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CHAOTIC BEHAVIOR OF HOLE MIXING TUNNELING IN ASYMMETRIC COUPLED QUANTUM WELLS

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Coherent oscillatory motion of hole mixing tunneling in asymmetric coupled quantum well structures collapses if the heavy hole state in the first well is aligned with the light hole state in the second well under a significant in-plane vector $k_{\parallel}$. The tunneling probability obtained by the time-dependent Schrödinger operator with the Luttinger Hamiltonian in the oscillation collapse region is shown to be a chaotic time series using the simplex projection method. This effect is attributed to the nonlinear interaction of mixing tunnelings between HH to the LH state in the first well and HH to the LH state in the second well. © 1997 Elsevier Science Ltd. All rights reserved

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The possibility of utilizing interwell coherent tunneling in coupled quantum wells which consist of two quantum wells located sufficiently close together has been first proposed by Luryi [1]. Considerable efforts have been devoted to this oscillation effect due to its rich physical natures and possible device applications in the range of terahertz radiation [2–6]. By applying the external electric field across coupled quantum wells, resonant condition can be achieved and an enhancement in tunneling time has been observed using time-resolved luminescence spectroscopy [3–4]. A real-time coherent oscillation of an electron wave packet in a coupled quantum well structure has been reported using the pump and probe technique and the time-domain terahertz spectroscopy [5–6]. In addition, the interplay between tunneling and chaos in a coupled quantum well potential has become an interesting subject. Lin and Ballentine [7] have established chaotic zone of spatial oscillatory tunneling in a double well potential under a driven anharmonic oscillator. The coherent oscillation is maintained in spite of the intervening of chaotic zone. Roncaglia *et al.* [8] have shown the size effects of chaotic zone on the tunneling rate under periodically perturbed double-well potential. Müller *et al.* [9] have observed a transition to chaos resulting from resonant tunneling spectroscopy of a quantum well in a tilted magnetic field.

For the valence band, in addition to the spatial hole tunneling (from one well to the other) [10], mixing tunneling (between heavy (HH) and light hole (LH) states) are also involved in the process due to the band mixing effects ($k_{\parallel} \neq 0$) [11–12]. The mixing tunneling which causes the oscillatory motion between two states have been verified using the pump and probe technique and the time-domain terahertz spectroscopy. In this letter we further suggest that a new kind of chaotic behavior could occur in the valence band of the mixing tunneling if the heavy hole state in the first well is aligned with the light hole state in the second well. The oscillatory motion has been described by the time-dependent Schrödinger operator with the Luttinger Hamiltonian [13]. By calculating the tunneling probability for each case, the mixing tunneling and spatial tunneling which happen at the same time can be clearly resolved. For a small in-plane vector $k_{\parallel}$, the tunneling probability shows an oscillation between heavy hole band and light hole band. However, as the $k_{\parallel}$ increases, the oscillatory motion between heavy and light hole tunneling collapses. The oscillation collapse is attributed to the nonlinear interaction of mixing tunneling between HH to the LH state in the first well and HH to the LH state in the second well. The tunneling probability in the oscillation collapse region can be shown to be a chaotic time series using the simplex projection method [14–15]. This method uses a reconstructed trajectory vector to make short and long term predictions about future behaviors based on the previous observed information. If the correlation coefficient between the predicted and observed values falls as the prediction extends further into the future, this time series is thus regarded as a chaotic time series.

The time-dependent Schrödinger equation with the reduced 2×2 Luttinger Hamiltonian H_h is written by [13, 16]

$$H_h \begin{pmatrix} \phi^1(x,t) \\ \phi^2(x,t) \end{pmatrix} = \begin{pmatrix} P + Q + V_h(z) & \tilde{R} \\ \tilde{R}^* & P - Q + V_h(z) \end{pmatrix} \begin{pmatrix} \phi^1(x,t) \\ \phi^2(x,t) \end{pmatrix} = i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \phi^1(x,t) \\ \phi^2(x,t) \end{pmatrix} \quad (1)$$

