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A study of the confined 2D isotropic harmonic oscillator in terms of the annihilation and creation operators and the infinitesimal operators of the SU(2) group

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Abstract
The eigenspectral properties of the 2D isotropic harmonic oscillator, centrally enclosed in the symmetric box with impenetrable walls, are studied for the first time using the annihilation and creation operators and the infinitesimal operators of the SU(2) group. It is shown explicitly how the imposition of the Dirichlet boundary condition at a certain uniquely prescribed confinement radius leads to the energy difference of two harmonic oscillator units between all successive *pairs* of the confined states, defined by the projection angular momentum quantum numbers $[m, m \pm 2]$ such that the lowest energy state corresponding to the chosen m is excluded in the first pair.

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1. Introduction

Models of spatially confined quantum systems are of great contemporary interest due to their applications in many areas of physics. Increasing interest in the confined systems is due to achievement in fabrication and investigation of mesoscopic scale semiconductor structures like quantum dots containing one, few or a finite countable number of spatially confined electrons [1]. The confined harmonic oscillator model has been successfully applied in the study of vibronic spectra of point defects, impurities or luminescence centers in solids, molecular vibrations in solids and the magnetic properties of an electron gas confined in the semiconductor nanostructures. In these investigations it is assumed that electronic energy sheets are represented by one or more dimensional harmonic oscillators. It is also useful for modeling the influence of the environment on atom and molecule vibrations on surfaces, into nanotubes and fullerenes. A detailed list of the relevant references can be found in review articles available in the literature [2]. The importance of the harmonic confinement potential is due to the fact that it is finite and gradually increasing in nature.

A majority of the theoretical studies reported so far have dealt with the computation of the changes in energy levels as a function of the parameters defining the confining potential. It is of interest to obtain the general rules and conditions which govern the eigenspectrum structure in terms of the well-defined characteristic features. An analysis of the characteristic patterns in the eigenspectrum has been addressed only in a few quantum systems [3–6].

In this work we deal with an isotropic harmonic oscillator (IHO) in two dimensions which is centrally confined by an impenetrable boundary of radius ρ_c (2D CHO model). Computationally, the CHO model with impenetrable walls has been studied by solving the radial Schrödinger equation together with the Dirichlet boundary condition imposed on the radial wavefunction. As compared to the 2D IHO, such confinements significantly affect the eigenspectral properties of the CHO. In particular, the equidistant separation between the adjacent energy levels (n, m) and $(n\mp1, m+1)$ and the $2n+|m|+1$ degeneracy of corresponding energy levels are both disturbed as a consequence of confinement. The imposition of the radially symmetric boundary is expected to lower the symmetry of 2D CHO. Here, it is important to examine whether some kind of symmetry and its resulting systematic degeneracy, are preserved or not. For comparison purposes, the spherically confined hydrogen atom (CHA) can be considered as another model system whose unconfined counterpart exhibits a high order of degeneracy of the energy levels due to its SO(4) symmetry. In this case it has been argued that some kind of symmetry (so-called conditional symmetry) and degeneracy of the energy levels are still conserved at finite values of the confinement radius [3–5]. To the best of our knowledge, a comparable analysis involving the symmetry arguments for the 2D CHO is not yet available. In this direction, very recently, the eigenspectral characteristics of constant separation among corresponding levels with the specific value of the radius of confinement have been examined [7] using the Gauss identities for the confluent hypergeometric function.

The purpose of this paper is to show that the algebraic method based on the formalism of annihilation and creation operators provides a useful tool in studying the characteristic properties of the eigenspectrum of the 2D CHO. Such an analysis also leads to a deeper understanding of the origin of these features. In section 2, the CHO model with the boundary condition is introduced and the resulting requirement imposed on the first derivative of the confined radial wavefunction is derived. In section 3, the behavior of the energy levels as a function of the confinement radius is discussed along with the reason for complete removal of any systematic degeneracy in the 2D CHO. Section 4 deals with application of the creation and annihilation operators on the radial wavefunction of a 2D CHO state. Finally, in section 5 the main results are summarized.

2. The model

A centrally confined harmonic oscillator in two dimensions is the particle of mass μ ($\mu = 1$ in h.o. units; in this system also $\hbar = 1$ and $\omega = 1$) moving in the xy-plane in the potential

$$V(\rho) = \begin{cases} \frac{1}{2}\rho^2, & \rho < \rho_c \\ \infty, & \rho \geqslant \rho_c. \end{cases} \tag{1}$$

Since the potential is axially symmetric, the projection of the angular momentum on the symmetry axis (z-axis), L_z, is constant of motion and the wavefunction of the 2D CHO stationary state is of the form

$$\Psi_{Em}(\rho, \varphi) = R_{Em}(\rho)\, \mathrm{e}^{\mathrm{i}m\varphi}, \tag{2}$$

where m is the quantum number characterizing L_z and it takes the values $m = 0, \pm 1, \pm 2, \ldots$. Using wavefunction (2) in the Schrödinger equation

$$H\Psi_{Em} \equiv \left[-\tfrac{1}{2}\Delta + V(\rho)\right]\Psi_{Em} = E\Psi_{Em}, \tag{3}$$

we obtain the radial Schrödinger equation for the radial wavefunction R_{Em}

$$\frac{d^2 R_{Em}}{d\rho^2} + \frac{1}{\rho}\frac{dR_{Em}}{d\rho} + \left[2E - \frac{m^2}{\rho^2} - \rho^2\right] R_{Em} = 0. \tag{4}$$

As is the case with 2D IHO, the 2D CHO states with quantum numbers m and $-m$ have the same energy and corresponding radial wavefunctions are identical $R_{Em}(\rho) = R_{E,-m}(\rho)$ due to the appearance of the term with m^2 in radial Schrödinger equation (4).

