Typeset with jjap2.cls <ver.1.1> **Regular Paper**

Theoretical study of the time-dependent phenomena on a two-dimensional electron gas weakly coupled with a discrete level

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We theoretically study a time evolution of the electron density distribution on a two-dimensional electron gas, which suddenly couples with a discrete level. Depending on the relative position between a discrete level and the Fermi level (E_f), a "dip" or a "peak" of electron density appears after a discrete level couples with the two-dimensional electron gas. Moreover, we clarify the mechanism of dip and peak formation by using a projection analysis.

KEYWORDS: tunneling phenomena, quantum interference, time-dependent Schrödinger equation, two-dimensional electron gas

1. Introduction

One of the central issues in semiconductor device is a precise control of tunneling phenomena which appear many situations such as a charge injection into floating gates of memory devices[1,2] and a leakage current in MOSFET.[3–5] These phenomena intimately related to reliability issues and channel technologies of modern semiconductor devices.[6–10] As for the theoretical studies of tunneling phenomena, a remarkable progress has recently been reported by solving Schrödinger equation with open boundary conditions.[11–13] However, a wide variety of dynamical processes such as electron dynamics at the interfaces of semiconductors becomes important especially in the aggressively scaled modern semiconductor devices. Thus, to consider an explicit trace of the dynamical process of electron wave functions is necessary to obtain a deeper understanding of tunneling phenomena.

In the present work, we investigate the tunneling phenomena from a two-dimensional electron gas to a discrete level which describes a quantum dot (QD) floating gate or a defect level in a dielectric material. We study the time-dependent electron density distribution of the two-dimensional electron gas, which suddenly couples with a spatially localized discrete level. We find that the time evolution of the electron density distribution is significantly different depending on the relative position between the connecting discrete level and the Fermi level of the two-dimensional electron gas. A clear dip of electron density on the two-dimensional electron gas is formed just below the connecting site during electron tunneling.

The content of this paper is as follows. In §2, we give the model of our study and the brief description of the calculational method. In §3, we review the time dependent behavior of

the electron density distribution on the two-dimensional electron gas by varying the relative energy level position between a discrete level and the Fermi level of the two-dimensional electron gas. Depending on the energy level position of the connecting site, a "dip" or a "peak" of electron density distribution appears on the two-dimensional electron gas. In §4, we clarify the mechanism of dip and peak formation by using a projection analysis. A summary is given in §5.

2. Model and Method

A time-evolution of electron wave functions is calculated by solving the time-dependent Schrödinger equation.[14–16] In this study, we employ a tight binding approximation, where two-dimensional electron gas and a discrete level are represented by the two-dimensional periodic tight binding lattice and a weakly coupled additional site, respectively [Fig. 1(a)].

We assume that the wave function of the k-th orbital $[\psi_k(t)]$ is expanded by the basis function $[\chi_i(x)]$ which is localized at each site,

$$\psi_k(x,t) = \sum_{i=1,\ldots,n,d} c_i^k(t)\chi_i(x), \tag{1}$$

where the notation i shows a position of the sites. The matrix elements of the tight binding Hamiltonian are expressed as

$$\begin{aligned} H_{i,j} \equiv & \int \chi_i^* H \chi_j dx \\ = & E_0\delta_{i,j} + E_d\delta_{i,j}\delta_{j,d} + (\gamma\delta_{i,j\pm1} + \text{c.c.}) + (\gamma_{kd}\delta_{i,0}\delta_{j,d} + \text{c.c.}). \end{aligned} \tag{2}$$

where, on-site energies (E_0, E_d) and transfer integrals (γ, γ_{kd}) are represented as follows;

$$E_0 = \int \chi_i^* H \chi_i dx \ , \ E_d = \int \chi_d^* H \chi_d dx, \tag{3}$$

$$\gamma = \int \chi_i^* H \chi_{i\pm1} dx = \int \chi_{i\pm1}^* H \chi_i dx, \tag{4}$$

$$\gamma_{kd} \int \chi_0^* H \chi_d dx. \tag{5}$$

where the notations i and d show the positions of two-dimensional lattice sites and an additional site, respectively. Note that $i \pm 1$ expresses the adjecent sites of the i-th site in the two dimensional lattice. We set that the additional site is connected to the one of the sites on the two-dimensional lattice whose position and transfer integral are 0 and γ_{kd}, respectively. The transfer integral between the nearest neighbor sites (γ) set to 1. Hereafter, we scaled the values of on-site energies and the transfer integrals by γ. In this study, time is scaled by $1/\gamma$.