where

$$P = \frac{1}{2}\left(\frac{\hbar^2}{m_0}\right)\gamma_1 k_\parallel^2 - \frac{1}{2}\left(\frac{\hbar^2}{m_0}\right)\frac{\partial}{\partial z}\gamma_1\frac{\partial}{\partial z},$$

$$Q = \frac{1}{2}\left(\frac{\hbar^2}{m_0}\right)\gamma_2 k_\parallel^2 + \left(\frac{\hbar^2}{m_0}\right)\frac{\partial}{\partial z}\gamma_2\frac{\partial}{\partial z},$$

$$\tilde{R} = \left(\frac{\hbar^2}{m_0}\right)\left(\frac{\sqrt{3}}{4}(\gamma_2+\gamma_3)k_\parallel^2 - \frac{\sqrt{3}}{2}k_\parallel\left(\gamma_3\frac{\partial}{\partial z} + \frac{\partial}{\partial z}\gamma_3\right)\right) \quad (2)$$

and $V_h(z)$ is the potential profile of the coupled quantum well structures, $\phi^1(x,t)$ and $\phi^2(x,t)$ are HH and LH state envelop wave functions respectively, γ_1, γ_2, γ_3 are the Luttinger parameters and are position-dependent in the heterojunction structures, m_0 is the electron rest mass, the in-plane vector $k_\parallel^2 = k_x^2 + k_y^2$. The discretization of equation (1) with respect to time gives [13, 17]

$$\left(1 + \frac{i\delta}{2\hbar}H_h\right)\begin{pmatrix} \phi_{n+1}^1 \\ \phi_{n+1}^2 \end{pmatrix} = \left(1 - \frac{i\delta}{2\hbar}H_h\right)\begin{pmatrix} \phi_n^1 \\ \phi_n^2 \end{pmatrix}, \quad (3)$$

where δ and n are the time spacing and time index respectively. This discrete-time technique preserves normalization of the wave function and introduces no extra nonlinear effect to the system. This difference equation can be written in a linear $Ax = b$ matrix equation with A being a complex symmetry matrix. The matrix is then solved using the L-U decomposition technique. Asymmetric coupled quantum well systems of 25-15-49 (first well width-barrier width-second well width in Angstroms) with a barrier height of 0.2506 eV are investigated. In this structure, the HH state in the first well is aligned with the LH state in the second well. The Luttinger parameters $(\gamma_1, \gamma_2, \gamma_3)$ are chosen to be (6.85, 2.1, 2.9) in the well region and (5.15, 1.39, 2.10), which are obtained by a linear interpolation of the Luttinger parameters of GaAs and AlAs, in the barrier region. Also, the space interval ϵ and time interval δ are chosen to be 1 Å and 1 femto second (10^{-15}). The initial wave functions are the heavy hole wave functions in the first well and the tunneling process is initiated at $t = 0$ without any driven force.

Mixing tunneling occurs between heavy and light hole states due to band mixing effects. This tunneling is significantly enhanced if the heavy hole state in the first well is aligned with the light hole state in the second well. To characterize the properties of the heavy to light hole mixing tunneling, one can define a mixing tunneling probability $F(t)$ as the probability of finding the heavy hole in the heavy hole band,

$$F(t) = \langle \phi^1(x,t) | \phi^1(x,t) \rangle_{hh}, \quad (4)$$

where $\phi^1(x,t)$ is the heavy hole wave function. When $F(t)$ approaches to one, the wavepacket is mainly located in the heavy hole band. When $F(t)$ is small, the wavepacket has left the heavy hole band and tunnels into the light hole band, in particular, the second well of light hole band.

Figure 1 shows the mixing tunneling probability $F(t)$ of 25-15-49 asymmetric coupled quantum well when $k_\parallel = 0.01$ and 0.03. When $k_\parallel = 0.01$, the wavepacket tunnels back and forth between heavy and light hole band. The oscillatory character of the mixing tunneling can be sustained over a long period of time (almost constant period and amplitude). When $k_\parallel = 0.03$, the wavepacket still tunnels back and forth between heavy and light hole band. However, the oscillatory character no longer exists. The period and amplitude of the mixing tunneling become disordered.

