Quantum tunnelling time and the adiabatic theorem

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We study the probability of a spin-flip of a particle when it is transmitted through the potential barrier with the spatially rotating field interacting with its spin. According to the adiabatic theorem, the probability depends on the velocity of the particle inside the barrier. The probability decreases as the height of the barrier increases due to the decrease of the velocity inside the barrier. However, it is numerically observed that the probability starts to increase again when the height of the barrier becomes close to the kinetic energy of the particle and exceeds it to enter the tunnelling regime. We suggest that this apparent increase in nonadiabaticity in the tunnelling regime can be caused by the limitation of the measurement of time by the time-of-flight method and preferred transmission of the higher energy modes at the end of the barrier.

The adiabatic theorem in quantum mechanics [1] has been applied to a wide range contexts, such as quantum phase transitions [2][8], geometric phase [9], quantum computations [10], chemical reactions [11] and atomic or molecular collision theory [12][14].

In the adiabatic theorem, the concept of time plays a crucial role. However the role of time occasionally becomes ambiguous in quantum mechanics [14][17]. In particular, the problem of quantum tunnelling time, i.e., “How long does quantum tunnelling take?”, has been a long-standing controversial issue of quantum mechanics [18][25]. Quantum tunnelling has been studied in various fields, including superconductors [20], spintronics [27], micromaser fields [28], nuclear fusion [29] and biological or chemical processes [30][31]. Many attempts have been made to define quantum tunnelling time, including the phase times [18][19], the dwell time [32], the Larmor time [33], or by using the time-dependent potential barrier [34], paths integrals [35] and weak measurements [36][37]. It has now become possible to address the problem experimentally using strong field tunnelling ionization [38] or ultracold atoms [39][40].

Here we consider the adiabatic theorem for a spin of a particle which propagates through the region with a gradual rotation of the direction of the field interacting with the spin. The model could be relevant to the electronic transport through a domain wall in a ferromagnetic [41][43]. First, we show that the probability of a spin flip of the particle after the propagation depends on its velocity due to the adiabatic theorem. We then introduce a rectangular potential barrier in addition to the field to investigate the adiabatic theorem during quantum tunnelling. The increased probability of a spin flip is numerically observed in the tunnelling regime. Finally, we suggest that the increase in the probability can be caused by the limitation of the measurement of time by the time-of-flight method and preferred transmission of the higher energy modes at the end of the barrier.

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1 The situation relevant to our toy model could be a conduction electron locally exchange coupled to electrons in a fixed configuration responsible for the magnetization of domains (separated by a domain wall).
Eq. (4) for a comparison. In other words, the reorientation of the field. In other words, the perspective of the spin state so that the spin can track the probability of a spin flip can be calculated as \[ \psi_s(y) = \frac{1}{\sqrt{2}} \psi_s(y_0) + \frac{1}{\sqrt{2}} \psi_s(y_0) \] or \[ \psi_s(y) = \frac{1}{\sqrt{2}} \psi_s(y_0) - \frac{1}{\sqrt{2}} \psi_s(y_0) \] respectively. This is the probability for finding the spin state \( \downarrow \) or \( \uparrow \) along the direction of the field in \( y \gg D \) when the state is initially prepared in \( \uparrow \) or \( \downarrow \) respectively along the direction of the field in \( y \approx -D \) before the propagation.

By repeating the above numerical computations with different \( k_0 \) so that \( \omega_0/E_0 = [0.01, 0.2] \), we obtain the result in Fig. 1. When \( \omega(v)/\omega_0 \geq 1 \), it can be seen that the result agrees well with the analytical plot from Eq. (4) represented by the solid grey line. This confirms that, in the regime of the weak field, the probability of a spin flip for the particle propagating through the spatially rotating field can be estimated by the adiabatic theorem where the adiabaticity is determined by the velocity of the particle \( v = k_0/m \). On the other hand, the strong field modifies the dynamics of the particle significantly. As a result, the time evolution of the particle becomes different depending on the initial spin state, and the numerical result deviates from the analytical estimate \( \text{Eq. (4)} \) when \( \omega(v)/\omega_0 < 1 \).

In this model, the spin interacting with the field may be considered to be able to measure the propagation time \( T \approx 2D/v = \pi \tau_D \) by observing the velocity of the particle. However, we have \( \mathcal{P} \rightarrow 0 \) and \( \mathcal{P} \rightarrow 1 \) when \( \tau_D \gg \tau_0 \) and \( \tau_D \ll \tau_0 \) respectively. Therefore, for a reasonable resolution of the time, it is necessary to have \( T \approx \tau_0 \). This indicates that the energy transfer between the spin and the particle should be large when \( T \) is small. Since the uncertainty of the momentum of the particle becomes \( \Delta k \sim \omega_0/v \sim 1/2D \) by the energy transfer, only measurements on the particle with \( k_0 \gg 1/2D \) would have reasonable accuracy. This is an inherent limitation of the time-of-flight method. Other ways of measuring time of propagation using a coupling to a physical clock also cannot avoid this limitation [14, 33].