We note here that (a) the radial wavefunction R_{Em} of the 2D CHO stationary state satisfies the Dirichlet boundary condition

$$R_{Em}(\rho_c) = 0, \tag{5}$$

and (b) in order that the radial Schrödinger equation (4) has a nontrivial solution the first-order derivative of R_{Em} follows the condition:

$$\left(\frac{dR_{Em}}{d\rho}\right)_{\rho=\rho_c} \neq 0. \tag{6}$$

We conclude this section by stating that the elements of the radial Hilbert space of the 2D CHO are square-integrable radial functions on $(0, \rho_c)$ with weight ρ satisfying conditions (5) and (6)

$$\mathcal{L}^2((0,\rho_c);\rho) = \left\{ R_{Em} : \rho \to \mathbb{C} \;\middle|\; \int_0^{\rho_c} |R_{Em}(\rho)|^2 \rho \, d\rho < \infty, R_{Em}(\rho_c) = 0 \right\}. \tag{7}$$

3. Degeneracy of 2D CHO energy levels

It is well known that $2n + |m|$ degeneracy of 2D IHO emerges from the symmetry, higher than the geometrical SO(2) symmetry responsible for the degeneracy of the states with quantum numbers m and $-m$. Confining this system even inside the radially symmetric boundary with impenetrable walls breaks the degeneracy and lowers the symmetry characteristic for 2D IHO.

Our aim in this section is to investigate if some kind of systematic degeneracy is still present when confinement is imposed. In order to establish the criterion for 2D CHO energy levels degeneracy, it will be convenient to study the energy levels as a function in confinement radius $E(\rho_c)$. In the remainder of this section only the levels with quantum numbers $m \geqslant 0$ will be considered due to the fact we have already discussed. We will start with solving radial Schrödinger equation (4) [7]

$$R_{Em}(\rho) = \rho^m e^{-\rho^2/2} F\left(\frac{m+1-E}{2}, m+1, \rho^2\right). \tag{8}$$

According to (5) energies of 2D CHO states are given by the zeros of the equation

$$F\left(\frac{m+1-E}{2}, m+1, \rho_c^2\right) = 0. \tag{9}$$

The first zero determines the energy of the lowest state with quantum number m whose radial wavefunction has no nodes, i.e. its radial quantum number is $n = 0$; the subsequent zero gives the energy of the 2D CHO state whose radial wavefunction has one node, i.e. its radial quantum number is $n = 1$. Due to this reason, throughout this work, the 2D CHO states are classified by the pairs of quantum numbers (nm) instead of (Em).

Table 1. Energies of the 2D CHO stationary states (00), (21) and (32) for small values of the confinement radius ρ_c and their discrepancy, in %, from the values calculated according to (12).

ρ_c	E_{00}	$\delta(\%)$	E_{21}	$\delta(\%)$	E_{32}	$\delta(\%)$
0.05	1156.637 46	0.000 49	20 699.891 20	0.000 02	43 784.038 26	0.000 03
0.1	289.160 39	0.000 85	5174.974 36	0.000 01	10 946.011 17	0.000 04
0.2	72.294 18	0.006 52	1293.749 84	0.000 49	2736.509 21	0.000 28
0.3	32.138 62	0.032 65	575.011 97	0.001 99	1216.238 68	0.000 63
0.4	18.089 90	0.097 00	323.462 46	0.008 22	684.152 99	0.004 03
0.5	11.593 62	0.236 03	207.040 58	0.020 11	437.883 19	0.009 80
0.6	8.071 42	0.488 78	143.809 24	0.041 72	304.117 46	0.020 30
0.7	5.954 56	0.906 27	105.693 36	0.076 70	223.471 86	0.036 91
0.8	4.587 73	1.541 36	80.965 64	0.131 92	171.141 00	0.064 11
0.9	3.657 85	2.466 81	64.023 60	0.210 74	135.274 64	0.102 00
1.0	3.000 00	3.749 51	51.916 48	0.322 20	109.631 37	0.156 50

3.1. Energy levels for small values of confinement radius

In the limit $\rho_c \to 0$ the third term in the squared brackets in the radial Schrödinger equation (4) can be neglected and (4) becomes the radial equation for the particle in infinite 2D potential well

$$\frac{d^2 R_{nm}}{d\rho^2} + \frac{1}{\rho}\frac{dR_{nm}}{d\rho} + \left[2E - \frac{m^2}{\rho^2}\right] R_{nm} = 0 \tag{10}$$

with Bessel function of integer order as a solution [8, 9]

$$R_{nm} = J_m(k\rho), \tag{11}$$

where $k = \sqrt{2E}$. Imposing Dirichlet boundary condition (5) gives the equation for determination of the energy E_{nm}

$$J_m(\rho_c\sqrt{2E_{nm}}) = 0, \tag{12}$$

in other words the energy levels are given by the zeros of the Bessel function with corresponding m value.

Since the Bessel function has no multiple zeros, the energy spectrum of 2D CHO is non-degenerated at small ρ_c values. The order of the energy levels (nm) is determined by the order of the Bessel function zeros [8]

$$\begin{aligned}&(00), (01), (02), (10), (03), (11), (04), (12), (20), (05), (13), (06), (21),\\&(14), (07), (22), (30), (08), (15), (23), (31), (16), (24), (32), (40), \ldots .\end{aligned} \tag{13}$$

Table 1 contains the numerical values for the energies of 2D CHO states (00), (21) and (32) obtained by the Numerov–Cooley method [10, 11]. Computation was performed with 30 000 grid nodes and following values of the parameters $\epsilon = 1 \times 10^{-5}$, $P = 4$ and $M = 100$–1000 (details can be found in [12]). The discrepancies δ, measuring the differences between the computed energy values and values determined according to (12) and data from table 9.5 in [8], are given too. Entries in table 1 confirm our supposition that 2D CHO energy levels coincide with the energy levels of infinite 2D potential well as well as the ordering of 2D CHO levels for small values of the confinement radius. We note here that the term 'small confinement radius' corresponds to different numerical values of ρ_c for the different 2D CHO states.

