

**Rotating harmonic oscillator: Its general solution and the lack of ground-state energy equipartition**

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Analytically and numerically we give the general solution of the rotating harmonic oscillator. Our solution verifies the resolution of a disagreement in the literature, and can be understood physically. We point out that the solution demonstrates the incorrectness of the "energy equipartition theorem" for the ground state of all quantum oscillators.

The rotating - harmonic-oscillator (RHO) potential

$$V(r) = \frac{1}{2} m \omega^2 (r - r_0)^2 = \hbar \omega \left[ \frac{1}{2} (z - z_0)^2 \right] , \tag{1}$$

$$z \equiv \left( \frac{m \omega}{\hbar} \right)^{1/2} r = ar, \quad z_0 = ar_0 , \tag{2}$$

has a history which can arguably be traced back a century in the development of quantum theory.<sup>1-10</sup> Even so, the properties of the potential continue to be studied<sup>11-16</sup>—this study even including a disagreement on the properties of its solutions.<sup>12-16</sup>

In this Brief Report we will give the general solution showing how the eigenvalues change continuously from the three-dimensional harmonic oscillator ( $z_0 \rightarrow 0$ ) to the RHO "diatomic molecule" ( $z_0 \gg 0$ ). In doing so we can verify the proper resolution<sup>13,15,16</sup> of the above disagreement, which resolution can be understood on physical grounds.

To define the problem, start with the Schrödinger equation. Reduce out the angular variable, write the wave function as  $\chi(r) = r\psi(r)$ , change variables to  $z$ , and write all energies in terms of units of  $\hbar\omega$ :

$$\left[ \frac{d^2}{dz^2} - (z - z_0)^2 - \frac{l(l+1)}{z^2} + 2\epsilon \right] \chi = 0 . \tag{3}$$

First consider the large- $z_0$  case. Physically, this case is important. If the RHO potential is taken as a model diatomic-molecule potential,  $z_0$  can be written as

$$z_0 = 5.446114 (\mu_a k_{ic})^{1/2} r_A , \tag{4}$$

$$k_{ic} = 1/\lambda = v_{ic}/c = \omega_{ic}/2\pi c , \tag{5}$$

where  $\mu_a$  is the reduced mass in atomic mass units,  $k_{ic}$  is

the wave number for transition to the first vibrationally excited state in  $1000 \text{ cm}^{-1}$ , and  $r_A$  is the equilibrium distance of the atoms in angstroms. Thus, even for the hydrogen molecule,  $z_0$  is 6.01, and for other molecules it is larger. Now by writing the function of  $z$  in Eq. (3) as a McLaurin series about  $z_0$ , we can approximate the Schrödinger equation as

$$\left[ \frac{d^2}{dY^2} + Y^2 + \left( \frac{2\epsilon - \delta^2 - l(l+1)/(z_0 + \delta)^2}{[1 + 3l(l+1)/(z_0 + \delta)^4]^{1/2}} \right) \right] \chi = 0 , \tag{6}$$

$$Y = (z - z_0 - \delta) [1 + 3l(l+1)/(z_0 + \delta)^4]^{1/2} , \tag{7}$$

$$\delta = l(l+1)/z_0^3 . \tag{8}$$

For  $z_0 \gg 0$  the effect of the boundary condition at  $z = 0$  is negligible, so this is a one-dimensional harmonic oscillator. Thus we have the approximate eigenvalues ( $l = 0, 1, 2, \dots; \nu = 0, 1, 2, \dots$ )

$$\epsilon = \left( \nu + \frac{1}{2} \right) \left[ 1 + \frac{3l(l+1)}{(z_0 + \delta)^4} \right]^{1/2} + \frac{\delta^2}{2} + \frac{l(l+1)}{2(z_0 + \delta)^2} \tag{9}$$

$$\approx \left( \nu + \frac{1}{2} \right) + \frac{l(l+1)}{2z_0^2} + \left( \nu + \frac{1}{2} \right) \frac{3l(l+1)}{2z_0^4} + \dots . \tag{10}$$

In essence, the above is a variant of what Schrödinger did,<sup>8</sup> exhibiting the first three terms in a power series in  $z_0^{-2}$ . In the 1930's, papers appeared<sup>9,10</sup> using WKB and perturbation methods which carried out this power series higher, agreeing up to order  $(z_0^{-2})^4$ .

