Collapse of electron band gaps in periodical structures dressed by a high-frequency field

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It is demonstrated theoretically that the strong interaction between electrons in periodical structures and a high-frequency electromagnetic field suppresses the Bragg reflection of the electrons. As a result, the band gaps in electron energy spectra of the structures (the Bragg gaps) are collapsed. This quantum phenomenon can take place in various periodical structures, including both natural crystalline solids and artificial superlattices.

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Introduction.— Advances in laser physics and microwave techniques have made possible using a strong high-frequency electromagnetic field as a tool to manipulate electronic properties of various quantum systems. Since the interaction between electrons and the strong field cannot be described within the conventional perturbation theory, the system “electron + field” should be considered as a whole. Such a bound electron-field object, which is known as an “electron dressed by field” (dressed electron), became commonly used model in modern physics [1, 2]. The field-induced modification of energy spectrum of dressed electrons was studied in both atomic systems [1, 2] and various condensed-matter structures, including bulk semiconductors [4–6], graphene [6–10], quantum wells [11–14], quantum rings [15–17], etc. In studies of periodical structures dressed by a high-frequency field, the research activity was focused substantially on the dynamic localization of electrons [18–21]. As to the effect of the field on electron band gaps in the structures, it still awaited for detailed study. Performing theoretical analysis of this open problem, I found that the field can collapse the gaps.

It is well-known that the band gaps are the characteristic property of electron energy spectra of all periodical structures. Physically, they arise from the Bragg reflection of electron waves, which was discovered at the dawn of quantum mechanics (Nobel prize, 1937) and determines all electronic properties of crystalline solids. It follows from the announced effect that a high-frequency field suppresses the Bragg reflection of electrons. As a consequence, periodical structures can be almost transparent for electrons strongly coupled to the field. The present Letter is devoted to the first theoretical analysis of this unexpected quantum phenomenon which has direct relation to the basic principles of condensed-matter physics.

The Schrödinger problem.— In order to simplify calculations, let us consider a homogeneous dressing electric field, \( \mathbf{E}(t) = E_0 \sin \omega t \), where \( E_0 \) is the amplitude of the field, and \( \omega \) is the frequency of the field. If an electron subjected to this dressing field is in vacuum (or, generally, in a homogeneous medium), the Hamiltonian of the dressed electron is

\[
\hat{H}_0 = \frac{1}{2m} \left[ \mathbf{p} - \frac{e}{c} \mathbf{A}(t) \right]^2,
\]

where \( \mathbf{p} \) is the operator of electron momentum, \( m \) is the electron mass, \( e \) is the electron charge, and \( \mathbf{A}(t) = (eE_0/\omega) \cos \omega t \) is the vector potential of the considered dressing field. The accurate solving of the Schrödinger equation with the Hamiltonian [1], \( i\hbar \partial \psi_k(r, t)/\partial t = \hat{H}_0 \psi_k(r, t) \), leads to the exact wave function of the dressed electron [22],

\[
\psi_k(r, t) = \exp \left[ -i \left( \frac{e k + e A_0}{\hbar} t + \frac{E_0^2 e^2}{8 m \omega^3 \hbar} \sin 2\omega t \right) - \frac{e E_0 k}{m c^2 \omega^2} \sin \omega t \right] \phi_k(r),
\]

where \( \phi_k(r) = V^{-1/2} \exp(i k r) \) is the plane electron wave, \( k \) is the electron wave vector, \( r \) is the electron radius-vector, \( V \) is the normalization volume, \( c_k = \hbar^2 k^2 / 2m \) is the energy spectrum of free electron, and \( A_0 = E_0^2 e^2 / 4 m \omega^2 \) is the field-induced shift of the zero point of energy, which will be omitted in what follows. It should be stressed that the Hamiltonian [1] with the same vector potential \( \mathbf{A}(t) \) describes a low-dimensional (two- or one-dimensional) electron system subjected to a plane linearly polarized monochromatic electromagnetic wave with the frequency \( \omega \) and the amplitude \( E_0 \), which propagates perpendicularly to the system. As a consequence, the theory developed below is directly applicable, particularly, to electrons in various nanostructures (semiconductor quantum wires, carbon nanotubes, semiconductor quantum wells, etc) irradiated by light.