The formal solution of the time-dependent Schrödinger equation is expressed as

$$\psi_k(t + \Delta t) = \exp(-iH\Delta t)\psi_k(t), \tag{6}$$

where Δt is a small increment of time. We employ the second order differencing scheme for

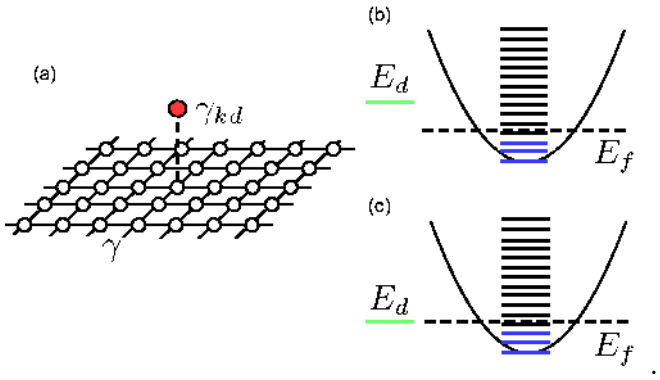

Fig. 1. (a) Schematic illustration of the two-dimensional tight-binding lattice (open circle) with a weakly coupled additional site (closed circle). The coupling constant between a two-dimensional lattice and the additional site (γ_{kd}) is set to 0.1γ. On the other hand, we varied the on-site energy of the discrete level. The number of site (N) is 255×255. We considered two cases. One is the case of (b) $E_d > E_f$ and the other is (c) $E_d = E_f$, respectively. The electrons initially occupy five states from the ground state of two-dimensional lattice assuming the low carrier density.

representing the time propagator as,

$$\psi_k(t + \Delta t) = \psi_k(t - \Delta t) - 2i\Delta t H\psi_k(t). \tag{7}$$

This scheme is accurate up to $(H\Delta t)^2$.[17,18] Moreover, this scheme is symmetric in time and known to be conditionally stable. We use $\Delta t = 1/256$ and $\Delta x = 1$ for satisfying the stable condition of $\Delta t/\Delta x^2 \leq 0.25$.

Under the above assumptions, we study dynamical properties of the electron density distribution in the two-dimensional lattice which suddenly couples with the discrete level. **In order to clarify the local modulation of the electron density distribution, caused by the tunneling from the electron gas to the discrete level, we define the differential density between the initial density distribution and the time-developed density distribution ($\Delta\rho(t)$) as follows,**

$$\Delta\rho(t) = \rho(x, 0) - \rho(x, t), \tag{8}$$

where $\rho(x,t)(\equiv \sum_{k=1}^{N} \psi_k(x,t)|^2)$ is the electron density distribution in the two dimensional lattice. We investigate two cases in this study. One is $E_d > E_f$ [Fig. 1(b)], the other is $E_d = E_f$ [Fig.1(c)]. **In order to obtain the precise picture of electron dynamics for these different conditions, we employ a projection analysis, where the initial wave function ψ_k which is the k-th eigenstate of the condition $\gamma_{kd} = 0$ $(t = 0)$ are expanded by the eigenstates (ϕ_i) of the condition $\gamma_{kd} \neq 0$ $(t > 0)$. A projection**

probability of initial states (P_i) can be described as follows:

$$P_i = \sum_{k=1}^{N} | \int \phi_i^* \psi_k d\mathbf{x}|^2. \tag{9}$$

We expect that the value of P_i and the spatial density distributions of each eigenstate ϕ_i enable us to reveal the detailed feature of the time evolution of electron density distributions.

We set that five electrons initially occupy five lowest eigenstates of the two-dimensional lattice. Thus, E_f is about -4.00γ in this situation. **The carrier density of electron gas is about $1.4\times10^{11}/\mathrm{cm}^2$ when the lattice constant of the tight binding lattice coincides with the length of Si-Si bond. This condition corresponds to the typical carrier density of weak inversion layer of MOSFET. We investigate a time evolution as follows. At $t = 0$, a discrete level suddenly begins to couple ($\gamma_{kd} \neq 0$) with the two-dimensional lattice, though γ_{kd} is 0 when t is smaller than 0. In the present work, we neglect the electron-electron interaction for simplicity.**

