# SPECTRAL DISTRIBUTION OF A NONLINEAR OSCILLATOR PERFORMING BROWNIAN MOTION IN A DOUBLE-WELL POTENTIAL

### M.I. DYKMAN, S.M. SOSKIN

Institute of Semiconductors, Academy of Sciences of the UkrSSR, Kiev, USSR

and

#### M.A. KRIVOGLAZ

Institute of Metal Physics, Academy of Sciences of the UkrSSR, Kiev, USSR

#### Received 11 March 1985

The spectral distribution  $Q(\omega)$  of the coordinate fluctuations is studied for an oscillator performing Brownian motion in a double-well potential at low damping. The most detailed analysis is given for the Duffing oscillator with potential energy  $U(q) = -\frac{1}{2}\omega_0^2q^2 + \frac{1}{4}\gamma q^4$ . The important features of  $Q(\omega)$  are shown to be related to the slowing-down of the motion in the vicinity of the local potential maximum. In a certain range of the noise intensity,  $Q(\omega)$  has three distinct peaks. They are due to fluctuational transitions between potential wells and to vibrations near the minima of U(q) and above the barrier. A typical feature of  $Q(\omega)$  is the exponential tail in the region  $\omega < \omega_0$  passing into a plateau at still smaller  $\omega$  (but  $\omega \gg \Gamma$ ). The plateau depends on the friction coefficient  $\Gamma$  nonanalytically (as  $\sqrt{\Gamma}$ ).

#### 1. Introduction

The Brownian motion of the oscillator whose potential energy has two minima has been studied in many papers. The interest to the problem is due to large effects that may result when the oscillator is subjected to even a weak random force. In particular the noise causes transitions between stable states (see ref. 1) as well as transitions from unstable stationary state (the local maximum of the potential) to one of the stable states (see refs. 2 and 3 and references cited therein). The transition probabilities depend nonanalytically on the noise intensity.

In the present paper the time correlation function of the oscillator coordinates

$$Q(t) = \langle q(t)q(0)\rangle \tag{1}$$

and its spectral distribution

0378-4371/85/\$03.30 © Elsevier Science Publishers B.V. (North-Holland Physics Publishing Division)

$$Q(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \exp(i\omega t) Q(t)$$
 (2)

are investigated for the oscillator with a double-well potential.

Analysis of the distribution  $Q(\omega)$  is of interest for a number of problems of spectroscopy (in particular, for the spectroscopy of crystals with impurities that have several equilibrium positions in the elementary cell) and for radiophysics. The system under consideration is also of general interest from the viewpoint of the investigation of the nonlinearity influence on the oscillator relaxation and fluctuations. Such an investigation was fulfilled in detail for the van der Pol<sup>4</sup>) and Duffing<sup>5</sup>) oscillators. For the Duffing oscillator whose nonlinearity is due to the form of the potential (not of the friction force as in the case of the van der Pol oscillator) the case of a single-well potential was studied.

The existence of two minima of the potential energy results in specific features of the oscillator spectral distribution. They may be understood easily by considering a simple double-well potential (that for the double-well Duffing oscillator)

$$U(q) = -\frac{1}{2}\omega_0^2 q^2 + \frac{1}{4}\gamma q^4. \tag{3}$$

The function U(q) is shown in fig. 1. It has minima at

$$q = \pm q_0, \qquad q_0 = \sqrt{\frac{\omega_0^2}{\gamma}}. \tag{4}$$

The Brownian motion in potential (3) is described by the generalized Langevin equation

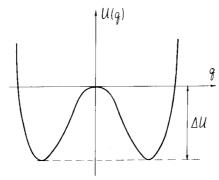


Fig. 1. Potential energy U(q) of the double-well Duffing oscillator.

$$\ddot{q} - \omega_0^2 q + \gamma q^3 + 2\Gamma \dot{q} = f(t), \quad \langle f(t)f(t') \rangle = 2B\Gamma \delta(t - t'). \tag{5}$$

Here  $\Gamma$  is the friction coefficient, while the parameter B characterizes the intensity of the white noise f(t) (in the case when the random force f(t) and friction result from the coupling of the oscillator to a bath B = 2kT).

The stationary distribution of the oscillator for the model (5) is Gibbsian:

$$W_{\rm st} = W_{\rm st}(E) = Z^{-1} \exp\left(-\frac{2E}{B}\right). \tag{6}$$

The oscillator energy E and the statistical integral Z are given by the standard expressions

$$E = \frac{1}{2}p^2 + U(q), \quad Z = \iiint dp \, dq \, \exp\left(-\frac{2E}{B}\right). \tag{7}$$

The form of the distribution  $Q(\omega)$  in the model (3), (5) depends on the parameter

$$\beta = \frac{B}{8\Delta U} = \frac{\gamma B}{2\omega_0^4}, \quad \Delta U = \frac{1}{4} \frac{\omega_0^4}{\gamma}. \tag{8}$$

( $\Delta U$  is the potential barrier height, see fig. 1). It is obvious from eq. (6) that at  $\beta \ll 1$  the oscillator with overwhelming probability is located near one of the minima and "jumps" to another minimum very rarely. The spectral distribution in the case of sufficiently small friction,

$$\Gamma \leqslant \omega_0$$
, (9)

has two sharp peaks. One of them is located at the frequency of the eigenoscillations near the potential minima  $\omega_0\sqrt{2}$  and is described by the Lorentzian distribution with the half-width  $\Gamma$  at  $\beta \ll \Gamma/\omega_0$ . The other peak is caused by fluctuational transitions between the minima. It is placed at  $\omega = 0$  and its width is exponentially small  $(\sim \Gamma \exp(-\frac{1}{4}\beta^{-1}))$ .

With increasing  $\beta$  (e.g. due to increasing noise intensity B) the form of  $Q(\omega)$  changes substantially. For the case of small friction (9) the shape of the peak at  $\omega \approx \omega_0 \sqrt{2}$  is distorted already at relatively small  $\beta$ ,

$$1 \gg \beta \geqslant \frac{\Gamma}{\omega_0}$$

due to specific modulational spectrum broadening<sup>6</sup>). The latter is caused by the dependence of the frequency of a nonlinear oscillator on its energy. The typical frequency straggling due to nonlinearity  $\delta \omega$  may be estimated allowing for the width of the oscillator energy distribution being of the order of B (according to (6)). We thus obtain

$$\delta\omega \sim B\left(\frac{\partial\omega(E)}{\partial E}\right)_{E_m}, \quad \delta\omega \sim \omega_0\beta, \quad \beta \leqslant 1.$$
 (10)

Here  $\omega(E)$  is the frequency of the vibrations at energy E in the absence of friction and a random force,  $E_{\rm m}$  is the characteristic energy ( $\omega(E_{\rm m})$  coincides with the position  $\omega_{\rm m}$  of the spectral distribution maximum).

When  $\delta\omega$  is of the same order as the uncertainty in frequency  $\Gamma$  due to friction, the shape of the peak of  $Q(\omega)$  in the vicinity of  $\omega_0\sqrt{2}$  is determined by competition between the frequency smearing mechanisms. To calculate the peak shape for arbitrary  $\beta\omega_0/\Gamma$  (but for  $\beta\ll 1$ ) one may use the results obtained in ref. 7 for the low-damped single-well Duffing oscillator.

