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Brief Reports

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Rotating harmonic oscillator: Violation of an equipartition theorem

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The rotating harmonic oscillator in three dimensions (owing its relevance to the diatomic molecule) has been reinvestigated by Nieto and Gutschick. They have demonstrated that the ground-state energy, which is expected (on the basis of naive arguments involving the uncertainty principle) to acquire a contribution $\frac{1}{2}\hbar\omega$ from each degree of freedom, and hence should have a value $\frac{3}{2}\hbar\omega$, does, on the contrary, in the limit of large equilibrium separation (between the atoms), go to the asymptotic value of only $\frac{1}{2}\hbar\omega$, thereby violating what these authors called a "quantum folk theorem." The present Brief Report consists of showing that these conclusions can be elucidated analytically and further extended through the $1/N$ expansion (N being the dimensionality of the space), leading, in particular, to the result that for the case $N=2$ the approach to the asymptotic limit ($\frac{1}{2}\hbar\omega$) is, surprisingly, from below, thereby providing an even stronger violation of this type of "equipartition theorem."

The history of the rotating harmonic oscillator, as pointed out, by Nieto and Gutschick,[1] goes back to the early days of quantum mechanics when Schrödinger[2] obtained a perturbative solution to the problem. The study of this system derives its importance from the consideration of the energy levels of the diatomic molecule, the systematics of the spectral terms of which were investigated almost a century ago by Deslandres.[3] The rotating harmonic oscillator, nevertheless, has continued to attract attention.[4-8]

The rotating harmonic oscillator is governed by the potential $V(r)=\frac{1}{2}m\omega^2(r-a)^2$ where m, ω, and a are the mass, frequency, and equilibrium displacement parameters, respectively. On the basis of some physical reasoning substantiated by analytical calculations and the numerical solution of the corresponding Schrödinger equation in N dimensions, Nieto and Gutschick[1] arrived at the conclusion that as $a\rightarrow 0$ the ground-state energy, as should be the case in this oscillator limit, goes to $\frac{1}{2}N\hbar\omega$, while in the limit $a\rightarrow\infty$ the ground-state energy approaches the asymptotic value $\frac{1}{2}\hbar\omega$ (from above), a result which appears to violate the usual expectation ("folklore") that the uncertainty principle would imply a contribution $\frac{1}{2}\hbar\omega$ per degree of freedom for an oscillator. Of course, as these authors pointed out, the radial part of the wave function $R(r)$, in three dimensions, written as $u(r)/r$, results in the radial function $u(r)$ satisfying an equation identical to that in one dimension but with the difference in the condition that $u(r)$ must vanish at the origin, which leads to the result that the ground-state energy for a three-dimensional oscillator has the energy which would correspond to the first odd-wave function of the one-dimensional oscillator, namely, $\frac{3}{2}\hbar\omega$. However, since the wave function has a maximum near $r=a$ for this oscillator, the boundary condition at the origin is automatically satisfied in the asymptotic limit ($a\rightarrow\infty$) and, consequently, due to this relaxation, the ground-state energy turns out to be $\frac{1}{2}\hbar\omega$. The same conclusion may also be arrived at by observing that the Laplacian operator in three dimensions differs from that in one dimension by the term $(2/r)dR(r)/dr$, which for asymptotic a contributes vanishingly compared with the curvature of the wave function $(d^2/dr^2)R(r)$.

The present study demonstrates that the $1/N$ expansion (where N is the dimensionality of the space) is particularly efficacious for the explication of the aforementioned results and indeed goes further to indicate for two dimensions ($N=2$) an even more interesting consequence, in that the asymptotic limit of the ground-state energy $\frac{1}{2}\hbar\omega$ is approached from below, a conclusion which is supported by the variational approach and borne out by explicit numerical calculations, thereby indicating an even stronger violation of this type of "equipartition theorem."

Several authors[9-15] have developed the $1/N$ expansion, in general, and for the solutions of the Schrödinger equation, in particular, by considering the radial part of the wave function for a particle moving in a suitably defined potential[10] in N dimensions. In units where $m=1=\hbar$ the kinetic-energy operator in a state of angular momentum l becomes

$$-\frac{1}{2}\left[\frac{d}{dr^2}+\frac{N-1}{r}\frac{d}{dr}\right]+\frac{l(l+N-2)}{2r^2}\ .$$

Setting the radial part of the wave function $R(r)=r^{(N-1)/2}u(r)$ the radial equation becomes

$$-\frac{1}{2}\frac{d^2}{dr^2}u+k^2\left[\frac{(1-1/k)(1-3/k)}{8r^2}+V(r)\right]u=Eu\ , \qquad (1)$$

where $k=N+2l$. In the limit of large k (large N) the eigenfunctions $u(r)$ have a maximum about the minimum

r_0 of the effective potential $\frac{1}{8}r^{-2}+V(r)$ and the spectrum becomes concentrated around $E^{(-2)}=1/8r_0^2+V(r_0)$, where $k^2E^{(-2)}$ is the energy of a classical particle of angular momentum $L_{\rm cl}=\frac{1}{2}k$ executing circular motion in the potential and constituting the lowest-order approximation to the eigenvalue. A systematic expansion of the eigenvalue has been developed[10] by these authors in powers of $1/k$ and involve the solution of algebraic equations. This expansion is, in effect, nonperturbative (in the sense that power series in the coupling constant are not involved) and even the leading order of the series (as will clearly emerge in the present case) may exhibit qualitative features of the problem that are not readily evident in other approximations. Moreover, in being most effective for low-lying states, the method is complementary to the Wentzel-Kramers-Brillouin (WKB) approach.

