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1998 J. Phys. A: Math. Gen. 31 L501

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LETTER TO THE EDITOR

Quantum oscillator of quartic anharmonicity

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Received 18 February 1998, in final form 17 April 1998

Abstract. A Taylor series method is derived to construct an analytical solution for the quantum anharmonic oscillator. The expression presented is found to yield in a rather natural way the corresponding special result obtained by using perturbation theoretic techniques. Attempts are made to give a possible physical interpretation for the various terms originating from nonlinear effects. Numerical results are presented to develop a feeling for their relative importance.

A wide variety of physical phenomena ranging from problems in Newtonian mechanics to those quantum field theory can be understood and visualized by using the so-called harmonic oscillator (HO) model. This model describes small oscillations of a system about the mean position of equilibrium under the action of a linear restoring force. For real systems, however, one needs to accommodate in the theory the effect of anharmonicity and go beyond the simple-minded HO model. The Morse potential in molecular physics [1] serves as a typical example in respect of this. Again, the concept of anharmonic oscillator finds a potential use in the condensed matter physics [2]. Our interest in this work is to develop an analytical method for solving the quantum quartic anharmonic oscillator problem which also plays a role in several areas of physics including the response of nonlinear media to electromagnetic radiation. We shall see that the merit of this approach is its simplicity. For example, restricting ourselves to the first-order correction of the anharmonic effect we could use a few difference equations to obtain a closed form solution of the problem starting from an assumed Taylor series solution.

The nonlinear equation for the classical anharmonic oscillator with quartic anharmonicity is given by

$$\ddot{X} + \omega^2 X + \lambda X^3 = 0 \quad (1)$$

with ω , the frequency of oscillation and λ , the anharmonic constant. Here the dots denote differentiation with respect to time t . For $X(t)$ to be bounded one will require λ to be positive. Understandably, the cubic nonlinearity in (1) has its origin in the $X^4(t)$ term associated with the corresponding Hamiltonian. The same equation as in (1) can also describe the quantum oscillator if we demand that $X(t)$ and $\dot{X}(t)$ are no longer numbers but become operator-valued functions in the Hilbert space satisfying the equal time commutation relation. Thus, as opposed to the numerical initial condition of the classical problem, here one has to deal with a general operator initial condition. This tends to pose some new complication in constructing a solution for quantum-mechanical anharmonic oscillator.

In all problems of physical interest, the anharmonicity acts only as a small perturbation over the harmonic motion. We therefore, assume that λ in (1) is very small compared with

unity. It should be noted that while the change in the equation of motion or Hamiltonian may be small, the eventual effect on the perturbation on the motion may be quite significant. Keeping these in mind we try a Taylor series solution for (1) written as

$$X(t) = X(0) + t\dot{X}(0) + \frac{t^2}{2!}\ddot{X}(0) + \frac{t^3}{3!}\dddot{X}(0) + \frac{t^4}{4!}\dots + \dots \quad (2)$$

Admittedly, the chosen solution in (2) will be strictly valid only for sufficiently small values of t . Here $X(0)$ and $\dot{X}(0)$ stand for the operator initial conditions satisfying the canonical commutation relation $[X(0), \dot{X}(0)] = i(\hbar = 1)$ is used throughout the text). From (1) and (2) we obtain the approximate solution up to the linear power of λ in the form