The vibration nonlinearity results also at finite  $\beta$  in the weak (for  $\beta \le 1$ ) peaks in the oscillator spectrum at the frequencies that are multiples of  $\omega_0 \sqrt{2}$ .

With a further increase in  $\beta$  the oscillator frequency straggling becomes of the same order of magnitude as  $\omega_m$ . To calculate the shape of the broad peak of  $Q(\omega)$  near the maximum in the case

$$\delta \omega \gg \Gamma$$
 (11)

damping may be neglected (similar approximation was used in ref. 8 for the single-well Duffing oscillator).

Let us consider now the spectral distribution  $Q(\omega)$  in the range  $4\beta \ge 1$  (corresponding to temperatures  $kT \ge \Delta U$  for the system coupled to a bath). In this range  $Q(\omega)$  is formed both by vibrations near the potential minima and those above the barrier. The features of the distribution are due to the following: for small energies  $|E| \le \Delta U$  (the energy is measured relative to the local potential maximum at q=0) the oscillator motion is evidently slow near the maximum and the period of vibrations is large (the classical oscillator "sticks" to the point q=0), while the dispersion of the vibration frequencies  $\omega(E)$  is strong. As a result the peak corresponding to the motion above the barrier may appear in  $Q(\omega)$  parallel with the peak corresponding to the vibrations near  $q=\pm q_0$ . At  $4\beta \le 1$  the first peak intensity is exponentially small. When  $4\beta \approx 0.4$ , the peaks are of the same order of magnitude, i.e. the spectrum has a characteristic two-humped structure in the range  $\omega \ge \Gamma$  (the "central" peak at  $\omega=0$  with the width  $\sim \Gamma$  remains in  $Q(\omega)$  for  $4\beta \ge 1$ ). The peak caused by the

overbarrier motion increases with increasing  $\beta$  and in the range  $4\beta \approx 1.5$  it overlaps the peak caused by the vibrations near the minima. The slowing-down of the motion near the local potential maximum results also in another effect, the appearance of the characteristic low-frequency tail of  $Q(\omega)$  that decreases as  $\exp(-\text{const.} \cdot \omega^{-1})$  in the range  $\omega < \omega_0$ .

In the range of still lower frequencies,  $\omega \ll \omega_0$  (but  $\omega \gg \Gamma$ ), the shape of  $Q(\omega)$  is influenced essentially by the motion aperiodicity due to dissipative and fluctuational effects. These effects are of primary importance for the range of small  $\omega(E)$  since the phase diffusion coefficient diverges at  $\omega(E) \to 0$ . The aperiodic motion gives rise to the flatness of the spectral distribution (the plateau) at  $\omega \ll \omega_0$ , the height of the plateau depending nonanalytically on the noise intensity  $\Gamma B$  at  $\Gamma \to 0$ .

In section 2 the motion of the Duffing oscillator with a double-well potential is considered neglecting dissipation. In section 3 the general expressions for Q(t) and  $Q(\omega)$  are obtained in the form of series, the results of numerical calculations of the spectral distribution at various  $\beta$  and analytical expressions for  $Q(\omega)$  in the limiting cases of small and large  $\beta$  are presented. In section 4 the spectral distribution is obtained explicitly in the frequency range  $\omega < \omega_0$  for arbitrary  $\beta$  and its structure is analyzed. The results of section 4 are generalized to the case of an arbitrary double-well potential in section 5. In section 6 the plateau of  $Q(\omega)$  in the low-frequency range  $\Gamma \ll \omega < 2\pi\omega_0 \ln^{-1}(\omega_0 \Delta U/\Gamma B)$  is investigated by analyzing the Einstein-Fokker-Planck equation. In the appendix the smallness of the dissipation-induced corrections to  $Q(\omega)$  at  $\omega \geqslant \omega_0$  is shown.

### 2. The motion of the isolated Duffing oscillator with a double-well potential

At sufficiently small friction  $(\Gamma \ll \delta \omega)$  one may neglect the damping of the oscillator vibrations when calculating the spectral distribution peak shape in the frequency range  $\omega \geqslant \omega_0$ , because for the time  $(\delta \omega)^{-1}$  during which the peak is formed, the motion is quasiconservative. Accordingly, to find the time correlation function Q(t) one may first solve the problem of the free motion of the oscillator with a given energy E and then average over the energy and phase with the weight (6) (this method is justified in the Appendix on the basis of the Einstein–Fokker–Planck equation corresponding to the stochastic equation (5)).

The solution of the equation of free motion

$$\ddot{q} - \omega_0^2 q + \gamma q^3 = 0 \tag{12}$$

in the range of positive energies is of the form

$$q(t) = \omega_0 \gamma^{-1/2} (1 + b_E^2)^{1/2} \operatorname{cn} \left( \frac{2K}{\pi} \varphi \right), \quad \varphi \equiv \varphi(t) = \omega(E) t + \varphi(0),$$

$$\omega(E) = \frac{\pi}{2K} b_E \omega_0, \quad k^2 \equiv m = \frac{1}{2} (1 + b_E^{-2}), \quad b_E = \left( 1 + \frac{E}{\Delta U} \right)^{1/4},$$

$$\Delta U = \frac{\omega_0^4}{4\gamma}, \quad E > 0.$$
(13)

Here, cn  $u \equiv \operatorname{cn}(u|m)$  is the Jacobi elliptic cosine, k is the module (m) is the parameter),  $K \equiv K(k)$  is the elliptic integral of the first kind,  $\varphi(0)$  is the initial phase.

For negative energies E the oscillator can vibrate with the same energy either in the left or in the right potential well (see fig. 1). Therefore eq. (12) has two solutions:

$$q_{l}(t) = (-1)^{l} \omega_{0} \gamma^{-1/2} (1 + b_{E}^{2})^{1/2} \operatorname{dn} \left(\frac{K}{\pi} \varphi_{l}\right), \quad \varphi_{l} \equiv \varphi_{l}(t) = \omega(E) t + \varphi_{l}(0),$$

$$\omega(E) = \frac{\pi}{\sqrt{2}K} \omega_{0} (1 + b_{E}^{2})^{1/2}, \quad k^{2} \equiv m = 2(1 + b_{E}^{-2})^{-1},$$

$$b_{E} = \left(1 + \frac{E}{\Delta U}\right)^{1/4}, \quad E < 0, l = 1, 2.$$
(14)

Here, dn  $u = \operatorname{dn}(u|m)$  is the amplitude delta,  $\varphi_l(0)$  are the initial values of the phases  $\varphi_l$  of the vibrations in the left (l=1) and right (l=2) wells.

The quantity  $\omega(E)$  in (13), (14) is determined in such a way that it equals the eigenfrequency of the vibrations (this follows from the properties of the functions cn u, dn u, see ref. 9. At  $|E| \rightarrow 0$  the frequency  $\omega(E)$  tends to zero according to the inverse logarithmic law

$$\omega(E) \approx \begin{cases} \pi \omega_0 [\ln(64 \Delta U/E)]^{-1}, & E > 0, \\ 2\pi \omega_0 [\ln(64 \Delta U/|E|)]^{-1}, & E < 0, \end{cases} |E| \ll \Delta U.$$
 (15)

The divergence of the oscillation period at  $|E| \rightarrow 0$  is obvious from fig. 1.

