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LETTER TO THE EDITOR

# Precise determination of the energy levels of the anharmonic oscillator from the quantization of the angle variable

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**Abstract.** Using an ansatz motivated by the classical form of $e^{i\phi}$, where $\phi$ is the angle variable, we construct operators which satisfy the commutation relations of the creation–annihilation operators for the anharmonic oscillator. The matrix elements of these operators can be expressed in terms of *entire* functions in the position complex plane. These functions provide solutions of the Ricatti equation associated with the time-independent Schrödinger equation. We relate the normalizability of the eigenstates to the global properties of the flows of this equation. These exact results yield approximations which complement the WKB approximation and allow an arbitrarily precise determination of the energy levels. We give numerical results for the first 10 levels with 30 digits. We address the question of the quantum integrability of the system.

In recent years, many interesting questions regarding the quantum behaviour of systems which classically exhibit sensitive dependence on the initial conditions have been raised [1]. Classically integrable systems with a perturbation [2] provide rich sequences of transitions to chaos when the parameter controlling the perturbation is increased. Recent studies [3] of the energy spectra of the quantum version of such systems have provided unexpected results. Ultimately, the questions raised in this context may become relevant for quantum field theory on a space lattice, i.e. a system of coupled anharmonic oscillators. It would be interesting to understand whether the tool which is used classically to control the effects of the perturbation, namely the analysis of small denominators, can also be used for the quantum problem. The prerequisite for such a discussion is to have at hand a quantum version of the action-angle variables for classically nonlinear problems. Due to the ordering problem this is a non-trivial issue.

In this letter, we construct a quantum operator corresponding to the classical quantity $e^{i\phi}$, $\phi$ being the angle variable, for one of the simplest nonlinear problems with one degree of freedom, namely the anharmonic oscillator with an energy operator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \tfrac{1}{2}m\omega_0^2\hat{x}^2 + \lambda\hat{x}^4. \tag{1}$$

We assume $\lambda > 0$, but the sign of $\omega_0^2$ is not crucial for the calculations which follow. The method proposed can indeed be extended straightforwardly to the case where $V$ is any even polynomial bounded from below. Classically, the angle variable $\phi$ satisfies the Poisson bracket relation $\{H, e^{i\phi}\} = -ie^{i\phi}\omega(H)$, where $\omega$ is one over the derivative of the action with respect to the energy. A quantum version of this equation reads as

$$[\hat{H}, \hat{A}] = \hbar\hat{A}\Delta(\hat{H}) \tag{2}$$

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where $\Delta$ is a function which remains to be specified. In order to construct an operator $\hat{A}$ satisfying equation (2), we use an ansatz which, in the classical case, provides an explicit expression for $e^{i\phi}$ in terms of $p$ and $x$. The form of the classical ansatz can be obtained directly from the well known expression of the angle variable in terms of the position and the energy. In addition, we pick a special type of ordering, namely

$$\hat{A} = \sum_{n=0}^{\infty} \hat{x}^{2n}(i\hat{p}K_n(\hat{H}) + \hat{x}L_n(\hat{H})). \tag{3}$$

With this choice of ordering, a solution $A$ multiplied on the right by an arbitrary function of $H$ is another solution. In the classical theory, this ambiguity is raised by imposing that $e^{i\phi}$ be on the unit circle. In the case of the potential given in equation (1), we obtain a formal solution of equation (2) provided that for $n \geqslant 0$

$$\begin{aligned}
&\frac{\hbar^2}{m}(n+2)(n+1)(2n+3)K_{n+2}(\hat{H}) \\
&\qquad = \Bigg[ -(2\hat{H} + \hbar\Delta(\hat{H}))2(n+1)K_{n+1}(\hat{H}) \\
&\qquad\quad + \left((2n+1)m\omega_0^2 - \frac{m(\Delta(\hat{H}))^2}{2n+1}\right) K_n(\hat{H}) + \lambda 4nK_{n-1}(\hat{H}) \Bigg] \\
&L_n(\hat{H}) = -\frac{m\Delta(\hat{H})}{2n+1}K_n(\hat{H}) - \hbar(n+1)K_{n+1}(\hat{H}).
\end{aligned} \tag{4}$$

If $\hbar$ is set to zero in equation (4) and $\hat{H}$ replaced by a numerical value $E$, one recovers the difference equations for the corresponding classical equation mentioned above. Our starting equation (2) can be compared with the operator equation $[F(\hat{x}, \hat{p}), \hat{H}] = i\hbar$, a quantum version of $\{\phi/\omega(H), H\} = 1$, solved by Bender [4] with a different type of ansatz (which requires negative powers of $\hat{p}$ or $\hat{x}$).