3. Results and Discussion

3.1 Time Evolution

Figures 2 (a) and (b) show the snapshots of the time-dependent electron density distributions against the time in the condition of $E_d > E_f (E_d = -3.95\gamma)$ and $E_d = E_f$, respectively. The time evolution of the electron density distributions on the two-dimensional lattice show the different features that depend on the relative position of the energy levels. When $E_d = -3.95\gamma$, a tunneling from the two-dimensional lattice to the discrete level is rare due to the sufficient energy difference [Fig. 2(c)]. Noticeable feature is that the electron density distribution has a peak around the connecting site and the modulation oscillatory spreads outwards from the connecting site during time development. **The maximum value of the electron density at the peak is about 30% larger than the initial density.** In the condition of $E_d = E_f$, however, the time evolution of the electron density distribution is completely different. A "clear dip" instead of a peak is formed around the site which connects to the discrete level and this dip region becomes deeper and wider during tunneling event [Fig. 4(c)]. **The minimum value of the density at the dip is about 40% smaller than the initial density.** Note that the tunneling probability to the discrete level at t=200 in Fig.2(d) is about 15 times larger than the peak at t=50 in Fig.2(c) caused by the large mixing between the two-dimensional lattice and the discrete level.

These phenomena can be regarded as a time dependent version of the Friedel oscillation. Electrons initially on the eigenstates of the two-dimensional lattice are perturbed by coupling with the discrete level. Consequently, the initial states are no longer being an eigenstate of this system and a mixed state is formed, where electron wavefunctions are expanded by the

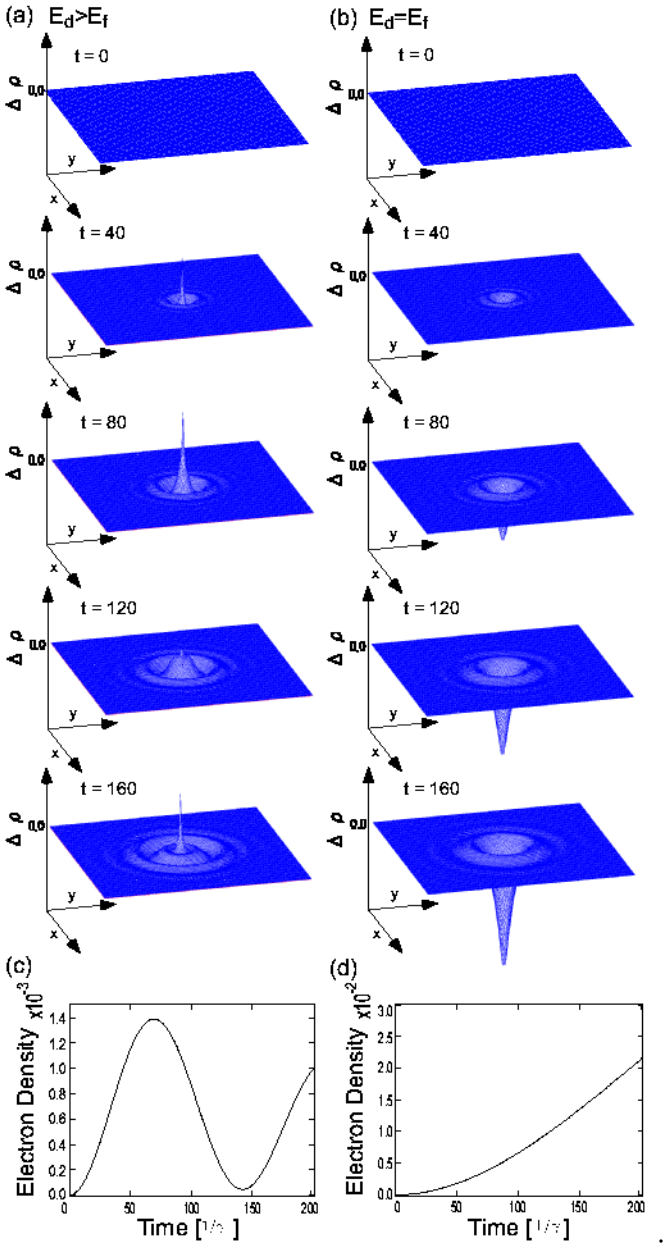

Fig. 2. Snapshots of time-dependent electron density distribution under the condition of (a) $E_d = -3.95\gamma$ and (b) $E_d = -4.00\gamma$. Fermi level corresponds to $E_d = -4.00\gamma$. At $t = 0$, the two-dimensional lattice and the discrete level is connected by the strength of $\gamma_{kd} = 0.1\gamma$. The time dependency of the electron density in the discrete level for the condition of (c) $E_d = -3.95\gamma$ and (d) $E_d = -4.00\gamma$, respectively. Note that the longitudinal axis of (d) is twenty times larger than (c).

