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Time evolutions of quantum mechanical states in a symmetric double-well potential

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The time evolution of quantum mechanical states in a square well of infinite depth with a Dirac δ function at its center has been examined for cases where the initial state was localized in one of the wells. Let well A denote the well in which the initial state is localized, and let $P(t)$ denote the integrated probability density $\Psi^*\Psi$ in well A. For opaque barriers the time-dependent system is adequately described by a two-state model in which only the pair of stationary states of even and odd parity are considered whose wave functions in well A, apart from an arbitrary phase factor, are largely identical with the wave function of the initial state. For $P(t)$ a harmonic oscillation is observed whose frequency ν_t is well approximated by the well-known formula for the tunneling frequency $\nu_t \simeq \Delta E/h$, where ΔE represents the energy separation among the pair of states in the model. For the present model of a symmetric double well it has been shown that for highly transparent barriers a three-state model can describe the time evolution adequately. The three stationary states involved in this model are a state of odd parity whose wave function in well A is largely the same as the wave function of the initial state and a pair of stationary states of even parity which on the energy scale are immediately above and below the first state. In this three-state model the function $P(t)$ is a superposition of two sinusoidal functions with nearly identical amplitudes and frequencies plus a constant. As a consequence, the amplitude of $P(t)$ changes harmonically. In the present model a δ function has been used as a barrier in order to minimize the mathematical detail involved in the time-dependent treatment. It is to be expected that the beating in $P(t)$ can be observed also in the time evolution of a state localized in one of the wells of a symmetric double-minimum potential with a more realistic "low" barrier if the density of energy levels near the energies of the levels to be considered in the corresponding three-state model varies slowly with energy.

I. INTRODUCTION

In discussions of patterns in the energies of stationary states of a symmetric double well the simplest model in use is the infinite square well with a Dirac δ function at its center

$$V(x) = (\hbar^2/m)\Omega\delta(x), \qquad (1)$$

for $|x| < a$ and V is infinite for $|x| > a$. Using the abbreviation $k_n^{\pm} = (2mE_n^{\pm})^{1/2}/\hbar$, the wave functions for the stationary states can be formulated as follows:[1,2]

$$\psi_n^+(x) = \begin{cases} -A_n^+ \sin[k_n^+(x+a)] & \text{for } -a \leqslant x \leqslant 0, \quad (2a) \\ A_n^+ \sin[k_n^+(x-a)] & \text{for } 0 \leqslant x \leqslant a, \quad (2b) \end{cases}$$

and

$$\psi_n^-(x) = A_n^- \sin(k_n^- x) \quad \text{for } -a \leqslant x \leqslant a, \qquad (3)$$

where ψ_n^+ and ψ_n^- are states of even and odd parity, respectively. For levels of odd parity the solutions turn out to remain unaffected by the presence of the barrier at $x = 0$ and we obtain $k_n^- = n\pi/a$ with $n = 1,2,3,...$ and $A_n^- = a^{-1/2}$.[1]

For levels of even parity the first derivative of the wave functions ψ_n^+ is discontinuous at the location of the δ function and the appropriate boundary conditions give rise to a quantization of the energy levels as follows:[1,2]

$$\zeta_n \cot \zeta_n = -\Omega a, \qquad (4)$$

where $\zeta_n = k_n^+ a$. The levels obtained from (4) as a function of Ωa are shown in Fig. 1. The normalization factors for the levels of even parity are

$$A_n^+ = \{a[1 - \sin(2\zeta_n)/2\zeta_n]\}^{-1/2}. \qquad (5)$$

The present work is concerned with the time evolution of a

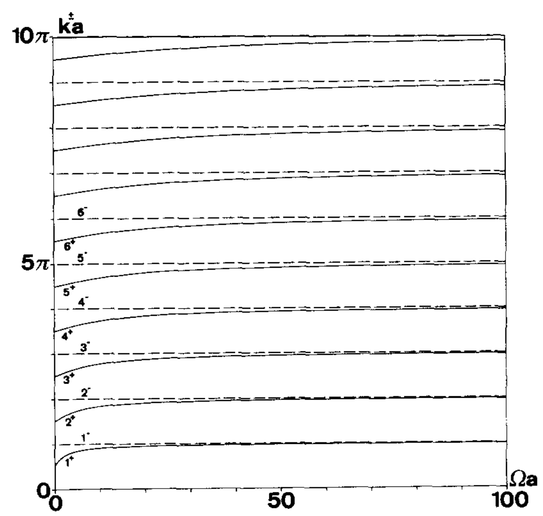

Fig. 1. Level positions for δ functions of different strengths. Full lines even, broken lines odd parity.