Now consider the small- $z_0$  case. There, one can use standard first-order perturbation theory about the  $z_0 = 0$  three-dimensional - harmonic-oscillator limit to obtain ( $l = 0, 1, 2, \dots, n = l, l+2, l+4, \dots$ )

$$\epsilon = \left( n + \frac{3}{2} \right) + \frac{1}{2} z_0^2 - z_0 \sum_{k=0}^{(n-l)/2} (-1)^k \frac{\Gamma(\frac{1}{2}(n-l) - k - \frac{1}{2})}{\Gamma(\frac{1}{2}(n-l) - k + 1)} \frac{\Gamma(l+k+2)}{\Gamma(l+k+\frac{3}{2})} \frac{1}{\Gamma(-k-\frac{1}{2})\Gamma(k+1)} . \tag{11}$$

For the general solution, first consider  $l = 0$ . Changing variables in Eq. (3) to  $y = z - z_0$ , one has the standard one-dimensional - harmonic-oscillator equation, but with the boundary conditions  $\chi(\infty) = 0$  and  $\chi(-z_0) = 0$ . Such a solution is well known analytically. It is the parabolic cylinder function  $D_\mu(y\sqrt{2})$ , with eigenvalue  $\mu + \frac{1}{2}$  deter-

mined by the boundary condition  $D_\mu(-z_0\sqrt{2}) = 0$ .<sup>17</sup> The eigenvalues  $\epsilon_{l=0}(z_0)$  are shown as the thick lines of Fig. 1.

For arbitrary  $l$ , one can numerically integrate the Schrödinger Eq. (3) to obtain the eigenvalues. Start by observing that at the origin and infinity, the wave function behaves as  $(z)^{l+1}$  and  $\exp[-\frac{1}{2}(z - z_0)^2]$ , respectively.

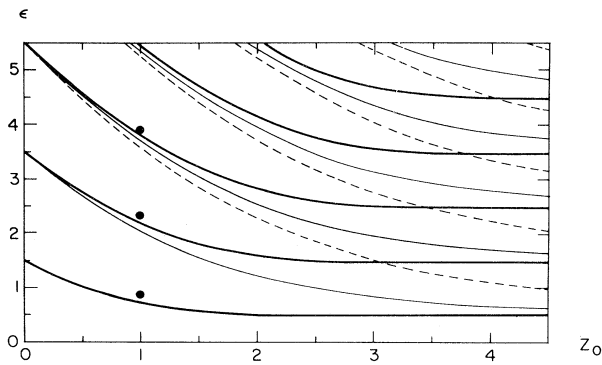


FIG. 1. Eigenvalues of the RHO potential as a function of  $z_0$ . The thick lines are for  $l=0$ , thin lines for  $l=2$ , and dashed lines for  $l=4$ . The heavy circles show first-order-perturbation-theory predictions for  $l=0$  about the  $z_0=0$  three-dimensional-harmonic-oscillator limit. [See Eq. (11).]

Thus, by using the standard numerical-integration techniques of splitting the Schrödinger equation into two first-order differential equations satisfying the above boundary conditions, integrating out from zero, and demanding that the wave function be small for  $z \gg z_0$ , one can obtain the eigenvalues for all  $l$  and  $z_0$ . We show these eigenvalues for  $l=2$  and 4 in Fig. 1 and  $l=1$  and 3 in Fig. 2.

Figures 1 and 2 allow us to see the general properties of the solutions. For the transition from the small- $z_0$  to the large- $z_0$  case, the solutions change as

$$\lim_{z_0 \rightarrow 0} \text{Curve}(n, l) \rightarrow \lim_{z_0 \rightarrow \infty} \text{Curve}(v = \frac{1}{2}(n-l), l) . \quad (12)$$

By Eq. (12) we mean that in the two limits of  $z_0$  shown, the two eigenvalue levels connect. This is reminiscent of the transition from  $L, S$  to  $J, S$  coupling.