several eigenstates of H described in eq. (2) whose γ_{kd} is finite. As a result, the electron density distribution **is modulated by the mixing of these eigenstates.** From another viewpoint, this modulation is understood in terms of the transitions among the unperturbed states via the discrete level. In this perspective, we could see that the second order perturbation produces

the modulation of the electron density in the electron gas. Further details of this consideration are discussed in our previous work.[19)]

Recently, Ikeda *et al.* have reported the collective motion of electrons occurs during electron injection into Si-QDs in the MOS memory transistor system, where many electrons collectively tunnel into the Si-QDs within a very short period.[1)] The results of our time-dependent calculations in the $E_f = E_d$ [Fig. 2 (b)] enable us to propose a possible mechanism of this **collective motion of electrons**. Once tunneling event occurs, a dip of electron density is formed in the two-dimensional gas just below the discrete level. The tunneling probability between a localized state and a discrete level is much larger than that between a delocalized level and a discrete level. Accordingly, after one tunneling event occurs, the tunneling probability of second tunneling is expected to be remarkably enhanced, which leads to the occurrence of successive electron tunneling.

3.2 Projection Analysis

In the previous subsection, we found that the time-evolution of the electron density distribution sensitively depends on the relative position between E_d and E_f. In the condition $E_d = E_f$, a clear dip of electron density on the two-dimensional lattice appears around the connecting site, however, in the condition $E_d > E_f$, a peak appears around it. In this subsection, we discuss these characteristic time-evolutions in terms of the superposition of the eigenstates for H with $\gamma_{kd} \neq 0$.

Figure 3 is the schematic illustrations of the time evolution for two-state system, where the wave function is expanded by two states of ϕ_1 and ϕ_2. We assume that both two states have the peak (dip) of electron density distribution around the center of the system. Further, these two states have different eigenvalues each other, which leads to the different phase velocity in time evolution. The superpositions of these states for different time are shown in the right row of Figs. 3(a) and (b). We also assume that the relative phase between the two states is initially π for satisfying the uniform distribution of electron density at $t = 0$ [Fig. 3(a)]. The time-development of this wavefunction shows the modulation of the density distribution, because the relative phase difference between the two states changes in time evolution. Fig. 3(b) describes the system at $t = t_1$, where the relative phase between the two states is 0. As shown in this figure, the electron density distribution has the clear peak (dip) around the center of the system at $t = t_1$. Thus, the "hidden structures" of the electron state inevitably emerge during the time evolution as shown in Figs. 3 (a) and (b). Based on this consideration,

The electron density distributions of the eigenstates of H with $\gamma_{kd} = 0.1\gamma$ in the two-dimensional lattice are shown in Figs. 4 (a) and (b) for the conditions of $E_d > E_f$ ($E_d = -3.95\gamma$) and $E_d = E_f$, respectively. Here, the wave functions having cosine waves for both x and y directions mix with a discrete level because of the symmetry. We classify these states into two groups by their spatial distributions of electron density, where we assign the eigenstate

