T_n^+ D_n^+\left[\frac{(n - 1/2)^2}{(n + 1/2)^2} - 1\right]H \\
& + D_n^+ \frac{n - 1/2}{n + 1/2}\left(\alpha_n - \frac{1}{n + 1/2}\right)\frac{\kappa}{r}\,\frac{i}{\hbar}\,\mathbf{r}\cdot\mathbf{p} \\
& + D_n^+ \frac{n - 1/2}{n + 1/2}\left[1 + \frac{\alpha_n}{2} - \frac{\beta_n + 1}{n + 1/2}\right]\frac{\kappa}{r} \\
& + 2D_n^+ \frac{(n - 1/2)^2}{(n + 1/2)^2}\left[H + \frac{\kappa}{2a}\,\frac{1}{(n - 1/2)^2}\,(n + 1/2)\alpha_n\right]
\end{aligned} \tag{28}$$

When (28) acts on $|\psi_n\rangle$, we set

$$\alpha_n - \frac{1}{n + 1/2} = 0, \qquad 1 + \frac{\alpha_n}{2} - \frac{\beta_n + 1}{n + 1/2} = 0$$
$$\left[H + \frac{\kappa}{2a}\frac{1}{(n - 1/2)^2}(n + 1/2)\alpha_n\right]|\psi_n\rangle = 0 \tag{29}$$

i.e., $\alpha_n = 1/(n + 1/2)$, $\beta_n = n$, $E_n = -(\kappa/2a)/(n - 1/2)^2$; therefore, (28) becomes

$$[H, Q_n^+] = Q_n^+ F^+, \qquad \left[F^+ = \left(\frac{(n - 1/2)^2}{(n + 1/2)^2} - 1\right)H\right]|\psi_n\rangle = (E_{n+1} - E_n)|\psi_n\rangle \tag{30}$$

Based on the definition (4), Q_n^+ is the sought raising operator. By the same Ansatz method, the lowering operators can also be determined. They are

$$Q_1^- = T_1^- = -\frac{i}{\hbar}\mathbf{r}\cdot\mathbf{p} - \frac{2r}{a}, \qquad Q_n^- = T_n^- D_n^- \qquad (n \geq 2)$$
$$T_n^- = -\frac{i}{\hbar}\mathbf{r}\cdot\mathbf{p} - \frac{r}{a}\frac{1}{(n - 1) - 1/2} + n - 1 \tag{31}$$

From $\mathbf{r}\cdot\mathbf{p} = -i\hbar r\ \partial/\partial r$, $T_1^- R_{10}(r) = 0$, $Q_n^- R_{n,n-1}(r) = 0$, $Q_n^+ R_{n,l}(r) = R_{n+1,l}(r)$, and $Q_n^- R_{n,l}(r) = R_{n-1,l}(r)$, we can obtain all the radial parts of the wave functions $R_{n,l}(r)$.

In conclusion, based on hints from the raising and lowering operators of a 2D harmonic oscillator, we have established $Q_n^{\pm}$ for a 2D hydrogen atom by an Ansatz method. The n-dependent operators $Q_n^{\pm}$ can be expressed in a unified formula as (for $n \geq 2$):

$$Q_n^{\pm} = T_n^{\pm} D_n^{\pm} = \pm\left(\frac{i}{\hbar}\mathbf{r}\cdot\mathbf{p} + \frac{1}{2}\right)D_n^{\pm} - \frac{r}{a}D_n^{\pm}\frac{1}{(n \pm 1) - 1/2} + D_n^{\pm}\left(n - \frac{1}{2}\right) \tag{32}$$

If we introduce the operator

$$\hat{\mathcal{N}} = \sqrt{-\frac{\kappa}{2a}\frac{1}{H}} \tag{33}$$

then

$$\hat{\mathcal{N}}|\psi_n\rangle = \sqrt{-\frac{\kappa}{2a}\frac{1}{E_n}}\,|\psi_n\rangle \tag{34}$$

which can be written in terms of n as $\hat{\mathcal{N}}|\psi_n\rangle = (n - 1/2)|\psi_n\rangle$. The dilatation operator can be expressed as

$$D_n^{\pm} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{\hbar} \mathbf{r} \cdot \mathbf{p} + 1 \right)^n \left(\ln \frac{n - 1/2}{(n - 1/2) \pm 1} \right)^k \tag{35}$$

When $D_n^{\pm}$ acts on $|\psi_n\rangle$, its effect is the same as that of

$$D^{\pm} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{\hbar} \mathbf{r} \cdot \mathbf{p} + 1 \right)^k \left(\ln \frac{\hat{\mathcal{N}}}{\hat{\mathcal{N}} \pm 1} \right)^k \tag{36}$$

Based on the above analysis, from (32) the n-independent raising and lowering operators $Q^{\pm}$ are given by

$$Q^{\pm} = \pm \left(\frac{i}{\hbar} \mathbf{r} \cdot \mathbf{p} + \frac{1}{2} \right) D^{\pm} - \frac{r}{a} D^{\pm} \frac{1}{\hat{\mathcal{N}} \pm 1} + D^{\pm} \hat{\mathcal{N}} \tag{37}$$

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