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Dressed-band theory for semiconductors in a high-intensity infrared laser field

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Under the illumination of intense off-resonant laser light, the electronic states of semiconductors are strongly modified, or dressed, by the oscillating electric field. We present a framework using linear combination of atomic orbital band theory to calculate the dressed band structure and optical absorption spectrum of covalent semiconductors in an intense off-resonant laser field. The interaction with the laser field is taken into account exactly from the beginning of the band calculation. It is shown that the irradiation of an intense infrared laser gives rise to a blueshift of the absorption edge as well as the emergence of a new absorption band below the edge, in agreement with recent experimental data for GaAs crystals.

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I. INTRODUCTION

Technical developments in laser physics in recent years have made possible the production of high intensity monochromatic light with a wide range of wavelengths comparatively easily. This has opened a new possibility in the use of lasers as a tool to manipulate electronic wave functions of atoms and molecules through coherent modulations. An electronic system under an intense and coherent electromagnetic field is strongly modified and forms an intermixed state of the electronic configuration and photons called a dressed state.[1] In atoms and molecules, this effect induces peculiar optical properties such as the dynamic Stark effect,[2] the Mollow triplet in light scattering,[3] and electromagnetically induced transparency.[4] In solids, it is expected that the irradiation of intense laser light will give rise to coherent modification of the energy band structures and that the energy bands are intermingled with the radiation field to form *dressed bands*, analogous to the case of atoms.

In regard to the solid case, Kono and co-workers[5] have recently performed a pump-probe experiment on semiconductors using a high intensity off-resonant pump laser and reported that an additional absorption band is observed below the original band edge in the near infrared region only when the pump and probe laser field temporally overlap each other. In addition, detailed investigation[6] revealed that the band edge recedes to the high energy side under the pump laser field. In this phenomenon, real excitations of carriers and thermal effects do not play any essential role, because the induced change of the absorption is observed only in the presence of the pump pulse. The crucial point is the use of intense midinfrared laser, which allows to minimize the interband absorption and sample damage while maximizing the ponderomotive energy U_p given by

$$U_p = \frac{e^2 E_0^2}{4m\omega^2}, \tag{1}$$

where e is the magnitude of the electric charge, m is the mass of the electron, and E_0 is the intensity of the electric field oscillating with frequency ω.

From theory, a number of studies have been devoted to the investigation of the modulation of the electronic states of crystals by an intense electromagnetic field. For example, Dunlap and Kenkre[7] obtained a rigorous solution for the model of an electron in a one-dimensional lattice under an oscillating electric field and showed that the electron may be localized around the initial state by applying the field with a suitable ratio of the amplitude and frequency. This phenomenon is called dynamic localization. Holthaus *et al.*[8,9] calculated quasi-energies of the superlattice under an intense laser field by the Floquet theory[10,11] and predicted the collapse of quasi-energy minibands. These phenomena are closely related with the coherent destruction of tunneling in confined systems.[12]

The effect of the interaction with an intense electromagnetic field in semiconductors has been studied theoretically in a series of early works.[13–15] Here, the energy quantum of the electromagnetic field has been assumed to be *resonant*, i.e., larger than the band gap energy. It was predicted that an extra gap would open in the quasi-energy spectrum due to the strong mixing between the valence band and the conduction band.

For the interaction with an off-resonant field, the induced change of the linear absorption spectrum at the absorption edge due to an intense infrared laser field has been calculated for bulk crystals[16] and for mesoscopic systems.[17] In both cases, a two-band model with field-induced mixing due to the Franz-Keldysh effect[18,19] is assumed. On the other hand, Miranda[20] has shown that the effective band gap reduces linearly with increasing intensity of the field within the framework of nearly free electron model.

We would like to stress here that, in actual semiconductors, both the conduction and valence bands consist of the same set of the atomic orbitals of the component atoms. In Si or GaAs, for example, the ns and np states ($n=3$ for Si and

$n=4$ for GaAs) of the outermost valence levels are hybridized to form sp^3 orbitals. These orbitals at nearest neighboring atoms are then hybridized with each other to form covalent bonds. The band gap of these materials corresponds essentially to the energy difference between the bonding state and the antibonding state. In order to investigate the effect of an intense off-resonant radiation field on the band structure of semiconductors quantitatively, it is necessary to begin with the atomic orbital of the basis and treat quantum mechanical hybridization and interaction with the intense electromagnetic field on the same footing. In other words, a new theoretical framework for the dressed-band calculations of semiconductors, which are the band calculations for the electronic system *exactly* including the interaction with the electromagnetic field, should be developed.

Furthermore, because of the highly nonstationary character of the electronic state under the intense electromagnetic field, the traditional method to calculate the optical response based on the perturbation theory from the equilibrium distribution cannot be applied, and the linear response theory for the probe light should be reformulated in order to analyze the experimental data.

Since the coherent control of the electronic properties of solids by external radiation fields may lead to a novel principle of nonlinear optical devices, it is highly desirable to establish a theoretical framework which enables us to analyze the phenomena quantitatively. In previous work,[21] we proposed a simplified one-dimensional model of semiconductors as a prototype of covalent semiconductors under an intense off-resonant electromagnetic field. We have calculated dressed band structure and reformulated the line shape function of the absorption spectrum for the system. The calculated absorption spectrum shows peculiar features with a blue shift of the band edge and the emergence of an additional structure below the edge, in qualitative agreement with the experimental data.[6]

In the present work, we propose a theory of dressed-band-calculation based on the realistic three-dimensional model of semiconductors under an intense off-resonant laser field. The electronic system for zincblende crystal is described by an linear combination of atomic orbital (LCAO) approximation for a three-dimensional tight-binding Hamiltonian. The interaction with the intense pump laser is treated rigorously by the Floquet formalism. The dressed band structures are calculated by combined application of the Bloch theory and the Floquet theory to the spatiotemporal periodic Hamiltonian. The absorption spectrum for a weak probe field is reformulated by the generating function method. The calculated pump-probe signals in the band edge of GaAs crystals are in good agreement with the experimental observation.

In the next section, the model is presented and the formulation of the calculation of the optical responses is given. The numerical results are shown in Sec. III together with discussions. Concluding remarks are given in Sec. IV.

II. MODEL AND FORMULATION

We consider a model for the electronic states of semiconductors under intense off-resonant laser field described by the Hamiltonian in the Coulomb gauge

$$H(t) = H_S + H_I(t), \tag{2}$$

$$H_S = \frac{\boldsymbol{p}^2}{2m} - e\phi, \tag{3}$$

$$H_I(t) = e\boldsymbol{r} \cdot \boldsymbol{E}(\boldsymbol{r},t), \tag{4}$$

where $\boldsymbol{p}$ is the momentum operator of an electron with the electric charge $-e(<0)$ and the mass m, $\boldsymbol{E}(\boldsymbol{r},t)$ is the electric field of the pump laser, and ϕ is the Coulomb potential which has the periodicity of the crystal. For the interaction Hamiltonian with the weak probe light, we adopt simply,

$$H'(t) = \frac{e}{m}\boldsymbol{A}(\boldsymbol{r},t) \cdot \boldsymbol{p}, \tag{5}$$

in which $\boldsymbol{A}(\boldsymbol{r},t)$ are the vector potential of the probe light field. For later convenience, we have expressed the interaction with the intense pump field in terms of the electric field, while that with the weak probe field in terms of the vector potential. Note that the interaction with the pump field is exactly taken into account in $H_I(t)$.[22] The interaction with the probe light is, on the other hand, is treated in $H'(t)$ to the first order of $\boldsymbol{A}(\boldsymbol{r},t)$, neglecting the quadratic term as usual.

A. Tight-binding Hamiltonian for the electronic system

The electronic system is treated within the tight binding approximation. We assume a zinc blende structure crystal that consists of two kind of atoms (atom 1 and atom 2) with an s orbital and p orbitals of x, y, and z symmetry for each atom. The spin-degree of freedom is neglected. These atoms are located at

$$\boldsymbol{r}_{1,l_1,l_2,l_3} = l_1\boldsymbol{a} + l_2\boldsymbol{b} + l_3\boldsymbol{c}, \tag{6}$$

$$\boldsymbol{r}_{2,l'_1,l'_2,l'_3} = \left(l'_1 + \frac{1}{4}\right)\boldsymbol{a} + \left(l'_2 + \frac{1}{4}\right)\boldsymbol{b} + \left(l'_3 + \frac{1}{4}\right)\boldsymbol{c}, \tag{7}$$

for the atom 1 and atom 2, respectively. In the above equations, $\boldsymbol{a}=(\boldsymbol{i}_x+\boldsymbol{i}_y)a/2$, $\boldsymbol{b}=(\boldsymbol{i}_y+\boldsymbol{i}_z)a/2$, and $\boldsymbol{c}=(\boldsymbol{i}_z+\boldsymbol{i}_x)a/2$ are the primitive basis vectors, where $\boldsymbol{i}_x$, $\boldsymbol{i}_y$, and $\boldsymbol{i}_z$ are unit vectors in the x, y, and z directions, respectively, and a is the lattice constant. The atomic basis function at the atomic position $\boldsymbol{r}_{j,l_1,l_2,l_3}$ with the symmetry ξ ($\xi=s$, p_x, p_y, or p_z, hereafter) is denoted by $|\boldsymbol{r}_{j,l_1,l_2,l_3},\xi\rangle$, and these functions make orthonormal basis set for the LCAO calculation.

