

Resonance excitation and hysteresis in a quantum anharmonic oscillator

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The problem of resonance excitation of a quantum anharmonic oscillator by an external force is solved. A periodic force is shown to have a hysteresis and oscillations. A new branch appears between the "classical" branches on the resonance curve of a quantum oscillator.

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An interest in hysteresis effects produced as a result of the influence of optical radiation on different objects has increased recently.^{1,2} A quantum anharmonic oscillator can be used as the basic device for this purpose. Such a model can be used for a wide range of problems, including the description of the buildup of molecular oscillations by laser radiation.^{3,4} Although hysteresis for the classical case is well known,⁵ hysteresis involving the solution of the Schrödinger equation remains open. In fact, an analogy with the classical hysteresis has been noticed in the quasi-classical limit ($\hbar \rightarrow 0$).⁶ It was concluded in Ref. 7, however, by taking into account the following terms in \hbar that the quantum oscillator, in contrast to the classical oscillator, can exist in only one state (with higher energy).

Let us examine the Schrödinger equation ($\hbar = m = 1$)

$$i \frac{\partial \psi}{\partial t} + \frac{1}{2} \frac{\partial^2 \psi}{\partial x^2} - \frac{1}{2} \omega^2(t) x^2 \psi + f(t) x \psi - U_{\text{NL}}(x) \psi = 0. \quad (1)$$

Here $f(t)$ is the external force with the characteristic frequency ω_f and $U_{\text{NL}}(x) = \alpha x^3 + \beta x^4$ is the anharmonic addition to the potential $|\omega^2(t)/\omega_f^2 - 1| \ll 1$. We shall select as the zeroth approximation the coherent states of the free harmonic oscillator^{8,9} (H_n are the Hermite polynomials)

$$\begin{aligned} \psi_n^{(\circ)} = \Phi_n(x_1) \exp[i (\dot{\eta}^{(\circ)} x_1 - \epsilon_n t + \sigma_n^{(\circ)}(t))], \quad \Phi_n(x_1) = \left[\frac{1}{2^n n!} \sqrt{\frac{\omega_f}{\pi}} \right]^{1/2} \\ \times \exp\left(-\frac{1}{2} \omega_f x_1^2 \right) H_n(\sqrt{\omega_f} x_1), \end{aligned} \quad (2)$$

where

$$\begin{aligned} x_1 = x - \eta^{(\circ)}(t), \quad \ddot{\eta}^{(\circ)} + \omega_f^2 \eta^{(\circ)} = 0, \quad \dot{\sigma}^{(\circ)} = \frac{1}{2} (\dot{\eta}^{(\circ)})^2 - \omega_f^2 \eta^{(\circ)2}, \\ \epsilon_n = \left(n + \frac{1}{2} \right) \omega_f, \quad n = 0, 1, 2, \dots \end{aligned}$$

This solution corresponds to a wave packet whose center of mass moves along the classical trajectory of the harmonic oscillator with an arbitrary oscillation amplitude because of the linear oscillator. We shall use the variables $x_1 = x - \eta(t)$, t in Eq. (1) and seek a solution in the form

$$\psi_n = \phi_n(x_1, t) \exp[a(t) x_1 - i \epsilon_n t + i \sigma(t)], \quad a(t) = i \dot{\eta} - \frac{3}{4 \omega_f^2} (a + 4 \beta \eta). \quad (3)$$

Using the recurrence relations for Φ_n in the first approximation for the small parameters proportional to α, β, f , and $\omega^2(t) - \omega_f^2$, we obtain

$$i \frac{\partial \phi_n}{\partial t} + \frac{1}{2} \frac{\partial^2 \phi_n}{\partial x_1^2} - \frac{1}{2} [\omega^2(t) + 6 \alpha \eta + 12 \beta \eta^2] x_1^2 \phi_n + \epsilon_n \phi_n + X(t) x_1 \phi_n + Y(t) \phi_n = Z, \quad (4)$$

where

$$X(t) = f(t) - \ddot{\eta} - \omega^2(t) \eta - 3 \alpha \eta^2 - 4 \beta \eta^3 - (a + 4 \beta \eta) \frac{3 \left(n + \frac{1}{2} \right)}{2 \omega_f} - i \frac{3 \beta}{\omega_f^2} \dot{\eta}, \quad (5)$$

$$Y(t) = -\dot{\sigma} + \frac{1}{2} \dot{\eta}^2 - \frac{1}{2} \omega^2(t) \eta^2 + f(t) \eta - \alpha \eta^3 - \beta \eta^4 - \frac{3 \beta}{4 \omega_f^2} (2n^2 + 2n + 1). \quad (6)$$

Although the value of X is of the first order in smallness, it cannot be taken into account in the standard perturbation theory since it contains resonance terms. We must therefore set $X(t) = 0$, which gives the equation of motion for $\eta(t)$. The quantity Z contains nonresonance terms—a small addition of the states $\phi_{n \pm 2, n \pm 3, n \pm 4}$. They can be accounted for by using a well-known method,⁸ but they do not contribute to the equation of motion. The term with $Y(t)$ can be eliminated by an appropriate selection of $\sigma(t)$. The solution of the remaining Schrödinger equation for the harmonic oscillator with a variable frequency is given in Ref. 9. Note that our treatment is valid if ϕ_n are close to the unperturbed Φ_n functions. This condition requires additional substantiation in the region of the parametric resonance.⁹ We can show that this case for an anharmonic oscillator effectively reduces to the nonresonance case as a result of additional, slight modification of the wave function. The equation of motion in this case does not change.