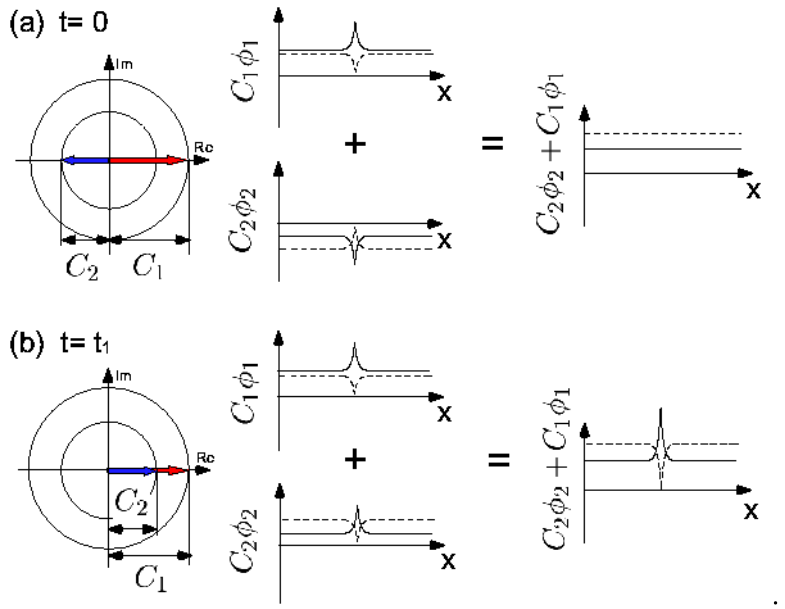

Fig. 3. The schematic illustrations of the time evolution for two-state system, where both states have the peak (solid line) or the dip (broken line) of electron density distribution around the center of the system. Further, these two states have the different eigenvalues each other, which leads to the different phase velocity in time evolution. The relative phase between these states is π at $t = 0$ (a) and the one is 0 at $t = t_1$ (b).

having a peak on the two-dimensional lattice around the connecting site as a "peaked state" and the one having a dip as a "dipped state", respectively. On the other hand, the wave functions having a sine form (odd symmetry) cannot mix with the discrete level and does not change its density distribution even in the condition $\gamma_{kd} \neq 0$. We assign these states as "the odd states". We can see that the electron density distributions of the eigenstates of the condition $\gamma_{kd} \neq 0$ show the completely different features depending on the relative position between E_d and E_f. In the condition $E_d = -3.95\gamma$ [Fig.4(a)], we can only find peaked and odd states; The first, second, sixth states can be categorized into peaked states and the other six states are odd states as clearly shown in Fig. 4 (a). In the condition $E_d = E_f$ [Fig. 4(b)], however, most of the states are dipped and odd states except the ground state (peaked state); The second, sixth, and tenth states can be categorized into dipped state and the threefold degenerate states (the third to fifth and the seventh to ninth states) are classified as odd states. Only the ground states can be assigned as a peaked state in this condition. It is noted that the ground state has very small amplitude on the two-dimensional lattice whereas large amplitude on the discrete level reflecting the large mixing between the two-dimensional lattice and the discrete level.

To investigate the role of these eigenstates in the time evolution, we project the initial states into these eigenstates as defined above. The projection probabilities for each condition