# 3. Time correlation function of the coordinates and its spectral distribution in the absence of damping

When damping is neglected the correlator Q(t) (1) is

$$Q(t) = \iiint_{\infty} dq(0) dp(0) q(t)q(0) W_{st}(E), \qquad (16)$$

where  $W_{\rm st}(E)$  and q(t) are determined by (6), (13) and (14) (cf. ref. 8). In calculating the integral (16) it is convenient to transform to new canonical variables: the action I and phase  $\varphi$ , and then to the energy and phase (the action depends only on the energy)

$$dp dq = dI d\varphi, \quad dI = \omega^{-1}(E) dE. \tag{17}$$

Thus the averaging over the initial coordinates and momenta in (16) reduces to integration over E and over the initial phase  $\varphi(0)$  (for E>0) or  $\varphi_1(0)$ ,  $\varphi_2(0)$  (for E<0). The averaging over  $\varphi(0)$  ( $\varphi_{1,2}(0)$ ) may be easily performed using the expansion of the functions  $\operatorname{cn}(2K\varphi/\pi)$  and  $\operatorname{dn}(K\varphi/\pi)$  in the Jacobi parameter  $q_J$  (see ref. 9),

$$\operatorname{cn}\left(\frac{2K}{\pi}\varphi\right) = \frac{2\pi}{kK} \sum_{n=0}^{\infty} c_{2n+1} \cos(2n+1)\varphi,$$

$$\operatorname{dn}\left(\frac{K}{\pi}\varphi\right) = \frac{\pi}{2K} + \frac{2\pi}{K} \sum_{n=1}^{\infty} c_{2n} \cos n\varphi,$$

$$c_n \equiv c_n(k) = q_J^{n/2} (1 + q_J^n)^{-1}, \quad q_J \equiv q_J(k) = \exp\left(-\pi \frac{K'(k)}{K(k)}\right),$$

$$K'(k) = K(\sqrt{1-k^2}).$$
(18)

Substituting expressions (13), (14), (18) into (16) and allowing for (6) and (17) we obtain

$$Q_{1}(t) = \frac{32\pi}{\gamma Z} \int_{0}^{\infty} dE \,\omega(E) \exp\left(-\frac{2E}{B}\right) \sum_{n=0}^{\infty} c_{2n+1}^{2} \cos(2n+1)\omega(E)t, \tag{19}$$

$$Q_2(t) = \frac{2\pi}{\gamma Z} \int_{-\Delta U}^{0} dE \,\omega(E) \exp\left(-\frac{2E}{B}\right) \left\{1 + 8 \sum_{n=1}^{\infty} c_{2n}^2 \cos n\omega(E)t\right\}.$$

 $Q(t) = Q_1(t) + Q_2(t).$ 

Taking into account eqs. (6) and (17), the statistical integral Z may be

presented also as the integral over the energy only. The terms  $Q_1(t)$  and  $Q_2(t)$  in (19) are determined by the ranges of positive and negative oscillator energies, respectively.

The integrands in  $Q_{1,2}(t)$  present the series of harmonics. These series converge fast in the energy range  $E \gg \Delta U$  where the Jacobi parameter  $q_J \approx \exp(-\pi) \ll 1$ , and in the range  $E + \Delta U \ll \Delta U$ , where  $q_J \approx ((E + \Delta U)/64 \Delta U)^{1/2} \ll 1$ . At small |E| the series for  $Q_{1,2}(t)$  are slowly convergent.

In the approximation adopted, when relaxation and fluctuations are not taken into account explicitly, the oscillator with E < 0 does not change from one potential minimum into another and vibrates about one of the equilibrium positions (4). This causes the time-independent term in Q(t). This term decays when the transitions are taken into account.

The spectral distribution of the time correlation function (19) is

$$Q(\omega) = Q_{1}(\omega) + Q_{2}(\omega),$$

$$Q_{1}(\omega) = \sum_{n=0}^{\infty} \psi_{2n+1}(\omega), \quad Q_{2}(\omega) = \psi_{0}\delta(\omega) + 2\sum_{n=1}^{\infty} \psi_{2n}(\omega),$$

$$\psi_{0}(\omega) = \frac{2\pi}{\gamma Z} \int_{-\Delta U}^{0} dE \,\omega(E) \exp\left(-\frac{2E}{B}\right),$$

$$\psi_{n}(\omega) = \frac{16\pi\omega c_{n}^{2}(k_{n})}{\gamma Z n^{2}} \exp\left(-\frac{2E_{n}}{B}\right) \left|\frac{d\omega(E_{n})}{dE_{n}}\right|^{-1}, \quad n \ge 1,$$

$$(20)$$

where  $k_n \equiv k(E_n)$ , while the energies  $E_n$  are determined from the equations

$$\omega(E_{2n+1}) = \frac{\omega}{2n+1} \quad (n = 0, 1, 2, \dots; E_{2n+1} > 0),$$

$$\omega(E_{2n}) = \frac{\omega}{n} \qquad (n = 1, 2, \dots; E_{2n} < 0)$$
(21)

(it may be shown that  $d\omega(E)/dE$  does not vanish anywhere, hence,  $\psi_n(\omega)$  in (20) are finite).

The terms  $Q_1(\omega)$  and  $Q_2(\omega)$  in eq. (20) describe the contributions to the spectral distribution from the vibrations with positive and negative energy, respectively. According to (8), (13), (14),  $\gamma \omega_0^{-1} Q(\omega)$  depends only on the dimensionless parameter  $\beta$  and the variable  $\omega/\omega_0$ . The distribution  $Q(\omega)$  is expressed in (20) by special functions and may be found with the aid of a computer. The results of calculation for several values of the parameter  $\beta$  (8)

are presented in fig. 2. It is not hard to obtain  $Q(\omega)$  in a simple analytical form for the ranges of small and large values of  $\beta$ .

At  $\beta \leqslant 1$ , as already mentioned, the oscillator motion presents mainly the weakly nonlinear vibrations about the potential minima  $(E + \Delta U \leqslant \Delta U)$  with frequencies  $\omega(E) \approx \omega_0 \sqrt{2}$ . The dominant contribution to  $Q(\omega) \approx Q_2(\omega)$  in the range of the peak  $(\omega \approx \omega_0 \sqrt{2})$  is made by the term  $2\psi_2(\omega)$  in (20). Taking into account only terms linear in  $(E + \Delta U)/\Delta U$  in the expressions (14), (18) for  $\omega(E)$ ,  $c_2$  we obtain from eqs. (20), (21)

$$Q(\omega) \approx Q_2(\omega) \approx \frac{\omega_0 \sqrt{2}}{6\gamma} \Omega \exp(-\Omega) \theta(\Omega) ,$$

$$\Omega = -\frac{4}{3\sqrt{2}} \frac{\omega - \omega_0 \sqrt{2}}{\beta \omega_0} , \quad \theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x \le 0, \end{cases}$$

$$\omega \approx \omega_0 \sqrt{2}, \quad \frac{\Gamma}{\omega_0} \ll \beta \ll 1.$$
(22)