In the tight-binding picture, the system Hamiltonian is written as

$$H_S = H_0 + H_{111} + H_{1\bar{1}\bar{1}} + H_{\bar{1}1\bar{1}} + H_{\bar{1}\bar{1}1}, \tag{8}$$

where H_0 represents the diagonal energy of the s and p orbitals, ε_{s_j} and ε_{p_j} of each atom, and H_{111}, $H_{1\bar{1}\bar{1}}$, $H_{\bar{1}1\bar{1}}$, and $H_{\bar{1}\bar{1}1}$ represent interatomic hopping between nearest neighbor atoms for each directions. These Hamiltonians are explicitly written as

$$H_0 = \sum_{j=1}^{2} \sum_{l_1,l_2,l_3} (\varepsilon_{s_j} |\boldsymbol{r}_{j,l_1,l_2,l_3}, s\rangle\langle \boldsymbol{r}_{j,l_1,l_2,l_3}, s| + \varepsilon_{p_j} |\boldsymbol{r}_{j,l_1,l_2,l_3}, p_x\rangle \times \langle \boldsymbol{r}_{j,l_1,l_2,l_3}, p_x| + \varepsilon_{p_j} |\boldsymbol{r}_{j,l_1,l_2,l_3}, p_y\rangle\langle \boldsymbol{r}_{j,l_1,l_2,l_3}, p_y| + \varepsilon_{p_j} |\boldsymbol{r}_{j,l_1,l_2,l_3}, p_z\rangle\langle \boldsymbol{r}_{j,l_1,l_2,l_3}, p_z|), \tag{9}$$

$$H_{111} = \sum_{l_1,l_2,l_3} \sum_{\xi,\xi'} t^{111}_{\xi,\xi'} |\boldsymbol{r}_{1,l_1,l_2,l_3}, \xi\rangle\langle \boldsymbol{r}_{2,l_1,l_2,l_3}, \xi'| + (\mathrm{H.c.}), \tag{10}$$

$$H_{1\bar{1}\bar{1}} = \sum_{l_1,l_2,l_3} \sum_{\xi,\xi'} t^{1\bar{1}\bar{1}}_{\xi,\xi'} |\boldsymbol{r}_{1,l_1,l_2,l_3}, \xi\rangle\langle \boldsymbol{r}_{2,l_1,l_2-1,l_3}, \xi'| + (\mathrm{H.c.}), \tag{11}$$

$$H_{\bar{1}1\bar{1}} = \sum_{l_1,l_2,l_3} \sum_{\xi,\xi'} t^{\bar{1}1\bar{1}}_{\xi,\xi'} |\boldsymbol{r}_{1,l_1,l_2,l_3}, \xi\rangle\langle \boldsymbol{r}_{2,l_1,l_2,l_3-1}, \xi'| + (\mathrm{H.c.}), \tag{12}$$

$$H_{\bar{1}\bar{1}1} = \sum_{l_1,l_2,l_3} \sum_{\xi,\xi'} t^{\bar{1}\bar{1}1}_{\xi,\xi'} |\boldsymbol{r}_{1,l_1,l_2,l_3}, \xi\rangle\langle \boldsymbol{r}_{2,l_1-1,l_2,l_3}, \xi'| + (\mathrm{H.c.}), \tag{13}$$

where $t^{d}_{\xi\xi'}$ [$d=(111),(1\bar{1}\bar{1}),(\bar{1}1\bar{1})$, or $(\bar{1}\bar{1}1)$, hereafter] is the hopping integral between the ξ orbital of atom 1 and the ξ' orbital of atom 2 in the d direction. All hopping integrals are calculated by giving only the values $(ss\sigma)$, $(sp\sigma)_{1,2}$, $(sp\sigma)_{2,1}$, $(pp\sigma)$, and $(pp\pi)$.[23] The energy band structure of GaAs calculated in the tight-binding model is shown in Fig. 1. The parameter values for the energies of atomic orbitals are $\varepsilon_{s,\mathrm{Ga}}=-10.48$ eV, $\varepsilon_{p,\mathrm{Ga}}=-4.01$ eV for Ga and $\varepsilon_{s,\mathrm{As}}=-16.44$ eV, $\varepsilon_{p,\mathrm{As}}=-7.02$ eV for As, and the hopping integrals between the nearest neighbor atoms are $(ss\sigma)=-1.547$ eV, $(sp\sigma)_{\mathrm{Ga,As}}=1.729$ eV, $(sp\sigma)_{\mathrm{As,Ga}}=2.184$ eV, $(pp\sigma)=3.1304$ eV, and $(pp\pi)=-0.8099$ eV, where $(sp\sigma)_{\mathrm{Ga,As}}$ represents the hopping between the s orbital of Ga and p orbital of As. In order to fit the band gap E_g to experimental results $E_g=1.42$ eV, the hopping integrals are modified by multiplying 0.91 to the parameters of Harrison.[24] The agreement of the near edge structure with more elaborate band calculations[24–26] is fairly good.

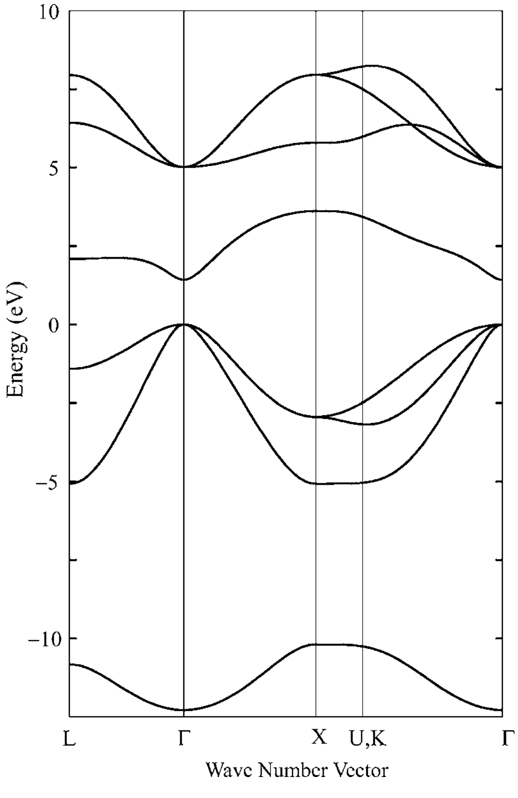

FIG. 1. Energy band structure of GaAs calculated by the tight-binding model.

B. Interaction with the radiation fields

In accordance with the former works,[7–9,16,17] we treat the pump laser field as an oscillating electric field with a uniform intensity. This is justified when the field intensity is high enough and the photon energy is much less than the typical energy scale of the system. The electric field is written as

$$\boldsymbol{E}(t) = E_0 \cos(\omega t) \boldsymbol{e}_\nu, \tag{14}$$

where E_0 and ω are the amplitude and frequency of the field, respectively, and $\boldsymbol{e}_\nu = e_x \boldsymbol{i}_x + e_y \boldsymbol{i}_y + e_z \boldsymbol{i}_z$ ($|\boldsymbol{e}_\nu|=1$) is the polarization vector, in which ν is the suffix of the direction. In order to expand the interaction Hamiltonian with the tight-binding basis, we decompose the dipole moment into two parts. The one is the interatomic component which takes part in the oscillation of the relative energies of the atoms as a whole depending on the atomic site. The other is the intra-atomic component which induces the internal Stark effect within each atom. Then the interaction Hamiltonian $H_I(t)$ is given by

$$H_I(t) = \sum_{j=1}^{2} \sum_{l_1,l_2,l_3} (\boldsymbol{e}_\nu \cdot e\boldsymbol{r}_{j,l_1,l_2,l_3} I_{j,l_1,l_2,l_3} - M_{\mu,j,l_1,l_2,l_3}) \times E_0 \cos(\omega t), \tag{15}$$

with

$$I_{j,l_1,l_2,l_3} = |\boldsymbol{r}_{j,l_1,l_2,l_3}, s\rangle\langle \boldsymbol{r}_{j,l_1,l_2,l_3}, s| + |\boldsymbol{r}_{j,l_1,l_2,l_3}, p_x\rangle\langle \boldsymbol{r}_{j,l_1,l_2,l_3}, p_x| + |\boldsymbol{r}_{j,l_1,l_2,l_3}, p_y\rangle\langle \boldsymbol{r}_{j,l_1,l_2,l_3}, p_y| + |\boldsymbol{r}_{j,l_1,l_2,l_3}, p_z\rangle\langle \boldsymbol{r}_{j,l_1,l_2,l_3}, p_z| \tag{16}$$

and

$$M_{\nu,j,l_1,l_2,l_3} = -e\alpha_j |\boldsymbol{r}_{j,l_1,l_2,l_3}, s\rangle\langle \boldsymbol{r}_{j,l_1,l_2,l_3}, p_\nu| + (\mathrm{H.c.}), \tag{17}$$

where the first term represents the interatomic Stark effect and the second term the intra-atomic Stark effect, respectively. In the above equations,

$$\alpha_j = \langle \boldsymbol{r}_{j,l_1,l_2,l_3}, s | x | \boldsymbol{r}_{j,l_1,l_2,l_3}, p_x\rangle \tag{18}$$

$$= \langle \boldsymbol{r}_{j,l_1,l_2,l_3}, s | y | \boldsymbol{r}_{j,l_1,l_2,l_3}, p_y\rangle \tag{19}$$

$$= \langle \boldsymbol{r}_{j,l_1,l_2,l_3}, s | z | \boldsymbol{r}_{j,l_1,l_2,l_3}, p_z\rangle \tag{20}$$

is the parameter of the intra-atomic Stark effect and

$$|\boldsymbol{r}_{j,l_1,l_2,l_3},p_\nu\rangle = e_x|\boldsymbol{r}_{j,l_1,l_2,l_3},p_x\rangle + e_y|\boldsymbol{r}_{j,l_1,l_2,l_3},p_y\rangle + e_z|\boldsymbol{r}_{j,l_1,l_2,l_3},p_z\rangle \tag{21}$$

represents the projection of the p orbital in the ν direction. The other terms vanish due to symmetry.

On the other hand, the vector potential of the probe laser light is written in the photon picture as

$$\boldsymbol{A}(t,\Omega) = A(be^{-i\Omega t} + b^\dagger e^{i\Omega t})\boldsymbol{e}_{\nu'}, \tag{22}$$

where b ($b^\dagger$) is the annihilation (creation) operator of the photon of the probe laser light with the frequency Ω. The amplitude A is written as $A=\sqrt{\hbar/2\varepsilon_0 V\Omega}$ for the system with volume V and dielectric constant ε_0.

