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1986 J. Phys. A: Math. Gen. 19 L1137

(http://iopscience.iop.org/0305-4470/19/18/004)

J. Phys. A: Math. Gen. 19 (1986) L1137-L1140. Printed in Great Britain

LETTER TO THE EDITOR

The coherent tunnelling propagator and chaotic bistability

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Received 11 August 1986

Abstract. The tunnelling propagator is determined by means of an explicit evaluation of the small energy level splittings for ground state as well as excited state doublets in a symmetric double-well potential. Squeezing the initial state is shown to generate considerable chaotic tunnelling features, which are conjectured to involve a fractal dimension.

In a previous letter [1] the energy level splitting ΔE_0 for the lowest lying doublet in a bistable potential $U(x)$ has been obtained by means of a simple explicit formula rather than by either employing a subtly detailed asymptotic connection procedure for the wavefunctions in between the potential minima and the barrier peak or by applying the contextually rather awkward instanton method [2]. If the system (the particle, say) is prepared at time $t=0$ in precisely one of the two local ground states, then the particle travels back and forth between the potential minima as† $x(t)=x(0)\cos(\Delta\omega_0 t)$, where $x(0)=\pm a$ and $\Delta\omega_0\equiv\Delta E_0/\hbar$. The classic microscopic example is the ammonia inversion, but modern dissipation-free superconducting Josephson interference devices (SQUID) should present a promising macroscopic paradigm [3].

However, the level splitting, which is due to the finiteness of the barrier, is of course not restricted to the local vacuum but also exists for the excited states. If the width of the initially prepared local wave packet is squeezed [4] in comparison with the ground state Gaussian, the excited state splittings are necessarily involved in the ensuing tunnelling dynamics.

It will be shown that the method of [1] is perfectly tailored to the determination of the higher tunnelling frequencies, which do not seem to be available elsewhere. Using these results, the tunnelling propagator is evaluated. Although throughout the observed $x(t)$ is given by a coherent‡ superposition of cosine functions, the spectrum is such that a plot of position against time acquires substantial chaotic features [5] upon squeezing the initial state.

For a barrier with a height§ U_0 which is large compared to the local ground state energies $E_1\approx E_0\approx\hbar\omega_0$, where ω_0 represents the harmonic oscillator frequency of the potential wells, it suffices to use the semiclassical wavefunctions (see e.g. [6]) in the barrier peak region. Through first order in $\hbar\omega_0/U_0\ll 1$, one may readily present the globally even and odd solutions in the following form:

$$\begin{aligned}\psi_{2n}(x)&=[2U(x)]^{-1/4}\cosh[-(n+\tfrac{1}{2})\omega_0\tau(x)+\tfrac{1}{2}S(x)/\hbar]\\ \psi_{2n+1}(x)&=[2U(x)]^{-1/4}\sinh[-(n+\tfrac{1}{2})\omega_0\tau(x)+\tfrac{1}{2}S(x)/\hbar]\end{aligned}\qquad(1)$$

† As it is unlikely to be misunderstood, the quantum mechanical brackets on $x(t)$ have been omitted.
‡ Coherent is used in this context in the sense of non-stochastic, non-dissipative, time reversible.
§ Throughout the particle mass $m=1$, for convenience, so that potential height equals energy difference.

where $n=0, 1, 2, \ldots$, and

$$S(x) \equiv \int_{-x}^{x} (2U(x'))^{1/2} \mathrm{d}x' \qquad \tau(x) \equiv \int_{0}^{x} \mathrm{d}x'/(2U(x'))^{1/2}. \tag{2}$$

By symmetry one may confine oneself to, say, positive x. When $x \to a$, i.e. towards a potential minimum, it suffices to keep only the leading exponential $\exp(\frac{1}{2}S_0/\hbar)$, with $S_0 \equiv S(a)$, from the hyperbolic functions. In addition, it is important to observe that in this region $\tau(x)$ behaves like

$$\tau(x) \to \tau_0 + \omega_0^{-1} \ln[a\omega_0/(2U(x))^{1/2}] \tag{3}$$

which implicitly defines τ_0. Inserting all this into (2.1), setting $U(x) \approx \frac{1}{2}\omega_0^2(x-a)^2$ in the logarithm in (2.3) and defining the local coordinate $\eta \equiv (\omega_0/\hbar)^{1/2}(x-a)$, it is easily seen that $\psi_{2n}(x) \approx \psi_{2n+1}(x)$ acquires a prefactor proportional to η^n upon the approach of the parabolic well region. Hence, both functions smoothly connect with the local eigenfunction belonging to the nth excited local oscillator state, as follows:

$$\psi_{2n}(x) = \tfrac{1}{2}(a\omega_0)^{-1/2}\left[\frac{1}{2a}\left(\frac{\hbar}{\omega_0}\right)^{1/2}\right]^n H_n(\eta) \exp[-\tfrac{1}{2}\eta^2 - (n+\tfrac{1}{2})\omega_0\tau_0 + \tfrac{1}{2}S_0/\hbar] \tag{4}$$

where $H_n(\eta)$ is the nth degree Hermite polynomial, while $\psi_{2n+1}(x) = \psi_{2n}(x)$ here. This is as much as is needed for the evaluation of the level splitting by means of the method of [1].

