Formation process of quantized states in electromagnetic fields

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We theoretically investigate formation process of quantized electronic states in electromagnetic fields. By using the path-integration theory, we first follow time-evolution of an electronic state which is initially regarded as an extended band state. Next, we show that an eigenstate in an electromagnetic field is expressed as a superposition of states which the electron has undergone. We may regard this effect as an afterimage, i.e., an electronic state is a time average over the path of history. This is a viewpoint that reflects the nature of electrons. We show that the Landau states and Stark ladders are formed as a consequence of the afterimage effect.

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I. INTRODUCTION

The purpose of this paper is to describe the process of how eigenstates in electromagnetic fields are formed from the band states. It is well known that electronic eigenstates in static electromagnetic fields are localized wave packet.[1,2] In a magnetic field, such states are called Landau levels. In an electric field, localized Stark ladders are formed as well. These wave functions and eigen energies are easily obtained by solving the Schrödinger equations including electromagnetic potential.[2,3]

Let us think that a steplike electromagnetic field is applied to a crystalline solid in which band states are eigenstates. How do the band states change into localized wave packet? As far as we know, there are no clear answers to this question.

Recent development of measurement technologies enables us to observe phenomena in very short time scales. Therefore, it will be important to describe transformation process in order for better understanding of electron nature as well as for device applications.

II. ELECTRONIC MOTION AND FORMATION OF EIGENSTATE

In order to show how eigenstates are formed from free electronic states, we first consider simple one-dimensional motion in harmonic potential $V(x)=m\omega^2x^2/2$. Let $\psi(x_0,t_0)$ the initial state at the time t_0 given by

$$\psi(x_0,t_0)=\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-(\alpha/2)x_0^2+ik_0x_0}, \tag{1}$$

where k_0 is a wave number and $\alpha^{-1/2}$ is extension length of this state. This is a wave packet put at the origin with velocity k_0/m. The energy of this state is $E=\hbar^2k_0^2/2m$, which is retained during the process of oscillatory motion as is in the classical harmonic oscillator. We note that the value of α is introduced so as to show the oscillation in the real space clearly. In order to describe transformation from band states to localized eigenstate, α must be small enough. When α is small, this state is well regarded as a free electronic state with a continuous energy spectrum.

By using the path-integration theory,[4–7] the time evolution of the state is described as

$$\psi(x',t')=\int_{-\infty}^{\infty}K(x't',x_0t_0)\psi(x_0,t_0)dx_0, \tag{2}$$

where $K(x't',x_0t_0)$ is the Feynman kernel. For the harmonic potential, we can write down the Feynman kernel as

$$K(x't',x_0t_0)=\left[\frac{m\omega}{2\pi i\hbar\sin\omega(t'-t_0)}\right]^{1/2}\times\exp\left\{\frac{im\omega}{2\pi\hbar\sin\omega(t'-t_0)}[(x'^2+x_0^2)\times\cos\omega(t'-t_0)-2x'x_0]\right\}. \tag{3}$$

By inserting Eqs. (1) and (3) into Eq. (2), we can calculate the wave function at time t' as

$$\psi(x',t')=\left(\frac{\alpha}{\pi}\right)^{1/4}\left(\frac{i}{\cos\omega t+i\xi\sin\omega t}\right)^{1/2}\times\exp\left\{\frac{-\alpha/2[x'-x(t')]^2+ik(t')x'+i\eta\sin2\omega t'}{\cos^2\omega t+\xi^2\sin^2\omega t}\right\}, \tag{4}$$

with $\xi=\alpha\hbar/m\omega$ and $\eta=(\alpha^2x'^2-k_0^2)\hbar/m\omega-m\omega x'^2/\hbar$. In Eq. (4),

$$x(t')=\hbar k_0\frac{\sin\omega t'}{m\omega} \tag{5}$$

and

$$k(t')=k_0\cos\omega t' \tag{6}$$

are the central position and the momentum at the time t', respectively. Figure 1 shows the calculated states evolved from the initial-state with $(\hbar/m\omega)^{1/2}k_0=5$. One period of evolution of the initial state is plotted. We can see that