The spectral distribution (22) is strongly asymmetric. Its maximum lies at the frequency

$$\omega_{\rm m} = \omega_0 \sqrt{2} (1 - \frac{3}{4}\beta) \tag{23}$$

and its integral width is

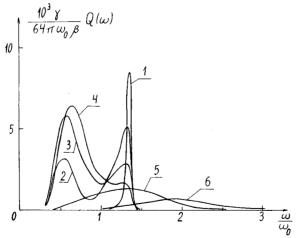


Fig. 2. Spectral distribution  $Q(\omega)$  for the Duffing oscillator in the range  $\omega \gg \omega_0 \ln^{-1}(\omega_0/\Gamma) \gg \Gamma$ . The curves 1 to 6 refer to the parameter values  $4\beta = 0.1$ , 0.3, 0.5, 0.8, 10.0, 40.0. Curve 1 is reduced along the y-axis by a factor of 2.

$$\delta\omega_{\rm I} \equiv Q^{-1}(\omega_{\rm m}) \int_{0}^{\infty} d\omega \ Q(\omega) \approx \frac{3\sqrt{2}}{4} \beta\omega_{0} \, {\rm e} \ . \tag{24}$$

Both the width of the peak and the shift of its maximum relative to  $\omega_0\sqrt{2}$  are proportional to intensity of the random force acting upon the oscillator (to temperature, for the case of coupling to a bath). For very small  $\beta$  when  $\beta\omega_0 \leq \Gamma$  expression (22) is not valid and to calculate the peak shape one should use the theory<sup>7</sup>) that takes into account the spectrum broadening due both to the frequency straggling of the nonlinear oscillator and to the dissipative processes\*.

For  $\beta \gg 1$ , the main contribution to the broad peak of the spectral distribution  $Q(\omega)$  comes from the range of high positive energies  $(E \gg \Delta U, E \sim B)$  and the shape of the peak for the double-well oscillator under consideration appears to coincide with that for the single-well oscillator studied in ref. 8,

$$Q(\omega) \approx \frac{\xi_1 \omega}{\gamma} \tilde{\Omega}^3 \exp(-\xi_2 \tilde{\Omega}^4) , \quad \tilde{\Omega} = \left(\frac{2}{\gamma B}\right)^{1/4} \omega ,$$

$$\xi_1 \approx 0.60 , \quad \xi_2 \approx 0.49 , \quad \omega \sim (\gamma B)^{1/4} \sim \beta^{1/4} \omega_0 , \quad \beta \gg 1$$
(25)

(cf. curve 6 in fig. 2 and curve 5 in fig. 1 of ref. 8 obtained for the same  $\beta$ ). Note that the distribution (25) is independent of  $\omega_0$ .

The analytical expression for  $Q(\omega)$  in the frequency range  $\omega_0 \ln^{-1}(\omega_0/\Gamma) \le \omega \le \omega_0$  may be obtained for arbitrary  $\beta$ . It is presented in section 4 and allows one to understand the "two-humped" structure of the curves 2–4 in fig. 2 corresponding to the range  $4\beta \le 1$ .

# 4. Structure of the low-frequency wing of the spectral distribution in the absence of damping

The spectral distribution  $Q(\omega)$  in the range of relatively low frequencies  $\omega \ll \omega_0$  is formed mainly by vibrations with small |E|,  $|E| \ll \Delta U$ . Since the vibration frequency  $\omega(E)$  decreases with decreasing |E| as  $\ln^{-1}(64 \Delta U/|E|)$  according to (15), the effective density of states for low-frequency vibrations is small,  $|dE/d\omega(E)| \sim \pi |E|\omega_0 \omega^{-2}(E) \ll \Delta U \omega_0^{-1}(|E| \ll \Delta U)$ . It decreases with

<sup>\*</sup> When using the results of ref. 7 (see also ref. 5) for the description of the peak at frequency  $\omega_0\sqrt{2}$  one should take into consideration that in the expansion of the oscillator potential energy near  $q_0$  there are the terms  $\propto (q-q_0)^3$ . Therefore the fourth-order anharmonicity parameter in the expressions for correlators given in ref. 7 should be renormalized (as well as  $\omega_0$ ):  $\tilde{\omega}_0 = \omega_0\sqrt{2}$ ;  $\tilde{\gamma} = -4\gamma$ .

decreasing |E|. This provides fast convergence of the series (20) in the range  $\omega \ll \omega_0$  since for the *n*th overtone at small |E| we have according to (21) and (15)

$$\left| \frac{\mathrm{d}\omega(E_n)}{\mathrm{d}E_n} \right| \propto \exp\left(-\frac{\pi\omega_0}{\omega}n\right).$$
 (26)

If the conditions

$$\varepsilon \equiv \exp\left(-\pi \frac{\omega_0}{\omega}\right) \ll 1 \,, \tag{27}$$

$$\beta > 16 \exp\left(-\pi \frac{\omega_0}{\omega}\right) \frac{\omega}{\pi \omega_0} \tag{28}$$

are fulfilled the main contribution to  $Q(\omega)$  comes from the term with n=1 in (20) which corresponds to the over-barrier motion. At  $\varepsilon < 10^{-2}$ , allowing for (15) we obtain

$$Q(\omega) \approx Q_1(\omega) \approx \left(\frac{8\pi}{\gamma}\right)^2 \frac{\omega_0^5}{\omega} Z^{-1} \operatorname{ch}^{-2}\left(\frac{\pi\omega}{2\omega_0}\right) \exp\left(-\pi \frac{\omega_0}{\omega} - 16\beta^{-1} \exp\left(-\pi \frac{\omega_0}{\omega}\right)\right).$$
(29)

It is seen from eq. (29) that at  $16\beta^{-1} \gg 1$  in the wing of the spectral distribution  $Q(\omega)$  in the range  $\omega < \omega_0$  the additional peak is manifested. This is due to the competition of two factors forming the spectral distribution, namely to the decrease in the state population with increasing E and the simultaneous increase in density of the vibrational states. This peak is sharp at  $\beta < 0.1$  since these competing dependences are exponentially sharp (in energy and frequency, respectively).

It follows from eq. (29) that when the conditions (27), (28) are fulfilled the peak is located at

$$\tilde{\omega}_{\rm m} = \pi \omega_0 / \ln(16/\beta) , \quad \ln(16/\beta) \gg 1 . \tag{30}$$

Eq. (30) within an error <10% describes the position of the left maximum of the curves 2 to 4 in fig. 2. For the curves 2, 3 the left to the right peak amplitude ratio calculated according to eqs. (29), (30), (22) is also in good agreement with the results of numerical calculations. This ratio grows as  $\beta$  increases. For sufficiently large  $\beta$  (when  $\beta \ge 0.3$ ) the peak caused by the intrawell motion cannot be separated. At the same time eq. (29) becomes inapplicable in the range where the maximum of the distribution (29) is located. To calculate the shape of the peak of  $Q(\omega)$  near the maximum in this range of  $\beta$  the complete expression (20) should be used.