Now let us consider the situation where there exists the potential barrier in addition to the field (Fig. 2). The Hamiltonian can be written as

\[ H = \frac{k^2}{2m} + \frac{\omega_0}{2} \hat{f} \cdot \hat{r} + U(y) \] (6)

where we introduce the rectangular potential barrier such that \( U(y) = U_0 \) for \( |y| < L \) and \( U(y) = 0 \) otherwise, and \( L \geq D \). In addition to the conditions stated in [2], we assume that \( \hat{f} = 0 \) when \( |y| > L \). However, the discussions below also apply to the case where the uniform field \( \hat{f} = \frac{1}{2} \hat{r} \) is...
The dashed grey line is given by Eq. (4) with the approximate velocity \( v = \sqrt{2m(E_0 - U_0)/m} \). Since \( \omega_0 \) is disregarded, the analytic estimates of \( P \) for \( \ket{\uparrow} \) and \( \ket{\downarrow} \) are the same. The dashed grey line is plotted in the range where the analytical expression of \( v \) is well-defined, \( U_0/E_0 \leq 1 \). When \( L \) and \( D \) are large and the interaction time between the field and the spin can be long, it is possible to measure the nonadiabaticity of the propagation with a small \( \omega_0 \) (upper panel). However, in this regime, the tunnelling probability becomes extremely low, \( e^{-4\kappa L} \approx 10^{-9} \) for \( U_0/E_0 \approx 1.001 \) with \( \kappa = \sqrt{2m(U_0 - E_0)} \). In order to obtain a reasonably high tunnelling probability, the length of the barrier \( 2L \) should be around \( 1/\kappa \). With this length, the appropriate resolution for the measurement of the nonadiabaticity can be obtained with \( \omega_0 \) which causes the momentum transfer \( \Delta k \approx 1/2D \geq \kappa \). In other words, the energy transfer \( \Delta E \geq \kappa^2/2m \) is necessary in exchange for the reasonable resolution. In the lower panel, the tunnelling probability can be estimated as \( e^{-4\kappa L} \approx 5 \times 10^{-3} \) for \( U_0/E_0 \approx 1.2 \), and it can be seen that \( \omega_0 \) should be increased to measure the nonadiabaticity for a short \( L \). However, a large \( \omega_0 \) has a great effect on the dynamics of the particle instead and can alter it significantly. In both the upper and lower panels, \( P \) decreases as \( U_0/E_0 \) increases when \( U_0/E_0 \) is sufficiently smaller than 1 since \( v \) decreases inside the potential barrier. However, as \( U_0 \) approaches to \( E_0 \) and exceeds it to enter the tunnelling regime (\( U_0/E_0 \geq 1 \), \( P \) starts to increase again. This behaviour can be seen in both \( \ket{\uparrow} \) and \( \ket{\downarrow} \) initial spin states. Similar results were obtained in experiments attempting to measure quantum tunnelling time using the Landau clock [39, 40] and the results were interpreted as the tunnelling taking less time for higher barriers.

These results may be understood as follows. Due to the initial spatial localization of the wave packet and the energy transfer from the spin, the wave packet is broadened in momentum space and modes with higher energies than the barrier can exist even when \( U_0/E_0 \) is greater than 1. The constructive interference between these modes and the modes with lower energies than the barrier form the wave packets propagating through the barrier from left to right. When the wave packets arrive at the right edge of the barrier and are transmitted out of the barrier, some modes get reflected at the boundary of the barrier. As the energy of the barrier increases, the higher energy modes are selectively transmitted at the boundary. Therefore, the wave packets which propagated non-adiabatically are preferentially transmitted and it appears that the probability of a spin-flip increases for higher barriers in the tunnelling regime when the measurements are performed on the right side of the barrier.

FIG. 3: The probability of a spin flip \( P \) as the function of \( U_0/E_0 \) evaluated numerically. The initial spin state is prepared in \( \ket{\uparrow} \) (navy squares) and \( \ket{\downarrow} \) (pink triangles) respectively. The dashed grey line is given by Eq. (4) with the approximate velocity \( v = \sqrt{2m(E_0 - U_0)/m} \) for a comparison. In the lower panel, \( L \) is shorter and \( \omega_0 \) is larger than in the upper panel.

\[ -\text{sgn}(y)\hat{x} \text{ exists outside the potential barrier } |y| > L. \]