state that originally is localized in one of the wells. For this, the following wave function is used:

$$\Psi(x,0) = (2/a)^{1/2} \sin[(N\pi/a)(x+a)] \quad (6)$$

for $-a \leqslant x \leqslant 0$ and $\Psi(x,0) = 0$ otherwise. N is a positive integer. The time-dependent wave function can then be constructed from the initial wave function $\Psi(x,0)$ and the wave functions for the stationary states as follows:[3]

$$\Psi(x,t) = \sum_n (C_n^+ \psi_n^+(x) e^{-iE_n^+ t/\hbar} + C_n^- \psi_n^-(x) e^{-iE_n^- t/\hbar}), \quad (7)$$

where

$$C_n^\pm = \int_{-a}^{0} \psi_n^\pm(x)\Psi(x,0)dx. \quad (8)$$

With the wave function of the initial state formulated as shown in (6) all C_n^-, except C_N^-, vanish, where $C_N^- = (-1)^N 2^{-1/2}$.

The time evolution of the system for the wave function o the initial state as shown in (6) will be examined with th help of the degree of localization of the particle in the tw wells as a function time

$$P(t) = \int_{-a}^{0} \Psi^*(x,t)\Psi(x,t)dx, \quad (9)$$

where Ψ^* denotes the complex conjugate of Ψ. In what follows the time t will be replaced by the dimensionless variable τ, where $\tau = (\hbar/2ma^2)t$. The probability of localization in the left-hand well as a function of τ can readily be computed as follows:

$$P(\tau) = 1/4 + N^2\pi^2 \sum_n \xi_n [1 + 2\cos(u_{Nn}\tau)], \quad (10)$$

where $u_{Nn} = (N\pi)^2 - \zeta_n^2$ and

$$\xi_n = (1 - \sin 2\zeta_n/2\zeta_n)^{-1}(\sin\zeta_n/u_{Nn})^2. \quad (11)$$

II. APPROXIMATE RESULTS FOR OPAQUE BARRIERS

If Ωa is large, i.e., if the barrier is opaque, then the coefficients ξ_n in the sum in (10) are small with the exception of ξ_N such that P becomes a sinusoidal function of τ and the particle oscillates among the wells. For Ωa large we obtain from (4)

$$\zeta_N \simeq N\pi[1 - (\Omega a)^{-1}]. \quad (12)$$

Then $u_{NN} \simeq 2N^2\pi^2/\Omega a$. Let τ_0^{-1} denote the tunneling frequency. The period of the oscillation among the wells becomes then $2\pi/u_{NN}$ such that

$$\tau_0 \simeq \Omega a/N^2\pi. \quad (13)$$

In Fig. 2 the probability of localization of the particle in the left-hand well is shown for two cases. In both cases $N = 1$ in the initial state but in one case the barrier is fairly transparent in which case the oscillations in P are somewhat irregular and the tunneling frequency is high. For the opaque barrier where $\Omega a = 64P$ follows a regular sinusoidal curve whose period of oscillation expressed in the dimensionless measure of time τ is roughly 20. This is in fair agreement with the result of the above analysis because Eq. (13) gives $\tau_0 \simeq 64/\pi = 20.4$.

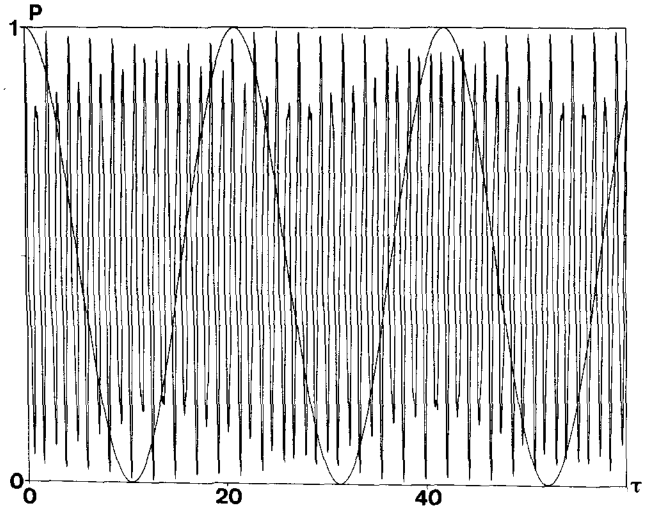

Fig. 2. Probability of localization in the left-hand well as defined in (9) as a function of the time τ with $N = 1$ in $\Psi(x,0)$. The curve with the high frequency of oscillation is for $\Omega a = 1$ and the one with the low frequency of oscillation is for an opaque barrier with $\Omega a = 64$.