3.2. Energy levels for large values of confinement radius

It is obvious that 2D CHO energy spectrum approaches the energy spectrum of unconfined 2D harmonic oscillator in the limit $\rho_c \to \infty$. Let us define the quantity

$$\Delta E_{nm} = E_{nm} - E^0_{nm} \to 0 \qquad \text{for} \quad \rho_c \to \infty \tag{14}$$

measuring the difference between the energy E_{nm} of the 2D CHO state (nm) for large values of confinement radius and the energy $E^0_{nm} = 2n + |m| + 1$ of the 2D IHO state with the same quantum numbers. When ρ_c takes the large values, we can use the asymptotic form for confluent hypergeometric function (relation (13.5.1) in [8] or equation (7) in [3]) and give (9) the form

$$\frac{\Gamma(b)}{\Gamma(b-a)}(-1)^{-a}\rho_c^{-2a} + \frac{\Gamma(b)}{\Gamma(a)}\rho_c^{2(a-b)}\,\mathrm{e}^{\rho_c^2} = 0, \tag{15}$$

where the abbreviations are used

$$b = m+1, \qquad a = \frac{m+1-E}{2} \to -n \qquad \text{when} \quad \rho_c \to \infty. \tag{16}$$

Applying the asymptotic form for parameter a from the former relation and calculating $\Gamma(a) \to \Gamma\left(-n - \frac{\Delta E_{nm}}{2}\right) = \frac{2(-1)^{n+1}}{n!\Delta E_{nm}}$, (15) gives

$$\Delta E_{nm} = \frac{2\rho_c^{2(2n+m+1)}\,\mathrm{e}^{-\rho_c^2}}{n!\Gamma(n+m+1)} > 0 \tag{17}$$

and subsequent ratios follows immediately

$$\frac{\Delta E_{n-2,m+4}}{\Delta E_{nm}} = \frac{n(n-1)}{(n+m+2)(n+m+1)} < 1, \qquad \frac{\Delta E_{n-1,m+2}}{\Delta E_{nm}} = \frac{n}{n+m+1} < 1$$
$$\frac{\Delta E_{n-2,m+4}}{\Delta E_{n-1,m+2}} = \frac{n-1}{n+m+2} < 1, \tag{18}$$

so that

$$E_{n-2,m+4} < E_{n-1,m+2} < E_{nm}. \tag{19}$$

This ordering implies that among the number of states with the same energy in the case of 2D IHO, the state with the maximal value of m has the lowest energy value when confinement is present. Also, the greater the azimuthal quantum number value is, the greater the energy will be when the radial quantum number is held unchanged and relation (19) can be completed

$$E_{n-2,m+3} < E_{n-2,m+4} < E_{n-1,m+2} < E_{nm} < E_{n,m+1} \tag{20}$$

so that the ordering of the 2D CHO states emerges

$$\begin{aligned}&(00), (01), (02), (10), (03), (11), (04), (12), (20), (05), (13), (21), (06)\\&(14), (22), (30), (07), (15), (23), (31), (08), (16), (24), (32), (40), \ldots .\end{aligned} \tag{21}$$

The 2D CHO level ordering (19) for the states (05), (13) and (21) have been numerically tested using the direct evaluation of the roots of the confluent hypergeometric function as described earlier [7]. The results presented in table 2 show the validity of the relative ordering prescribed above. Also, it is evident that in large ρ_c limit energy levels are almost degenerated and the same levels are in question as in the 2D IHO case.

Table 2. Energies of the 2D CHO stationary states (05), (13) and (21) for the large values of the confinement radius.

ρ_c	E_{05}
5.0	6.000 042 098 390 945 921 308 952 970 171 344 118 800 534 011 079 790
5.5	6.000 000 737 485 437 045 982 738 093 457 260 284 542 442 155 656 496
6.0	6.000 000 006 961 517 781 540 063 047 675 542 665 733 851 586 712 602
6.5	6.000 000 000 036 242 387 387 224 421 743 027 851 641 470 042 951 557
7.0	6.000 000 000 000 105 772 826 759 875 012 021 835 066 769 477 337 582
7.5	6.000 000 000 000 000 175 166 030 654 432 831 756 705 617 370 006 178
8.0	6.000 000 000 000 000 000 166 158 663 384 612 655 493 849 819 102 564
9.0	6.000 000 000 000 000 000 000 000 028 907 103 419 034 816 684 052 584
10.0	6.000 000 000 000 000 000 000 000 000 000 000 582 406 859 878 536 201
11.0	6.000 000 000 000 000 000 000 000 000 000 000 000 000 001 401 652 447
	E_{13}
5.0	6.000 144 905 921 532 840 636 370 663 382 961 467 832 209 610 207 531
5.5	6.000 002 736 942 048 351 459 373 748 636 726 789 347 034 523 551 667
6.0	6.000 000 027 250 180 453 131 316 739 092 227 623 635 469 424 776 267
6.5	6.000 000 000 147 601 395 056 888 961 984 901 507 166 561 594 893 087
7.0	6.000 000 000 000 444 086 723 003 420 721 469 694 274 723 533 704 497
7.5	6.000 000 000 000 000 753 278 727 339 579 418 370 644 268 398 626 831
8.0	6.000 000 000 000 000 000 728 440 374 769 224 304 475 078 950 121 100
9.0	6.000 000 000 000 000 000 000 000 130 426 331 885 694 627 752 138 226
10.0	6.000 000 000 000 000 000 000 000 000 000 002 681 294 579 686 515 238
11.0	6.000 000 000 000 000 000 000 000 000 000 000 000 000 006 548 594 180
	E_{21}
5.0	6.000 240 164 070 584 093 071 607 358 629 252 525 639 636 962 983 465
5.5	6.000 004 713 329 122 358 486 775 294 827 979 215 044 270 766 111 538
6.0	6.000 000 048 208 656 503 779 360 560 598 412 465 646 108 526 666 006
6.5	6.000 000 000 266 381 288 153 680 920 388 833 763 959 933 186 054 658
7.0	6.000 000 000 000 813 801 622 919 847 108 736 195 250 575 679 166 609
7.5	6.000 000 000 000 001 397 100 974 853 729 298 722 471 591 890 913 621
8.0	6.000 000 000 000 000 001 364 135 975 659 157 523 035 142 164 796 218
9.0	6.000 000 000 000 000 000 000 000 247 789 425 360 339 870 130 321 812
10.0	6.000 000 000 000 000 000 000 000 000 000 005 145 700 772 566 859 987
11.0	6.000 000 000 000 000 000 000 000 000 000 000 000 000 012 660 321 422