$$\begin{aligned} X(t) = & X(0) \cos \omega t + \frac{1}{\omega} \dot{X}(0) \sin \omega t \\ & - \frac{\lambda}{\omega^2} X^3(0) \left\{ \frac{\omega^2 t^2}{2!} - 4 \frac{\omega^4 t^4}{4!} + 25 \frac{\omega^6 t^6}{6!} - 208 \frac{\omega^8 t^8}{8!} + 1849 \frac{\omega^{10} t^{10}}{10!} \dots \right\} \\ & - \frac{\lambda}{\omega^3} [\dot{X}(0) X^2(0) + X(0) \dot{X}(0) X(0) + X^2(0) \dot{X}(0)] \\ & \times \left\{ \frac{\omega^3 t^3}{3!} - 8 \frac{\omega^5 t^5}{5!} + 69 \frac{\omega^7 t^7}{7!} - 616 \frac{\omega^9 t^9}{9!} + 5537 \frac{\omega^{11} t^{11}}{11!} - \dots \right\} \\ & - \frac{2\lambda}{\omega^4} [X(0) \dot{X}^2(0) + \dot{X}(0) X(0) \dot{X}(0) + \dot{X}^2(0) X(0)] \\ & \times \left\{ \frac{\omega^4 t^4}{4!} - 11 \frac{\omega^6 t^6}{6!} + 102 \frac{\omega^8 t^8}{8!} - 922 \frac{\omega^{10} t^{10}}{10!} + \dots \right\} \\ & - \frac{6\lambda}{\omega^5} \dot{X}^3(0) \left\{ \frac{\omega^5 t^5}{5!} - 11 \frac{\omega^7 t^7}{7!} + 102 \frac{\omega^9 t^9}{9!} - 922 \frac{\omega^{11} t^{11}}{11!} + \dots \right\}. \quad (3) \end{aligned}$$

It is possible to extend the solution for higher power of λ . Interestingly, the infinite series in the curly brackets can be expressed in terms of the circular functions by using the difference equations

$$t_r = (-1)^{r+1} (9t_{r-1} - 6r + 7) \quad (4a)$$

$$t_r = (-1)^{r+1} (9t_{r-1} - 2r + 3) \quad (4b)$$

$$t_r = (-1)^{r+1} (9t_{r-1} + 2r) \quad (4c)$$

and

$$t_r = (-1)^{r+1} (9t_{r-1} + 6r) \quad (4d)$$

the solutions of which are given by

$$t_r = (-1)^{r+1} \frac{1}{32} [9^r + 24r - 1] \quad (5a)$$

$$t_r = (-1)^{r+1} \frac{1}{32} [3 \times 9^r + 8r - 3] \quad (5b)$$

$$t_r = (-1)^{r+1} \frac{1}{32} [9 \times 9^r - 8r - 9] \quad (5c)$$

and

$$t_r = (-1)^{r+1} \frac{3}{32} [9 \times 9^r - 8r - 9] \quad (5d)$$

respectively. t_r is the r th term of the infinite series under the curly brackets of equation (4). For example, $t_3 = 25$ and $t_4 = -208$ under the first curly bracket. We thus have

$$X(t) = X(0) \cos \omega t + \frac{1}{\omega} \dot{X}(0) \sin \omega t - \frac{\lambda}{32\omega^2} X^3(0) [\cos \omega t - \cos 3\omega t + 12\omega t \sin \omega t]$$

$$\begin{aligned}
& + \frac{\lambda}{32\omega^3} [\dot{X}(0)X^2(0) + X(0)\dot{X}(0)X(0) + X^2(0)\dot{X}(0)] \\
& \times [\sin 3\omega t - 7 \sin \omega t + 4\omega t \cos \omega t] \\
& - \frac{\lambda}{32\omega^4} [X(0)\dot{X}^2(0) + \dot{X}(0)X(0)\dot{X}(0) + \dot{X}^2(0)X(0)] \\
& \times [\cos 3\omega t - \cos \omega t + 4\omega t \sin \omega t] \\
& - \frac{\lambda}{32\omega^5} \dot{X}^3(0) [\sin 3\omega t + 9 \sin \omega t - 12\omega t \cos \omega t]. \tag{6}
\end{aligned}$$