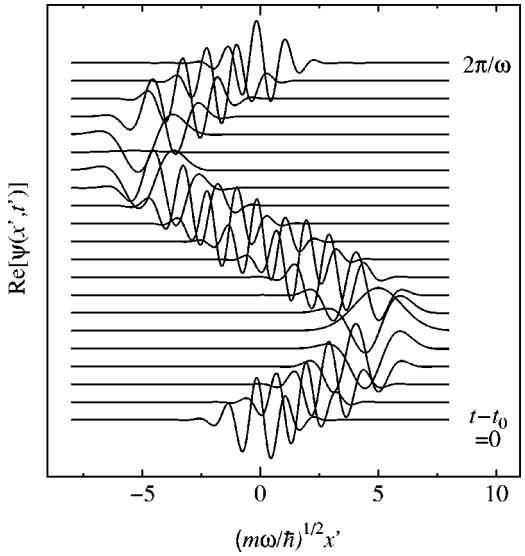

FIG. 1. Time evolution of initial state in harmonic potential. Real part of the wave function is plotted over one period of oscillation. Initial wave number is set as $(\hbar/m\omega)^{1/2}k_0=5$.

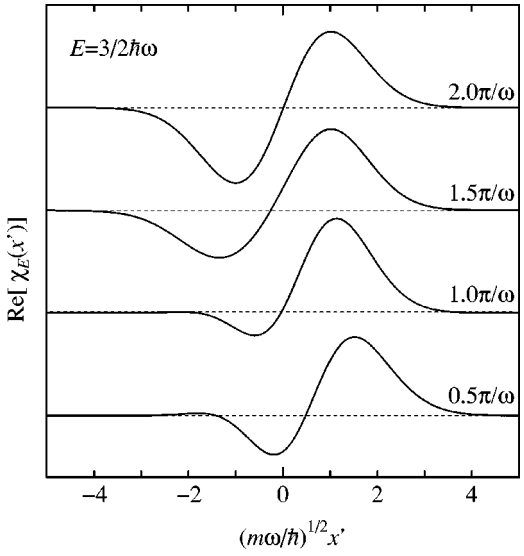

FIG. 2. Formation process of the eigen wave function. Since the energy of the oscillator is $(3/2)\hbar\omega$, $\chi_E(x')$ approaches the eigenstate with $n=1$.

$\psi(x',t')$ is oscillating with change of wavelength as well as position. We note that the state is not quantized at this stage, that is, continuous value of energy $E=\hbar^2k_0^2/2m$ is possible for such an oscillator.

Here we make a superposition of the oscillating states as

$$\chi_E(x',t)=\frac{1}{\sqrt{t-t_0}}\int_{t_0}^{t} e^{iE(t'-t_0)/\hbar}\psi(x',t')dt'. \qquad (7)$$

The factor $1/\sqrt{t-t_0}$ has been added for normalization of $\chi_E(x',t)$. Mathematically, Eq. (7) is a Fourier transformation from time representation to energy representation.[8] In our interpretation, this can be called afterimage effect. In other words, $\chi_E(x',t)$ is a superposition of electron over the history, i.e., what we see is an electron in the past. Although it may sound spooky, the function $\chi_E(x',t)$ is a reality as a time-integrated probability amplitude, i.e., the probability of finding an electron at energy E during the period $t_0\sim t$. In this sense, this is a wave function changing gradually from a band state to an eigenstate in an applied potential.

The exponential factor in Eq. (7) cancels the time-dependent phase factor of $\psi(x',t')$, $e^{-iEt'/\hbar}$. Such a cancellation is necessary to obtain a rational result. When we consider a superposition of states belonging to different times, if additional constant potential is applied, relative phase difference between the states changes, and resulting wave function becomes quite different. Such a situation is irrational and undesirable. Therefore, from the viewpoint of the gauge invariance of wave functions, the time-dependent phase factor should be excluded from the superposition as shown in Eq. (7).

In Fig. 2, we show $\chi_E(x',t)$ calculated at $t-t_0=0.5\pi/\omega\sim 2\pi/\omega$ for an oscillator with energy $E=(3/2)\hbar\omega$. This energy corresponds to the eigen energy of the $n=1$ state. At first, the oscillator moves rightward as shown in Fig. 1, and at this stage the peak at $(m\omega/\hbar)^{1/2}x\simeq 1$ grows. As time increases, the oscillator turns around, the dip in the left grows, and $\chi_E(x',t)$ approaches the eigen wave function of $n=1$.