A remarkable feature of the distribution (29) is its exponential decrease at

low frequencies:

$$Q(\omega) = A \exp\left(-\pi \frac{\omega_0}{\omega}\right), \quad A = \text{const } \frac{\omega_0}{\omega}, \quad \omega \ll \omega_0.$$
 (31)

For small  $\beta$  the tail of  $Q(\omega)$  is located in the range  $\omega < \tilde{\omega}_{\rm m}$ , but as  $\beta$  grows it spreads over the entire range of  $\omega$  where the criterion  $\varepsilon < 10^{-2}$  ( $\omega < 0.7\omega_0$ ) is fulfilled.

# 5. Structure of the low-frequency wing of the spectral distribution in case of oscillator with an arbitrary double-well potential

It is seen from (29) that the shape of the spectral distribution wing in the region  $\omega < \omega_0$  for the Duffing oscillator depends only on the parameter  $\omega_0$ , while the nonlinearity parameter  $\gamma$  enters only the constant coefficient  $\gamma^{-2}Z^{-1}$ . The parameter  $-\omega_0^2$  is equal to the curvature of the potential at the local maximum (see fig. 1). We shall show that for an arbitrary oscillator whose potential U(q) has a local maximum where  $U(q) = -\frac{1}{2}\omega_0^2q^2$  (the coordinate q is counted off from the maximum position) the spectral distribution in the tail of its broad peak is proportional to  $\exp[-\pi\omega_0/\omega - \theta^{-1}\exp(-\pi\omega_0/\omega)]$  ( $\theta$  is given below).

In the general case the cyclic frequency  $\omega(E)$  of vibrations with E > 0 (the energy E is measured relative to the value U(0)) is

$$\omega(E) = \pi \left( \int_{q_1}^{q_2} dq \left[ 2E - 2U(q) \right]^{-1/2} \right)^{-1}, \tag{32}$$

where  $q_1$  and  $q_2$  are the turning points that limit the motion,  $U(q_i) = E$   $(i = 1, 2), q_1 < 0, q_2 > 0$ . For low energies the main contribution to the integral (32) comes from the range  $|q| \le E^{1/2}/\omega_0$  ( $|q_{1,2}| \ge E^{1/2}/\omega_0$ ), where the integrand is large. As a result of integration we obtain

$$\omega(E) \approx \pi \omega_0 \ln^{-1} \left(\frac{C}{E}\right), \quad C \sim \omega_0^2 q_i^2, \quad E \to 0 \quad (E > 0).$$
 (33)

When relaxation is neglected the time correlation function of a Brownian vibrating particle may be put into the form similar to (19),

$$Q(t) = \int dE \exp\left(-\frac{2E}{B}\right) \sum_{n=0}^{\infty} \varphi_n(E) \cos n\omega(E)t, \qquad (34)$$

where the functions  $\varphi_n(E)$  depend on details of the potential. Let us perform the Fourier-transform over time in (34) and change from integration over E to that over  $\omega(E)$ . Then at small E there appears the factor

$$\frac{\mathrm{d}E}{\mathrm{d}\omega(E)} \approx \pi \omega_0 C \omega^{-2}(E) \exp\left(-\pi \frac{\omega_0}{\omega(E)}\right), \quad E \to 0 \quad (E > 0)$$
(35)

under the integral sign. Keeping only the term with n=1 in (34) at  $\exp[-\pi\omega_0/\omega(E)] \le 1$  (as was done in deriving (29)) and taking (35) into account we obtain

$$Q(\omega) \approx C' \exp\left[-\pi \frac{\omega_0}{\omega} - \theta^{-1} \exp\left(-\pi \frac{\omega_0}{\omega}\right)\right], \quad \theta = \frac{B}{2C}, \quad \exp\left(-\pi \frac{\omega_0}{\omega}\right) \ll 1$$
(36)

(the term with  $\theta^{-1}$  should be allowed for only if  $\theta \le 1$ ). The coefficient C' in (36) depends on a power of  $\omega_0/\omega$ . In (36) just as in (29) the corrections  $\sim \exp(-n\pi\omega_0/\omega)$  with n>1 are neglected. Such corrections are caused in particular by the motion with E<0.

Just as the distribution (29), the function  $Q(\omega)$  (36) has the maximum at  $\omega = \omega_{\rm m} = \pi \omega_0/\ln \theta^{-1}$  if  $\theta \ll 1$ , and in the tail it decreases exponentially with decreasing frequency (cf. (31)). Thus, the low-frequency structure of the distribution of the oscillator with an arbitrary double-well potential is universal and is determined by the curvature of the potential near the local maximum.

The results obtained above may be easily extended to the case of a potential with N local maxima. If the height and curvature of the maxima are identical, relationships similar to (36) are valid with the only difference that  $\omega_0/N$  should be substituted for  $\omega_0$ , and C, C' depend on N. If the heights or curvatures of the local maxima are different the pattern is somewhat more complicated.  $Q(\omega)$  is then represented by a superposition of expressions similar to (36) with the appropriate weight factors. In this case, additional in  $Q(\omega)$  maxima may appear.

## 6. Analysis of the effects caused by dissipation and motion stochasticity

It follows from eq. (31) that in the range of very small frequencies  $\omega \ll \omega_0$  the spectral distribution  $Q(\omega)$  calculated with neglect of dissipation and motion stochasticity is exponentially small. The main contribution to  $Q(\omega)$  in this range is due to the vibration periodicity breaking by the dissipation processes and random forces acting on the oscillator. To analyse  $Q(\omega)$  at  $\omega \ll \omega_0$  and to substantiate the approach used above in calculating the peak of  $Q(\omega)$  at  $\omega \gg \omega_0$ 

(it allowed for the friction and random forces only as for the cause of the Gibbsian energy distribution formation) one may apply the Einstein-Fokker-Planck (EFP) equation.

The estimate of the corrections to  $Q(\omega)$  at  $\omega \ge \omega_0$  that are due to dissipation is given in the appendix. They are proportional to the friction coefficient  $\Gamma$  and are as small as  $\max[\Gamma\omega^{-1}(Q(\omega), \Gamma \partial Q(\omega)/\partial \omega]]$  at  $\Gamma \le \delta\omega$ ,  $\omega$ ,  $\omega_0$ .

A peculiar situation arises in the low-frequency range  $\omega \ll \omega_0$  (but  $\omega \gg \Gamma$ ). The main contribution to  $Q(\omega)$  at these frequencies is due to the oscillator motion with small |E|. The perturbation theory given in the appendix cannot be applied here. This is obvious formally if one substitutes the expression (A.8) for  $V_l^{(1)}$  calculated by the perturbation theory into expression (A.5) for  $Q(\omega)$ . According to eq. (A.1)  $V_l^{(1)}$  contains terms  $\propto \Gamma B \ \partial^2 \omega(E)/\partial E^2$  which are due to the diffusion terms in the EFP-equation. At  $\omega(E) \ll \omega_0$  these terms are proportional to  $E^{-2}$  and thus cause the divergence of the integral over energy in eq. (A.5).