To characterize the time series $F(t)$ under various

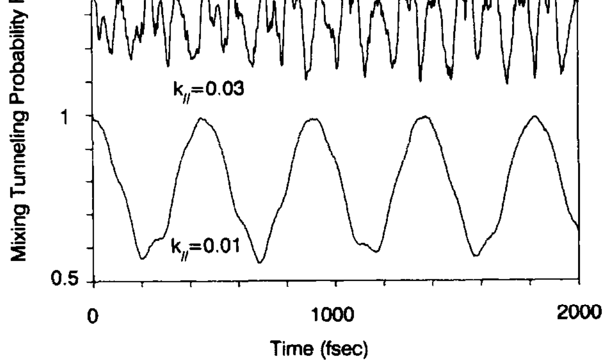

Fig. 1. The heavy to light hole mixing tunneling probability $F(t)$ of 25-15-49 asymmetric coupled quantum well when $k_\parallel = 0.01$ and 0.03

$k_{\|}$s, the simplex projection method is used [14–15]. The approach is designed for making short-term predictions about the trajectories of chaotic dynamical systems. The short-term prediction is based on a piecewise-linear approximation of the past patterns in a time series. By comparing the predicted and actual trajectories, chaotic behavior can be established if the accuracy of the prediction falls off as the prediction time increases. The algorithm is summarized as follows:

(i) Divide the time series into two parts: a fitting set $x_1, \ldots, x_N$ and an observed set $x_{N+1}, \ldots, x_{2N}$.

(ii) Choose an embedding dimension m, a delay time τ and a prediction time T.

(iii) Choose a delay vector $\mathbf{X}_i = (x_i, \ldots, x_{i-(m-1)\tau})$ for $i \geqslant N$.

(iv) Compute the distance d_{ij} of the test vector $\mathbf{X}_j$ from the delay vector $\mathbf{X}_i$, $N - T \geqslant i \geqslant 1 + (m-1)\tau$, using the maximum norm.

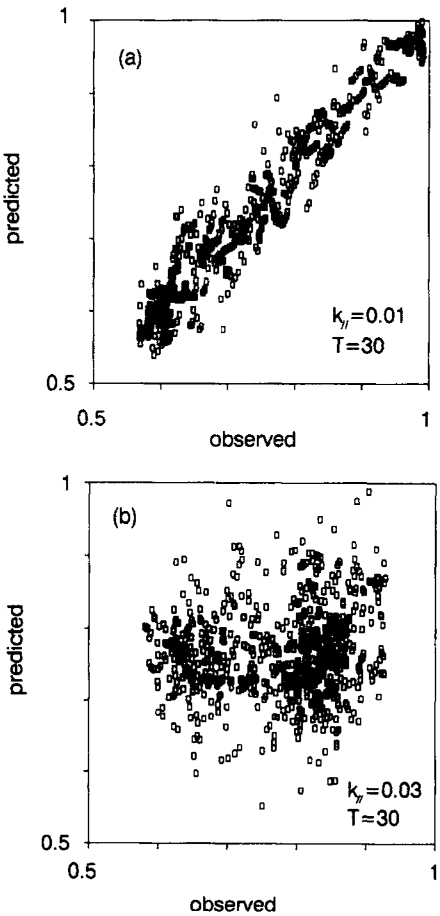

Fig. 2. (a) and (b) Predictions 30 time step into the future ($T = 30$) vs observed values for $k_{\|} = 0.01$ and 0.03 respectively. The first 1000 time points and the second 1000 time points of Fig. 1 are taken to be a fitting set and an observed set ($N = 1000$) with the embedding dimension $m = 3$ and delay time $\tau = 1$

(v) Find the k nearest neighbors of $\mathbf{X}_{i(1)}, \ldots, \mathbf{X}_{i(k)}$ of $\mathbf{X}_j$ and fit an affine model, where the parameters $\alpha_0, \ldots, \alpha_m$ are computed by least squares.

(vi) Repeat step (i) to (v) for all i to estimate a T step ahead prediction value.

(vii) Compute the linear correlation coefficient γ between the observed set and the predicted set.