Our results verify the conclusions of Refs. 13, 15, and 16 in the disagreement<sup>12-16</sup> mentioned above. Contrary to Refs. 12 and 14, for  $l \neq 0$ , there is a continuous change in all the eigenvalues which is dependent on the value of  $z_0$ .

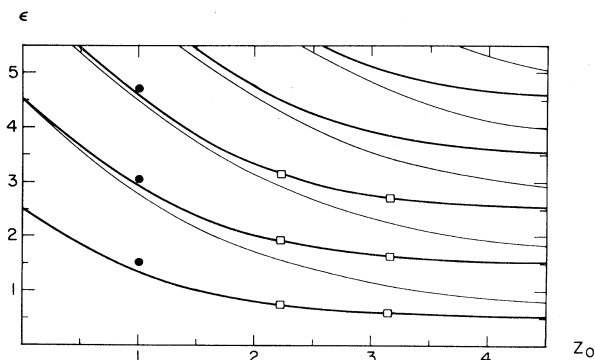


FIG. 2. Eigenvalues of the RHO potential as a function of  $z_0$ . The thick lines are for  $l=1$  and the thin lines for  $l=3$ . The heavy circles show first-order-perturbation-theory predictions for  $l=1$  about the  $z_0=0$  three-dimensional-harmonic-oscillator limit. [See Eq. (11).] The small squares are specific values for  $l=1$  given in Table 2 of Ref. 13.

There is no solution which is independent of  $z_0$  with eigenvalues  $(n + \frac{1}{2})$ . From our point of view this makes sense intuitively. As  $z_0$  gets larger, we are changing continuously from the three-dimensional-harmonic-oscillator problem to the one-dimensional-harmonic-oscillator problem. The change is a continuous perturbation from one limit to the other, and is nonsingular.

Further, our figures show where the special-case exact results of Ref. 16 fit in. In Ref. 16 it was shown by continued-fraction methods that for certain specific values of  $z_0$ , the continued-fraction solution terminates to give exact eigenvalues  $(\frac{1}{2} + l + \text{positive integer})$ . [These methods also specifically exclude the predicted exact solutions of Refs. 12 and 14,  $\epsilon = (l + \frac{3}{2})$ ,  $l \neq 0$ , supposedly true for all  $z_0$ .] The above intuitively is not in disagreement with us. For any given  $(n, l)$ , as  $z_0$  increases the eigenvalue curves always decrease and thus can cross the value  $(\frac{1}{2} + l + \text{positive integer})$ .

In particular, Ref. 16 derives<sup>18</sup>

$$\epsilon = l + \frac{5}{2} \text{ at } z_0 = 1/(l+2)^{1/2} , \quad (13)$$

and

$$\epsilon = l + \frac{7}{2} \text{ at } z_0 = \left[ \frac{(4l+9)}{(l+2)(l+3)} \right]^{1/2} . \quad (14)$$

Table I shows the  $l=0, 1, 2$ , and 3 special-case eigenvalues of Eqs. (13) and (14) that are contained in and agree with Figs. 1 and 2.

Finally, this brings up the<sup>19</sup> quantum "folk theorem," that a confined oscillator has  $\frac{1}{2}$  quantum per degree of freedom as a ground-state energy. For the  $z_0=0$  three-dimensional harmonic oscillator, this is correct. But as  $z_0$  gets larger, the ground-state energy goes down to  $\frac{1}{2}$  (as Figs. 1 and 2 show) for all  $l$ . Further, if we consider the  $N$ -space-dimensional rotating harmonic oscillator, the same phenomena will occur, with the even higher ground-state energy of  $N/2$  also going down to  $\frac{1}{2}$ .

What is going on? Descriptively, in the one-dimensional problem, the ground-state Gaussian is large, approximately between some  $-x_T$  and  $+x_T$ . In the three-dimensional case, the boundary condition at the origin means that the

TABLE I. Special-case exact eigenvalues of Eqs. (13) and (14) that are contained in our Figs. 1 and 2.