C. Formulation of the absorption spectrum

The optical susceptibility should have time-dependence due to the oscillatory driving force. Experimentally observed spectrum corresponds to the stationary component with the oscillatory component averaged out. In order to treat such a situation, we reformulate the expression of the absorption spectrum as follows.[27] Consider the pump and probe laser field are switched on at the time $t=0$. By using Feynman's disentangling theorem and treating $H'(t,\Omega)$ in the lowest order perturbation, the density matrix of the system describing the time-evolution that, initially in the state $\rho_0=|i\rangle\langle i|$, it is in the excited state at time t after absorbing a probe photon, is given by

$$\rho(t,\Omega) = \frac{1}{\hbar^2}\int_0^t dt_1 \int_0^t dt_2 F(t,t_1)H'(t_1,\Omega)F(t_1,0) \times \rho_0 F^\dagger(t_2,0)H'^\dagger(t_2,\Omega)F^\dagger(t,t_2). \tag{23}$$

In the above equation, $F(t_f,t_i)$ is the operator for the time-evolution from t_i to t_f driven by the unperturbed Hamiltonian $H(t)=H_S+H_I(t)$, which is given by

$$F(t_i,t_f) = \exp_+\left\{-\frac{i}{\hbar}\int_{t_i}^{t_f} H(\tau)d\tau\right\}, \tag{24}$$

with $\exp_+$ meaning the time-ordered exponential. The diagrammatic representation of the process is shown in Fig. 2. In the consideration of the transition probability, the final state $|f\rangle$ is also driven by the pump laser field, and evolves into $|f(t)\rangle=F(t,0)|f\rangle$ at time t.

Then, the probability of the transition to the final state is given by

$$P(t,\Omega) = \langle f(t)|\rho(t,\Omega)|f(t)\rangle \tag{25}$$

$$= \frac{1}{\hbar^2}\int_0^t dt_1 \int_0^t dt_2 \langle f|F^\dagger(t_1)H'(t_1,\Omega)F(t_1)|i\rangle \times \langle i|F^\dagger(t_2)H'^\dagger(t_2,\Omega)F(t_2)|f\rangle, \tag{26}$$

where $F(t)\equiv F(t,0)$.

In the usual case of band calculations, Bloch's theorem plays a crucial role to exploit the translational symmetry of the crystal. In the present case, the translational symmetry is broken because of the presence of the external electric field. This difficulty can be overcome by applying a gauge transformation as follows. Define a unitary operator $U(t)$ by

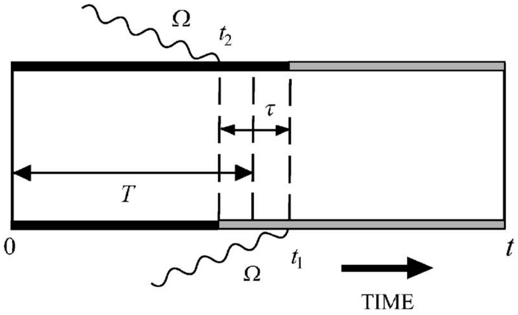

FIG. 2. Feynman diagram for the density matrix $\rho(t,\Omega)$.

$$U(t) \equiv \exp\left\{-\frac{i}{\hbar}\int_0^t H_I(\tau)d\tau\right\} \tag{27}$$

$$= \sum_{j=1}^{2}\sum_{l_1,l_2,l_3} \exp\left\{\frac{i}{\hbar}eA_1(t)(\boldsymbol{e}_\nu\cdot\boldsymbol{r}_{j,l_1,l_2,l_3})\right\} \times \exp\left\{-\frac{i}{\hbar}A_1(t)M_{\nu,j,l_1,l_2,l_3}\right\}, \tag{28}$$

with $A_1(t)=-(E_0/\omega)\sin(\omega t)$, and transform the Hamiltonian as $\widetilde{H}(t)=U^\dagger(t)H_S U(t)$. The transformed Hamiltonian is given by

$$\widetilde{H}(t) = U_1^\dagger(t)H_0U_1(t) + U_2^\dagger(t)H_0U_2(t) + \sum_d \{f_d(t)U_1^\dagger(t)H_dU_2(t) + (\mathrm{H.c.})\}, \tag{29}$$

where

$$U_j(t) = \sum_{l_1,l_2,l_3} \exp\left\{-\frac{i}{\hbar}A_1(t)M_{\nu,j,l_1,l_2,l_3}\right\} \tag{30}$$

and

$$f_{111}(t) = \exp\left\{\frac{i}{\hbar}eaA_1(t)(e_x+e_y+e_z)/4\right\}, \tag{31}$$

$$f_{1\bar{1}\bar{1}}(t) = \exp\left\{\frac{i}{\hbar}eaA_1(t)(e_x-e_y-e_z)/4\right\}, \tag{32}$$

$$f_{\bar{1}1\bar{1}}(t) = \exp\left\{\frac{i}{\hbar}eaA_1(t)(-e_x+e_y-e_z)/4\right\}, \tag{33}$$

$$f_{\bar{1}\bar{1}1}(t) = \exp\left\{\frac{i}{\hbar}eaA_1(t)(-e_x-e_y+e_z)/4\right\}. \tag{34}$$

Thus the translational symmetry is recovered in $\widetilde{H}(t)$.

Introduce new basis vectors

$$|\varphi_{\boldsymbol{k}},\xi\rangle = \frac{1}{\sqrt{N}}\sum_{l_1,l_2,l_3}^{N} |\boldsymbol{r}_{1,l_1,l_2,l_2},\xi\rangle e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{1,l_1,l_2,l_3}}, \tag{35}$$

$$|\psi_{\boldsymbol{k}},\xi'\rangle = \frac{1}{\sqrt{N}}\sum_{l_1,l_2,l_3}^{N} |\boldsymbol{r}_{2,l_1,l_2,l_3},\xi'\rangle e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{2,l_1,l_2,l_3}}, \tag{36}$$

for the wave number vector $\boldsymbol{k}=k_x\boldsymbol{i}_x+k_y\boldsymbol{i}_y+k_z\boldsymbol{i}_z$ $(-\pi/a < k_x,k_y,k_z \leqslant \pi/a)$, where N is the number of unit cells, and decompose the Hamiltonian as $\widetilde{H}(t)=\Sigma_{\boldsymbol{k}}\widetilde{H}_{\boldsymbol{k}}(t)$. The time-evolution operator is transformed into the form

$$\widetilde{F}(t_1,t_0) = U^{\dagger}(t_1)F(t_1,t_0)U(t_0) \tag{37}$$

$$= \exp_{+}\left\{-\frac{i}{\hbar}\int_{t_0}^{t_1}\widetilde{H}(\tau)d\tau\right\}, \tag{38}$$

which can be decomposed as $\widetilde{F}(t_1,t_0)=\Sigma_{\boldsymbol{k}}\widetilde{F}_{\boldsymbol{k}}(t,t_0)$ with

$$\widetilde{F}_{\boldsymbol{k}}(t,t_0) = \exp_{+}\left\{-\frac{i}{\hbar}\int_{t_0}^{t_1}\widetilde{H}_{\boldsymbol{k}}(\tau)d\tau\right\}. \tag{39}$$

In order to apply the unitary transformation to $H'(t,\Omega)$, we use the relation

$$\boldsymbol{p} = i\frac{m}{\hbar}[\boldsymbol{p}^2/2m,\boldsymbol{r}], \tag{40}$$

and rewrite the interaction Hamiltonian as

$$H'(t,\Omega) = -i\mu[H_S,M_{\nu'}]be^{-i\Omega t} + (\text{H.c.}), \tag{41}$$

where $\mu=A/\hbar=1/\sqrt{2\varepsilon_0 V\hbar\Omega}$, and $M_{\nu'}$ is the transition dipole moment which causes the intra-atomic $s\rightarrow p_{\nu'}$ transition, given by

$$M_{\nu'} = \sum_{j=1}^{2}\sum_{l_1,l_2,l_3} M_{\nu',j,l_1,l_2,l_3}. \tag{42}$$

We find that

$$U^{\dagger}(t)[H_S,M_{\nu'}]U(t) = \sum_{\boldsymbol{k}}[\widetilde{H}_{\boldsymbol{k}}(t),M_{\nu'\boldsymbol{k}}], \tag{43}$$

where

$$\begin{aligned} M_{\nu'\boldsymbol{k}} = {} & -e\alpha_1(|\varphi_{\boldsymbol{k}},s\rangle\langle\varphi_{\boldsymbol{k}},p_{\nu'}| + |\varphi_{\boldsymbol{k}},p_{\nu'}\rangle\langle\varphi_{\boldsymbol{k}},s|) \\ & - e\alpha_2(|\psi_{\boldsymbol{k}},s\rangle\langle\psi_{\boldsymbol{k}},p_{\nu'}| + |\psi_{\boldsymbol{k}},p_{\nu'}\rangle\langle\psi_{\boldsymbol{k}},s|). \end{aligned} \tag{44}$$

Therefore, the probability of transition from $|i\rangle\langle i| = \Sigma_{\boldsymbol{k}}|i_{\boldsymbol{k}}\rangle\langle i_{\boldsymbol{k}}|$ to $|f\rangle\langle f| = \Sigma_{\boldsymbol{k}}|f_{\boldsymbol{k}}\rangle\langle f_{\boldsymbol{k}}|$ is decomposed as $P(t,\Omega) = \Sigma_{\boldsymbol{k}}P_{\boldsymbol{k}}(t,\Omega)$, where

$$\begin{aligned} P_{\boldsymbol{k}}(t,\Omega) = {} & \frac{\mu^2 n_p}{\hbar^2}\int_0^t dt_1\int_0^t dt_2\langle f_{\boldsymbol{k}}|\widetilde{F}_{\boldsymbol{k}}^{\dagger}(t_1)[\widetilde{H}_{\boldsymbol{k}}(t_1),M_{\nu'\boldsymbol{k}}]\widetilde{F}_{\boldsymbol{k}}(t_1)|i_{\boldsymbol{k}}\rangle \\ & \times\langle i_{\boldsymbol{k}}|\widetilde{F}_{\boldsymbol{k}}^{\dagger}(t_2)[M_{\nu'\boldsymbol{k}},\widetilde{H}_{\boldsymbol{k}}(t_2)]\widetilde{F}_{\boldsymbol{k}}(t_2)|f_{\boldsymbol{k}}\rangle e^{-i\Omega(t_1-t_2)}. \end{aligned} \tag{45}$$

