Ultrasharp Crossover from Quantum to Classical Decay in a Semiconductor Heterostructure

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The decay of metastable states is dominated by quantum tunneling at low temperatures and by thermal activation at high temperatures. The escape rate of a particle out of a square well is calculated within a semi-classical approximation and exhibits an 'ultrasharp' crossover: a kink in the decay rate separates a *purely quantum* regime at low temperatures from a *purely thermal* regime at high temperatures. An experimental system – a semiconductor heterostructure – that may be used to check the prediction, along with necessary experimental conditions, are described.

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The decay of metastable states[1] is a phenomenon of great generality, with realizations ranging from the creep of vortices in superconductors[2] to the decay of false vacua[3] in cosmology[4]. A particular interest of the decay phenomenon resides in the fact that it relates quantum to classical metastability: the decay rate is highly sensitive to temperature, it is dominated by quantum tunneling at low temperatures and by thermal activation at high temperatures.

A canonical example consists of a quantum mechanical particle in an asymmetric potential well, as illustrated in Fig. 1. Because of energetic metastability, sooner or later the particle leaves the well and escapes to the right. The decay rate Γ, defined as the inverse lifetime, depends on the form of the effective action at temperature T. At low T the particle occupies its ground state most of the time and escapes through quantum tunneling, so that $\Gamma \propto e^{-S(0)/\hbar}$, where $S(0)$ is the quantum mechanical action, while at high T the decay is Arrhenius-like, with $\Gamma \propto e^{-V_0/T}$.

Here, we calculate the decay rate of a particle initially residing in the well of Fig. 1, and find that the transition from quantum to classical behavior is 'ultrasharp': a singularity separates a purely quantum regime from a purely classical regime. From a theoretical point of view, this example is valuable as its semi-classical treatment is asymptotically exact for large V_0. It also serves as a natural model to study an experimentally realizable object, namely a semiconductor heterostructure. Below, we define the object in question more precisely and discuss the specific experimental conditions needed to observe an ultrasharp crossover.

Before deriving specific results, we briefly describe general properties of the decay rate Γ. Mathematically, metastability may be encoded in imaginary corrections to the energy levels $E_n = \mathrm{Re}E_n - i\hbar\Gamma_n/2$. Here $\mathrm{Re}E_n$ are the energy levels in the large V_0 limit, in which the rates Γ_n are small (limit of 'true metastability'). The probability $\mathcal{P} \propto \left|e^{-iE_nt/\hbar}\right|^2$ that the system occupies a given state then decays exponentially in time, according to $e^{-\Gamma_n t}$. If the lifetimes $1/\Gamma_n$ are larger than the local thermal equilibrium time, the initial preparation of the system is irrelevant; the particle fluctuates in low-energy states according to the Boltzmann distribution. Decay occurs because of rare fluctuations that drive the particle through the energy barrier. In field-theoretic language, these fluctuations correspond to imaginary time trajectories (instantons)[5] that come about as solutions to saddle-point equations and, as a result, impose an exponential dependence $\Gamma = A(T)e^{-S(T)/\hbar}$, where $S(T)$ is an effective action. For true metastability $S(T)/\hbar \gg 1$ and the main dependence of the decay rate upon temperature comes from the action as, typically, the temperature dependence of the prefactor $A(T)$ is weak.

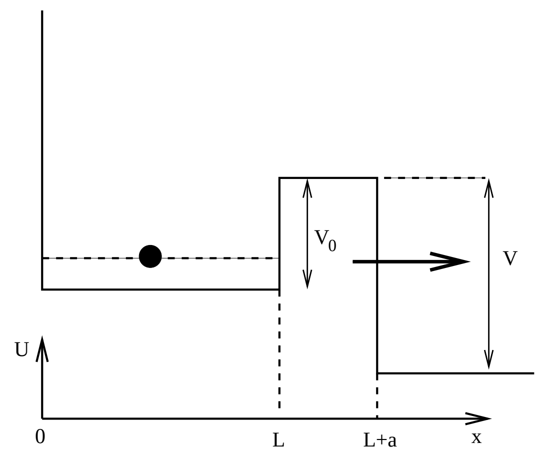

FIG. 1: Illustration of our simple theoretical model, consisting of a particle in a square well. Decay of the metastable state occurs by escape to the right (represented by the bold arrow).

Generically, the action $S(T)$ varies from the ground state action $S(0)$ at $T = 0$ to the high T Arrhenius limit $\hbar V_0/T$, where V_0 is the height of the energy barrier to overcome. This crossover, nevertheless, may occur in qualitatively different ways[6–12], depending on the shape of the trapping potential and the metastable dynamics[13], as illustrated on Fig. 2. For some metastable systems, the function $S(T)$ is smooth within the whole temperature range, but its second derivative is discontinuous at a critical temperature T_c (curve (a) on Fig. 2). Phase tunneling in a Josephson junction[14] constitutes a typical example of such a behavior. It may also happen that the derivative of S with respect to T has a discontinuity, resulting in a kink beyond which the behavior becomes purely classical (with $S \propto 1/T$) (curve (b) on Fig. 2). Such a singular temperature dependence was observed in Mn_{12} molecular magnets[15]. Our example yields yet another type of crossover, in which the quantum and classical behaviors are completely separated (curve (c) on Fig. 2): as before the decay rate is purely classical above the kink but, what is more, it is controlled by quantum tunneling *only* (with a *temperature-independent* action $S(0)$) below the kink. Such ultrasharp transitions are easier to detect experimentally, and might serve as useful tools for future investigations of macroscopic quantum phenomena.