Two useful checks on the solution in (6) are now in order. For example, if we assume $\dot{X}(0) = 0$ then the simple-minded perturbation theoretic result of Bhaumik and Dutta-Ray [3] is reproduced. Further, we can go to the classical limit if $X(0)$ and $\dot{X}(0)$ commute. In that case we obtain

$$\begin{aligned}
x(t) = & \alpha \cos(t + \beta) + \lambda\alpha^3 \left[-\frac{3}{8}t \sin(t + \beta) + \frac{1}{32} \cos(3t + 3\beta) + \frac{3}{8} \cos(t + 3\beta) \right. \\
& \left. - \frac{1}{8} \cos(t - 3\beta) + \frac{1}{16} \cos(t + \beta) - \frac{1}{16} \cos(t - \beta) \right] + \tag{7}
\end{aligned}$$

where we have introduced $X(0) = \alpha \cos \beta$, $\dot{X}(0) = -\alpha \sin \beta$, $\omega = 1$ and lowercase $x(t)$ as the classical equivalent of the operator $X(t)$. A few extra terms have appeared in (7) in comparison with that of the classical solution (i.e. equation (4.45) of [4]) obtained by perturbative techniques.

It is clear that the nonlinear contribution to the solution in (6) consists of four parts. The first part, namely the coefficient of $X^3(0)$, confirms the presence of higher harmonics. Here only the third harmonic has been generated because our constructed solution is linear in λ . Had we considered the terms containing λ^2 the fifth harmonic would be generated. A similar physical interpretation may be given for the remaining three parts. It may be of considerable interest to examine the relative contribution of these parts in producing the nonlinear effects. In figure 1 we plot the values of such contributions (after making dimensionless) as a function of the dimensionless quantity ωt . For small values of ωt the contributions for all the four parts are comparable. However, for large values of ωt the contribution of coefficient of $X^3(0)$ dominates over the contribution made by the remaining three parts. This is because the denominators of those three parts increase faster compared with the denominator of the first one. Thus, the leading contribution of the nonlinear effects will come from the coefficients of $X^3(0)$ for moderately large (as long as solution (2) permits) values of ωt . Curve (a) is oscillatory and its amplitude increases rapidly as ωt increases. The reason for this may be attributed to the secular term $\omega t \sin \omega t$ present in the coefficient of $X^3(0)$.

It is interesting to note that we can remove the secular term from the classical solution (7) by using the following relations

$$\sin\left(\frac{3}{8}\lambda\alpha^2 t\right) = \frac{3}{8}\lambda\alpha^2 t + h(0) \tag{8a}$$

$$\cos\left(\frac{3}{8}\lambda\alpha^2 t\right) = 1 + h(0). \tag{8b}$$

In the above equations we have limited ourselves up to the linear power of λ by neglecting the terms containing higher powers $h(0)$ of the same. Thus equation (7) takes the form

$$\begin{aligned}
x(t) = & \alpha \cos\left(t + \frac{3}{8}\lambda\alpha^2 t + \beta\right) + \lambda\alpha^3 \left[\frac{1}{32} \cos(3t + 3\beta) + \frac{3}{8} \cos(t + 3\beta) \right. \\
& \left. - \frac{1}{8} \cos(t - 3\beta) + \frac{1}{16} \cos(t + \beta) - \frac{1}{16} \cos(t - \beta) \right] + . \tag{9}
\end{aligned}$$

The first term shows the usual frequency shift of $\frac{3}{8}\lambda\alpha^2$. The same approach is adopted for