In the above equation, n_p is the number of photon which corresponds to the transition of the photon state from $|n_p\rangle$ to $|n_p-1\rangle$ in the absorption process of the probe photon, and is associated with the intensity of probe laser I_0 as $n_p = I_0 V/\hbar\Omega c$. With the use of definition of time-ordered exponential

$$i\hbar\frac{\partial}{\partial t}\widetilde{F}_{\boldsymbol{k}}(t) = \widetilde{H}_{\boldsymbol{k}}(t)\widetilde{F}_{\boldsymbol{k}}(t), \tag{46}$$

a part of representation in Eq. (45) is rewritten as

$$\begin{aligned} & \langle f_{\boldsymbol{k}}|\widetilde{F}_{\boldsymbol{k}}^{\dagger}(t_1)[\widetilde{H}_{\boldsymbol{k}}(t_1),M_{\nu'\boldsymbol{k}}]\widetilde{F}_{\boldsymbol{k}}(t_1)|i_{\boldsymbol{k}}\rangle \\ & = -i\hbar\frac{\partial}{\partial t_1}\langle f_{\boldsymbol{k}}|\widetilde{F}_{\boldsymbol{k}}^{\dagger}(t_1)M_{\nu'\boldsymbol{k}}\widetilde{F}_{\boldsymbol{k}}(t_1)|i_{\boldsymbol{k}}\rangle. \end{aligned} \tag{47}$$

In order to calculate $P(t,\Omega)$, we use the Floquet theory.[10,11] Since $\widetilde{H}_{\boldsymbol{k}}(t)$ has a periodicity in time, we can write

$$\langle u|\widetilde{F}_{\boldsymbol{k}}(t)|v\rangle = \sum_{l=-\infty}^{\infty}\langle\langle u,l|\exp(-iH_{F\boldsymbol{k}}t/\hbar)|v,0\rangle\rangle e^{il\omega t}, \tag{48}$$

where $|u\rangle$ is a time-independent state, and $|u,l\rangle\rangle$ is the corresponding Floquet state. The quasienergies form *dressed bands*, and are given by solving the eigenvalue equation

$$H_{F\boldsymbol{k}}|\phi_{\boldsymbol{k},j,l}\rangle\rangle = (\varepsilon_{\boldsymbol{k},j} + l\hbar\omega)|\phi_{\boldsymbol{k},j,l}\rangle\rangle, \tag{49}$$

where j is the band index which runs over the same number as the number of original bands. The index l corresponds to the photon number measured from a very large average number.[10] With the use of Eq. (48) and the relation

$$\langle\langle u,q|\phi_{\boldsymbol{k},j,l}\rangle\rangle = \langle\langle u,q-l'|\phi_{\boldsymbol{k},j,l-l'}\rangle\rangle, \tag{50}$$

Eq. (45) is transformed into

$$\begin{aligned} P_{\boldsymbol{k}}(t,\Omega) = {} & \frac{\mu^2 n_p}{\hbar^2}\sum_{j_1,j_2,j_3,j_4}\int_0^t dt_1\int_0^t dt_2\sum_{l_1,l_2,l_3,l_4}\langle\langle f_{\boldsymbol{k},0}|\phi_{\boldsymbol{k},j_1,l_1}\rangle\rangle \\ & \times\langle\langle\phi_{\boldsymbol{k},j_2,l_2}|i_{\boldsymbol{k},0}\rangle\rangle\langle\langle i_{\boldsymbol{k},0}|\phi_{\boldsymbol{k},j_3,l_3}\rangle\rangle\langle\langle\phi_{\boldsymbol{k},j_4,l_4}|f_{\boldsymbol{k},0}\rangle\rangle \\ & \times\sum_{m_1,m_2}\{(\varepsilon_{\boldsymbol{k},j_1}-\varepsilon_{\boldsymbol{k},j_2})-(m_1-m_2)\hbar\omega\} \\ & \times\langle\langle\phi_{\boldsymbol{k},j_1,0}|M_{\nu',\boldsymbol{k},m_1,m_2}|\phi_{\boldsymbol{k},j_2,0}\rangle\rangle\exp[i\{(\varepsilon_{\boldsymbol{k},j_1}-\varepsilon_{\boldsymbol{k},j_2})/\hbar \\ & -(m_1-m_2)\omega\}t_1]\sum_{m_3,m_4}\{(\varepsilon_{\boldsymbol{k},j_4}-\varepsilon_{\boldsymbol{k},j_3}) \\ & -(m_4-m_3)\hbar\omega\}\langle\langle\phi_{\boldsymbol{k},j_3,0}|M_{\nu',\boldsymbol{k},m_3,m_4}|\phi_{\boldsymbol{k},j_4,0}\rangle\rangle \\ & \times\exp[-i\{(\varepsilon_{\boldsymbol{k},j_4}-\varepsilon_{\boldsymbol{k},j_3})/\hbar \\ & -(m_4-m_3)\omega\}t_2]e^{-i\Omega(t_1-t_2)}, \end{aligned} \tag{51}$$

where

$$\begin{aligned} M_{\nu',\boldsymbol{k},m,m'} = {} & -e\alpha_1(|\varphi_{\boldsymbol{k}},s,m\rangle\rangle\langle\langle\varphi_{\boldsymbol{k}},p_{\nu'},m'| + |\varphi_{\boldsymbol{k}},p_{\nu'},m\rangle\rangle \\ & \times\langle\langle\varphi_{\boldsymbol{k}},s,m'|) - e\alpha_2(|\psi_{\boldsymbol{k}},s,m\rangle\rangle\langle\langle\psi_{\boldsymbol{k}},p_{\nu'},m'| \\ & + |\psi_{\boldsymbol{k}},p_{\nu'},m\rangle\rangle\langle\langle\psi_{\boldsymbol{k}},s,m'|) \end{aligned} \tag{52}$$

and

$$|u_{\boldsymbol{k},0}\rangle\rangle = \sum_{\xi}(|\varphi_{\boldsymbol{k}},\xi,0\rangle\rangle\langle\varphi_{\boldsymbol{k}},\xi| + |\psi_{\boldsymbol{k}},\xi,0\rangle\rangle\langle\psi_{\boldsymbol{k}},\xi|)|u_{\boldsymbol{k}}\rangle, \tag{53}$$

in which $|u_{\boldsymbol{k}}\rangle=|i_{\boldsymbol{k}}\rangle$ or $|u_{\boldsymbol{k}}\rangle=\rangle f_{\boldsymbol{k}}|$.

Introduce the relative and the center-of-mass time variables $\tau=t_1-t_2$ and $T=(t_1+t_2)/2$, respectively. The time-dependent part of $P(t,\Omega)$ is given by

$$\begin{aligned}&\int_0^t dt_1\int_0^t dt_2 \exp[i\{(\varepsilon_{\boldsymbol{k},j_1}-\varepsilon_{\boldsymbol{k},j_2})/\hbar-(m_1-m_2)\omega\}t_1]\\&\quad\times\exp[-i\{(\varepsilon_{\boldsymbol{k},j_4}-\varepsilon_{\boldsymbol{k},j_3})/\hbar-(m_4-m_3)\omega\}t_2]e^{-i\Omega(t_1-t_2)}\\&\quad=\left(\int_0^{t/2}dT\int_{-2T}^{2T}d\tau+\int_{t/2}^{t}dT\int_{-2(t-T)}^{2(t-T)}d\tau\right)e^{i\Omega_{1,\boldsymbol{k}}T}e^{i\Omega_{2,\boldsymbol{k}}\tau},\end{aligned}\tag{54}$$

with $\Omega_{1,\boldsymbol{k}}=(\varepsilon_{\boldsymbol{k},j_1}-\varepsilon_{\boldsymbol{k},j_2}+\varepsilon_{\boldsymbol{k},j_3}-\varepsilon_{\boldsymbol{k},j_4})/\hbar-(m_1-m_2+m_3-m_4)\omega$ and $\Omega_{2,\boldsymbol{k}}=\{(\varepsilon_{\boldsymbol{k},j_1}-\varepsilon_{\boldsymbol{k},j_2}-\varepsilon_{\boldsymbol{k},j_3}+\varepsilon_{\boldsymbol{k},j_4})/\hbar-(m_1-m_2-m_3+m_4)\omega\}/2-\Omega$. Note that, in the integrand, the optical frequency Ω appearers only in the relative-time component. The T dependent terms of the integrand generally give rise to the oscillatory contribution to $P(t,\Omega)$.