We emphasize that the curves in Fig. 2 are qualitatively different. Curve (a) corresponds to the continuous deformation of a given instanton as the temperature is increased. By contrast, curve (b) results from the balance of two instantons, whose associated actions become equal at T_c. We note that below T_c, thermal fluctuations play a role as the effective action depends upon the temperature. Curve (c) is a limiting case of curve (b), in which the minimal action is the pure quantum action (corresponding to tunneling out of the ground state) up to T_c.

For the well of Fig. 1, the imaginary correction to the nth energy level E_n is proportional to $\exp(-S_{E_n}/\hbar)$, with S_{E_n} the usual semi-classical (WKB) action

$$S_{E_n} = 2\sqrt{2m\,(V_0 - E_n)}a. \tag{1}$$

If local thermal equilibrium is achieved fast enough, the particle in the well occupies states that are very close to stable ($V_0 \to \infty$) ones, with probabilities given by the Boltzmann weight. Thus, the decay rate reads

$$\Gamma \propto \sum_n \Gamma_n e^{-E_n/T}, \tag{2}$$

with $\Gamma_n \propto e^{-S_{E_n}/\hbar} = e^{-2\sqrt{2m(V_0-E_n)}a/\hbar}$. In the limit of true metastability, the sum in Eq. (2) runs over a large number of terms and is dominated by the largest contribution, to wit the one that minimizes the function

$$f(E) = \frac{S_E}{\hbar} + \frac{E}{T}. \tag{3}$$

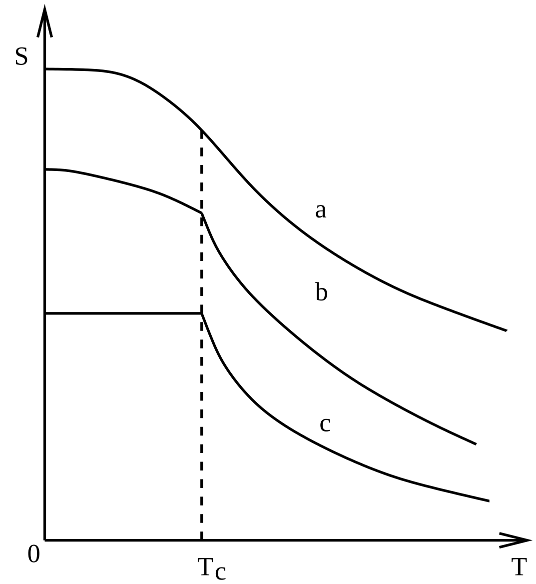

FIG. 2: Different types of crossover from quantum to classical decay: (a) smooth, (b) sharp, and (c) ultrasharp. At high T, thermal activation dominates and $S(T) \propto 1/T$ in all three curves.

It is easy to see that f has no local minimum in $[0, V_0]$ as its second derivative $\partial^2 f/\partial E^2$ is negative everywhere in the interval. Consequently, $f(E)$ takes its smallest value either at $E = 0$ (at low T) or at $E = V_0$ (at high T). Precisely,

$$\ln\left(\frac{1}{\Gamma}\right) \propto \frac{S(T)}{\hbar} = \begin{cases} \frac{2\sqrt{2mV_0}a}{\hbar}, & T < \frac{\hbar}{2a}\sqrt{\frac{V_0}{2m}} \equiv T_c, \\ \frac{V_0}{T}, & T > T_c. \end{cases} \tag{4}$$

Hence decay results either from purely quantum tunneling or from thermal activation out of the ground state. The ultrasharp crossover between the two is signaled by a kink in $S(T)$, as in curve (c) of Fig. 2.

We now turn to possible experimental realizations of our theoretical model. The temperature dependence of the decay rate may be extracted from current measurements, as the current is proportional to $\exp(-S(T)/\hbar)$. The required potential barrier may be 'chiseled' in a semiconductor heterostructure[16]. Using, *e.g.*, Si doped $Al_xGa_{1-x}As$, one can modulate spatially the concentration x in order to generate a rectangular barrier and one can tune the Si doping in order to control the concentration of carriers. Finally, one can apply an external electric field in order to bias current (Fig. 3(a)). We note, however, that a large electric field significantly distorts the potential away from a rectangular shape, and invalidates the form of the action $S(T)$ given in Eq. (4). (In that case, one has to take a non-vanishing electric field into account. While still sharp, the crossover becomes less abrupt and may not be classified as 'ultrasharp' in the presence of large enough electric fields[17].)