III. APPROXIMATE RESULTS FOR HIGHLY TRANSPARENT BARRIERS

For transparent barriers with Ωa small and/or large values of N the oscillations in P are modulated as shown in Fig. 3. In this case two of the coefficients ξ_n in (10) turn out to be relatively large and of roughly equal size, namely ξ_N and ξ_{N+1}. This can be inferred from (11) and the energy levels depicted in Fig. 1. For small values of Ωa and/or N large we obtain

$$\zeta_n \simeq (n - \tfrac{1}{2})\pi[1 + \Omega a/(n - \tfrac{1}{2})^2\pi^2]. \quad (14)$$

It can then be shown that[4]

$$P(\tau) \simeq \text{const} + \alpha\cos[(\pi^2/4 + 2\Omega a)\tau]\cos(N\pi^2\tau), \quad (15)$$

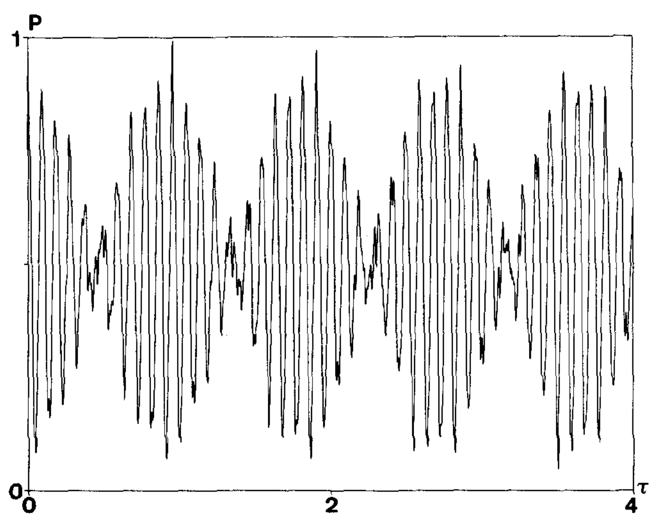

Fig. 3. Probability of localization in the left-hand well defined in (9) as a function of τ for $\Omega a = \frac{1}{2}$ and with $N = 7$ in the initial state.

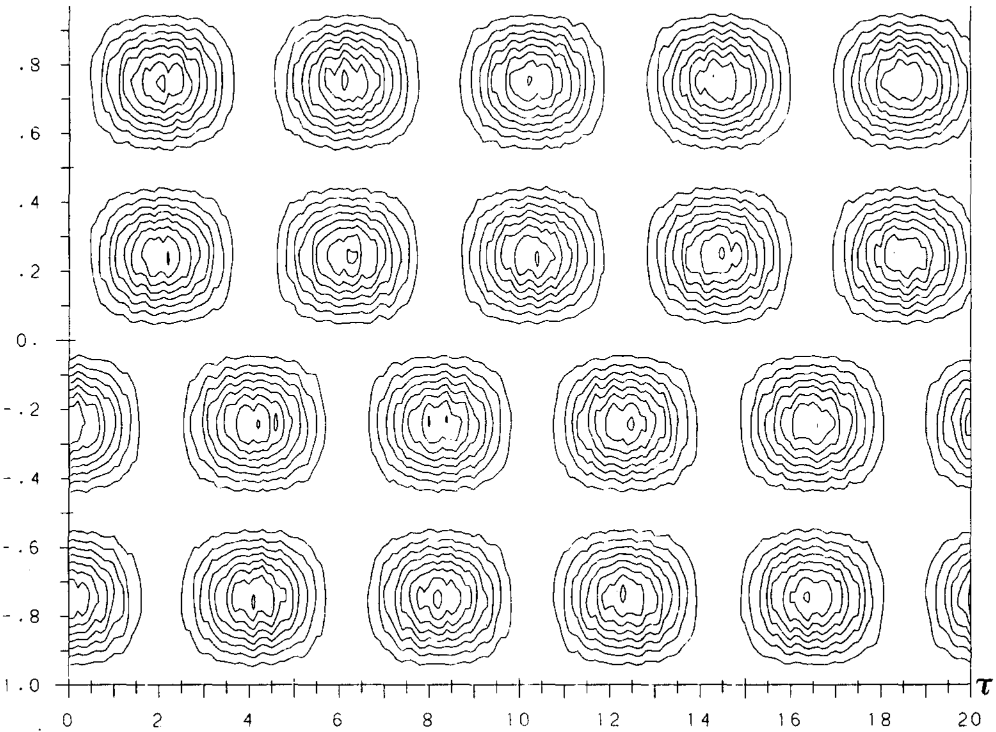

Fig. 4. Contour plot of the probability density $\Psi^*\Psi$ as a function of τ (horizontal axis) and the location x (vertical axis) for $\Omega a = 50$ and $N = 2$ in $\Psi(x,0)$. The vertical separation among neighboring contours is 0.25.