When \( E_0 > U_0 + \omega_0/2 \), it is known that the velocity inside the barrier can be approximated by \( v \approx k_{\text{fin}}/m = \sqrt{2m(E_0 - U_0 + \omega_0/2)/m} \) where \( k_0 \) and \( k_1 \) correspond to the momentum of the particle with the up spin state and the down spin state respectively. However \( k_{\text{fin}} \) inside the barrier in the tunnelling regime \( E_0 < U_0 + \omega_0/2 \) is imaginary. We use this model to investigate the nonadiabaticity of the propagation of the particle in the tunnelling regime. Fig. 3 shows the probability of a spin flip \( P \) of the transmitted parts after the propagation through the potential barrier evaluated numerically using the time-dependent Schrödinger equation with the Hamiltonian [40] and the initial wave packet \( |\Psi_{\text{in}}\rangle \) (navy squares) or with \( |\psi\rangle = |\downarrow\rangle \) (pink triangles). Here \( P = \int_{-\infty}^{\infty} \psi^*(y)\psi(y)dy \sum_{\sigma \neq \tau} \int_{-\infty}^{\infty} \psi_{\sigma}(y)\psi_{\tau}(y)dy \) with \( |\Psi_{\text{out}}\rangle = e^{-iHt}|\Psi_{\text{in}}\rangle = \sum_{\sigma \neq \tau} \psi_{\sigma}(y)|\psi\rangle \) and \( P \) is plotted as the function of \( U_0/E_0 \). We chose \( \sigma_0/D = 1 \), \( L/D = 2 \) and \( \omega_0/E_0 = 0.01 \) in the upper panel and \( \sigma_0/D = 5 \), \( L/D = 1 \) and \( \omega_0/E_0 = 0.1 \) in the lower panel respectively. The dashed grey line is given by Eq. (4) with the approximate velocity \( v = \sqrt{2m(E_0 - U_0)/m} \). Since \( \omega_0 \) is disregarded, the analytic estimates of \( P \) for \( |\uparrow\rangle \) and \( |\downarrow\rangle \) are the same. The dashed grey line is plotted in the range where the analytical expression of \( v \) is well-defined, \( U_0/E_0 \leq 1 \). When \( L \) and \( D \) are large and the interaction time between the field and the spin can be long, it is possible to measure the nonadiabaticity of the propagation with a small \( \omega_0 \) (upper panel). However, in this regime, the tunnelling probability becomes extremely low, \( e^{-4\kappa L} \approx 10^{-9} \) for \( U_0/E_0 \approx 1.001 \) with \( \kappa = \sqrt{2m(U_0 - E_0)} \). In order to obtain a reasonably high tunnelling probability, the length of the barrier \( 2L \) should be around \( 1/\kappa \). With this length, the appropriate resolution for the measurement of the nonadiabaticity can be obtained with \( \omega_0 \) which causes the momentum transfer \( \Delta k \approx 1/2D \geq \kappa \). In other words, the energy transfer \( \Delta E \geq \kappa^2/2m \) is necessary in exchange for the reasonable resolution. In the lower panel, the tunnelling probability can be estimated as \( e^{-4\kappa L} \approx 5 \times 10^{-3} \) for \( U_0/E_0 \approx 1.2 \), and it can be seen that \( \omega_0 \) should be increased to measure the nonadiabaticity for a short \( L \). However, a large \( \omega_0 \) has a great effect on the dynamics of the particle instead and can alter it significantly. In both the upper and lower panels, \( P \) decreases as \( U_0/E_0 \) increases when \( U_0/E_0 \) is sufficiently smaller than 1 since \( v \) decreases inside the potential barrier. However, as \( U_0 \) approaches to \( E_0 \) and exceeds it to enter the tunnelling regime (\( U_0/E_0 \geq 1 \), \( P \) starts to increase again. This behaviour can be seen in both \( |\uparrow\rangle \) and \( |\downarrow\rangle \) initial spin states. Similar results were obtained in experiments attempting to measure quantum tunnelling time using the Landau clock [39, 40] and the results were interpreted as the tunnelling taking less time for higher barriers.

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To conclude, we investigated the adiabatic theorem during quantum tunnelling using the model of a particle propagating through the potential barrier with the spatially rotating field, whose spin is interacting with the field. In the model, the non-adiabatic transition probability of the spin state can be related to the velocity of the
particle inside the barrier. It was presented numerically that the probability decreases as the height of the barrier increases and the velocity slows down when \( U_0/E_0 \ll 1 \). On the other hand, when the particle propagates through the barrier in the tunnelling regime (\( U_0/E_0 > 1 \)), an increase of the non-adiabatic transition probability is observed. However, we pointed out that the time-of-flight method has an inherent limitation that the energy transfer \( \Delta E > \kappa^2/2m \) is necessary in order to investigate the dynamics inside the barrier of length \( 2L \sim 1/\kappa \). This indicates that this method is not sensitive enough to analyze the dynamics of modes whose wavelengths are longer than the length of the barrier. We suggest that the apparent increase of the non-adiabatic transition probability for higher barriers is caused by the existence of modes whose energies are higher than the barrier even when \( U_0/E_0 > 1 \), due to the initial localization of the wave packet in position space and the energy transfer from the spin. When the wave packet exits the barrier after the propagation, they leave the barrier without reflection if the barrier is low. On the other hand, the higher barrier reflects the lower energy modes at the right end and the higher energy modes get selectively transmitted. As a result, the latter can appear to have propagated more non-adiabatically.

We demonstrated that the spatially varying field with the potential barrier can provide a new platform to investigate the quantum tunnelling phenomena with the adiabatic theorem. However, this method, like other time-of-flight methods such as the Larmor clock, cannot avoid its inherent limitation. If the length of the barrier is shortened so that the tunnelling has a reasonable probability, the amount of energy transfer required to obtain an appropriate resolution of time of propagation would increase. As a result, this method can modify the dynamics significantly and may not be suitable for analyzing the dynamics of modes with wavelengths longer than the barrier.

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