3.3. Simultaneous degeneracy

The symmetry group of the 2D IHO Hamiltonian is SU(2) group with three infinitesimal operators of the symmetry transformations. These mutually independent operators, commuting with the Hamiltonian, can be represented in terms of the products $a_i^\dagger a_j (i, j = x, y)$, where $a^\dagger$ and a are the creation and annihilation operators, respectively. There are different choices of the infinitesimal operators in the literature [13–15]. It will be convenient to use the operators given in [15]

$$S_+ = S_x + \mathrm{i}S_y, \qquad S_- = S_x - \mathrm{i}S_y, \qquad S_z = \tfrac{1}{2}L_z \tag{22}$$

where

$$S_x = \tfrac{1}{2}(xy + p_x p_y), \qquad S_y = \tfrac{1}{4}\left(p_y^2 - p_x^2 + y^2 - x^2\right). \tag{23}$$

It is obvious from the commutation relations between the operators $S_\pm$ and the operator L_z: $[L_z, S_\pm] = \pm 2S_\pm$, that they are the ladder operators with respect to the angular momentum projection on the z axis. When it is applied on the wavefunction of the 2D IHO state the operator S_+ raises its value by 2 h.o. units, and the operator S_- lowers it by the same amount [15].

For our analysis it will be sufficient to consider operator S_+. In polar coordinates it is given by the expression

$$S_+ = \frac{1}{4}\,e^{2i\varphi}\left[i\left(\frac{\partial^2}{\partial\rho^2} - \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} - \rho^2\right) + \frac{2}{\rho^2}\frac{\partial}{\partial\varphi} - \frac{2}{\rho}\frac{\partial^2}{\partial\rho\partial\varphi}\right], \qquad (24)$$

and its application on the wavefunction, given by the product of radial function $R(\rho)$ (here R stands for radial wavefunction of the 2D IHO state, P_{nm}, and the radial wavefunction of the 2D CHO state, R_{nm}) and angular function $e^{im\varphi}$, results in

$$S_+(R\,e^{im\varphi}) = -\frac{i}{2}(m+1)\,e^{i(m+2)\varphi}\left(\frac{1}{\rho}\frac{d}{d\rho} - \frac{m}{\rho^2} + \frac{E}{m+1}\right)R = h(\rho)\,e^{i(m+2)\varphi}, \qquad (25)$$

where the radial function h is determined by the expression in the bracket and the radial Schrödinger equation is used to eliminate the second-order derivative. Repeated actions of k times ($k \geqslant 2$) of the operator S_+ lead to

$$S_+^k(R\,e^{im\varphi}) = e^{i(m+2k)\varphi}h_k(\rho) = e^{i(m+2k)\varphi}\left[h_k'(\rho,E)\frac{d}{d\rho} + h_k''(\rho,E)\right]R \qquad (26)$$

where h_k' and h_k'' are the polynomial functions in energy.

Let R be the radial wavefunction of the 2D IHO state: $R \equiv P_{nm}$. In this case, according to the commutation relations, $h_k \sim P_{n-k,m+2k}$, i.e. operator S_+^k performs the transformations between the pairs of 2D IHO states belonging to the same energy level and whose quantum numbers m differ for $2k (k \geqslant 1)$.

When radial function R is the radial wavefunction of the 2D CHO state: $R \equiv R_{Em}$, the application of the operator S_+ produces different results to in the previous case of 2D IHO since it is now the operator in a different radial Hilbert subspace. From (25) and (26) it follows that it could be $h_k \sim R_{n',m+2k}$ with $n' \neq n-k (k \geqslant 1)$. It is of interest to find the criterion for the states (nm) and $(n', m+2k)$ to have the same energy E. Due to the results from subsection 3.2, the following inequalities must be satisfied: $E > 2n+m+1$ and $E > 2n'+m+2k+1$. Also, in order for the boundary conditions (5) and (6) to be fulfilled, it must be $h_k'(\rho_c, E) = 0$. In other words, 2D CHO states (nm) and $(n', m+2k)$ have the same energy for given confinement radius value ρ_c, if the following conditions are fulfilled:

$$(1)\quad E > \max(2n+m+1, 2n'+m+k+1) \qquad (27)$$

$$(2)\quad h_k'(\rho_c, E) = 0. \qquad (28)$$

It is clear from (25) and (28) that the conditions for degeneracy cannot be fulfilled for $k = 1$, in other words, the 2D CHO states (nm) and $(n', m+2)$ cannot have the same energy for any finite ρ_c value. When $k = 2$, the 2D CHO states (nm) and $(n', m+4)(n' \neq n-2)$ will have the same energy E if (1) $E > \max(2n+m+1, 2n'+m+5)$ and

$$h_2'(\rho_c, E) \equiv -\frac{2}{\rho_c}(m+2)\left(\frac{(m+1)(m+3)}{\rho_c^2} - E\right) = 0. \qquad (29)$$

The explicit appearance of energy term, E, in the above equation implies that the solution of equation (29) depends on energy, which suggests that different states might have the same energy at different values of confinement radius and simultaneous degeneracy can not arise. A similar conclusion is also valid for other values of k.

It is worth mentioning here that the above results can be obtained using the form of radial wavefunction (8) when the second condition for degeneracy (28) reduces to the requirement that for given ρ_c must be

$$F\left(a+k, b+2k, \rho_c^2\right) = F\left(a, b, \rho_c^2\right) = 0, \qquad (30)$$

where the arguments a and b are given by (16). When Gauss identities for confluent hypergeometric function are applied the same conclusions are obtained regarding the simultaneous degeneracy.

Therefore, it is proven that the degeneracy of energy levels with $\Delta m = 2k$, characteristic for 2D IHO and governed by SU(2) generators, is completely removed when the confinement is present. This is the expected result since the 2D IHO and 2D CHO Hamiltonians are different operators, although they are formally given by the same expressions, due to the fact that their domains are two different Hilbert spaces: $\mathcal{L}^2((0, \infty); \rho)$ and $\mathcal{L}^2((0, \rho_c); \rho)$, respectively.