Let an electron be in a periodical structure in the presence of the same dressing field \( \mathbf{A}(t) \). Then the wave function of the electron, \( \Psi(r, t) \), satisfies the Schrödinger equation

\[
i\hbar \frac{\partial \Psi(r, t)}{\partial t} = [\hat{H}_0 + U(r)] \Psi(r, t),
\]

where \( U(r) \) is the periodical potential of the structure. Since the functions [2] with different wave vectors \( k \) form
the complete function system for any time \( t \), one can seek
solution of the Schrödinger equation (3) as an expansion
\[
\Psi(r, t) = \sum_{k'} a_{k'}(t)\psi_{k'}(r, t). \tag{4}
\]

Substituting the expansion (4) into the Schrödinger equation (3), we arrive at the expression
\[
i\hbar \frac{\partial a_k(t)}{\partial t} = \sum_{k'} a_{k'}(t)e^{i(\varepsilon_{k'} - \varepsilon_k)t/\hbar} e^{i\mathbf{k}_{k' - k}\cdot \mathbf{r}} \sin \omega t U_{k' - k}, \tag{5}
\]
where \( U_k = (1/V) \int \psi(k) e^{i\mathbf{k}\cdot \mathbf{r}} d^3 \mathbf{r} \) is the Fourier transform of the potential, and \( \mathbf{j}_k = e\mathbf{E}_k \mathbf{k}/m\omega^2 \).

It follows from the conventional Floquet theory of quantum systems driven by an oscillating field \( \mathbf{E}(t) \) that the wave function (11) has the form \( \Psi(r, t) = e^{-i\varepsilon_k t / \hbar} \phi(r, t) \), where the function \( \phi(r, t) \) periodically depends on time, \( \phi(r, t) = \phi(r, t + 2\pi/\omega) \), and \( \varepsilon(k) \) is the quasi-energy of an electron. It is well-known that the quasi-energy (the energy of dressed electron) is the physical quantity which plays the same role in quantum systems driven by an oscillating field as the usual energy in stationary ones. Therefore, the present analysis of the Schrödinger problem (3) is aimed to find the energy spectrum, \( \varepsilon(k) \). It follows from the periodicity of the function \( \phi(r, t) \) that one can seek the coefficients \( a_k(t) \) in Eq. (4) as a Fourier expansion,
\[
a_k(t) = e^{i\varepsilon_k t / \hbar} \sum_{n = -\infty}^{\infty} a_n(k) e^{in\omega t}. \tag{6}
\]

Substituting the expansion (6) into the expression (5) and applying the Jacoby-Anger expansion, \( e^{i\varepsilon \sin \theta} = \sum_{n = -\infty}^{\infty} J_n(\varepsilon) e^{in\theta} \), to transform the exponent in the right side of this expression, one can seek the Schrödinger equation (5) as
\[
\sum_{n = -\infty}^{\infty} \sum_{g} \mathcal{H}_{n'n'}(g) a_{n'}(k + g) = \varepsilon(k) a_n(k), \tag{7}
\]
where
\[
\mathcal{H}_{n'n'}(g) = (\varepsilon_k + n\hbar\omega)\delta_{n,n'}\delta_{g,0} + J_{n-n'} (e\mathbf{E}_0 \mathbf{g}) \mathcal{U}_g \tag{8}
\]
is the Hamiltonian of dressed electron in the representation of wave vectors, \( J_n(z) \) is the Bessel function of the first kind, \( \mathbf{g} \) are periods of part of the reciprocal lattice of the considered periodical structure, and \( \delta_{n,n} \) is the Kronecker symbol. It should be noted that the Schrödinger equation (7) describes still exactly the initial Schrödinger problem (3). Next we will make some approximations.