The inapplicability of the perturbation theory at  $\omega(E) \leq \omega(E_c) \leq \omega_0$ , i.e. at  $|E| \leq E_c$ .

$$E_{\rm c} = \left(\frac{\Gamma}{\omega_0}\right)^{1/2} (\mathrm{B} \,\Delta \,U)^{1/2} \,, \quad \Delta \,U = \frac{\omega_0^4}{4\gamma} \,, \tag{37}$$

follows directly from eq. (A.1) since the term  $\Gamma B\omega_l(E)[\partial(p_l\,\partial q_l/\partial E)/\partial E]\times\partial W_{lj}/\partial \varphi$  in the operator  $\Gamma \hat{L}W_{lj}$  in eq. (A.1) at  $|E|\approx E_c$  appears to be of the same order as the term  $\omega_l(E)\,\partial W_{lj}/\partial \varphi$  describing the conservative motion (to obtain this estimate, (A.9) and (35) were used). It is essential that  $E_c$  depends nonanalytically on the random force intensity  $\Gamma B$ .

In the region  $|E| \le E_c$  the oscillator motion is complicated. This is due to a strong frequency dispersion at  $|E| \to 0$  (cf. (33)). At  $|E| \le E_c$ , the oscillator moves near the local potential maximum so slowly that the energy change caused by random forces over a run is sufficient for changing  $\omega(E)$  by an order of magnitude. Therefore, the motion becomes absolutely nonperiodic. The time scale characterizing such motion is determined by the time  $t_c$  needed for the oscillator to leave the region  $|E| \le E_c$ .

The quantity  $t_c$  may be estimated as the diffusion time,  $t_c \sim E_c^2 \bar{D}_{\rm EE}^{-1}$ , where  $\bar{D}_{\rm EE}$  is the characteristic value of the energy diffusion coefficient,  $D_{\rm EE} = \Gamma B p^2$  (it follows from (A.1) that the drift over energy in the range  $|E| \leq E_c$  is much slower than the diffusion). If we use for the estimation of  $D_{\rm EE}$  the value of  $p^2$  averaged over phase at  $E \approx E_c$ ,  $p^2 \sim I\omega(E_c)$  (I is the action,  $I \sim \Delta U/\omega_0$ ), then, taking (37) and (15) into account, we obtain

$$t_{\rm c} \sim \omega_0^{-1} \ln \frac{\Delta U}{E_{\rm c}} \tag{38}$$

According to (15), (37)  $t_c \sim \omega^{-1}(E_c)$ . In fact, the typical energy  $E_c$  itself may be defined as the energy for which the time  $t_c$  is of the same order of magnitude as the period of vibrations of the oscillator with energy  $E_c$ .

The aperiodic motion with the typical time of correlation decay  $t_c$  leads to the appearance of a plateau in the spectral distribution  $Q(\omega)$  at frequencies  $\omega \leq t_c^{-1}$ . The height of the plateau depends on the probability that the absolute value of the initial oscillator energy E does not exceed  $E_c$ . Consequently,

$$Q(\omega) \sim \frac{t_c E_c}{\omega_0 Z} \widetilde{q^2} \sim \frac{1}{Z} \frac{1}{\omega_0^4} \left(\frac{\Gamma}{\omega_0}\right)^{1/2} (B \Delta U)^{1/2} \Delta U, \quad \Gamma \ll \omega \ll t_c^{-1}, \quad 4\beta \geq 1. \quad (39)$$

Here  $\widetilde{q^2}$  denotes the squared amplitude of the vibrations with small  $E, \widetilde{q^2} \sim q_0^2$  (see eq. (4)). We have omitted in (39) the logarithmic factor  $\ln(\Delta U/E_c)$  (the allowance for this factor is beyond the accuracy of the present approach). The inequality  $\omega \gg \Gamma$  in (39) is connected with the presence of the peak of  $Q(\omega)$  at  $\omega \ll \Gamma$  due to interwell transitions.

According to (39), the low-frequency plateau of  $Q(\omega)$  depends nonanalytically on the random force intensity  $\Gamma B$  (in fact it was the friction coefficient  $\Gamma$  that was supposed small in deriving (39)). Just the nonanalyticity in  $\Gamma$  makes the perturbation theory inapplicable for the analysis of the plateau. At  $B \ll \Delta U$  the statistical integral  $Z \propto \exp(2\Delta U/B)$  in (39), and the nonanalytical (in  $\Gamma$ ) correction to  $Q(\omega)$  in the range  $\Gamma \ll \omega \ll \omega_0$  is exponentially small.

The nonanalytic (square root) dependence of  $Q(\omega)$  on  $\Gamma$  was obtained also<sup>7</sup>) in the problem of the single-well Duffing oscillator for the frequency range  $|\omega - \omega_0| \ll (\beta \omega_0 \Gamma)^{1/2}$  (at  $\Gamma \omega_0^{-1} \ll \beta \ll 1$ ). For the Brownian particle moving in a periodic potential the square root (in  $\Gamma$ ) correction to the mobility was obtained in ref. 10.

The fluctuation plateau (39) restricts the range where the exponential tail (31) is manifested by the inequality

$$\omega > 2\pi\omega_0/\ln\left(\frac{\omega_0}{\Gamma}\frac{\Delta U}{B}\right), \text{ i.e. } \omega > t_c^{-1}.$$
 (40)

(The expression (40) contains a weak inequality since the distribution (31) is exponentially sharp.)

#### 7. Conclusions

It follows from the results of the present paper that the presence of a local parabolic maximum in a potential energy curve gives rise to a number of specific features of the spectral distribution  $Q(\omega)$  of classical oscillator. Some of them are caused directly by the motion near the maximum and are determined by the character of this motion and by the curvature of the potential at the maximum  $-\omega_0^2$ , while their dependence on the shape of the potential near the minima is weak.

One of these features is the formation of the maximum of the function  $Q(\omega)$  at frequency  $\omega \leq \omega_0$  for relatively low noise intensity B (for relatively low temperatures in case of oscillator coupled to a thermostat; in this case B=2kT). This peak is connected with the exponential decrease of the oscillator state population with increasing energy on one hand and with the growth (exponential in frequency) of the vibrational state density for the overbarrier motion with increasing energy (and frequency) on the other hand. Therefore the maximum appears to be sufficiently narrow for small  $B/\Delta U$ .

Another feature of the spectral distribution  $Q(\omega)$  is the presence of the exponential tail in the frequency range  $\omega < \omega_0$  (see (27), (40)) for  $\Delta U \leq B$ . The shape of the tail reflects the exponential (for  $\omega(E) \leq \omega_0$ ) form of the vibrational state density for the overbarrier motion.

High sensitivity of the oscillator moving slowly near the potential maximum to external random force results in a nonanalytic (square root) dependence of  $Q(\omega)$  in the range of the low-frequency  $(\Gamma \ll \omega \ll 2\pi\omega_0/\ln(\omega_0 \Delta U/B\Gamma))$  plateau on the friction coefficient  $\Gamma$  at  $\Delta U \ll B$ .