The absorption spectrum $W(\Omega)$ is given by the stationary value of the rate of increase of $P(\Omega,t)$ per unit time as[27]

$$W(\Omega)=\lim_{t\to\infty}P(t,\Omega)/t.\tag{55}$$

The above expression automatically eliminates the effect of transient in the short time region and the effect of oscillation in the long time region. It can be shown that $W(\Omega)$ agrees with the conventional form of the absorption spectrum in the case of equilibrium initial state.[27] In the calculation of $W(\Omega)$, the T-dependent term of the integrand of Eq. (54) dies away in $P(t,\Omega)/t$ in the limit $t\to\infty$. Therefore, only terms with $\Omega_{1,\boldsymbol{k}}=0$ make finite contribution to the stationary response. This implies the conditions $m_1-m_2+m_3-m_4=0$ and either $j_1=j_2$ and $j_3=j_4$ or $j_1=j_4$ and $j_2=j_3$ should be satisfied. Carrying out the integral of Eq. (45), and rearranging the terms, we find

$$\begin{aligned}W(\Omega)=\;&2\pi\frac{I_0}{2\varepsilon_0\hbar^2c}\sum_{\boldsymbol{k}}\sum_{n}\left|\sum_{j}\sum_{k_1}\langle\langle f_{\boldsymbol{k}},0|\phi_{\boldsymbol{k},j,k_1}\rangle\rangle\sum_{m}\langle\langle\phi_{\boldsymbol{k},j,n}|\right.\\&\left.\times M_{\nu',\boldsymbol{k},m,m}|\phi_{\boldsymbol{k},j,0}\rangle\rangle\sum_{k_2}\langle\langle\phi_{\boldsymbol{k},j,k_2}|i_{\boldsymbol{k}},0\rangle\rangle\right|^2\delta(n\hbar\omega-\hbar\Omega)\\&+2\pi\frac{I_0}{2\varepsilon_0\hbar^2c}\sum_{\boldsymbol{k}}\sum_{n}\sum_{j_1\neq j_2}\left|\sum_{k_1}\langle\langle f_{\boldsymbol{k}},0|\phi_{\boldsymbol{k},j_1,k_1}\rangle\rangle\right|^2\\&\times\left|\sum_{m}\langle\langle\phi_{\boldsymbol{k},j_1,n}|M_{\nu',\boldsymbol{k},m,m}|\phi_{\boldsymbol{k},j_2,0}\rangle\rangle\right|^2\\&\times\left|\sum_{k_2}\langle\langle\phi_{\boldsymbol{k},j_2,k_2}|i_{\boldsymbol{k}},0\rangle\rangle\right|^2\delta\!\left(\frac{\varepsilon_{\boldsymbol{k}j_1}-\varepsilon_{\boldsymbol{k}j_2}}{\hbar}+n\hbar\omega-\hbar\Omega\right).\end{aligned}\tag{56}$$

The first term corresponds to the transition within the same Floquet subbands and is called the intradressed band transition, while the second term represents the interdressed band transitions. For the sake of completeness, we show explicit forms of the matrix elements of $\tilde{H}_{\boldsymbol{k}}(t)$ in Appendix A, and the corresponding matrix elements of the Floquet Hamiltonian $H_{F\boldsymbol{k}}$ in Appendix B.

III. NUMERICAL RESULTS AND DISCUSSION

We have performed numerical calculations of the absorption spectrum for GaAs crystals in the off-resonant laser field. Since we are concerned with the behavior of absorption spectrum near the band edge region, we have adopted three upper valence bands for the initial state and lowest conduction band for the final states. In actual calculations, we have divided the Brillouin zone into 101 mesh points for one direction, namely, 101^3 mesh points for the whole Brillouin zone, and the solved the eigenvalue problem for the Floquet matrix numerically. The infinite series of the expansion by the Floquet basis set is truncated at a large number of the Floquet index. The absorption spectra are calculated by Eq. (56), and are convoluted with a Gaussian function. The induced absorption coefficients are calculated by $\alpha(\Omega)=(\hbar\Omega/I_0n_1V)W(\Omega)$ with the refractive index n_1, and the induced transmission rates are calculated by $I_{\mathrm{tr}}(\Omega)=\exp\{-\alpha(\Omega)h\}$ with the sample width h. The parameter values are chosen in conformity with those for GaAs. The energies of the orbitals and the hopping integrals are the same as those described above. The lattice constant is $a=5.653\times10^{-1}$ nm, and the intra-atomic Stark parameters are calculated with the Cowan code $\alpha_{\mathrm{Ga}}=-6.718\times10^{-2}/\sqrt{3}$ nm and $\alpha_{\mathrm{As}}=-6.201\times10^{-2}/\sqrt{3}$ nm ($1/\sqrt{3}$ originates from the angular integration). The refractive index is $n_1=3.6$. The sample width is assumed to be $h=3.5$ μm in accordance with the experiment.[6] The polarization of the pump laser field is fixed in the [111] direction in the numerical results shown in this paper. It should be noted that, because of the cubic symmetry, the pump-probe signal depends only on the relative angle between the polarization vectors of the pump and the probe light.

In Fig. 3, an example of the dressed-bands, namely, the Floquet quasi energies, near the band gap are shown for the electric field amplitude $E_0=0.5\times10^9$ V/m and the photon energy $\hbar\omega=0.28$ eV of the pump light. The other parameter values are the same as Fig. 1. The original bands are plotted by the dashed lines.

In Fig. 4(a), the differential absorption coefficient, which is the difference of absorption coefficient between those with pump light and without pump light, near the band edge, and its dependence on the pump light intensity are shown. The photon energy of the pump light is fixed at $\hbar\omega=0.14$ eV and the electric field amplitude of the pump light is $E_0=1.0\times10^8$ V/m (solid line), $E_0=0.75\times10^8$ V/m (dashed line), $E_0=0.5\times10^8$ V/m (dash-dotted line), and $E_0=0.25\times10^8$ V/m (dotted line). The polarization of the probe light is in the [111] direction. The corresponding differential transmission spectra, normalized by the transmission without pump laser, are shown in Fig. 4(b).

In Fig. 5(a), dependence of differential absorption coefficient on the photon energy of the pump laser light is shown. The electric field amplitude of the pump light is fixed at $E_0=1.0\times10^8$ V/m, and the photon energy of pump light is $\hbar\omega=0.14$ eV ($\lambda\approx9$ μm, solid line), $\hbar\omega=0.21$ eV ($\lambda\approx6$ μm, dashed line), and $\hbar\omega=0.28$ eV ($\lambda\approx4.5$ μm, dotted line). The polarization of the probe light is in the [111] direction. The corresponding differential transmission spectra,

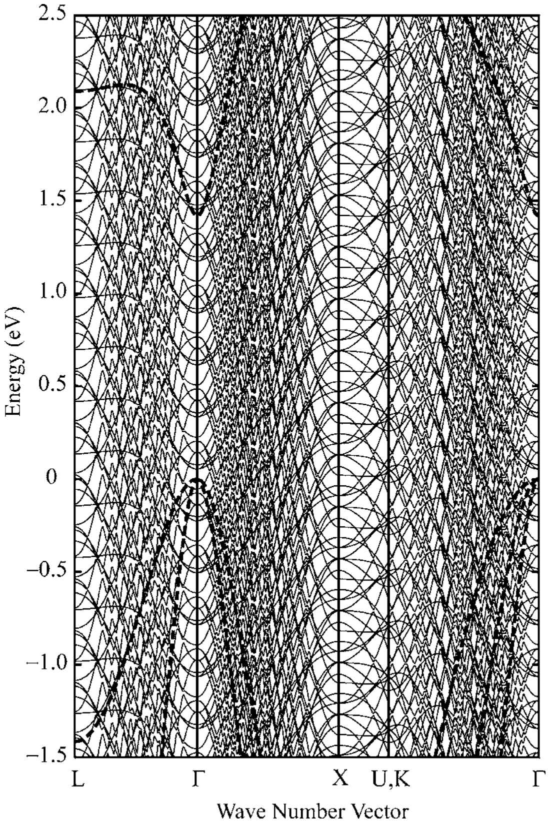

FIG. 3. Dressed bands for $E_0=0.5\times10^9$ V/m, $\hbar\omega=0.28$ eV and the polarization of the pump light in the [111] direction. The other parameter values are the same as Fig. 1. The dashed lines correspond to the original bands.

normalized by the transmission without pump laser, are shown in Fig. 5(b).

The dependence of the differential absorption coefficient on the relative angle of the polarization vector of the pump and probe laser light is shown in Fig. 6. The electric field amplitude and the photon energy of the pump light are fixed at $E_0=1.0\times10^8$ V/m and $\hbar\omega=0.14$ eV, respectively. The polarization of the probe laser light is in the direction [111] (0°, solid line), [201] (45°, dashed line), and $[1\bar{1}0]$ (90°, dotted line), respectively. Note that the effect of the modification of the band edge absorption spectrum is also observed in the right-angle configuration of the pump and the probe light, although it is most eminent in the parallel configuration.

As shown in Figs. 4–6 the applied pump laser field induced a drastic change in the transmission spectrum at the band edge. As far as the intensity of the pump laser is not extremely high, we can define the main dressed-band, which are the dressed bands that tend to the original bands in the limit of zero intensity of the applied field. Likewise, we can assign the Floquet indices (j,l) to each dressed band, where $(j,0)$ corresponds to the main dressed bands. Equation (56) tells us that the optical absorption spectrum consists of the transitions between pairs of dressed bands accompanying the change of (j,l). The dominant contribution comes from those between the main dressed bands corresponding to the band-to-band transitions of the unperturbed system. Therefore, the dramatic increase of the transmission above the band edge can be attributed to the virtual shrinkage of the width of the valence bands and the conduction bands. This can be seen more clearly in the previous results for a one-dimensional model.[21]

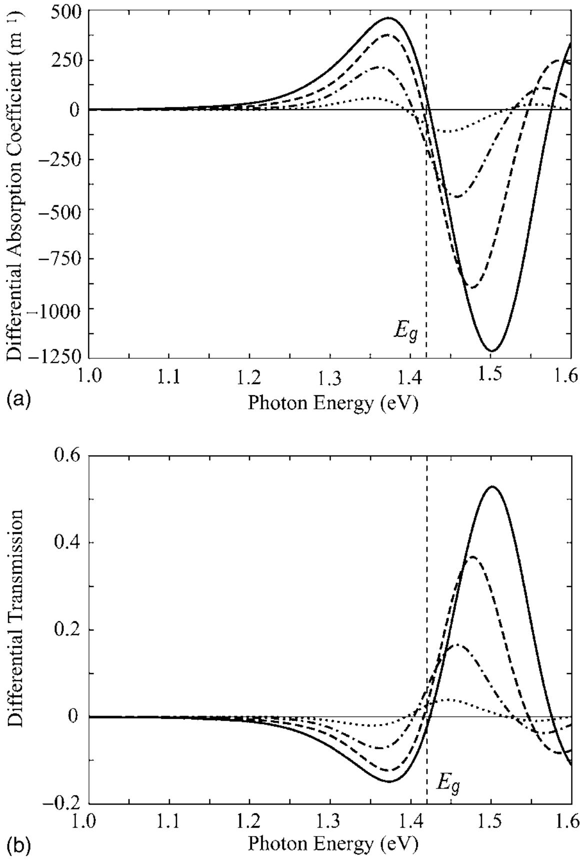

FIG. 4. (a) Dependence of the differential absorption coefficient on the intensity of the pump laser light. The energy of the pump light is $\hbar\omega=0.14$ eV with the polarization in the [111] direction. the other parameter values are the same as Fig. 1. The lines correspond to the electric amplitude of the pump laser light $E_0=1.0\times10^8$ V/m (solid line), $E_0=0.75\times10^8$ V/m (dashed line), $E_0=0.5\times10^8$ V/m (dash-dotted line), and $E_0=0.25\times10^8$ V/m (dotted line). $E_g=1.42$ corresponds to the unperturbed band gap energy. (b) Differential transmission normalized by the transmission without pump laser field. The width of the sample is 3.5 μm. The parameter values are the same as the corresponding lines of (a).