We now study the matrix element $\langle x|A|E\rangle = (\hbar K\mathrm{d}/\mathrm{d}x + L)\langle x|E\rangle$, where $L$ and $K$ are short for $\sum_{n=0}^{\infty} L_n(E)x^{2n+1}$ and $\sum_{n=0}^{\infty} K_n(E)x^{2n}$ respectively. In the following, the dependence of $L$, $K$ and $\Delta$ on $E$ is implicit and primes denote $x$ derivatives. Equation (2) is satisfied for an arbitrary potential provided that

$$\begin{aligned}
&\frac{\hbar}{2m}K'' + \frac{L'}{m} + K\Delta = 0 \\
&\frac{\hbar}{2m}L'' - 2K'(E-V) + KV' + L\Delta = 0.
\end{aligned} \tag{5}$$

In the case of the potential given in equation (1), these equations can be solved using the linear recursion relations given by equation (4) with $\hat{H}$ replaced by $E$. As a result, we get $\langle x|\hat{A}|E\rangle$ as a function of $E$, $\Delta(E)$, $K_0$ and $K_1$. If both $K_0$ and $K_1$ are zero, then $\langle x|\hat{A}|E\rangle = 0$, consequently we require at least one of them to be non-zero. In order to fix the ambiguity mentioned above, we shall impose that the first non-zero $K_n$ to be 1. One can prove rigorously that $|K_n| < C_1(C_2)^n(n!)^{-2/3}$ with $C_1$ and $C_2$ independent of $n$. This bound implies that $L$ and $K$ are *entire* functions of the position seen as a complex variable. This allows us to controllably approximate these functions in terms of their truncated power series. Note that in the classical case, the factorial suppression is absent and the functions $L$ and $K$ have a common finite radius of convergence which reflects the existence of turning points.

We are now in a position to construct formal solutions of the time-independent Schrödinger equation. First we notice that

$$L^2 - \hbar(L'K - K'L) - 2mK^2(V - E) = K_0(\hbar^2 K_1 + \hbar m \Delta K_0 + 2mK_0 E). \tag{6}$$

Recalling equation (4), the equality clearly holds at $x = 0$. In addition, equation (5) implies that the derivative of the left-hand side is zero, consequently it holds for any $x$. Adjusting the constants $K_0$ and $K_1$ in such a way that the left-hand side of equation (6) is zero, and dividing by $K^2$ (temporarily assuming that $K \not\equiv 0$), we obtain that $L/K$ satisfies the Ricatti equation

$$\hbar\left(\frac{L}{K}\right)' = \left(\frac{L}{K}\right)^2 - 2m(V - E). \tag{7}$$

A detailed study of equation (5) shows that equation (7) is also satisfied near a zero of $K$. Parametrizing the wavefunction as

$$\langle x|E\rangle \propto \exp\left\{\frac{1}{\hbar}\int_{x_0}^{x} \mathrm{d}y \frac{L(y)}{K(y)}\right\} \tag{8}$$

we find that equation (7) is the Ricatti form of the time independent Schrödinger equation. Note that equation (8) implies that $A|E\rangle = 0$. We still need to specify the conditions under which the right-hand side of equation (6) is zero. After fixing the arbitrariness in the coefficients as discussed above, there remain two possibilities. The first one is $K_0 = 1$ and $K_1 = -2mK_0/\hbar^2(\frac{1}{2}\Delta\hbar + E)$ which corresponds to an even eigenfunction $\langle x|E\rangle$. The second possibility is $K_0 = 0$ and $K_1 = 1$, which corresponds to an odd eigenfunction, and for which $L/K$ has automatically the $-\hbar/x$ singularity at the origin. In both cases, equation (4) defines uniquely $L(x)$ and $K(x)$ given $E$ and $\Delta$. From the uniqueness of the solution of the Ricatti equation, given a condition at $x = 0$ ($L/K = 0$ in the even case and $K/L = 0$ in the odd case), $L/K$ is indeed $\Delta$-independent as one can check order by order in the expansion of $L/K$ near $x = 0$. A particularly convenient choice is $\Delta = 0$, because in this case equations (5) and (8) imply that $|\langle x|E\rangle|^2 \propto |K(x)|$. We shall now use the formal solution of the Schrödinger equation to find sharp upper and lower bounds on the energy levels.

Our basic tool to find accurate upper bounds on the energy levels will be the theorem proven in [5] that for a Sturm–Liouville problem the $n$th eigenfunction divides the fundamental domain into $n$ parts by means of its nodal points. For the problem discussed here, the zeros of $\langle x|E\rangle$ are the poles of $L/K$ which is seen most easily by picking $\Delta = 0$. Consequently, if $K$ has more than $n$ zeros at finite $x$ (which are not zeros of $L$), then $E > E_n$. Furthermore, if $E$ is decreased continuously, the largest zero of $K$ increases continuously. When $E$ reaches $E_n$, a pair of zeros disappears at infinity. One can then monitor the 'entrance' of the zeros in the region $x \leqslant a$ while $E$ increases, by finding $E$ such that $K(a, E) = 0$. This can be done using Newton's method with an appropriate truncation in the expansion of $K$. One can then check whether the existence of the zero can be established despite the errors due to the truncation (which can be estimated using the bound mentioned above).