The contribution of the first approximation $\sim \alpha$ from the terms leads to an unessential, constant shift and to small oscillations $\eta(t)$. The second-order contribution $\sim \alpha^2$ can be determined from the variation of the β coefficient. We, therefore, set $\alpha = 0$ and $\omega^2(t) = \omega_0^2 = \text{const}$ in Eq. (5). The equation of motion becomes

$$\ddot{\eta} + \left[\omega_0^2 + 2\rho \left(n + \frac{1}{2} \right) \right] \eta + 4 \beta \eta^3 + i \frac{\rho}{\omega_f} \dot{\eta} = f(t), \quad \rho = \frac{3 \beta}{\omega_f} \left(= \frac{3 \beta \hbar}{m^2 \omega_f} \right). \quad (7)$$

According to Eq. (7), the trajectories of motion of the center of mass of a wave packet are complex. The classical Duffing equation can be derived from Eq. (7) if $\rho \rightarrow 0$ ($\hbar \rightarrow 0$). The quantum corrections are relatively small if the oscillation amplitude $\eta(t)$ exceeds considerably the characteristic width of the wave packet $\sim \omega^{-1/2}$.

Let us assume that the external force is monochromatic $f(t) = A \cos \omega_f t$. We shall seek the periodic solution of Eq. (7) in the form

$$\eta(t) = \frac{1}{2} (p e^{i \omega_f t} + q e^{-i \omega_f t}). \tag{8}$$

We obtain for the quantities $u = 3|\beta|pq$ and $v = 3|\beta|A^2$

$$[(u + d)^2 - \rho^2]u = v, \quad d = \text{sign}(\beta) \left[\omega_0^2 - \omega_f^2 + 2\rho \left(n + \frac{1}{2} \right) \right]. \tag{9}$$

For the stability of solutions it is required that $(d+u)(d+3u) \geq 0$. The complex solutions of (9) are unstable. The hysteresis dependence characterizing the oscillation intensity of the oscillator u as a function of detuning d is illustrated in Fig. 1. The quantum oscillator differs substantially from the classical oscillator in the resonance region ($d^2 \geq \rho^2$); however, this difference vanishes as $\rho \rightarrow 0$. A new branch ($u < 0$) appears between the "classical" branches ($u > 0$) which are separated by $\sim \rho$. The oscillation (8) can be represented in the form $\eta(t) = b \cos(\omega_f t + \phi_c)$, where the "phase" ϕ_c is imaginary. This made it impossible to detect a hysteresis in Ref. 7, in which the phase was assumed to be real. Note that the Schrödinger equation (1) corresponds to the omission of relaxation processes. The results, therefore, are generally justifiable for sufficiently large amplitudes of the force $A > \gamma\sqrt{\omega}$, where γ is the relaxation rate. This condition determines the minimum radiation power, which must be exceeded in order to realize the effects described by the resonance curve in Fig. 1.

The quantity u characterizes the steady states, which participate effectively in the decomposition of the coherent state, and hence the degree of excitation of the oscillator. We can see in Fig. 1 that the excitation increases sharply as the frequency difference d is reduced. The resonance excitation of higher excitation levels of molecules was analyzed in Refs. 10 and 11. The perturbation theory generally cannot be used for the external field under resonance conditions considered by us.

The indicated effects can be observed in infrared spectra of simple molecules

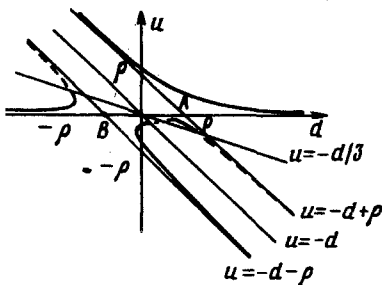


FIG. 1. Resonance curve for quantum anharmonic oscillator. The broken curve corresponds to unstable solutions. The points A and B correspond to auto-oscillations at frequencies $\omega_0^2 + 2\rho n + 1/2 \pm \rho^{1/2}$.

(for example, CO, NO, and HCl) due to the action of radiation from a tunable-frequency laser. The resonance width is characterized by the quantity $\rho(10 \text{ cm}^{-1})$. If the relaxation rate of an HCl molecule is $\gamma = 0.01 - 0.1 \text{ cm}^{-1}$ and its effective charge is $e^* = 0.1 e$ (Ref. 12) (e is the electron charge), then the minimum strength of the laser field will be $E \sim (\gamma/e^*)\sqrt{2m\hbar\omega} \sim 3 \times 10^4 - 3 \times 10^5 \text{ V/cm}$, i.e., the power density will be $1-100 \text{ MW/cm}^2$ (see also Ref. 13). These estimates can account for the excitation observed by Arnoldi *et al.*¹⁴ of HCl molecules to the second vibrational level by a relatively low-power chemical HCl laser, in spite of considerable anharmonism [$\omega_e x_e = 52 \text{ cm}^{-1}$ (Ref. 12)].

The dielectric constant of the medium, which is comprised of the anharmonic oscillators under consideration, may be an ambiguous function of the field intensity, which gives rise to peculiar optical hysteresis effects.¹⁵ Since a strange attractor appears in the classical analog (7) at $A > A_{\text{crit}}$,¹⁶ the Schrödinger equation (1) is expected to behave stochastically. The Duffing quantum equation (7) also describes a number of other nonlinear effects, including that produced due to nonmonochromatic excitation, as well as auto-oscillation. Since the Schrödinger equation (1) becomes a parabolic equation of propagation of optical beams after the substitution $t \rightarrow z$, the obtained results give a wave description of the fields in inhomogeneous wave guides and in optical cavities.

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