The first few terms in the $1/N$ expansion for the ground-state energy for the rotating harmonic oscillator in N dimensions is given by

$$E=N^2\frac{\Omega x}{8}\left[1+\frac{x^2}{4-3x^2}\right]+\frac{N\Omega}{2}(1-x)+\frac{\Omega x}{32}(1-x^2)(12-24x+11x^2)+\frac{1}{N}\frac{9\Omega x^2}{16}(1-x)(1+\cdots)+\cdots\ , \tag{2}$$

where $\Omega^2=\omega^2/N^2+\frac{3}{4}r_0^2$, with r_0 the minimum of the effective potential given by the solution of the equation

$$-\frac{N^2}{4\omega^2}+r_0^3(r_0-a)=0\ , \tag{3}$$

and the dimensionless parameter $x=1/\Omega r_0^2$. It is to be noted that while in the oscillator limit ($a\to 0\Rightarrow x\to 1$ and $\Omega\to 2\omega/N$) only the leading term in the energy expansion survives yielding $E=N(\hbar\omega/2)$; in the other extreme, the asymptotic limit ($a\to\infty\Rightarrow x\to 0$ and $\Omega\to\omega/N$) the ground-state energy (with only the second term contributing) becomes $E=\hbar\omega/2$. Thus the $1/N$ expansion exhibits in a particularly elegant fashion the different limits in agreement with numerical calculations. Furthermore, the approach to asymptopia is also correctly given as can be seen by retaining next to leading-order terms (up to x^2) yielding

$$E=\frac{1}{2}\omega+\frac{1}{8a^2}(N-1)(N-3)+\frac{3}{16a^4\omega}(N-1)(N-3)+\cdots\ , \tag{4}$$

(in units $\hbar=1$). It is immediately seen that for $N=3$ the approach to the asymptotic limit is in fact faster than any power of $1/a$, a conclusion which also follows from the asymptotic behavior of the parabolic cylindrical functions which are the solutions in that case. [Indeed

$$E=\tfrac{1}{2}\hbar\omega+(m\omega a/\sqrt{\pi}\hbar)e^{-m\omega a^2/\hbar}+\cdots$$

here.] However, for $N=2$ the approach is from below as the inverse square power. This behavior may be related to quantum fluctuations about the classical equilibrium position by considering the radial equations for values of the parameter a and $a+\delta a$ and constructing the Wronskian of the two solutions $u(r,a+\delta a)$ and $u(r,a)$ which vanishes at $r=0$ and $r\to\infty$ and yields in the limit $\delta a\to 0$ the result

$$\frac{\partial E}{\partial a}=-m\omega^2(\langle r\rangle-a)\ . \tag{5a}$$

A similar procedure with respect to ω gives

$$\frac{\partial E}{\partial\omega}=m\omega\langle(r-a)^2\rangle\ . \tag{5b}$$

Thus the qualitative difference in asymptotic behavior for $N=2$ and $N=3$ may be attributed to the relative magnitudes of $\langle r\rangle$ and a in the two cases arising from the nature of the wave function and the volume element. The particular case of $N=2$ exhibits peculiar asymptotic behavior, which is easily confirmed by employing the variational method with trial wave function of the form $\exp[-m\omega/\hbar(r-b)^2]$ with b as the parameter to be varied. Though the expectation value of the Hamiltonian involves error functions, nevertheless, the limit of large a may be studied analytically to yield a minimum energy $\frac{1}{2}\hbar\omega-1/8a^2+\cdots$ in agreement with the contention that the energy for $N=2$ goes below $\frac{1}{2}\hbar\omega$, a result which is borne out by explicit numerical calculations.

The genesis of differences in behavior of the ground-state energy as a function of the parameter a for different dimensionality may be traced to the starting point [Eq. (1)], wherein it may be observed that the "centrifugal" potential $(1-1/k)(1-3/k)/8r^2$ vanishes both for $N=1$ and $N=3$ giving an equation identical to that in one dimension though in the three-dimensional case the boundary condition at the origin is different. Again for $N=2$ this is attractive while for $N=4$, 5, it is repulsive. In fact this is basically why the approach to the asymptotic value is exponential for $N=3$ and power law for other N and is from below in the case $N=2$.

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