So far we have investigated the possibility of simultaneous degeneracy among the 2D CHO states whose azimuthal quantum numbers m differ by an even integer: $\Delta m = 2k$. We shall now study the remaining possibility of simultaneous degeneracy at some ρ_c value among the 2D CHO states whose azimuthal quantum numbers m differ for some odd integer: $\Delta m = 2k + 1$. We use the radial wavefunction (8) and the properties of confluent hypergeometric function. In this case the 2D CHO states (nm) and $(n', m + 2k + 1)$ have the same energy E if the following conditions are fulfilled:

$$(1) \quad E > \max(2n + m + 1, 2n' + m + 2k + 2), \tag{31}$$

$$(2) \quad F\left(a, b, \rho_c^2\right) = F\left(a + \frac{2k + 1}{2}, b + 2k + 1, \rho_c^2\right) = 0, \tag{32}$$

for given ρ_c value. Unlike the Gauss identities connecting $F(a + p, b + 2p, z)$ and $F(a, b, z)$ with p being an integer and valid for every a, b and z, condition (32) connects these functions with p being a half-integer and it can be fulfilled only for specific values of the arguments excluding, of course, the simultaneous degeneracy in this case as well.

3.4. Accidental degeneracy

In the preceding subsection we proved that simultaneous degeneracy cannot appear in 2D CHO. However, comparing (13) and (21) shows that there are intersections between the levels, which is reasonable since the energy values are the functions of the confinement radius as a parameter. According to that fact it can happen that there exists a value of ρ_c at which two energy levels can intersect; in other words accidental degeneracy between them occurs, in the sense that it is not of systematic character, but appears at different ρ_c values for different pairs of states. The confinement radius values at which the level intersections appear and corresponding energy values for a number of states, given in table 3, are obtained by the Numerov–Cooley method with 80 000 grid point and numerical parameters $\epsilon = 1 \times 10^{-8}$, $P = 4$ and $M = 100$–1000.

According to (29) we stated that 2D CHO states (nm) and $(n', m + 4)$ with $n' \neq n - 2$ could have the same energy E for a given ρ_c value if $E = (m + 1)(m + 3)/\rho_c^2$. But this condition is too specific to be realized as confirmed by orderings (13) and (21), respectively. Moreover, using the theorems on interlacing of Bessel function zeros [9], it can be shown that the relative positions among the states with $\Delta m = 2k$ are the same in both small and large ρ_c limits, leading to the conclusion that even accidental degeneracy is ruled out here.

The only possibility for degeneracy to appear is between the states with $\Delta m = 2k + 1$ ($k \geqslant 1$) at confinement radius and energy satisfying condition (32). If the properties of interlacing of the Bessel function zeros are used [9], along with the fact that $E_{nm} < E_{n,m+p}$, where $p \geqslant 1$ is an integer, it can be shown that, for the given ρ_c, states (km) and $(0, m + 2k + 1)$ are included in accidental degeneracy and that also the following relations among k and m must be fulfilled: $m \geqslant 5$ if $k = 1$, $m \geqslant 1$ if $k = 2$ and $m \geqslant 0$ for $k \geqslant 3$. It is worth mentioning that the energy separation between them is 1 h.o. unit in $\rho_c \to \infty$ limit.

Table 3. Energy and confinement radius at which the crossing between the corresponding states occurs.

ρ_c	States	E
2.002 437 18	(15), (08)	19.862 154 88
2.140 391 94	(21), (06)	12.067 328 90
2.477 050 94	(16), (09)	16.455 165 88
2.699 633 22	(22), (07)	10.553 190 90
2.860 192 44	(30), (07)	9.879 926 49
3.062 617 45	(23), (08)	10.771 306 42
3.264 235 93	(31), (08)	10.171 751 44
3.349 221 46	(24), (09)	11.383 064 14
3.570 086 35	(32), (09)	10.856 761 60
3.628 051 34	(40), (09)	10.748 580 38

We note here that a similar conclusion about the eigenspectrum of 3D CHO was made in [16] wherein only a qualitative analysis was presented.

Concluding, we state that the $2n + |m|$ degeneracy is completely removed in 2D CHO system, as it is expected, and that there is no simultaneous degeneracy (of course, we exclude the degeneracy of the states with quantum numbers m and $-m$) at any value of the confinement radius. This is in *contrast* to the confined hydrogen atom problem where systematic degeneracy between the levels with $\Delta l = 2$ is present when confinement radius has the value $l(l+1)$. This particular result is obtained from symmetry consideration based on the Lenz vector which, together with orbital angular momentum, generates the SO(4) group which is the symmetry group for the unconfined hydrogen atom [4].

4. Annihilation and creation operators

Another special feature of the 2D IHO eigenspectrum is given by the equal energy separation of 1 h.o. unit between its successive levels. The aim in this section is to check whether the similar condition holds for the 2D CHO eigenspectrum. To do so, we proceed with the spherical components of annihilation and creation operators

$$a_{\pm 1} = \frac{1}{\sqrt{2}}(a_x \pm \mathrm{i}a_y), \qquad a^\dagger_{\pm 1} = \frac{1}{\sqrt{2}}(a_x \mp \mathrm{i}a_y), \tag{33}$$

named left and right annihilation and creation operators in [15] and [17], where their applications on the 2D IHO states are considered, and also their powers. In polar coordinates they are given by the expressions

$$a_{\pm 1} = \frac{1}{2}\,\mathrm{e}^{\pm \mathrm{i}\varphi}\left(\frac{\partial}{\partial\rho} \pm \frac{\mathrm{i}}{\rho}\frac{\partial}{\partial\varphi} + \rho\right) \tag{34}$$

$$a^\dagger_{\pm 1} = -\frac{1}{2}\,\mathrm{e}^{\mp \mathrm{i}\varphi}\left(\frac{\partial}{\partial\rho} \mp \frac{\mathrm{i}}{\rho}\frac{\partial}{\partial\varphi} - \rho\right) \tag{35}$$

$$a^2_{\pm 1} = \frac{1}{4}\,\mathrm{e}^{\pm 2\mathrm{i}\varphi}\left\{\frac{\partial^2}{\partial\rho^2} + \left(2\rho - \frac{1}{\rho}\right)\frac{\partial}{\partial\rho} - \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \rho^2 \pm 2\mathrm{i}\left[\left(1 - \frac{1}{\rho^2}\right)\frac{\partial}{\partial\varphi} + \frac{1}{\rho}\frac{\partial^2}{\partial\rho\partial\varphi}\right]\right\} \tag{36}$$