Lower bounds can be found from the requirement that the wavefunction $\langle x|E\rangle$ is normalizable. Due to the fact that $\langle x|E\rangle$ has a definite parity, we will restrict the discussion to the positive $x$ part of the $(x, L/K)$ plane. This half plane can be divided into a region where $L/K$ increases and a region where $L/K$ decreases. The boundary between these two regions is characterized by $(L/K)' = 0$ which by equation (7) implies $(L/K) = \pm\sqrt{2m(V - E)}$. For this reason we call this curve the 'WKB curve'. For the

potential of equation (1), one finds that if a trajectory crosses the WKB curve $L/K$ continues to decrease when $x$ increases. In other words, the WKB curve is the boundary of a sink. Using bounds on $(L/K)'$ coming from equation (7) we can prove that, whenever the trajectory crosses the WKB curve, $\langle x|E\rangle$ defined by equation (8) is not normalizable. Consequently, if $\langle x|E\rangle$ has $n$ nodes and if the corresponding $L/K$ ultimately decreases (when $x$ becomes large enough), then $E < E_n$. Note that equation (7) shows that the poles of $L/K$ can only be simple and have a residue $-\hbar$. This implies that the Dunham condition [7] used in semiclassical calculations [8] is automatically satisfied. This also implies that for the potential of equation (1), a normalizable wavefunction cannot have a zero in the classically forbidden region (because $L/K$ could never reach the positive part of the WKB curve for $x$ larger than the location of the pole).

**Table 1.** The first ten energy levels $E_n$ and the number of (numerically) significant digits of the upper bound on $E_n$ (SD) in the case $\lambda = 1/10$, $m = 1/2$ and $\omega_0 = 2$.

| $n$ | $E_n$ | SD |
|---|---|---|
| 0 | 1.065 285 509 543 717 688 857 091 628 79 | 95 |
| 1 | 3.306 872 013 152 913 507 128 121 684 69 | 93 |
| 2 | 5.747 959 268 833 563 304 733 503 118 48 | 89 |
| 3 | 8.352 677 825 785 754 712 155 257 734 64 | 87 |
| 4 | 11.098 595 622 633 043 011 086 458 749 3 | 84 |
| 5 | 13.969 926 197 742 799 300 973 433 956 8 | 81 |
| 6 | 16.954 794 686 144 151 337 692 616 508 8 | 79 |
| 7 | 20.043 863 604 188 461 233 641 421 107 4 | 77 |
| 8 | 23.229 552 179 939 289 070 647 087 434 3 | 74 |
| 9 | 26.505 554 752 536 617 417 469 503 006 7 | 72 |

In summary, when $E$ is sufficiently close to $E_n$ and $x$ sufficiently large, $L/K$ follows closely the trajectory of the positive part of the WKB curve. When a certain value of $x$ is reached $L/K$ depends sensitively on small changes in $E$. A small increase in $E$ creates an additional zero of the wavefunction, a small decrease forces $L/K$ to cross the positive part of the WKB curve and to reach the negative part of it. This allows us to find sharp bounds on the energy levels. The only problem which remains is the control of the round-off errors. For a usual double precision computation, this is a serious issue, however since the linear recursion formula of equation (4) requires a number of operations which only grows linearly with the maximal order calculated, we can use 'slow' computational methods involving a very high precision. This can be implemented, for instance with MATHEMATICA, using the instruction 'SetPrecision[..., 100]' for numbers set with a precision of 100 digits. This method has allowed us to obtain the wavefunction with very good precision, at large $x$, far beyond the classical turning point, i.e. where the lowest-order WKB approximation works well.

Proceeding this way, we have calculated the first 10 energy levels in the case $m = 1/2$, $\omega_0 = 2$ and $\lambda = 1/10$. The results are displayed in table 1 with 30 significant digits. These numbers have been obtained by keeping 400 terms in the expansion of $L$ and $K$ and restricting the calculation to the interval $|x| \leqslant 7.5$ The starting precision was 100 digits. The difference between the upper and the lower bounds were required to be less than $10^{-32}$. These calculations have been performed independently using MATHEMATICA and MAPLE. Our numerical results are in agreement with the existing literature summarized in [6] and where numbers up to 15 significant digits can be found. Note that the numerical precision on the lower bounds obtained with Newton's methods (which can estimated from

the MATHEMATICA command 'Precision[...]') decreases approximately linearly when the level increases as shown in the last column of table 1. It is clear that these round-off errors are much smaller than the theoretical precision achieved. More generally, a preliminary analysis indicates that the enterprise of calculating a very large number of levels with a very large precision does not face prohibitive (i.e. exponential) growth of computer time. If this is effectively the case, we could say that the quantum anharmonic oscillator is 'numerically integrable'.

A more satisfactory outcome would be to find an operator which would be the analogue of the classical action which satisfies the Poisson bracket relation $\{I(H), e^{i\phi}\} = -ie^{i\phi}$. At the quantum level the corresponding relation implies an equally spaced spectrum. Equivalently, if we had an analytical expression for $\Delta(E)$ corresponding to $\hat{A}$ being the minimal creation operator (where $E$ is replaced by $E_n$ and $\hbar\Delta(E)$ by $E_{n+1} - E_n$ in the matrix elements), we could calculate the energy spectrum recursively. In both cases, it would mean that we would have at hand an implicit closed form expression for the energy spectrum. Despite interesting attempts [8], such an expression has not been found and discovering it is a challenge for the future.

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