Figures 2(a) and 2(b) show predictions 30 time steps into the future ($T = 30$) vs observed values for $k_{\|} = 0.01$ and 0.03 respectively. The first 1000 time points and the second 1000 time points of Fig. 1 are taken to be a fitting set and an observed set ($N = 1000$) with the embedding dimension $m = 3$ and delay time $\tau = 1$. Figure 3 illustrates the correlation coefficient γ as a function of prediction time for $k_{\|} = 0.01$ and 0.03. When $k_{\|} = 0.01$, the time series $F(t)$ shows periodical behavior since little decrease in the correlation coefficient with increasing prediction time interval. However, when $k_{\|} = 0.03$, the time series $F(t)$ shows chaotic behavior due to the loss of predictive power. A decrease in the correlation coefficient with increasing prediction time interval is a characteristic feature of chaos and can also give a rough measure of Lyapunov exponent. Thus, it is indicated that by varying $k_{\|}$ the coherent oscillatory motion in the coupled quantum well will collapse and turn into chaos.

The oscillation collapse is attributed to the nonlinear interaction between mixing tunneling to the first well (HH to the LH state in the first well) and mixing tunneling to the second well (HH to the LH state in the second well). In the asymmetric quantum well structure of 25-15-49, the HH state of the first well is aligned with the LH state of the second well. For a small $k_{\|}$ (0.01, for example), mixing tunneling occurs mainly between HH state of the first well and the LH state of the second well and gives rise to a periodic motion between HH and LH

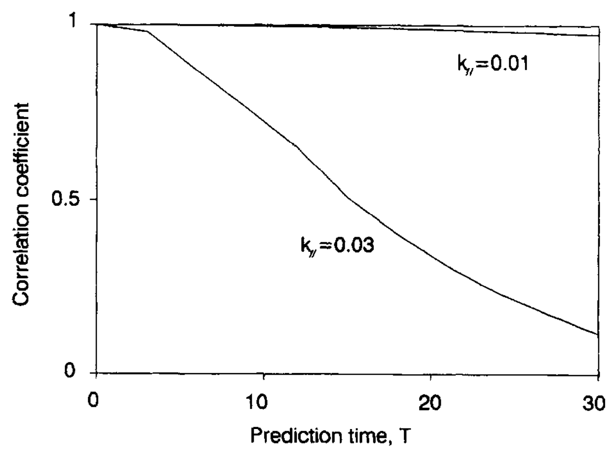

Fig. 3. The correlation coefficient γ as a function of prediction time for time series of Fig. 1 when $k_{\|} = 0.01$ and 0.03

states due to the alignment of the two states. If $k_{\parallel}$ approaches an extremely large number (1, for example), mixing tunneling would occur mainly between HH state of the first well and the LH state of the first well and give rise to a periodic motion between HH and LH states due to the strong mixing effect. However, for a medium $k_{\parallel}$ (0.03, for example), HH to LH in the first well and HH to LH in the second well become compatible (Note that these two factors have a completely different origin). Therefore, the nonlinear interaction of the two causes the collapse of the oscillatory motion between HH and LH states. To verify the collapse of the oscillatory motion due to the chaotic tunneling, the pump and probe technique and the time-domain terahertz spectroscopy can be used. Coupled-well samples should be carefully prepared so that the heavy hole state in the first well is aligned with the light hole state in the second well. Note that the alignment between HH state of the first well and LH state of the second well can be altered by an appropriate external electric field. Thus, it is expected that chaotic spectroscopy is shown without the electric field and terahertz oscillatory spectroscopy is shown with the electric field.

In conclusion, oscillatory motion of hole via the coherent tunneling in coupled quantum well structures have been known for its rich properties. One type of the oscillatory motion is the mixing tunneling which occurs between heavy and light hole states. By a proper design of a quantum well structure, the mixing tunneling can be driven by (1) HH to the LH state in the first well due to in-plane vector $k_{\parallel}$ and (2) HH to the LH state in the second well due to the alignment of the HH state in the first well and the LH state in the second well. If these two factors are compatible, the oscillation motion collapses. The simplex projection method has been used to show that the mixing tunneling in coupled quantum wells bears chaotic behavior.

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