Using $\psi_{2n}(0)$ and $\psi'_{2n+1}(0)$ from (1)† in the numerator, and inserting $\psi_{2n}(x)$ and $\psi_{2n+1}(x)$ from (4) into the integral in the denominator of the simple formula

$$\Delta E_{2n} = \tfrac{1}{2}\hbar^2[\psi_{2n}(0)\psi'_{2n+1}(0)]\left(\int_0^{\infty} \psi_{2n}(x)\psi_{2n+1}(x)\,\mathrm{d}x\right)^{-1} \tag{5}$$

for the level splitting $\Delta E_{2n} \equiv E_{2n+1} - E_{2n}$, one may write the result in the form

$$\Delta\omega_{2n} = (\bar{\omega}_{2n}/\pi)\exp(-S_0/\hbar) \tag{6}$$

where $\Delta\omega_{2n} \equiv \Delta E_{2n}/\hbar$, and where the attempt frequency [1] for the nth doublet will be

$$\bar{\omega}_{2n} = \bar{\omega}_0[a\exp(\omega_0\tau_0)(2\omega_0/\hbar)^{1/2}]^{2n}/n! \tag{7}$$

with $\bar{\omega}_0 = 2a\omega_0\exp(\omega_0\tau_0)(\pi\omega_0/\hbar)^{1/2}$. As it should, this $\bar{\omega}_0$ agrees with the result of [1].

The time evolution of any initial wave packet $\phi(x)$ is dictated by the propagator [6, 7]

$$K(x, t|x', 0) = \sum_{n=0}^{\infty} \psi_n(x)\psi_n^*(x')\exp(-\mathrm{i}E_n t/\hbar) \tag{8}$$

which can now be calculated by means of the results given above. For $\phi(x)$ we take the Gaussian wavepacket

$$\phi(x) = [\pi\hbar\exp(-2R)/\omega_0]^{-1/4}\exp[-\tfrac{1}{2}\eta^2\exp(2R)] \tag{9}$$

† In $\psi'_{2n+1}(0)$, the prime denoting differentiation WRT x, terms of relative order $\hbar\omega_0/U_0 \ll 1$ are disregarded.

which is centred at a potential minimum, and where R is a squeezing parameter [4]. Multiplying (8) by $\phi(x')$, integrating over x' using the normalised versions of (4) and invoking formula 7.374.4 from [8], one finds†

$$\phi(x, t) = \sum_{n=0}^{\infty} A_{2n}[\psi_{4n}(x)\exp(-\mathrm{i}E_{4n}t/\hbar) + \psi_{4n+1}(x)\exp(-\mathrm{i}E_{4n+1}t/\hbar)] \tag{10}$$

where $A_{2n} = \{[(2n)!]^{1/2}(\frac{1}{2}\tanh R)^n\}[n!(2\cosh R)^{1/2}]^{-1}$. Integrating the probability density $P(x, t) \equiv |\phi(x, t)|^2$ over either positive or negative values of the coordinate, and once more using the functions (4), it is easy to obtain the probability $P_0(t)$ to still or again find the particle in the initial well at time $t \geqslant 0$. In this letter we confine ourselves to presenting the ensuing expectation value‡ of $x(t)$.

As before dropping the expectation brackets for convenience, the result§ becomes

$$x(t)/x(0) = \sum_{n=0}^{\infty} 2A_{2n}^2 \cos(\Delta\omega_{4n}t) \tag{11}$$

where the coefficients (respectively the frequencies) can be found in (10) (respectively (6)). As it should, at zero squeezing (i.e. $R = 0$) all $A_{2n} = 0$ except $A_0 = 1/\sqrt{2}$ and (11) properly reduces to the well known single cosine.

The summations should be handled with discretion, primarily as they involve the parabolic approximation for the potential minima. But even if the global potential were a perfect double oscillator, the formulae for the level splittings should be expected to fail for levels above the barrier peak. Within the scope of this letter, however, the following should suffice.