$l$	$\epsilon$	$z_0$
0	$\frac{5}{2}$	$(\frac{1}{2})^{1/2} = 0.707$
0	$\frac{7}{2}$	$(\frac{3}{2})^{1/2} = 1.225$
1	$\frac{7}{2}$	$(\frac{1}{3})^{1/2} = 0.577$
1	$\frac{9}{2}$	$(\frac{13}{12})^{1/2} = 1.041$
2	$\frac{9}{2}$	$\frac{1}{2} = 0.5$
2	$\frac{11}{2}$	$(\frac{17}{20})^{1/2} = 0.922$
3	$\frac{11}{2}$	$(\frac{1}{5})^{1/2} = 0.447$

wave function must go to zero at the origin (this is like the first excited state in the one-dimensional problem) so that the ground-state energy is raised to  $\frac{3}{2}$ . However, as  $z_0$  gets large, on the left the wave function does not have to go to zero near  $z_0$ . Thus the distance in the radial direction over which the wave function can be large becomes effectively that of a one-dimensional problem (say, from  $-x_T + z_0$  to  $+x_T + z_0$ ). This allows the ground-state energy to approach that of a real one-dimensional oscillator.

Physically, one must realize that the above amounts to describing the results of analyzing the expectation values of the kinetic- and potential-energy terms of the Hamiltonian, minimizing the energy with respect to an  $x$ - $p$  uncertainty limit. This is the type of analysis that Messiah<sup>20</sup> applies to the hydrogen atom, and which must be done before a "theorem" is applied to any particular potential. To show this we repeat Messiah's analysis<sup>20</sup> for this system. (Note that all the arguments used to show the incorrectness of this "theorem" could be realized from any three-dimensional potential with many bound states and a minimum away from the origin, such as the Morse potential.)

Putting units back in, for  $r_0 = 0$ , the lowest state has  $l = 0$ . First consider the  $x$  direction. The average of the potential energy in the  $x$  direction around some classical turning points  $\pm x_T$  is  $m\omega^2 x_T^2/6$ . If we take  $\Delta x = x_T$  in the  $x$ - $p$  uncertainty relation, this yields a lower bound for  $\Delta p$  of  $\hbar/2x_T$ .

Take the kinetic energy as  $(\Delta p)^2/2m = \hbar^2/(4mx_T^2)$ . The sum of this kinetic energy and the average potential energy has a minimum at  $x_T^4 = 3\hbar^2/(4m^2\omega^2)$ , giving a value for the total minimum energy in this degree of freedom of

$$E_x = \frac{1}{2}\hbar\omega 3^{-1/2} . \quad (15)$$

(This answer is not precise, as it need not be.) However, now the total ground-state energy is predicted to be three times  $E_x$ , from all the  $x$ ,  $y$ , and  $z$  degrees of freedom.

Contrary to this, in the large  $r_0$  limit, the above argument goes through for one degree of freedom (the radial degree), but the angular coordinates give a vanishingly small number. To see this, consider the  $\theta$  coordinate. (We here ignore the complications of using the rigorous angular operators,<sup>21</sup> to make the arguments simpler.) At the position  $r_0$ , the potential energy is zero. The angle variable can vary over  $\pi$ . Taking this as  $\Delta\theta$ , the  $p_\theta$ - $\theta$  uncertainty relation says that  $\Delta p_\theta \geq \hbar/(2\pi)$ . Using  $\Delta p_\theta$  as  $p_\theta$  in the kinetic, and hence the total, energy gives<sup>22</sup>

$$E_\theta = \hbar\omega/(8\pi^2 z_0^2) , \quad (16)$$

which is vanishingly small as  $r_0$  gets larger.