where α represents some constant coefficient. We would then expect to observe oscillations with a period $2/N\pi$ which incidentally corresponds to the classical frequency of a particle with $ak = N\pi$ confined in a square well of length $2a$. According to (15) these oscillations are modulated with an oscillatory function whose period is $(\pi/8 + \Omega a/\pi)^{-1}$. For the case depicted in Fig. 3 we obtain for the period of oscillation $2/(7\pi) = 0.091$ in good agreement with what is observed in Fig. 3. For the period of the modulation we compute a value of 1.8 and the value observed in Fig. 3 is indeed located somewhere between 1.8 and 1.9.

IV. CONCLUSIONS

For opaque barriers the tunneling frequency ν_t is inversely proportional to the strength of the barrier. In this limit the tunneling frequency, i.e., the frequency with which the system shuttles back and forth between the wells, is related to the energy splitting ΔE among pairs of energy levels of even and odd parity and with the same n by the well-known formula $\nu_t = \Delta E/h$.[5,6] From (12) and noting that the corresponding level with odd parity is at $k_n^- a = N\pi$ we obtain for the period of tunneling $\tau_0 \simeq \Omega a/N^2\pi$ in agreement with the results obtained from (10) and (11).

For "low" barriers, the period of oscillations approaches the nonzero value $2/N\pi$ as $\Omega a \to 0$ and the oscillations are modulated by an oscillatory function whose period is roughly $(\pi/8 + \Omega a/\pi)^{-1}$. According to this, the modulation persists if $\Omega a \to 0$. Since (15) applies in the limit where N is large it would seem appropriate to introduce some purely classical concepts. For a particle confined in one of the wells with an energy for which $ak = N\pi$, the classical velocity is $\hbar N\pi/ma$ from which the period of oscillation in the double well of length $2a$ is obtained as $\tau_0 = 2/N\pi$ in agreement with the approximate result obtained for small values of Ωa.

Figure 4 shows a contour plot of the probability density $\Psi^*\Psi$ for an opaque barrier with $\Omega a = 50$ and with $N = 2$ in the initial state. The contour plot in Fig. 4 illustrates a regular pattern typical for opaque barriers where the particle oscillates between the wells. Figure 5 depicts the probability density for a fairly transparent barrier with $\Omega a = 0.5$ and with $N = 7$ in the initial state. There we can observe a basic pattern in which the particle is reflected at the walls at $x = -a$ and $x = a$. This regular pattern disappears in the region where the modulation vanishes; but later the oscillations resume with a phase shift of roughly π. This phase shift is due to the reversal of sign of the modulation. In the limit $\Omega a \to 0$ the coefficients C_n in the expansion of $\Psi(x,t)$ are zero or small with the exception of C_N^-, C_N^+, and C_{N+1}^+ where the coefficients for the stationary states of even parity are of roughly equal size. Interference in the evolution of the relevant pair of stationary states of even parity with wave functions $\psi_N^+(x)$ and $\psi_{N+1}^+(x)$ gives rise to a modulation of $P(\tau)$ whose frequency depends on the strength of the barrier but not on the integer N characterizing the initial state.

The reason why for small values of Ω only those three states are important can be seen from the fact that for $\Omega \to 0$ we have $\zeta_n = k_n^+ a \to (n - \frac{1}{2})\pi$, from which according to (11) we obtain the following:

$$\zeta_n \simeq \{\pi[N^2 - (n - 1/2)^2]\}^{-2}. \quad (16)$$

From the above formula it is apparent that in the expansion for $P(\tau)$ in (10) the terms with $n = N$ and $n = N + 1$ are roughly of equal size and much larger than the remaining