Consider from (6) the ratio $\Delta\omega_{2n+2}/\Delta\omega_{2n} \approx \beta$, where we have defined the parameter $\beta \equiv (2a^2\omega_0/\hbar)\exp(2\omega_0\tau_0)$. For the typical double oscillator $\tau_0 = 0$ [1], while $U_0 = \frac{1}{2}\omega_0^2 a^2$, which makes $\beta = 4U_0/\hbar\omega_0$. Obviously, $\beta \gg 1$. Next consider the sum in (11). The Nth term involves the $2N$th excited doublet, which is connected with the $2N$th excited oscillator states in the potential wells, i.e. with energy $E_{2N} \approx (2N + \frac{1}{2})\hbar\omega_0$. Requiring $E_{2N} \leqslant U_0$, one obtains the constraint $N \leqslant \frac{1}{8}\beta$ on the number of significant terms. On the other hand, cutting off at the energy $E_{2n} \approx U_0$ also implies a restriction on the amount of squeezing. Roughly keeping the energy contained in the squeezed initial state $\phi(x)$ below the barrier energy, i.e. $E(R) = \frac{1}{2}\hbar\omega_0\cosh(2R) \leqslant U_0$, one obtains the constraint $R \leqslant \frac{1}{2}\cosh^{-1}(\frac{1}{2}\beta)$.

In figure 1 the function $x(t)/x(0)$ has been computed‖ for $\beta = 46\pi/3 \approx 48.1711$, using $N = 6$, at $R = 1$ and 2. The timescale is in units where $\Delta\omega_0 = 1$. Each figure involves 51 sample points over 1.5 fundamental periods starting at $t = 0$. Hence, the sampling time interval equals $\Delta t = 3\pi/50$. As a consequence of the rather high ratio $\sim\beta^2$ of successive frequencies, it is obviously difficult to resolve anything beyond the coherent oscillation associated with the lowest lying doublet. In particular at somewhat increased squeezing, the higher doublets make the trajectory look rather chaotic. Improving the sampling frequency reveals ever more similar structure in the figure, as will be shown elsewhere [9]. This being a typical feature of fractal objects

† Concerning [8]: one should use the revised 1980 edition here. Concerning (10): the absence of odd-indexed A_{2n+1} is due to the symmetry of $\phi(x)$ about $\eta = 0$.

‡ Terms of relative order $(\hbar\omega_0/U_0)^{1/2} \ll 1$ are neglected.

§ Noticing that $(2n)!/n! = 2^{2n}(\frac{1}{2})_n$, using either a binomial series or an elementary result from the theory of Gauss hypergeometric series, and invoking a simple relation for hyperbolic functions, it is easily verified that the RHS of (11) indeed sums up to unity at $t = 0$, as it should.

‖ I am particularly grateful to Dr J A Boden for his generous assistance in this matter.

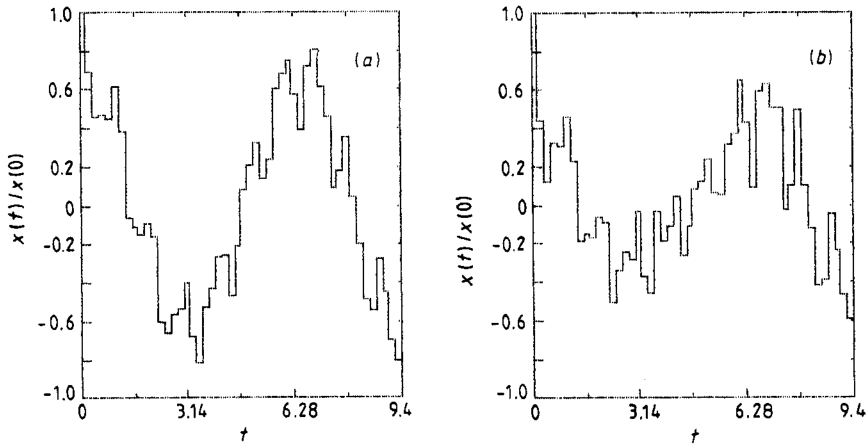

Figure 1. Expected normalised position against time of a particle tunnelling in a symmetric bistable potential, at two values ($R = (a)$ 1 and (b) 2) of the squeezing of the initial state, according to formula (11) of the text. $N = 6$ is the number of terms in the sum carried along in the actual calculations. Sampling time intervals amount to $\Delta t = 3\pi/50 \approx 0.1885$. The parameter $\beta(=46\pi/3 \approx 48.1711$ in this example) measures the height of the barrier. Details of such pictures (but not the conjectured fractal dimension) are particularly sensitive to the precise values of β and the sampling times, the sensitivity growing with increased squeezing. At $R = 0$ (no squeezing, i.e. 'ground state tunnelling') the figures reduce to the 'standard' single cosine.

[10] it is conjectured that the present tunnelling paths can be assigned a fractal dimension D, at least for not too small squeezing. Preliminary calculations seem to confirm this conjecture and yield, for example, $D \approx 1.86$ at $R = 1$ [9].

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