Figure 3 shows calculated $\chi_E(x',t)$ for $E=1.7\hbar\omega$. As this energy is not the eigen energy, the amplitude of $\chi_E(x',t)$ approaches zero with time. This is because, in this case, interference results in cancellation of amplitudes.

These results indicate that the formation process of eigenstates is described by the function $\chi_E(x',t)$. For $t<t_0$, the eigenstates are extended band states given by Eq. (1) (with $\alpha\simeq 0$). By applying the potential, the electronic motion shown in Fig. 1 occurs. As a result of self-interference, $\chi_E(x',t)$ changes gradually from a band states to a localized eigenstate for a particular value of E. Therefore, the function

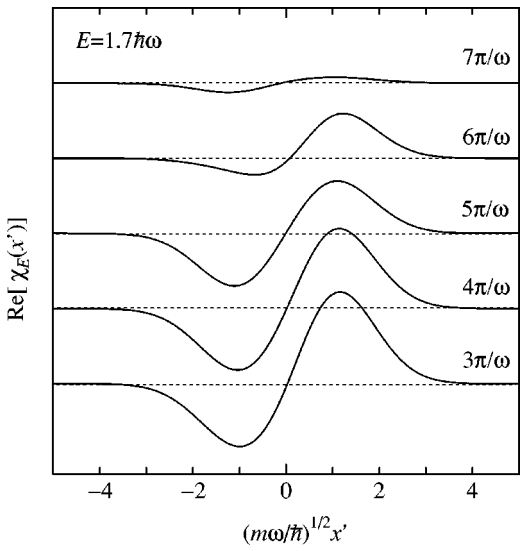

FIG. 3. Decay process of off-energy state. Since the energy of the oscillator is $1.7\hbar\omega$, $\chi_E(x')$ decays as time increases.

$\chi_E(x',t)$ describes the transformation from Bloch states (eigenstates for $V=0$) to localized eigenstates in electromagnetic fields.

Such behavior of $\chi_E(x',t)$ is also derived from an alternative expression of the Feynman kernel. We can express $K(x't',x_0t_0)$ by using the eigenstates of the system as[4,9]

$$K(x't',x_0t_0)=\sum_{n=0}^{\infty}\phi_n(x')\phi_n^*(x_0)e^{-iE_n(t'-t_0)/\hbar}. \quad (8)$$

In this equation, $\phi_n(x)$ and E_n are the wave function and the eigenenergy of a harmonic oscillator, respectively. Substituting Eqs. (2) and (8) into Eq. (7), we have

$$\chi_E(x',t)=\frac{1}{\sqrt{t-t_0}}\sum_n A_n\int_{t_0}^{t}e^{i(E-E_n)(t'-t_0)/\hbar}dt'\,\phi_n(x'), \quad (9)$$

where

$$A_n=\int_{-\infty}^{\infty}\phi_n^*(x_0)\psi(x_0,t_0)dx_0 \quad (10)$$

is an overlap between the initial state and the nth eigenstate. In the long-time limit, $\chi_E(x',t)$ becomes

$$\lim_{t\to\infty}\chi_E(x',t)=\frac{\pi A_n}{\hbar\sqrt{t-t_0}}\delta(E-E_n)\phi_n(x'), \quad (11)$$

where we used $\int_0^{\infty}\exp(iEt)dt=\pi\delta(E)$. This equation indicates that the superposition of the oscillating state approaches one of the eigenstates if the energy coincides with energy of corresponding eigenstate. On the other hand when the energy is different from any of eigen energies, the amplitude of $\chi_E(x',t)$ attenuates. This behavior of $\chi_E(x',t)$ is well understood in terms of the afterimage effect; if the phase change of the wave function after one cycle of motion is different from a multiple of 2π, the amplitudes are canceled out, and as a result, $|\chi_E(x',t)|$ decays with time.

Figure 4 shows the norm of $\chi_E(x',t)$ plotted as a function of energy. The curves are calculated for $t-t_0=2\pi/\omega \sim 20\pi/\omega$. We see that electronic states for any value of energy are possible for small value of t. With increasing t, quantization gradually occurs; peaks at $E_n=\hbar\omega(n+1/2)$ become sharper. The peak height in Fig. 4 depends on the choice of the initial state. Equations (9) and (10) indicate that the peak height is related to the overlap between the initial-state and resulting eigenstate. By setting α small enough, we can make the peak heights almost the same. Therefore, the curves in Fig. 4 show the quantization process from free electronic states to eigenstates in the harmonic potential. These results indicate that quantized eigenstates in harmonic potential are formed as a consequent of interference accompanied with electronic motion.