The emergence of a new absorption band below the edge is, on the other hand, due to the transitions between the dressed bands with different index l. This may be understood as the absorption of the probe photon assisted by the simultaneous absorption of the pump photons.

These field-induced modification becomes salient as the intensity of the pump laser field becomes high and/or the wave length of the pump laser becomes long, as can be seen from Figs. 4 and 5. Figures 4 and 5 should be compared with Fig. 3 in Ref. 6. The experimental features are well reproduced not only qualitatively but also quantitatively by the theory, except for the oscillatory structure in the induced absorption band. This is due to the effect of the multiple reflection of light in the sample, which is not considered in our model.

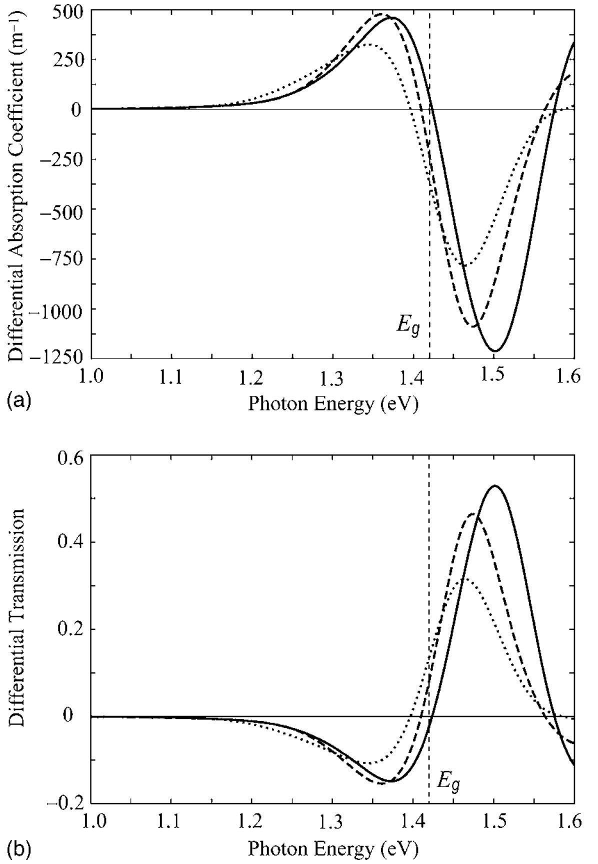

FIG. 5. (a) Dependence of the differential absorption coefficient on the photon energy of the pump laser light. The field intensity of the pump laser light is $E_0=1.0\times10^8$ V/m with the polarization in the [111] direction. The other parameter values are the same as Fig. 1. The lines correspond to the photon energy of the pump laser light $\hbar\omega=0.14$ eV ($\lambda\approx9$ μm, solid line), $\hbar\omega=0.21$ eV ($\lambda\approx6$ μm, dashed line), $\hbar\omega=0.28$ eV ($\lambda\approx4.5$ μm, dotted line). (b) Differential transmission normalized by the transmission without pump laser field. The width of the sample is 3.5 μm. The parameter values are the same as the corresponding lines of (a).

If one choose the sp^3-hybridized orbital localized on each atom for the basis functions of the band calculation, there appear terms in the Hamiltonian describing the intra-atomic hopping between these orbitals. The magnitude of the intra-atomic hopping integral is equal to $(\epsilon_{p,j}-\epsilon_{s,j})/4$ ($j=\mathrm{Ga,As}$). The origin of the shrinkage of the band widths is mainly attributed to the reduction of this hopping integral. As shown in Appendix B, the intra-atomic hopping integral in the main dressed bands is reduced by the zeroth order Bessel function with arguments proportional to $E_0/\hbar\omega$. Therefore, the magnitude of the blue shift of the absorption edge becomes large when E_0 becomes large and/or $\hbar\omega$ becomes small, as noted above.

On the other hand, the magnitudes of the off-diagonal matrix elements between the states with the difference of the Floquet index l is proportional to l-th Bessel function. Thus, the transition probability to the new absorption band below the edge increases as $E_0/\hbar\omega$ becomes large.

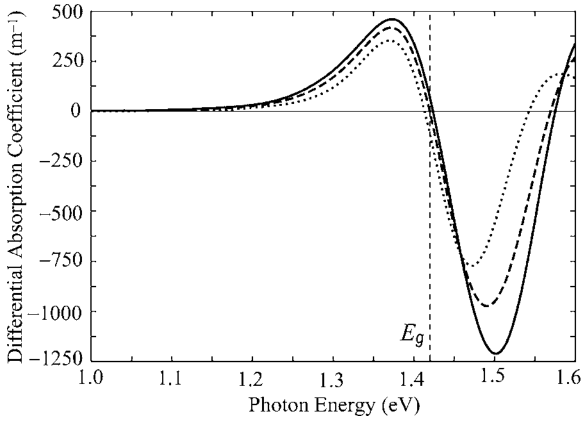

FIG. 6. Dependence of the differential absorption coefficient on the polarization of the probe laser light. The parameter values are $E_0=1.0\times10^8$ V/m, $\hbar\omega=0.14$ eV, and the polarization of the pump laser light is in the [111] direction. The other parameter values are the same as Fig. 1. The lines correspond to the polarization of probe laser light [111] (0°) (solid line), [201] (45°) (dashed line), $[1\bar{1}0]$ (90°) (dotted line).

IV. CONCLUDING REMARKS

In this work, we have presented a formalism to calculate the dressed-band structures of semiconductors in the intense off-resonant infrared laser field. We have carried out the calculation of the dressed-bands for a realistic model of band structures of GaAs crystals. Based on the tight-binding model with s and p orbitals, the quasi energies in the oscillating electric field have been obtained by applying the Bloch theory and the Floquet theory. A generating function theory of the linear absorption spectrum for the weak probe light has been formulated.

It has been shown that the irradiation of an intense off-resonant laser light results in the blueshift of the band edge and the emergence of an induced absorption below the edge, in agreement with the experimental observation, not only qualitatively but also quantitatively. These results are qualitatively in agreement with the results by Johnsen and Jauho,[17] in which a phenomenological two-band model with simple dispersion relations has been adopted for the description of the band structure. It should be noted that, in our theory, essentially all of the parameter values can be fixed by comparison with the band calculation for unperturbed system. This enables us to assess the effect of an intense electromagnetic field on the modification of optical properties of semiconductors quantitatively.

The formalism by the generating function, or the time-dependent density matrix, is essentially equivalent to that based on the nonequilibrium Green functions,[13,17] but is more appropriate for our purpose, because we need not start from the picture of two bands, a valence band and a conduction band. The use of the Floquet formalism is, on the other hand, is best suited for the dressed-band calculation. It is naturally adapted to the usual techniques of the band calculation as shown here. Furthermore, the explicit visualization of the dressed-bands will help the understanding the physical processes in the matter under an intense laser field.[21]

In Miranda's model in the nearly free electron picture, the origin of the band gap is the existence of weak scatterers distributed periodically in the free space. In an oscillating electric field, the effective scattering amplitude is reduced by a factor of zeroth order Bessel function with the argument proportional to $E_0/\hbar\omega$. It is predicted, therefore, that the application of an intense radiation field always reduces the band gap, in contradiction with the present result and the experimental observation.

We have investigated this problem by a one-dimensional *sp*-hybridized model in detail, and found that, roughly speaking, the effect of the oscillating electric field on the apparent band gap depends on the ratio of the original band gap E_g to $\hbar\omega$. When $E_g/\hbar\omega>1$, the apparent band gap energy increases, and when $E_g/\hbar\omega<1$, it decreases. The actual experimental situation in GaAs crystal belongs to the former case. Details will be presented elsewhere.[28]

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APPENDIX A

In Eq. (30), U_j is expanded as

$$\begin{aligned}U_j(t) = {}&[\cos\{g_j(t)\}-1]\sum_{l_1,l_2,l_3}(|\boldsymbol{r}_{j,l_1,l_2,l_3},s\rangle\langle\boldsymbol{r}_{j,l_1,l_2,l_3},s| \\ &+|\boldsymbol{r}_{j,l_1,l_2,l_3},p_\nu\rangle\langle\boldsymbol{r}_{j,l_1,l_2,l_3},p_\nu|) \\ &+i\sin\{g_j(t)\}\sum_{l_1,l_2,l_3}(|\boldsymbol{r}_{j,l_1,l_2,l_3},s\rangle\langle\boldsymbol{r}_{j,l_1,l_2,l_3},p_\nu| \\ &+|\boldsymbol{r}_{j,l_1,l_2,l_3},p_\nu\rangle\langle\boldsymbol{r}_{j,l_1,l_2,l_3},s|)+\sum_{l_1,l_2,l_3}I_{j,l_1,l_2,l_3},\end{aligned} \tag{A1}$$

where $g_j(t)=-(eE_0\alpha_j/\hbar\omega)\sin(\omega t)$. Then, the transformed Hamiltonian in the $\boldsymbol{k}$ picture $\widetilde{H}_{\boldsymbol{k}}(t)$ is given as

$$\langle\varphi_{\boldsymbol{k}},s|\widetilde{H}_{\boldsymbol{k}}(t)|\varphi_{\boldsymbol{k}},s\rangle=[\varepsilon_{s_1}+\sin^2\{g_1(t)\}(\varepsilon_{p_1}-\varepsilon_{s_1})], \tag{A2}$$