$$a^{\dagger 2}_{\pm 1} = \frac{1}{4}\,\mathrm{e}^{\mp 2\mathrm{i}\varphi}\left\{\frac{\partial^2}{\partial\rho^2} - \left(2\rho + \frac{1}{\rho}\right)\frac{\partial}{\partial\rho} - \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \rho^2 \pm 2\mathrm{i}\left[\left(1 + \frac{1}{\rho^2}\right)\frac{\partial}{\partial\varphi} - \frac{1}{\rho}\frac{\partial^2}{\partial\rho\partial\varphi}\right]\right\} \tag{37}$$

with more involved relations for higher powers. To begin with, we restrict ourselves to the operators a_{+1}^k. Using (34), (36) and similar expressions for $k \geqslant 3$ it is obtained

$$a_{+1}^k (R\,\mathrm{e}^{\mathrm{i}m\varphi}) = \mathrm{e}^{\mathrm{i}(m+k)\varphi} g_k(\rho) = \mathrm{e}^{\mathrm{i}(m+k)\varphi} \left[g_k'(\rho, E) \frac{\mathrm{d}}{\mathrm{d}\rho} + g_k''(\rho, E) \right] R \tag{38}$$

where the functions g_k' and g_k'' are the polynomial functions of their arguments and radial Schrödinger equation (4) was used to eliminate second- and higher-order derivatives of the radial wavefunction.

With $R \equiv P_{nm}$ and the commutation relation valid in the case of 2D IHO: $\left[a_{+1}^k, H\right] = k a_{+1}^k$, it follows that $g_k \sim P_{n-k,m+k}$. In view of this and expression (38), when $R \equiv R_{nm}$ (radial wavefunction of the 2D CHO state) we have g_k as the radial wavefunction of the 2D CHO state $(n', m+k)$ with $n' \neq n-k$ and energy $E-k$, where E is the energy of the 2D CHO state (nm) $(E \equiv E_{nm})$. Starting from (38) we can find the criterion for the energy separation between the 2D CHO states (nm) and $(n', m+k)$ to be k h.o. units: $E_{nm} - E_{n',m+k} = k$. This is realized if the following conditions are fulfilled:

$$(1) \quad E > \max(2n + |m| + 1, 2n' + |m+k| + k + 1) \tag{39}$$

$$(2) \quad g_k'(\rho_c, E) = 0. \tag{40}$$

For $k = 1$ it is found that $g_1' = \frac{1}{2}$ and g_2 is not the function from the 2D CHO Hilbert space (7) and energy separation between the 2D CHO states (nm) and $(n', m+1)$ cannot be 1 h.o. unit at any finite ρ_c value. This is not a very surprising result considering the behavior of the energy levels examined in the preceding section. When $k = 2$, the second condition (40) is of the form

$$g_2'(\rho_c, E) \equiv -(m+1)\left(\frac{1}{\rho_c} - \frac{\rho_c}{m+1}\right) = 0 \tag{41}$$

and the solution follows immediately

$$\rho_c = \sqrt{m+1} \quad \text{and} \quad m \geqslant 0. \tag{42}$$

With this specific choice of the confinement radius (42) one has $E_{nm} - E_{n',m+2} = 2$ and since ρ_c does not depend on energy, this general property includes all the states with given quantum numbers m and $m+2$ with non-negative m.

Finally, the radial quantum number n' is left to be identified. In $\rho_c \to \infty$ limit energy separation between the 2D CHO states (nm) and $(n', m+2)$ can be 0 when $n' = n-1$, 2 when $n' = n-2$, 4 if $n' = n-3$, generally, any even integer $2p$ when $n' = n-p-1$. According to the discussion from the preceding section, there are no intersections between these states so that energy separation between them is greater than the values listed above when the confinement radius has the finite value, leading to the conclusion $n' = n-1$ as the only possibility. We stress here that 2D CHO states (nm) and $(n-1, m+2)$ belong to the degenerated energy level of 2D IHO ($\rho_c \to \infty$ limit).

An analogous analysis performed for other operators leads to the conclusion that only their second powers $(k = 2)$ produce the same results, acting on the 2D CHO state (nm). Here, we give just the brief review:

- Operator a_{-1}^2 lowers both energy and angular quantum number m by 2, leading to $E_{nm} - E_{n',m-2} = 2$ if the following conditions are fulfilled:

$$(1) \quad E > \max(2n + |m| + 1, 2n' + |m-2| + 3), \tag{43}$$

$$(2) \quad g_2'(\rho_c, E) \equiv (m-1)\left(\frac{1}{\rho_c} + \frac{\rho_c}{m-1}\right) = 0, \tag{44}$$

leading to the results $n' = n - 1$ and

$$\rho_c = \sqrt{1-m} \quad \text{and} \quad m \leqslant 0. \tag{45}$$

- Application of $a_{+1}^{\dagger 2}$ on the 2D CHO state (nm) produces the other 2D CHO state $(n', m-2)$ with the energy higher by 2 then the energy of the former state if

$$(1) \quad E > \max(2n + |m| + 1, 2n' + |m-2| - 1) \tag{46}$$

$$(2) \quad g_2'(\rho_c, E) \equiv (m-1)\left(\frac{1}{\rho_c} - \frac{\rho_c}{m-1}\right) = 0. \tag{47}$$

The second condition is fulfilled only for

$$\rho_c = \sqrt{m-1} \quad \text{and} \quad m \geqslant 2 \tag{48}$$

and following the discussion given above, it is found that $n' = n + 1$.