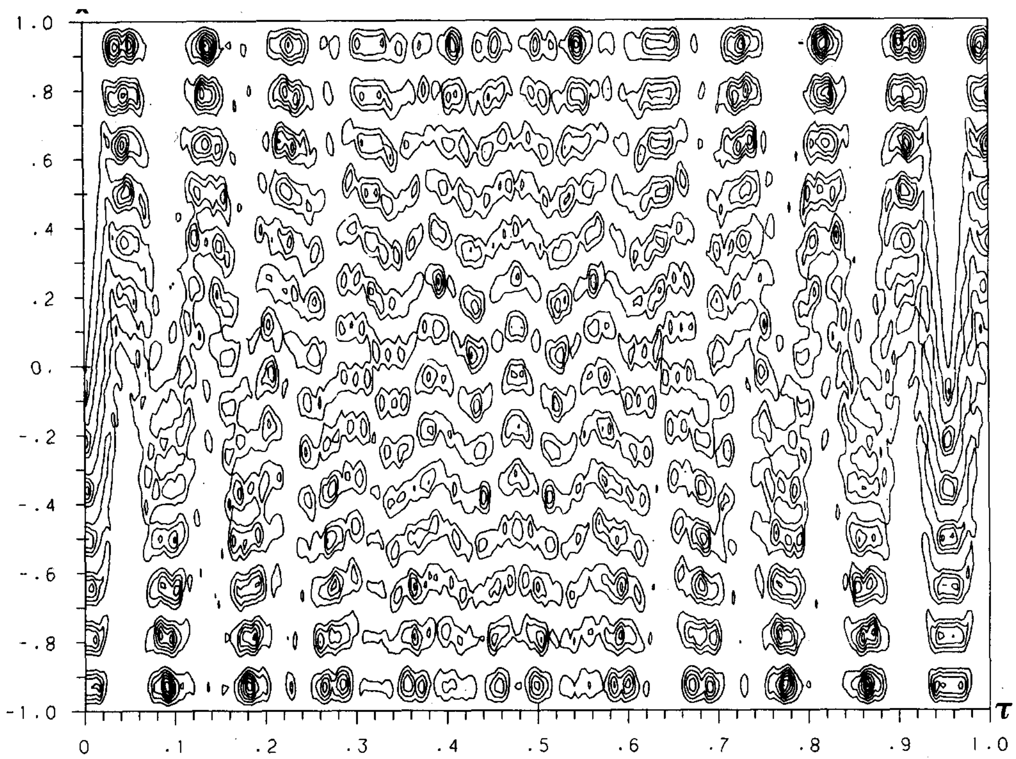

Fig. 5. Same as in Fig. 4 but for $\Omega a = \frac{1}{2}$ and $N = 7$ in $\Psi(x,0)$. The vertical separation among neighboring contours is 0.5.

terms. This is especially true if N is large. In a mathematical sense this means that in (10) we have a superposition of a pair of sinusoidal functions with nearly equal amplitudes. The periods u_{Nn} of these sinusoidal functions are nearly the same for large values of N. These conditions give rise to the observed beating in $P(\tau)$.[4] The coefficients C_n^+ in the expansion of the wave function $\psi(x,0)$ are closely related to the quantities ζ_n. In a physical sense this means that as a first approximation the three stationary states ψ_N^-, ψ_N^+, and ψ_{N+1}^+ are sufficient in the expansion of the time-dependent wave function $\psi(x,t)$ in (7). The stationary state ψ_N^- gives rise to a constant and the pair of neighboring states ψ_N^+ and ψ_{N+1}^+ of even parity give rise to terms with sinusoidal functions whose frequencies become $\pi^2(N \pm 1/4)$ if $\Omega \to 0$. For a superposition of a pair of sinusoidal functions the observed beating may arise if both the amplitudes and the periods of oscillation are nearly the same, which in the present example turns out to be the case for large values of N. For more realistic symmetric double-minimum potentials the time evolution of a state localized initially in a particular well is expected to give rise to beating in the integrated probability density $P(\tau)$ if the energies of the pair of stationary states of even parity to be considered in the corresponding three-state model are almost equal distances apart from the energy level of the stationary state of odd parity in between. Investigations of time evolutions of symmetric static double-wells have indeed uncovered patterns with regular alterations of collapse and revivals in $P(\tau)$ or related quantities if the wave function is not initially symmetric.[7] These so-called *quantum beats* disappear if the initial wave function is projected into each one of the invariant subspaces of the evolution operator, and each projection is considered separately.[7]

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[4]From (14) we obtain $u_{NN} \simeq (N - 1/4)\pi^2 - 2\Omega a$ and $u_{N,N+1} \simeq -(N + 1/4)\pi^2 - 2\Omega a$. Since ξ_N and ξ_{N+1} are roughly the same we can write $P(\tau) \simeq \text{const} + (\alpha/2)\ [\cos(u_{NN}\tau) + \cos(u_{N,N+1}\tau)]$ from which the result in (15) can readily be derived using the well-known trigonometric formula $\cos\alpha + \cos\beta = 2\cos[(\alpha + \beta)/2]\cos[(\alpha - \beta)/2]$.

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