### **Appendix**

It is convenient to write the EFP equation corresponding to the Langevin equation (5) in variables energy and phase,

$$\frac{\partial W_{ij}}{\partial t} = -\omega_{l}(E) \frac{\partial W_{ij}}{\partial \varphi} + \Gamma \hat{L} W_{ij},$$

$$\hat{L} W_{ij} = \omega_{l}(E) \frac{\partial}{\partial E} \left[ \omega_{l}^{-1}(E) p_{l}^{2} \left( 2 + B \frac{\partial}{\partial E} \right) W_{ij} - B p_{l} \frac{\partial q_{l}}{\partial E} \frac{\partial W_{ij}}{\partial \varphi} \right]$$

$$+ \frac{\partial}{\partial \varphi} \left[ -\omega_{l}(E) p_{l} \frac{\partial q_{l}}{\partial E} \left( 2 + B \frac{\partial}{\partial E} \right) W_{ij} + B \omega_{l}^{2}(E) \left( \frac{\partial q_{l}}{\partial E} \right)^{2} \frac{\partial W_{ij}}{\partial \varphi} \right],$$

$$W_{ij} \equiv W_{ij}(E, \varphi, t; E(0), \varphi(0), 0).$$
(A.1)

Here indices l, j run over the values 0, 1, 2. The value 0 refers to the overbarrier motion with energy E > 0 (the energy is relative to the local potential maximum), whereas the values 1, 2 refer to the motion in the left and

right potential wells (see fig. 1) with energy E < 0. The energy E, phase  $\varphi$  and l determine unambiguously the oscillator coordinate  $q \equiv q_l(E, \varphi)$  and momentum  $p \equiv p_l(E, \varphi)$ .

The function  $W_{ij}$  in (A.1) is the probability density for the oscillator transition from the point  $q_j(E(0), \varphi(0))$ ,  $p_j(E(0), \varphi(0))$  to the point  $q_i(E, \varphi)$ ,  $p_i(E, \varphi)$  for the time t. The initial condition for eq. (A.1) is

$$W_{li}(E, \varphi, 0; E(0), \varphi(0), 0) = \omega_l(E)\delta_{li}\delta(E - E(0))\delta(\varphi - \varphi(0)).$$

In fact for each j = 0, 1, 2 eq. (A.1) presents the set of three equations (l = 0, 1, 2). In addition to the initial condition it should be complemented with the conditions of continuity of the functions  $W_{ij}$  and their derivatives over  $p_l(E, \varphi)$ ,  $q_l(E, \varphi)$  at E = 0.

It is easy to see that the stationary solution of eq. (A.1) is of the form (6).

The time correlation function of the oscillator coordinates (1) is expressed in terms of the functions  $W_{ii}$  by the relation

$$Q(t) = \sum_{l} \int \int dE \, d\varphi \, \omega_{l}^{-1}(E) q_{l}(E, \varphi) V_{l}(E, \varphi, t) ,$$

$$V_{l}(E, \varphi, t) = \sum_{j} \int \int dE(0) \, d\varphi(0) \, \omega_{j}^{-1}(E(0)) q_{j}(E(0), \varphi(0)) W_{st}(E(0))$$

$$\times W_{li}(E, \varphi, t; E(0), \varphi(0), 0)$$
(A.2)

(in fact (A.2) is a definition of the procedure of averaging denoted in eq. (1) by the brackets  $\langle \cdots \rangle$ ). The auxiliary function  $V_l(E, \varphi, t)$  introduced here satisfies evidently eq. (1) with the initial condition

$$V_l(E, \varphi, 0) = q_l(E, \varphi) W_{sl}(E) \tag{A.3}$$

and the appropriate joining conditions at E = 0.

The influence of dissipation and fluctuations on the oscillator motion is described by the operator  $\Gamma \hat{L} W_{ij}$  in (A.1) for  $W_{ij}$  (or  $\Gamma \hat{L} V_l$  in the corresponding equation for  $V_l$ ). To analyse the spectral distribution  $Q(\omega)$  in the range  $\omega \ge \omega_0$  with allowance for dissipation and fluctuations it is convenient to perform the Fourier transform over t and  $\varphi$  in the equation for  $V_l$  (obviously, the function  $V_l(E, \varphi, t)$  as well as  $q_l(E, \varphi)$  is periodic in  $\varphi$ ). Then one obtains from (A.1)–(A.3)

$$-\mathrm{i}(\omega - n\omega_l(E))V_l(E, n, \omega) = \frac{1}{2\pi}q_l(E, n)W_{\mathrm{st}}(E) + (\Gamma\hat{L}V_l(E, \varphi, \omega))_n,$$

$$V_l(E, \varphi, \omega) = \frac{1}{2\pi} \int_0^{\infty} dt \exp(i\omega t) V_l(E, \varphi, t),$$

$$V_l(E, n, \omega) = \frac{1}{2\pi} \int_{0}^{2\pi} d\varphi \, \exp(-in\varphi) V_l(E, \varphi, \omega), \qquad (A.4)$$

$$(\Gamma \hat{L} V_l(E, \varphi, \omega))_n = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \exp(-in\varphi) \Gamma \hat{L} V_l(E, \varphi, \omega),$$

$$q_l(E, n) = \frac{1}{2\pi} \int_{0}^{2\pi} d\varphi \exp(-in\varphi) q_l(E, \varphi).$$

According to eqs. (2), (A.2) and (A.4),

$$Q(\omega) = 4\pi \operatorname{Re} \sum_{l} \sum_{n} \int dE \,\omega_{l}^{-1}(E) q_{l}(E, -n) V_{l}(E, n, \omega) \,. \tag{A.5}$$

The solution of (A.4) to zeroth order in  $\Gamma$  is of the form

$$V_l^{(0)}(E, n, \omega) = \frac{i}{2\pi} q_l(E, n) W_{st}(E) (\omega - n\omega_l(E))^{-1}. \tag{A.6}$$

In case of the Duffing oscillator

$$q_{0}(E, 2n - 1) = 2\sqrt{2} \frac{\omega(E)}{\sqrt{\gamma}} c_{2n-1}, \quad q_{0}(E, 2n) = 0, \quad q_{0}(E, 0) = 0,$$

$$q_{0}(E, -n) = q_{0}(E, n) \quad (E > 0)$$

$$q_{l}(E, 2n - 1) = 0, \quad q_{l}(E, 2n) = (-1)^{l} \sqrt{2} \frac{\omega(E)}{\sqrt{\gamma}} c_{2n},$$

$$q_{l}(E, 0) = (-1)^{l} \omega(E)(2\gamma)^{-1/2}, \quad q_{l}(E, -n) = q_{l}(E, n), \quad l = 1, 2 \quad (E < 0)$$

$$n = 1, 2, \dots$$

(see (13), (14), (18)). Eqs. (A.5)-(A.7) result in expression (20).

Below when estimating the corrections we imply the Duffing oscillator model although the analysis may be generalized easily to the case of oscillator with an arbitrary double-well potential. We consider the case also when the noise intensity parameter B is of the same order or greater than the potential well depths  $(\beta \ge 1)$ . This case is of the most interest for the analysis of the low-frequency plateau of  $Q(\omega)$ .