$$\langle\varphi_{\boldsymbol{k}},s|\widetilde{H}_{\boldsymbol{k}}(t)|\varphi_{\boldsymbol{k}},p_\eta\rangle=-i\sin\{g_1(t)\}\cos\{g_1(t)\}(\varepsilon_{p_1}-\varepsilon_{s_1})e_\eta, \tag{A3}$$

$$\langle\varphi_{\boldsymbol{k}},p_\eta|\widetilde{H}_{\boldsymbol{k}}(t)|\varphi_{\boldsymbol{k}},s\rangle=i\sin\{g_1(t)\}\cos\{g_1(t)\}(\varepsilon_{p_1}-\varepsilon_{s_1})e_\eta, \tag{A4}$$

$$\begin{aligned}\langle\varphi_{\boldsymbol{k}},p_{\eta_1}|\widetilde{H}_{\boldsymbol{k}}(t)|\varphi_{\boldsymbol{k}},p_{\eta_2}\rangle={}&-\sin^2\{g_1(t)\}(\varepsilon_{p_1}-\varepsilon_{s_1})e_{\eta_1}e_{\eta_2} \\ &+\varepsilon_{p_1}\delta_{\eta_1,\eta_2},\end{aligned} \tag{A5}$$

$$\langle\psi_{\boldsymbol{k}},s|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},s\rangle=[\varepsilon_{s_2}+\sin^2\{g_2(t)\}(\varepsilon_{p_2}-\varepsilon_{s_2})], \tag{A6}$$

$$\langle\psi_{\boldsymbol{k}},s|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},p_\eta\rangle=-i\sin\{g_2(t)\}\cos\{g_2(t)\}(\varepsilon_{p_2}-\varepsilon_{s_2})e_\eta, \tag{A7}$$

$$\langle\psi_{\boldsymbol{k}},p_\eta|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},s\rangle=\langle\psi_{\boldsymbol{k}},s|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},p_\eta\rangle^\dagger, \tag{A8}$$

$$\begin{aligned}\langle\psi_{\boldsymbol{k}},p_{\eta_1}|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},p_{\eta_2}\rangle={}&-\sin^2\{g_2(t)\}(\varepsilon_{p_2}-\varepsilon_{s_2})e_{\eta_1}e_{\eta_2} \\ &+\varepsilon_{p_2}\delta_{\eta_1,\eta_2},\end{aligned} \tag{A9}$$

$$\begin{aligned}&\langle\varphi_{\boldsymbol{k}},s|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},s\rangle \\ &\quad=\sum_d\Bigg[\cos\{g_1(t)\}\cos\{g_2(t)\}t^d_{ss} \\ &\qquad-i\sin\{g_1(t)\}\cos\{g_2(t)\}\sum_\zeta t^d_{p_\zeta s}e_\zeta \\ &\qquad+i\cos\{g_1(t)\}\sin\{g_2(t)\}\sum_\zeta t^d_{sp_\zeta}e_\zeta \\ &\qquad+\sin\{g_1(t)\}\sin\{g_2(t)\}\sum_{\zeta_1,\zeta_2}t^d_{p_{\zeta_1}p_{\zeta_2}}e_{\zeta_1}e_{\zeta_2}\Bigg]f_d(t)e^{-ik_da},\end{aligned} \tag{A10}$$

$$\begin{aligned}&\langle\varphi_{\boldsymbol{k}},s|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},p_\eta\rangle \\ &\quad=\sum_d\Bigg[i\cos\{g_1(t)\}\sin\{g_2(t)\}t^d_{ss}e_\eta \\ &\qquad+\sin\{g_1(t)\}\sin\{g_2(t)\}\sum_\zeta t^d_{p_\zeta s}e_\zeta e_\eta+\cos\{g_1(t)\} \\ &\qquad\times[\cos\{g_2(t)\}-1]\sum_\zeta t^d_{sp_\zeta}e_\zeta e_\eta-i\sin\{g_1(t)\} \\ &\qquad\times[\cos\{g_2(t)\}-1]\sum_{\zeta_1,\zeta_2}t^d_{p_{\zeta_1}p_{\zeta_2}}e_{\zeta_1}e_{\zeta_2}e_\eta+\cos\{g_1(t)\}t^d_{sp_\eta} \\ &\qquad-i\sin\{g_1(t)\}\sum_\zeta t^d_{p_\zeta p_\eta}e_\zeta\Bigg]f_d(t)e^{-ik_da},\end{aligned} \tag{A11}$$

$$\begin{aligned}&\langle\varphi_{\boldsymbol{k}},p_\eta|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},s\rangle \\ &\quad=\sum_d\Bigg[-i\sin\{g_1(t)\}\cos\{g_2(t)\}t^d_{ss}e_\eta+[\cos\{g_1(t)\}-1] \\ &\qquad\times\cos\{g_2(t)\}\sum_\zeta t^d_{p_\zeta s}e_\zeta e_\eta+\sin\{g_1(t)\}\sin\{g_2(t)\} \\ &\qquad\times\sum_\zeta t^d_{sp_\zeta}e_\zeta e_\eta+i[\cos\{g_1(t)\}-1]\sin\{g_2(t)\} \\ &\qquad\times\sum_{\zeta_1,\zeta_2}t^d_{p_{\zeta_1}p_{\zeta_2}}e_{\zeta_1}e_{\zeta_2}e_\eta+\cos\{g_2(t)\}t^d_{p_\eta s} \\ &\qquad+i\sin\{g_2(t)\}\sum_\zeta t^d_{p_\eta p_\zeta}e_\zeta\Bigg]f_d(t)e^{-ik_da},\end{aligned} \tag{A12}$$

$$\begin{aligned}\langle\varphi_{\boldsymbol{k}},p_{\eta_1}|\widetilde{H}_{\boldsymbol{k}}(t)|\psi_{\boldsymbol{k}},p_{\eta_2}\rangle = \sum_d \Bigg[& \sin\{g_1(t)\}\sin\{g_2(t)\}t^d_{ss}e_{\eta_1}e_{\eta_2} + i[\cos\{g_1(t)\}-1]\sin\{g_2(t)\}\sum_\zeta t^d_{p_\zeta s}e_\zeta e_{\eta_1}e_{\eta_2} - i\sin\{g_1(t)\}[\cos\{g_2(t)\}-1] \\ & \times\sum_\zeta t^d_{sp_\zeta}e_\zeta e_{\eta_1}e_{\eta_2} + [\cos\{g_1(t)\}-1][\cos\{g_2(t)\}-1]\sum_{\zeta_1,\zeta_2} t^d_{p_{\zeta_1}p_{\zeta_2}}e_{\zeta_1}e_{\zeta_2}e_{\eta_1}e_{\eta_2} - i\sin\{g_1(t)\}t^d_{sp_{\eta_2}}e_{\eta_1} \\ & + [\cos\{g_1(t)\}-1]\sum_\zeta t^d_{p_\zeta p_{\eta_2}}e_\zeta e_{\eta_1} + i\sin\{g_2(t)\}t^d_{p_{\eta_1}s}e_{\eta_2} + [\cos\{g_2(t)\}-1]\sum_\zeta t^d_{p_{\eta_1}p_\zeta}e_\zeta e_{\eta_2} + t^d_{p_{\eta_1}p_{\eta_2}}\Bigg]f_d(t)e^{-ik_d a},\end{aligned} \tag{A13}$$

where $d=111,1\bar{1}\bar{1},\bar{1}1\bar{1},\bar{1}\bar{1}1$ is the index of direction and

$$k_{111} = (k_x + k_y + k_z)/4, \tag{A14}$$

$$k_{1\bar{1}\bar{1}} = (k_x - k_y - k_z)/4, \tag{A15}$$

$$k_{\bar{1}1\bar{1}} = (-k_x + k_y - k_z)/4, \tag{A16}$$

$$k_{\bar{1}\bar{1}1} = (-k_x - k_y + k_z)/4, \tag{A17}$$

and a is the lattice constant. In the above representations, η, η_1, η_2, ζ, ζ_1, and ζ_2 take x, y, or z.

APPENDIX B

The Floquet Hamiltonian is defined by

$$\langle\langle u,q|H_{F\boldsymbol{k}}|v,q-l\rangle\rangle = q\hbar\omega\delta_{u,v}\delta_{l,0} + \frac{\omega}{2\pi}\int_0^{2\pi/\omega}\langle u|\widetilde{H}_{\boldsymbol{k}}(\tau)|v\rangle e^{-il\tau}, \tag{B1}$$

where $|u\rangle$ is a time-independent state, and $|u,q\rangle\rangle$ $(-\infty<q<\infty)$ is the corresponding Floquet state. Explicitly, they are given by using lth order Bessel function $J_l(x)$ as

$$\begin{aligned}\langle\langle\varphi_{\boldsymbol{k}},s,q|H_{F\boldsymbol{k}}|\varphi_{\boldsymbol{k}},s,q-l\rangle\rangle = & -\frac{(\varepsilon_{p_1}-\varepsilon_{s_1})}{4}\{J_l(2A_1)+J_{-l}(2A_1)\} \\ & + \left\{\frac{(\varepsilon_{s_1}+\varepsilon_{p_1})}{2}+q\hbar\omega\right\}\delta_{l,0},\end{aligned} \tag{B2}$$

$$\begin{aligned}&\langle\langle\varphi_{\boldsymbol{k}},s,q|H_{F\boldsymbol{k}}|\varphi_{\boldsymbol{k}},p_\eta,q-l\rangle\rangle \\ &= -\frac{(\varepsilon_{p_1}-\varepsilon_{s_1})}{4}\{J_l(2A_1)-J_{-l}(2A_1)\}e_\eta,\end{aligned} \tag{B3}$$

$$\begin{aligned}&\langle\langle\varphi_{\boldsymbol{k}},p_\eta,q|H_{F\boldsymbol{k}}|\varphi_{\boldsymbol{k}},s,q-l\rangle\rangle \\ &= \frac{(\varepsilon_{p_1}-\varepsilon_{s_1})}{4}\{J_l(2A_1)-J_{-l}(2A_1)\}e_\eta,\end{aligned} \tag{B4}$$