The behavior of energy spectrum shown in Fig. 4 has been well known as the lifetime broadening due to the uncertainity principle $\Delta E\Delta t\geq\hbar$. In interpreting optical absorption spectra, we often attribute the linewidth to finite lifetime due to scattering. However, we note that a treatment based on the uncertainity principle is phenomenological and its validity is sometimes vague. On the other hand, the present theory has verified the origin of the broadened energy spectrum, and it brings about quantitatively the same results as the treatment by the uncertainity principle.

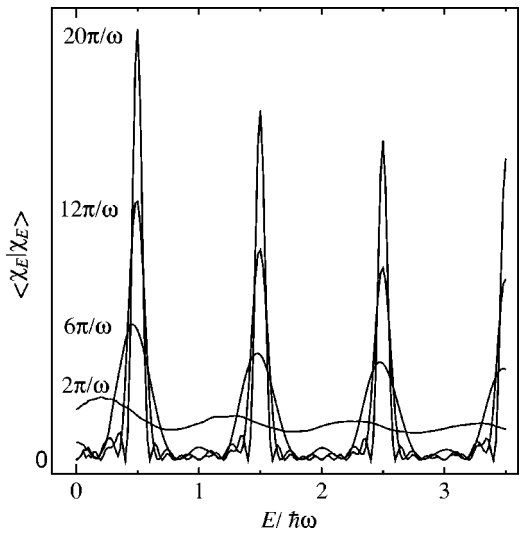

FIG. 4. Norm of the state $\langle\chi_E|\chi_E\rangle$ plotted as a function of energy. As the time increases, quantized states are formed and the peaks at $E=E_n$ become sharp.

It has been shown that an oscillating wave packet is expressed as a linear combination of time-dependent eigenfunctions of harmonic oscillator.[10] The procedure described above is just the reverse of it: an eigenfunction is expressed as a linear combination of an oscillating state.

III. LANDAU LEVELS IN A MAGNETIC FIELD

Electronic eigenstates in a crystalline solid in a magnetic field is called Landau levels. The Landau states are formed as a result of cyclic motion of band electrons. Thus, the results for the harmonic oscillator shown in the previous section is readily applicable to the Landau states formation. We consider a Hamiltonian with a static magnetic field applied along the z axis as

$$\mathcal{H}=\frac{1}{2m}(\mathbf{p}+e\mathbf{A})^2=\frac{\hbar^2k_x^2}{2m}+\frac{m\omega^2}{2}\left(x+\frac{\hbar k_y}{m\omega}\right)^2+\frac{\hbar^2k_z^2}{2m}, \quad (12)$$

where $\mathbf{A}$ is vector potential and $\omega=eB/m$. We have chosen the gauge as $\mathbf{A}=B(0,x,0)$ so as to give the magnetic field along the z axis. From Eq. (12), we see that the motion the xy plane is a one-dimensional oscillator deviated by $-\hbar k_y/m\omega$. This system is thus regarded as a harmonic oscillator with a degree of freedom along the z direction.

By applying the result shown in the previous part, we make a superposition of free states as

$$\chi_{E,\mathbf{k}}(\mathbf{r},t)=\frac{1}{\sqrt{t}}\int_0^t e^{iEt'-i\mathbf{k}(t')\cdot\mathbf{r}}dt', \quad (13)$$

where $E=\hbar^2(k_x^2+k_y^2+k_z^2)/2m$ and $\mathbf{k}(t)=(k_x\cos\omega t,k_y,k_z)$.

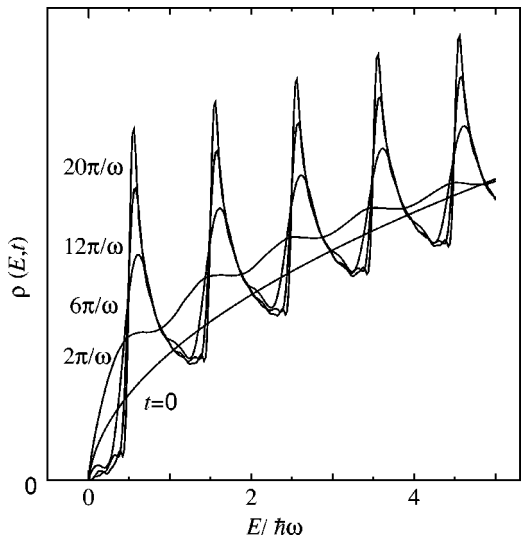

FIG. 5. The time-dependent density of states plotted as a function of energy.