To the first order in  $\Gamma$  the correction to  $V_l(E, n, \omega)$  is

$$V_{l}^{(1)}(E, n, \omega) = i(\omega - n\omega_{l}(E))^{-1} (\Gamma \hat{L} V_{l}^{(0)}(E, \varphi, \omega))_{n},$$

$$V_{l}^{(0)}(E, \varphi, \omega) = \sum_{n} \exp(in\varphi) V_{l}^{(0)}(E, n, \omega).$$
(A.8)

To calculate the contribution of the correction (A.8) to  $Q(\omega)$  at  $\omega \gg \omega_0$  it is expedient to single out in (A.5) the range of small |E| where  $\omega(E) \ll \omega_0 \ll \omega$ . Out of this range the functions  $\omega_l(E)$ ,  $q_l(E,n)$  are seen from (13), (14), (18), (A.7) to depend smoothly on the energy. As a result of the term-by-term action of the differential operator  $\hat{L}$  on the terms  $V_l^{(0)}(E,n,\omega) \exp(in\varphi)$ , the coefficients  $(\omega - n\omega_l(E))^{-2}$  and  $(\omega - n\omega_l(E))^{-3}$  appear. After integrating over energy in (A.5) with allowance for the well-known path-tracing rule (Im  $\omega \to +0$ ) the corresponding terms give the corrections  $\sim \Gamma \partial Q(\omega)/\partial \omega \sim \Gamma(\delta\omega)^{-1}Q(\omega)$  where  $\delta\omega$  is the characteristic width of the spectral distribution (see for details ref. 11). The term-by-term calculation of the right-hand side of (A.8) in the range  $\omega(E) \geq \omega_0$  appears to be convenient due to fast decrease of  $V_l^{(0)}(E,n,\omega)$  with increasing n in this range.

The range  $\omega(E) \ll \omega_0$  needs special consideration since  $|\partial \omega(E)/\partial E| \sim \omega^2(E)(\omega_0|E|)^{-1} \to \infty$  at  $|E| \to 0$  according to (15), (35). The derivatives  $\partial q/\partial E$ ,  $\partial \varphi/\partial E$  diverge also at  $|E| \to 0$ . According to (13),  $q_0(E, \varphi)$  is asymptotically at  $E \to 0$  (E > 0) of the form

$$q_0(E,\varphi) = \left(\frac{2E}{\omega_0^2}\right)^{1/2} \operatorname{sh}\left[\frac{\omega_0}{\omega(E)}\left(\varphi - \frac{\pi}{2}\right)\right], \quad \left|\varphi - \frac{\pi}{2}\right| \ll 1,$$

$$\omega(E) \ll \omega_0, \quad E > 0. \tag{A.9}$$

Eq. (A.9) is written for  $\varphi$  such that the oscillator is near the local potential maximum. This equation is valid for an arbitrary double-well potential. It is obvious from (A.9) that  $|\partial q/\partial E| \approx |q/E|$ .

The divergence of  $\partial \omega/\partial E$ ,  $\partial q/\partial E$  at  $E \to 0$  with allowance for (A.1) and (A.6) causes the divergent terms in the functions  $(\Gamma \hat{L} V_l^{(0)}(E, \varphi, \omega))_n$  in the right-hand side of eq. (A.8). However at  $\omega \gg \omega_0$  the correction to  $Q(\omega)$  due to the range  $\omega_l(E) \ll \omega_0$  appears to be small as a whole. Indeed, taking into account (A.6)

one may put the function  $V_l^{(0)}(E, \varphi, \omega)$  at  $\omega \gg \omega_0$ ,  $\omega(E)$  into the form

$$V_l^{(0)}(E,\varphi,\omega) = \frac{\mathrm{i}}{2\pi\omega} W_{\mathrm{st}}(E) \sum_{m=0}^{\infty} \left( -\mathrm{i} \frac{\omega_l(E)}{\omega} \frac{\partial}{\partial \varphi} \right)^m q_l(E,\varphi). \tag{A.10}$$

The first terms of the expansion (A.10) are respectively

$$\frac{\mathrm{i}}{2\pi\omega}W_{\mathrm{st}}(E)\Big(q_l-\mathrm{i}\frac{p_l}{\omega}+\cdots\Big).$$

In fact the expansion (A.10) is seen from (A.9) to present the series in  $\omega_0/\omega$  for the most "dangerous" range, the vicinity of the local potential maximum. Writing the operator  $\hat{L}$  as

$$\hat{L} = \frac{\partial}{\partial p} \left( 2p + B \frac{\partial}{\partial p} \right),$$

one sees from (A.9) and (A.10) that  $\hat{L}V_{l}^{(0)}(E,\varphi,\omega)$  presents the series in  $\omega_{0}/\omega$  also; this series does not contain the divergences at  $E \to 0$ .

It is easy to verify, taking (A.10) into account, that the contribution of  $V_l^{(1)}(E, n, \omega)$  to the integral (A.5) over the range E where  $\omega(E) \ll \omega_0$  is finite and  $\sim \Gamma \omega^{-1} Q(\omega)$ .

Thus the whole correction to  $Q(\omega)$  at  $\omega \ge \omega_0$  due to dissipation and fluctuations is  $\sim \max[\Gamma\omega^{-1}Q(\omega), \Gamma \partial Q(\omega)/\partial \omega]$ . This justifies the above calculation of  $Q(\omega)$  neglecting dissipation and fluctuations.

## Note added in proof

After the present paper was submitted for publication, we learned of the paper by Y. Onodera (Prog. Theor. Phys. 44 (1970) 1477) where in the zero-friction limit the general expression for the spectral distribution  $Q(\omega)$  of the Duffing oscillator similar to eq. (20) was obtained using another approach and its numerical analysis was carried out. In this paper, however, the peak at zero frequency was missed, the explicit asymptotic expressions for  $Q(\omega)$  (see eqs. (22)–(25), (29)–(31)) were not obtained and the above analysis of the features of  $Q(\omega)$  for the general case of systems with a double-well potential was not given as well.

### References

- 1) H.A. Kramers, Physica 7 (1940) 284.
- 2) N.G. van Kampen, J. Stat. Phys. 17 (1977) 71.
- 3) M. Suzuki, in: Synergetics. Far from Equilibrium, A. Pacault and C. Vidal, eds. (Springer, Berlin, 1979).
- 4) M. Lax, Fluctuation and Coherent Phenomena in Classical and Quantum Physics (Gordon and Breach, New York, 1968).
- 5) M.I. Dykman and M.A. Krivoglaz, in: Soviet Physics Reviews, vol. 5, I.M. Khalatnikov, ed. (Harwood Academic Publishers, New York, 1984).
- 6) M.A. Ivanov, L.B. Kvashnina and M.A. Krivoglaz, Fiz. Tverd. Tela 7 (1965) 2047.
- 7) M.I. Dykman and M.A. Krivoglaz, Phys. Stat. Sol. (b) 48 (1971) 497.
- 8) M.I. Dykman and M.A. Krivoglaz, Physica 104A (1980) 495.
- M. Abramovitz and I.A. Stegun, eds., Handbook of Mathematical Functions, National Bureau of Standards, Applied Mathematics Series 55 (US Govt. Printing Office, Washington. D.C., 1964).
- 10) H. Risken and H.D. Vollmer, Z. Physik B35 (1979) 177.
- 11) M.I. Dykman, S.M. Soskin and M.A. Krivoglaz, Preprint IMP 4.84, Kiev, 1984.