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<sup>1</sup>In 1886, one year after Balmer (Ref. 2) had empirically determined his form of the hydrogen spectra, Deslandres did the same for the diatomic molecule (Ref. 3). Later, in his fundamental old-quantum-theory papers, Bohr was able to solve the hydrogen atom (Ref. 4), but he could not obtain the Deslandres terms for the diatomic molecule (Ref. 5). That remained for the last paper of Schwarzschild (Ref. 6). Finally, although most people know that the first of Schrödinger's basic papers on quantum mechanics solved the hydrogen atom (Ref. 7), few know that in his second paper, he approximately solved the rotating harmonic-oscillator problem for the diatomic molecule (Ref. 8). A more detailed historical account will appear elsewhere.

<sup>2</sup>J. J. Balmer, Verh. Naturforsch. Ges. Basel 7, 548, 750 (1885); Ann. Phys. Chem. 25, 80 (1885).

<sup>3</sup>H. Deslandres, C. R. Acad. Sci. 103, 375 (1886).

<sup>4</sup>N. Bohr, Philos. Mag. 26, 1, 476 (1913).

<sup>5</sup>N. Bohr, Philos. Mag. 26, 857 (1913).

<sup>6</sup>K. Schwarzschild, Sitzungsber. K. Preuss. Akad. Wiss. 435, 538 (1916).

<sup>7</sup>E. Schrödinger, Ann. Phys. (Leipzig) 79, 361 (1926).

<sup>8</sup>E. Schrödinger, Ann. Phys. (Leipzig) 79, 489 (1926).

<sup>9</sup>J. L. Dunham, Phys. Rev. 41, 721 (1932).

<sup>10</sup>J. E. Rosenthal and L. Motz, Phys. Rev. 23, 259 (1937).

<sup>11</sup>N. Fröman and P. O. Fröman, Ann. Phys. (N.Y.) 115, 169 (1978).

<sup>12</sup>G. P. Flessas, Phys. Lett. 71A, 315 (1979).

<sup>13</sup>N. Fröman, P. O. Fröman, and F. Karlsson, Phys. Lett. 77A, 397 (1980).

<sup>14</sup>G. P. Flessas, Nuovo Cimento 64B, 358 (1981).

<sup>15</sup>F. Karlsson, P. O. Fröman, and A. Hökback, Nuovo Cimento 70B, 155 (1982).

<sup>16</sup>V. Singh, S. N. Biswas, and K. Datta, J. Math. Phys. 23, 1323 (1982).

<sup>17</sup>We found it convenient to derive and use a nonstandard representation of the parabolic cylinder function  $D_\mu(y\sqrt{2})$  to calculate the zeros of  $D_\mu(-z_0\sqrt{2})$  as a function of  $z_0$ . This representation is

$$2^{\mu/2} \exp(z^2/2) \sum_{n=0}^{\infty} [(-z^2)^n/\Gamma(n+1)] \\ \times [\cos(\pi\mu/2)\Gamma(n+\frac{1}{2}+\mu/2)/\Gamma(n+\frac{1}{2}) \\ + \sin(\pi\mu/2)\Gamma(n+1+\mu/2)/\Gamma(n+\frac{3}{2})] .$$

<sup>18</sup>Our Eq. (13) rectifies a crucial misprint three lines below Eq. (23) of Ref. 16. There, " $(l+2)/2$ " was written as " $1/2(l+2)$ ," with their  $\alpha = 1/2z_0^2$  and  $\lambda = \epsilon - \frac{1}{2}$  in our notation. We thank J. P. Ader for pointing this out to us.

<sup>19</sup>"Folk theorem" is a term which mathematical physicists like to use to describe widely known results which may, however, be incorrect. A definition perhaps can be taken from a quote at the end of the preface to R. F. Streater and A. S. Wightman, *PCT, Spin & Statistics, & All That* (Benjamin, New York, 1964). "... we have eliminated all theorems whose proofs are nonexistent."

<sup>20</sup>A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1966), Vol. 1, p. 413.

<sup>21</sup>See, for example, P. Carruthers and M. M. Nieto, Rev. Mod. Phys. 43, 277 (1971), and references therein.

<sup>22</sup>See, for example, T. T. Taylor, *Mechanics: Classical and Quantum* (Pergamon, Oxford, 1976), p. 50.