- Application of $a_{-1}^{\dagger 2}$ on the 2D CHO state (nm) raises both energy and quantum number m by 2: $E_{n',m+2} - E_{nm} = 2$, if the following conditions are satisfied

$$(1) \quad E > \max(2n + |m| + 1, 2n' + |m+2| - 1), \tag{49}$$

$$(2) \quad g_2'(\rho_c, E) \equiv -(m+1)\left(\frac{1}{\rho_c} + \frac{\rho_c}{m+1}\right) = 0, \tag{50}$$

giving results $n' = n + 1$ and

$$\rho_c = \sqrt{-m-1} \quad \text{and} \quad m \leqslant -2. \tag{51}$$

Expressions (42) and (45) can be written more concisely

$$\rho_c = \sqrt{|m|+1} \tag{52}$$

and expressions (48) and (51) can be given the form

$$\rho_c = \sqrt{|m|-1} \quad \text{and} \quad |m| \geqslant 2. \tag{53}$$

The above expressions give the same ρ_c value when the associated quantum numbers m are such that $\Delta|m| = 2$. Confinement radius value (52) is identical with the position of the node of the radial wavefunction corresponding to the 2D IHO state with the radial quantum number $n = 1$ and given projection angular momentum quantum number m. This last value is obtained from the form of the radial wavefunction of the unconfined 2D IHO state $R_{nm} = \rho^{|m|}\,\mathrm{e}^{-\rho^2/2}F(-n, |m|+1, \rho^2)$ and the definition of the confluent hypergeometric function [8]. In this case, according to the incidental degeneracy [3], the energy of the lowest-laying 2D CHO state $(0m)$ (whose radial wavefunction has no zeros) is the same as the energy of 2D IHO state $(1m)$ and its value is $E = |m| + 3$. This 2D CHO state cannot be transformed under the action of the operators $a_{\pm 1}^2$ since the first conditions in (39) (for $k = 2$) and (43) impose the requirement on its energy $E > |m| + 3$.

From the previous discussion it is clear that the operators a_{+1}^2 and $a_{+1}^{\dagger 2}$ mutually transform the wavefunctions of the 2D CHO stationary states with non-negative m values, and the operators a_{-1}^2 and $a_{-1}^{\dagger 2}$ do the same thing with the states having non-positive m values when the confinement radius is determined according to (52)

$$\Psi_{nm} \xrightarrow{a_{+1}^2} \Psi_{n-1,m+2} \xrightarrow{a_{+1}^{\dagger 2}} \Psi_{nm} \quad \text{only for the 2D CHO states with } m \geqslant 0, n \geqslant 1; \tag{54}$$

$$\Psi_{nm} \xrightarrow{a_{-1}^2} \Psi_{n-1,m-2} \xrightarrow{a_{-1}^{\dagger 2}} \Psi_{nm} \quad \text{only for the 2D CHO states with } m \leqslant 0, n \geqslant 1. \tag{55}$$

Table 4. Energies of the 2D CHO stationary states (10), (11) and (12) for different values of the confinement radius ρ_c.

ρ_c	E_{10}	E_{11}	E_{21}
0.1	1523.564 674 02	2460.924 482 63	3542.501 753 69
0.2	380.897 008 36	615.237 370 66	885.632 217 73
0.5	60.981 459 38	98.478 581 13	141.745 193 93
1.0	15.391 538 05	24.776 009 99	35.605 834 87
2.0	4.440 505 19	6.825 774 45	9.582 826 32
5.0	3.000 000 17	4.000 003 78	5.000 027 16
∞	3.000 000 00	4.000 000 00	5.000 000 00

For the higher k values, solution of the equation given by condition (40) depends on energy. Thus, the requirement $E_{nm} - E_{n',m+k} = k$ can be fulfilled at different ρ_c values for different pairs of 2D CHO states (nm) and $(n', m+k)$, even with the same m value, yielding the conclusion that this property is not of systematic character, contrary to that we have already discussed.

The main conclusions obtained in this section are summarized as follows:

- Applying the annihilation and creation operators $a_{\pm 1}$ and $a^{\dagger}_{\pm 1}$, determined in (34) and (35), on the wavefunction of the 2D CHO stationary state does not result in the wavefunction corresponding to some other stationary state of this quantum system. As a consequence the energy separation between states with adjacent values of the quantum numbers, m and $m \pm 1$, and the same value of quantum number n cannot be 1 h.o. at any finite radius of confinement as it is the case with 2D IHO. This situation can be achieved only for large values of confinement radius $\rho_c \to \infty$ when the eigenspectrum of the 2D CHO coincides with that of 2D IHO (as it was discussed in subsection 3.2). Numerical results, obtained by applying Numerov–Cooley method with $\epsilon = 1 \times 10^{-8}$, $P = 4$ and $M = 100$–1000 and presented in table 4, support that conclusion.
- When the value of the confinement radius is determined by $\rho_c = \sqrt{|m| + 1}$, then the lowest-laying 2D CHO state with given quantum number m, $(0m)$ state, has the energy value of $E = |m| + 3$, which is the energy of the 2D IHO state with radial quantum number $n = 1$ and that quantum number m.
- When the value of the confinement radius is determined by $\rho_c = \sqrt{|m| + 1}$, then there is the one-to-one correspondence between the 2D CHO states (nm) with energy E (with the exception of the lowest-laying one), and the states $(n - 1, m + 2)$ with energy $E - 2$. The entries in table 5, obtained by Numerov–Cooley integration of the radial Schrödinger equation (4) with $\epsilon = 1 \times 10^{-8}$, $P = 4$ and $M = 100$–1000, confirm that statement. The mutual transformation among the states with quantum numbers m and $m + 2$ when $m \geqslant 0$ is realized via the operators a^2_{+1} and $a^{\dagger 2}_{+1}$, and the operators a^2_{-1} and $a^{\dagger 2}_{-1}$ realize the mutual transformation among the states with quantum numbers m and $m - 2$ for $m \leqslant 0$. This is opposite to the case of 2D IHO where all the operators $a_{\pm 1}$ and $a^{\dagger}_{\pm 1}$ act on the wavefunctions with both non-negative and non-positive m values [15, 17].

Finally, let us consider the shell-confined 2D HO, which differs from what we have investigated up to now, in that the form of the potential energy operator is defined by

$$V(\rho) = \begin{cases} \infty, & \rho \leqslant \rho_{c1} \\ \frac{1}{2}\rho^2, & \rho_{c1} < \rho < \rho_{c2} \\ \infty, & \rho \geqslant \rho_{c2}. \end{cases} \tag{56}$$

Table 5. Energies of the 2D CHO stationary states with $|m| = 3$–6 at the values of the confinement radius given by (52).