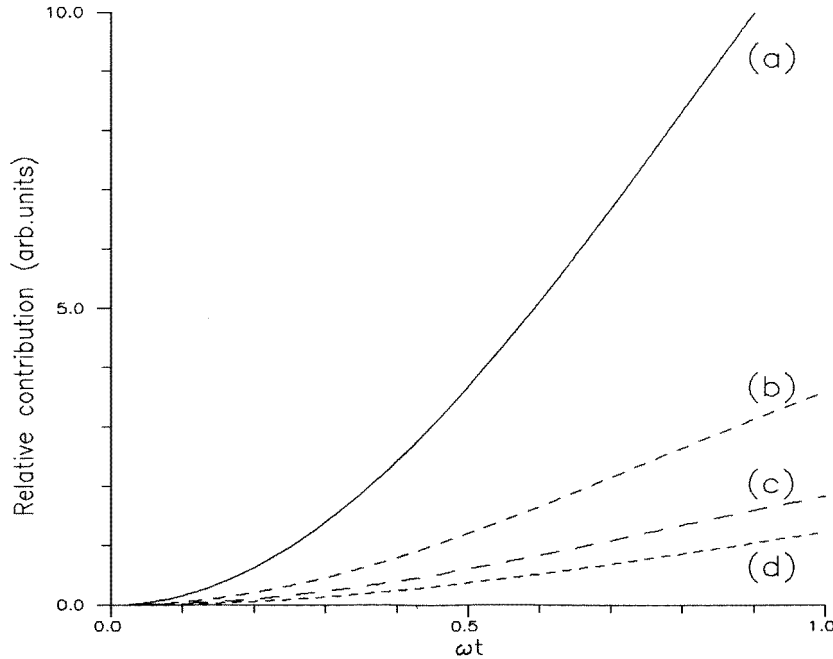


Figure 1. Relative contributions of the coefficients of curves: (a) $X^3(0)$; (b) $X^2(0)\dot{X}(0) + X(0)\dot{X}(0)X(0) + \dot{X}(0)X^2(0)$; (c) $\dot{X}^2(0)X(0) + \dot{X}(0)X(0)\dot{X}(0) + X(0)\dot{X}^2(0)$, and (d) $\dot{X}^3(0)$ to nonlinear effect as a function of ωt .

equation (6) to have the following relation

$$\begin{aligned}
 X(t) = \frac{1}{2 \cos(\frac{3}{8}\lambda t)} \left\{ \left[X(0) \cos\left(t + \frac{3\lambda t}{4} H_0\right) \right] + \left[\cos\left(t + \frac{3\lambda t}{4} H_0\right) X(0) \right] \right. \\
 \times \left[\dot{X}(0) \sin\left(t + \frac{3\lambda t}{4} H_0\right) \right] + \left[\sin\left(t + \frac{3\lambda t}{4} H_0\right) \dot{X}(0) \right] \\
 + \frac{3\lambda}{64} [X(0)\dot{X}^2(0) + \dot{X}^2(0)X(0)] \times (\cos t - \cos 3t) \\
 + \frac{3\lambda}{64} [\dot{X}(0)X^2(0) + X^2(0)\dot{X}(0)] \times (\sin 3t - 7 \sin t) \\
 \left. - \frac{\lambda}{32} (\sin 3t + 9 \sin t) \dot{X}^3(0) - \frac{\lambda}{32} (\cos t - \cos 3t) X^3(0) \right\} \quad (10)
 \end{aligned}$$

where $\omega = 1$ and $H_0 = \frac{1}{2}(X^2(0) + \dot{X}^2(0))$ is the Hamiltonian of the harmonic oscillator. The relations $\sin \alpha = \alpha$ and $\cos \alpha = 1$ for small α have been used. We obtain the solution of Bender and Bettencourt [5] if we drop the last three rows from our solution (10). The appearance of the third harmonic term is also explicit in (10). The quantum anharmonic oscillator has also been studied by using an integral approach [6]. Equivalent nonlinear operator integral equations were framed out of the differential form of the position and momentum operators. Finally an iterative approach was used to obtain the solution of the operator integral equation [6].

We conclude by noting that there are several examples where we come across a Hamiltonian of a quartic anharmonic oscillator. These include the interaction of light with nonabsorbing (lossless) inversion symmetric media if the third-order susceptibilities are

taken into account. The order of anharmonicities will increase as the orders of nonlinear susceptibilities increases. It is well known that the interaction of light with nonlinear media leads to the higher harmonic generation [7]. The orders of the generated higher harmonics are compatible with the order of the nonlinear susceptibilities. Clearly, the third harmonic term present in our solution tends to reflect this physical fact even in a model calculation.

Solution (6) which is obtained by using the Taylor series also has a drawback. The presence of the secular term proportional to $\omega t \sin \omega t$ rises rapidly with increasing ωt . Hence, the solution is nonuniform under the series expansion. Such a drawback is removed by using renormalization techniques.

This work was supported by the Department of Science and Technology, Government of India through the SERCYS project SR/SY/P-10/92. The author is grateful to Dr B Talukdar for his kind interest in this work.

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