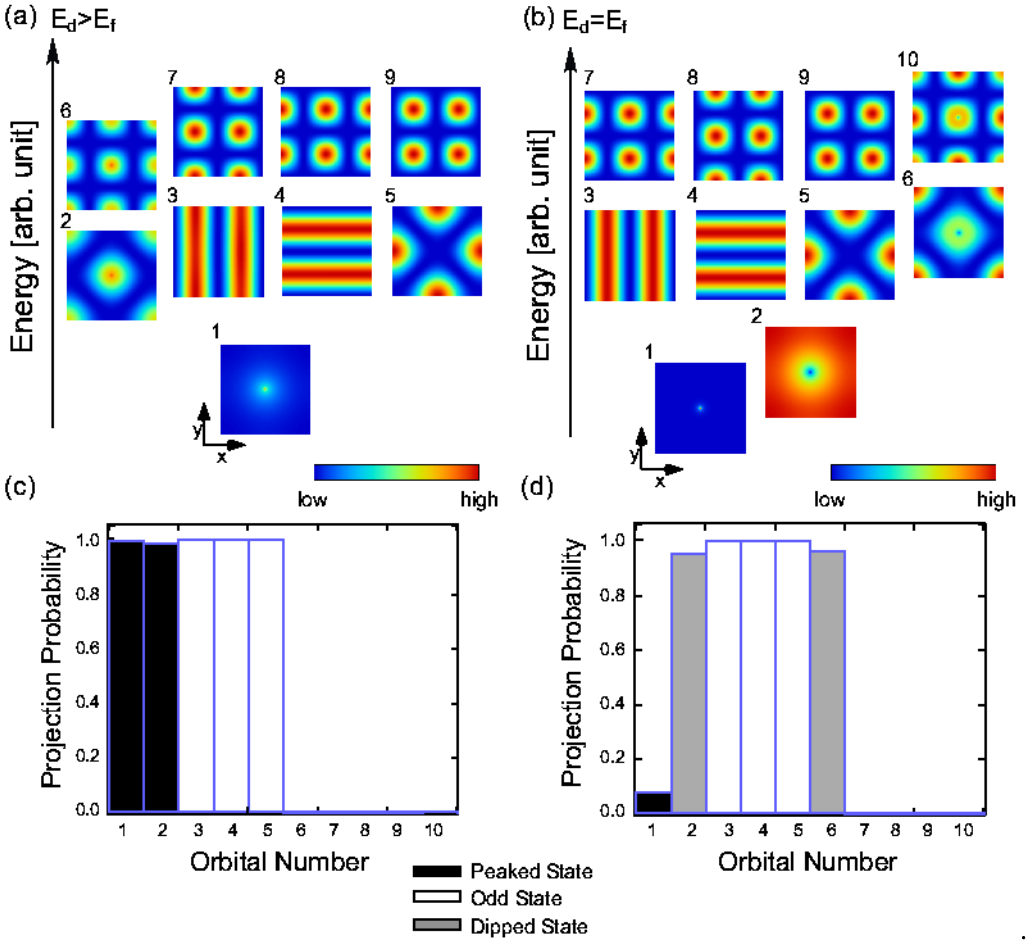

Fig. 4. The electron density distribution of eigenstates of the condition $\gamma_{kd} = 0.1\gamma$ in the two-dimensional lattice for (a) $E_d > E_F$ and (b) $E_d = E_f$. The eigenstates are assigned by sequential numbers and classified into three groups by their characteristics of the electron density distributions. The threefold degenerate states (3 to 5 and 7 to 9) are classified as the "odd states" on both conditions. The states 2, 6 and 10 in (b) are classified as the "dipped states". The other states [1, 2 and 6 in (a) and 1 in (b)] are the "peaked states". The projection probability of the initial states, where each wave function is decomposed into the eigenstates in the cases of (c) $E_d > E_f$ and (d) $E_d = E_f$, respectively. The filled, shade and open bars correspond to a peaked, a dipped and an odd state, respectively.

are shown in Figs. 4 (c) and (d). In the condition $E_d > E_f$ ($E_d = -3.95\gamma$), we find that the initial state is mainly expanded by two peaked states and three odd states. Here the coefficients of the basis functions (eigenstates of the condition $\gamma \neq 0$) are determined by satisfying the uniform distribution of electron density similar to the model of Fig 3(a). Thus, the time evolution of the electron density distribution inevitably shows the modulation of electron density caused by the fact that each eigenstates have a different phase velocity in time evolution. It is noticeable that there are only the peaked and the odd states around the

Fermi level in this condition. Therefore, the hidden structures of the electron state (peaked states) emerge during the time evolution as shown in Fig. 2(b). Note that the effect of the coupling on discrete level is rather small because E_d is sufficiently far from the Fermi level in this condition. Therefore, the mixing of the discrete level is limited and the electron tunneling hardly occurs.

Contrary to the condition of $E_d > E_f$, a clear tunneling is observed in the condition $E_d = E_f$ due to the large mixing between two-dimensional lattice and the discrete level. Here, the initial state is mainly expanded by the dipped and the odd states as shown in Fig.4(d). Thus, the hidden state is the dipped state instead of the peaked state in this condition. Accordingly, the resulting electron density distribution shows the dip formation as clearly seen in Fig. 2(b) reflecting the characteristics of these eigenstates.

4. Summary

We theoretically study the time-evolution of the modulation of electron density for the two-dimensional electron gas with a weakly coupled discrete level. We clearly show the tunneling event remarkably modifies the two-dimensional electron gas and the characteristics of modulation is sensitively depends on the relative position between Fermi level of the two-dimensional electron gas and a discrete level. In the condition $E_d > E_f$, the electron density distribution forms the peak around the connecting site in two-dimensional electron gas. In the condition $E_d = E_f$, the dip is generated due to the electron tunneling to the discrete level. The origin of generating the dip and the peak formation is investigated by using the projection analysis, where the initial wave functions (the eigenstates of H with $\gamma_{kd} = 0$ at $t = 0$) are expanded by the eigenstates of the condition $\gamma_{kd} \neq 0$ at $t > 0$. We show that the electron density distribution of the eigenstates near the Fermi level play significant roles for the characteristic modulations. In the condition $E_d > E_f$, the initial state is expanded by the peaked and the odd states, on the other hand, in the condition $E_d = E_f$, the one is mainly expanded by the dipped and the odd states. We reveal that these hidden structures of electron state emerge during time evolution. **These dynamical properties in two-dimensional electron gas could possibly affect the electron tunneling from the electron gas to the discrete level. It indicates that the time evolution of the electron state in electron gas is important issue for the precise control of electrons in the semiconductor devices.**.

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