$$\begin{aligned}&\langle\langle\varphi_{\boldsymbol{k}},p_{\eta_1},q|H_{F\boldsymbol{k}}|\varphi_{\boldsymbol{k}},p_{\eta_2},q-l\rangle\rangle \\ &= \frac{(\varepsilon_{p_1}-\varepsilon_{s_1})}{4}\{J_l(2A_1)+J_{-l}(2A_1)\}e_{\eta_1}e_{\eta_2} \\ &\quad + \left\{(\varepsilon_{p_1}+q\hbar\omega)\delta_{\eta_1,\eta_2}-\frac{(\varepsilon_{p_1}-\varepsilon_{s_1})}{2}e_{\eta_1}e_{\eta_2}\right\}\delta_{l,0},\end{aligned} \tag{B5}$$

$$\begin{aligned}\langle\langle\psi_{\boldsymbol{k}},s,q|H_{F\boldsymbol{k}}|\psi_{\boldsymbol{k}},s,q-l\rangle\rangle = & -\frac{(\varepsilon_{p_2}-\varepsilon_{s_2})}{4}\{J_l(2A_2)+J_{-l}(2A_2)\} \\ & + \left\{\frac{(\varepsilon_{s_2}+\varepsilon_{p_2})}{2}+q\hbar\omega\right\}\delta_{l,0},\end{aligned} \tag{B6}$$

$$\begin{aligned}&\langle\langle\psi_{\boldsymbol{k}},s,q|H_{F\boldsymbol{k}}|\psi_{\boldsymbol{k}},p_\eta,q-l\rangle\rangle \\ &= -\frac{(\varepsilon_{p_2}-\varepsilon_{s_2})}{4}\{J_l(2A_2)-J_{-l}(2A_2)\}e_\eta,\end{aligned} \tag{B7}$$

$$\begin{aligned}&\langle\langle\psi_{\boldsymbol{k}},p_\eta,q|H_{F\boldsymbol{k}}|\psi_{\boldsymbol{k}},s,q-l\rangle\rangle \\ &= \frac{(\varepsilon_{p_2}-\varepsilon_{s_2})}{4}\{J_l(2A_2)-J_{-l}(2A_2)\}e_\eta,\end{aligned} \tag{B8}$$

$$\begin{aligned}&\langle\langle\psi_{\boldsymbol{k}},p_{\eta_1},q|H_{F\boldsymbol{k}}|\psi_{\boldsymbol{k}},p_{\eta_2},q-l\rangle\rangle \\ &= \frac{(\varepsilon_{p_2}-\varepsilon_{s_2})}{4}\{J_l(2A_2)+J_{-l}(2A_2)\}e_{\eta_1}e_{\eta_2} \\ &\quad + \left\{(\varepsilon_{p_2}+q\hbar\omega)\delta_{\eta_1,\eta_2}-\frac{(\varepsilon_{p_2}-\varepsilon_{s_2})}{2}e_{\eta_1}e_{\eta_2}\right\}\delta_{l,0},\end{aligned} \tag{B9}$$

$$\begin{aligned}\langle\langle\varphi_{\boldsymbol{k}},s,q|H_{F\boldsymbol{k}}|\psi_{\boldsymbol{k}},s,q-l\rangle\rangle = \sum_d\sum_{\sigma_1,\sigma_2}\frac{1}{4}\Bigg[& J_l(B_d+\sigma_1A_1+\sigma_2A_2)t^d_{ss} - \sigma_1J_l(B_d+\sigma_1A_1+\sigma_2A_2)\sum_\zeta t^d_{p_\zeta s}e_\zeta \\ & + \sigma_2J_l(B_d+\sigma_1A_1+\sigma_2A_2)\sum_\zeta t^d_{sp_\zeta}e_\zeta - \sigma_1\sigma_2J_l(B_d+\sigma_1A_1+\sigma_2A_2)\sum_{\zeta_1,\zeta_2}t_{p_{\zeta_1}p_{\zeta_2}}e_{\zeta_1}e_{\zeta_2}\Bigg]e^{-ik_d},\end{aligned} \tag{B10}$$

$$\begin{aligned}\langle\langle\varphi_{\boldsymbol{k}},s,q|H_{F\boldsymbol{k}}|\psi_{\boldsymbol{k}},p_{\eta},q-l\rangle\rangle = \sum_{d}\sum_{\sigma_1,\sigma_2}\frac{1}{4}\Bigg[&\sigma_2 J_l(B_d+\sigma_1A_1+\sigma_2A_2)t^d_{ss}e_{\eta}+\{J_l(B_d+\sigma_1A_1+\sigma_2A_2)-J_l(B_d+\sigma_1A_1)\}\\ &\times\sum_{\zeta}t^d_{sp_{\zeta}}e_{\zeta}e_{\eta}-\sigma_1\sigma_2J_l(B_d+\sigma_1A_1+\sigma_2A_2)\sum_{\zeta}t^d_{p_{\zeta}s}e_{\zeta}e_{\eta}-\sigma_1\{J_l(B_d+\sigma_1A_1+\sigma_2A_2)\\ &-J_l(B_d+\sigma_1A_1)\}\sum_{\zeta_1,\zeta_2}t^d_{p_{\zeta_1}p_{\zeta_2}}e_{\zeta_1}e_{\zeta_2}e_{\eta}+J_l(B_d+\sigma_1A_1)t^d_{sp_{\eta}}-\sigma_1J_l(B_d+\sigma_1A_1)\sum_{\zeta}t^d_{p_{\zeta}p_{\eta}}e_{\zeta}\Bigg]e^{-ik_da},\end{aligned}\tag{B11}$$

$$\begin{aligned}\langle\langle\varphi_{\boldsymbol{k}},p_{\eta},q|H_{F\boldsymbol{k}}|\psi_{\boldsymbol{k}},s,q-l\rangle\rangle = \sum_{d}\sum_{\sigma_1,\sigma_2}\frac{1}{4}\Bigg[&-\sigma_1J_l(B_d+\sigma_1A_1+\sigma_2A_2)t^d_{\mathrm{ss}}e_{\eta}+\{J_l(B_d+\sigma_1A_1+\sigma_2A_2)-J_l(B_d+\sigma_2A_2)\}\sum_{\zeta}t^d_{p_{\zeta}s}e_{\zeta}e_{\eta}\\ &-\sigma_1\sigma_2J_l(B_d+\sigma_1A_1+\sigma_2A_2)\sum_{\zeta}t^d_{sp_{\zeta}}e_{\zeta}e_{\eta}+\sigma_2\{J_l(B_d+\sigma_1A_1+\sigma_2A_2)-J_l(B_d+\sigma_2A_2)\}\\ &\times\sum_{\zeta_1,\zeta_2}t^d_{p_{\zeta_1}p_{\zeta_2}}e_{\zeta_1}e_{\zeta_2}e_{\eta}+J_l(B_d+\sigma_2A_2)t^d_{p_{\eta}s}+\sigma_2J_l(B_d+\sigma_2A_2)\sum_{\zeta}t^d_{p_{\eta}p_{\zeta}}e_{\zeta}\Bigg]e^{-ik_da},\end{aligned}\tag{B12}$$

$$\begin{aligned}\langle\langle\varphi_{\boldsymbol{k}},p_{\eta_1},q|H_{F\boldsymbol{k}}|\psi_{\boldsymbol{k}},p_{\eta_2},q-l\rangle\rangle = \sum_{d}\sum_{\sigma_1,\sigma_2}\frac{1}{4}\Bigg[&-\sigma_1\sigma_2J_l(B_d+\sigma_1A_1+\sigma_2A_2)t^d_{ss}e_{\eta_1}e_{\eta_2}-\sigma_1\{J_l(B_d+\sigma_1A_1+\sigma_2A_2)-J_l(B_d+\sigma_1A_1)\}\\ &\times\sum_{\zeta}t^d_{sp_{\zeta}}e_{\zeta}e_{\eta_1}e_{\eta_2}+\sigma_2\{J_l(B_d+\sigma_1A_1+\sigma_2A_2)-J_l(B_d+\sigma_2A_2)\}\sum_{\zeta}t^d_{p_{\zeta}s}e_{\zeta}e_{\eta_1}e_{\eta_2}\\ &+\{J_l(B_d+\sigma_1A_1+\sigma_2A_2)-J_l(B_d+\sigma_1A_1)-J_l(B_d+\sigma_2A_2)+J_l(B_d)\}\sum_{\zeta_1,\zeta_2}t^d_{p_{\zeta_1}p_{\zeta_2}}e_{\zeta_1}e_{\zeta_2}e_{\eta_1}e_{\eta_2}\\ &-\sigma_1J_l(B_d+\sigma_1A_1)t^d_{sp_{\eta_2}}e_{\eta_1}+\{J_l(B_d+\sigma_1A_1)-J_l(B_d)\}\sum_{\zeta}t^d_{p_{\zeta}p_{\eta_2}}e_{\zeta}e_{\eta_1}+\sigma_2J_l(B_d+\sigma_2A_2)t^d_{p_{\eta_1}s}e_{\eta_2}\\ &+\{J_l(B_d+\sigma_2A_2)-J_l(B_d)\}\sum_{\zeta}t^d_{p_{\eta_1}p_{\zeta}}e_{\zeta}e_{\eta_2}+J_l(B_d)t^d_{p_{\eta_1}p_{\eta_2}}\Bigg]e^{-ik_da},\end{aligned}\tag{B13}$$

where $A_j=-\alpha_j eE_0/\hbar\omega$ and $B_{111}=-(eE_0/\hbar\omega)(e_x+e_y+e_z)a/4$, $B_{1\bar{1}\bar{1}}=-(eE_0/\hbar\omega)(e_x-e_y-e_z)a/4$, $B_{\bar{1}1\bar{1}}=-(eE_0/\hbar\omega)(-e_x+e_y-e_z)a/4$, $B_{\bar{1}\bar{1}1}=-(eE_0/\hbar\omega)(-e_x-e_y+e_z)a/4$. In the above representations, η, η_1, η_2, ζ, ζ_1, and ζ_2 take x, y, or z, and σ_1 and σ_2 take $+1$ or -1.

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