To show how quantization occurs and energy spectrum changes due to interference, we calculate

$$\rho(E,t)=\sum_{\mathbf{k}} \langle \chi_{E,\mathbf{k}}|\chi_{E,\mathbf{k}}\rangle \delta(E-E_{\mathbf{k}}). \tag{14}$$

This is density of states with weight of norm of $\chi_{E,\mathbf{k}}$. Figure 5 shows $\rho(E,t)$ plotted as a function of energy for various values of t. At $t=0$, the density of states is that of the three-dimensional free electron. With increasing time, interference accompanied with electronic motion occurs, and quantized density of states realizes.

IV. STARK LADDERS

In a static electric field $\mathbf{F}$, wave vectors increase as $\mathbf{k}(t)=k_0+e\mathbf{F}t/\hbar$. At the edge of the Brillouin zone, the electron is Bragg reflected due to crystalline potential. Accompanied with this motion, a ladderlike energy spectrum associated with localized wave functions realizes. This is known as a Stark ladder. We can describe the formation process of Stark ladders accompanied with the motion called the Bloch oscillation.

In principle, we should treat applied and crystal potential on an equal footing. Although it will be a hard task, we can apply the effective mass approximation where the effects from crystalline potential are included in a cosinelike dispersion curve.[1,2]

We consider a case where an electric field is applied along the z axis. In this case, we can make a superposition of Bloch states as[12,13]

$$\chi_{n\mathbf{k}}(\mathbf{r})=\sqrt{\frac{\Omega}{2\pi\Delta}}\int_{-\Delta/2}^{\Delta/2} d\kappa e^{-i/\hbar\int_0^t[\varepsilon_{k_z(\tau)}-eFLn]d\tau}\phi_{\mathbf{k}(t)}(\mathbf{r}), \tag{15}$$

where $\phi_{\mathbf{k}}(\mathbf{r})$ is a Bloch function, L is the lattice constant, Ω is the system size, $\mathbf{k}(t)=\mathbf{k}+e\mathbf{F}t/\hbar$, and $\kappa=eFt/\hbar$. We note that $eFLn$ in the exponential function is corresponding to the energy E in Eq. (7).

When Δ is much smaller than Brillouin zone width, we can set as $\Delta\simeq 2\pi/\Omega$, and $\chi_{n\mathbf{k}}(\mathbf{r})$ is regarded as a Bloch function. A bandlike energy spectrum realizes in this case. With increasing Δ, if n is not an integer, the amplitudes interfere with one another and cancel out. Whereas when n is an integer, $\chi_{n\mathbf{k}}(\mathbf{r})$ becomes a rung of the Stark ladder located at the nth position for $\Delta \gg 2\pi/L$. Therefore, a ladderlike spectrum associated with localized state is realized. Temporal behavior of energy spectrum is similar to that shown in Fig. 4 (but without the zero point energy).

The formation process of Stark ladder is important in terms of device applications. For high-field transport in nanoscale semiconductor devices, it has been pointed out that quantum effects are important. There have been a number of studies on quantum effects in transport phenomena.[11] Many of these studies employ the Green's functions, however, there are some attempts to describe transport phenomena by using half-localized Stark ladder state.[14,15]

V. CONCLUSION

In conclusion, we have described the quantization process in electromagnetic fields. We showed that an eigen wave function is formed as a superposition of electronic states over the path in which the electron has undergone. This means that the origin of quantization of an electron in motion is self-interference with electron itself in the past. We may call this effect as the afterimage, that is, an eigenstate is not just an image at each moment but a superposition of all images in the past. In other words, an eigenfunction is a time-integrated probability amplitude, i.e., the probability of finding an electron at energy E during the period $0\sim t$. This is a viewpoint which is essential for describing electron behavior as well as for a better understanding of the nature of electrons.

ACKNOWLEDGMENTS

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