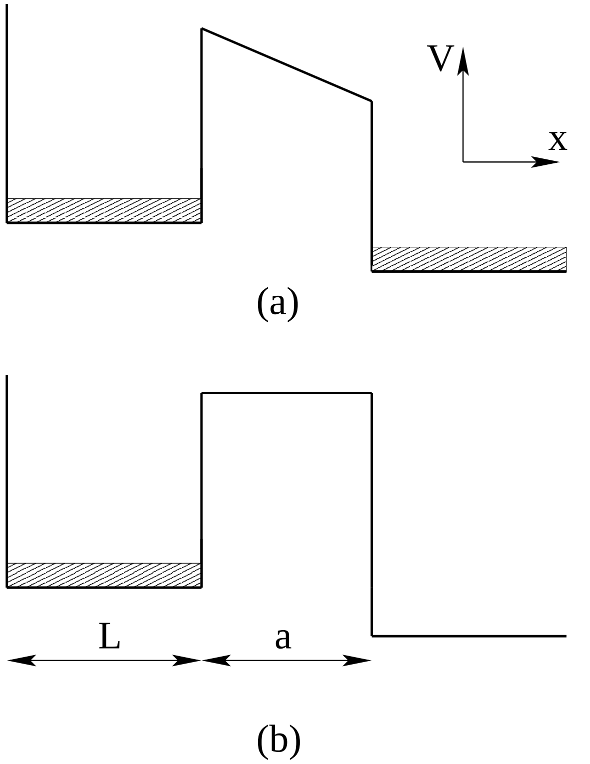

FIG. 3: Illustration of the experimental setups we propose in order to measure an ultrasharp crossover. (a) An applied electric field imposes a bias to the right. (b) Carriers in the left region are produced by ionization of deep donors (DX-centers). They are trapped in the metastable state and will eventually tunnel out to the right.

Thus, one requires that $a \ll L$. Alternatively, one may generate a linear potential, again using a semiconductor heterostructure[16], in order to 'compensate' for the effect of the electric field. As an aside, we remark that the setup just described may be realized best in vertical quantum dots[18].

Semiconductor heterostructures offer yet another possibility, which circumvents the use of electric fields altogether. In $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$, a high enough aluminium concentration x generates deep donors (the so called DX-centers)[16, 19]. One can ionize these donors with light and, hence, transfer their electrons into the conduction band. The carriers thus created do not reintegrate the ionized deep donors rapidly because of high barriers (of, typically, more than 0.1 eV). In effect, the relaxation time of carriers (associated with their reabsorption) may far exceed the tunneling time. Thus, in order to mimic the setup of Fig. 1, one can prepare a rectangular barrier in a Si-doped heterostructure (as in Fig. 3(a)) and then photoionize DX-centers to the left of the barrier (Fig. 3(b)) in order to bias current, instead of applying an electric field.

Experimental potentials are smeared in comparison to strictly rectangular barriers. Our theory is applicable if the characteristic size of the smearing is much smaller than the width a of the barrier, as the ultrasharp transition originates in the existence of a large enough region $L < x < L + a$ in which the potential does not vary substantially. We estimate the required value of a as follows. The characteristic value of the action $S_0/\hbar = V_0/T_c$ may be estimated as $2\sqrt{2m^* V_0}a/\hbar$, where the effective electron mass m^* relates to the free electron mass m_0 through $m^* \approx 0.1 m_0$. With $T_c \approx 5$ K and $V_0/T_c \approx 30$, we obtain $a \approx 160$ nm. Thus, a greatly exceeds the characteristic size of imperfections, typically comparable to atomic sizes of a few tenths of nanometers.

Before concluding, we point out that the metastability condition $S(T) \gg \hbar$ cannot be satisfied in practice arbitrarily well. If the action $S(T)$ is too large, the tunneling time exceeds the duration of experiments, and no current is detected. Typically, one requires $S(T)/\hbar \lesssim 30$ in order to observe decay. (One should ensure, though, that the thermal relaxation times of the carriers in the metastable well be much smaller than their characteristic lifetimes, so that quasiequilibrium hold.) Because of the finiteness of $S(T)$, the crossover from quantum to classical behavior is rounded over a narrow region, the width of which is estimated as follows. As long as the difference between classical and quantum actions, divided by $\hbar$, is of order 1, *i.e.*, as long as

$$\left| \frac{S_0}{\hbar} - \frac{V_0}{T} \right| \lesssim 1, \tag{5}$$

neither of the two processes dominates over the other. Assuming $V_0/T_c \gg 1$ and expanding $1/T$ in $\Delta T = T - T_c$, we find that the crossover is rounded over an interval $\Delta T \approx T_c^2/V_0 \ll T_c$.

In summary, we showed that the decay rate of a metastable electron in a rectangular well exhibits an ultrasharp transition from quantum to classical behavior: to exponential accuracy, decay results from quantum tunneling only, below a critical temperature T_c set by the barrier height, while above T_c, only thermal activation is relevant. Moreover, we described a semiconductor heterostructure that may be used to check our theoretical prediction, as well as some of the associated experimental restrictions.

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