	$\rho_c = 2$		$\rho_c = \sqrt{5}$	
n	$E_{n,3}$	$E_{n-1,5}$	$E_{n,4}$	$E_{n-1,6}$
0	6.000 000 00		7.000 000 00	
1	12.689 595 23	10.689 595 23	13.280 433 90	11.280 433 90
2	21.906 316 47	19.906 316 47	21.614 063 80	19.614 063 80
3	33.609 195 86	31.609 195 86	31.948 808 97	29.948 808 97
4	47.787 150 07	45.787 150 07	44.269 364 41	42.269 364 41
5	64.436 221 82	62.436 221 82	58.569 882 78	56.569 882 78

Table 6. Energies of the 2D shell-confined harmonic oscillator states with $|m| = 3$–6 for the values of the confinement radius ρ_{c1} given by the first relation in (58) and $\rho_{c2} = 30$.

	$\rho_{c1} = 2$		$\rho_{c1} = \sqrt{5}$	
n	$E_{n,3}$	$E_{n-1,5}$	$E_{n,4}$	$E_{n-1,6}$
0	6.000 000 00		7.000 000 00	
1	8.990 042 64	6.990 042 64	10.057 100 78	8.057 100 78
2	11.762 855 42	9.762 855 42	12.893 525 96	10.893 525 96
3	14.420 698 07	12.420 698 07	15.610 564 61	13.610 564 61
4	17.003 910 56	15.003 910 56	18.249 085 58	16.249 085 58
5	19.533 501 00	17.533 501 00	20.830 685 79	18.830 685 79

This leads to the imposition of the Dirichlet boundary condition at two boundary points. Thus, the conditions to be satisfied by the radial wavefunction now assume the form

$$R_{nm}(\rho_{c1}) = R_{nm}(\rho_{c2}) = 0, \qquad \left(\frac{\mathrm{d}R_{nm}}{\mathrm{d}\rho}\right)_{\rho=\rho_{c1}} \neq 0, \qquad \left(\frac{\mathrm{d}R_{nm}}{\mathrm{d}\rho}\right)_{\rho=\rho_{c2}} \neq 0. \tag{57}$$

Following the analysis given in section 3, it can be shown that the conclusions similar to those obtained for the 2D CHO are valid for the shell-confined 2D HO only if

$$\rho_{c1} = \sqrt{|m| + 1} \quad \text{and} \quad \rho_{c2} = \infty, \tag{58}$$

This conclusion is confirmed by the results of the numerical tests presented in table 6 and reproduced by the same method and the same values of the parameters as for table 5.

5. Summary

Study of the characteristic features in the eigen spectra of the 2D CHO have been realized, for the first time, by the algebraic method. Using the infinitesimal operators of the SU(2) group, which is the symmetry group of the 2D IHO Hamiltonian, we proved that not only the simultaneous degeneracy, but also any accidental degeneracy is impossible between the 2D CHO states whose quantum numbers m differ by an even integer. In the confined system under consideration here, only accidental degeneracy between the states whose projection angular momentum quantum numbers differ for odd integers can appear. Confinement causes the breaking of any systematic degeneracy, but preserves SO(2) symmetry and double degeneracy of each energy level (except the energy levels with $m = 0$).

Application of the second powers of the spherical components of the annihilation and creation operators leads to the explanation of the separation pattern of 2 h.o. units in energy when the confinement radius has a specific value. Also, it is approved that the different operators from the Hilbert space of 2D CHO perform the mutual transformation between the states with non-negative and non-positive values of quantum number m at that specific value of the confinement radius, contrary to the 2D IHO, where the application of all the operators given in section 4 does not depend on the sign of quantum number m.

The applied method enabled us to investigate the structure of the 2D CHO eigenspectrum. We have applied an analogous method, based on SU(3) group generators and formalism of annihilation and creation operators, to the 3D CHO to explain thoroughly the regularities in its energy spectrum. Also, analysis based on the SO(3) group has enabled us to establish the criterion for simultaneous degeneracy in the confined 2D hydrogen atom, and this result, to our knowledge, has not been reported in the literature yet. This is the contents of our forthcoming reports.

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References

[1] Heiss W D (ed) 2005 *Quantum Dots: A Doorway to Nanoscale Physics* (Berlin: Springer)
[2] Jaskólski W 1996 *Phys. Rep.* **271** 1
Fowler P W 1984 *Mol. Phys.* **53** 865
Fowler P W 1985 *Mol. Phys.* **54** 129
Buchachenko A L 2001 *J. Phys. Chem.* **105** 5839
Dolmatov V K, Baltenkov A S, Connerade J-P and Manson S T 2004 *Radiat. Phys. Chem.* **70** 417
Gravesen J, Willatzen M and Voon L L Y 2005 *Phys. Scr.* **72** 105
Lo J H M, Klobukowski M and Diercksen G H F 2005 *Adv. Quantum Chem.* **48** 59
[3] Scherbinin A V, Pupyshev V I and Ermilov A Yu 1997 *Physics of Clusters* (Singapore: World Scientific) p 273
[4] Pupyshev V I and Scherbinin A V 1998 *Chem. Phys. Lett.* **295** 217
[5] Pupyshev V I and Scherbinin A V 2002 *Phys. Lett.* A **299** 371
[6] Schmelcher P and Schweizer W (ed) 2002 *Atoms and Molecules in Strong External Fields* (New York: Kluwer) chapter 38
[7] Montgomery Jr. H E, Aquino N A and Sen K D 2007 *Int. J. Quantum Chem.* **107** 798
[8] Abramowitz M and Stegun I A (ed) 1972 *Handbook of Mathematical Functions* (New York: Dover)
[9] Watson G N 1944 *A Treatise on the Theory of Bessel Functions* 2nd edn (Cambridge: University Press)
[10] Numerov B 1933 *Publs. Observatoire Central Astrophys. Russ.* **2** 188
[11] Cooley J W 1961 *Math. Comput.* **15** 363
[12] Jensen P 1983 *Comput. Phys. Rep.* **1** 1
[13] Elliott J P and Dawber P G 1979 *Symmetry in Physics* (London: Macmillan)
[14] Liu Y F, Huo W J and Zeng J Y 1998 *Phys. Rev.* A **58** 862
[15] Mota R D, Granados V D, Queijeiro A and Garcí a J 2002 *J. Phys. A: Math. Gen.* **35** 2979
[16] Aquino N A 1997 *J. Phys. A: Math. Gen.* **30** 2403
[17] Granados V D and Aquino N A 1999 *J. Mol. Struct. (THEOCHEM)* **493** 37