In what follows, let us assume that the field frequency, \( \omega \), is high to satisfy the condition
\[
\left| \frac{\mathcal{H}_{00}(g)}{\varepsilon_k - \varepsilon_{k+g} + n\hbar\omega} \right| \ll 1 \tag{9}
\]
for \( n \neq 0 \). Physically, the condition (9) means that the field frequency lies far from resonant frequencies of the periodical structure at the considered wave vector \( \mathbf{k} \). Mathematically, this makes it possible to treat the terms \( \mathcal{H}_{n0}(g) \) in the Hamiltonian (5) as a small perturbation. Applying the conventional perturbation theory to analyze the Schrödinger equation (7) under the condition (9), we easily arrive at the estimation \( |\alpha_{n\neq0}(k)| \ll 1 \). Since \( a_n(k) \) is the quantum amplitude of the absorption (emission) of \( n \) photons by an electron, this estimation has the clear physical meaning: The considered nonresonant field can be neither absorbed nor emitted by the electron. As a consequence, the main contribution to Eq. (7) arises from the terms with \( n, n' = 0 \), which describe the elastic interaction between an electron and the field. Neglecting the small terms with \( n, n' \neq 0 \), Eq. (7) can be rewritten in the form
\[
[\varepsilon(k) - \varepsilon_{k} a_{0}(k) - \sum_{g} a_{0}(k + g)\tilde{U}_{g}] = 0, \tag{10}
\]
where
\[
\tilde{U}_{g} = J_0 \left( \frac{e\mathbf{E}_0 \mathbf{g}}{m\omega^2} \right) \mathcal{U}_g \tag{11}
\]
is the periodical potential renormalized by the high-frequency field. Within the coordinate representation, the renormalized potential (11) reads as
\[
\tilde{U}(r) = \sum_{g} J_0 \left( \frac{e\mathbf{E}_0 \mathbf{g}}{m\omega^2} \right) \mathcal{U}_g e^{i\mathbf{g}\cdot \mathbf{r}}. \tag{12}
\]
From the formal mathematical viewpoint, Eq. (10) exactly corresponds to the stationary Schrödinger problem with the potential (12),
\[
\left[ \frac{\hat{p}^2}{2m} + \tilde{U}(\mathbf{r}) \right] \psi_{\mathbf{k}}(\mathbf{r}) = \varepsilon(\mathbf{k}) \psi_{\mathbf{k}}(\mathbf{r}). \tag{13}
\]
Indeed, expanding the stationary wave function, \( \psi_{\mathbf{k}}(\mathbf{r}) \), on plane waves, \( \phi_{\mathbf{k}}(\mathbf{r}) \), and substituting this expansion, \( \psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{g}} a_{0}(k)\phi_{\mathbf{k}}(\mathbf{r}) \), into Eq. (13), we arrive at Eq. (10). Thus, the nonstationary Schrödinger problem (3) describing a periodical structure dressed by a high-frequency nonresonant field can be reduced to the conventional stationary Schrödinger problem (13) with the renormalized periodical potential (12). This makes it possible to find the energy spectrum of dressed electron in the periodical structure, \( \varepsilon(k) \), from the known energy spectrum of bare electron in the same structure, \( \varepsilon(k) \), with the formal replacement \( \mathcal{U}_g \rightarrow \tilde{U}_g \).

The Bragg problem.— The remarkable consequence of the renormalization (11)-(12) is the field-induced collapse of the electron band gaps which normally take place in electron energy spectra of periodical structures at the borders of the Brillouin zones. In order to demonstrate this effect, we will restrict the following analysis by the
simplest case of an one-dimensional periodical potential $U(x)$ with the period $d$ but the proper generalization for any periodical structure can be easily made. In the one-dimensional case, the band gaps take place at the electron wave vectors $k = g_n/2$, where $g_n = ( \pm 2 \pi n / d, 0, 0 )$ are vectors of the reciprocal lattice of the one-dimensional periodical structure, and $n = 1, 2, 3, ...$ is the number of the corresponding Brillouin zone (see Fig. 1a). Physically, the band gaps are originated in the scattering of an electron by a periodical potential between the two electron states with mutually opposite wave vectors, $k_\pm = \pm g_n/2$ (the Bragg reflection of the electron wave). Therefore, the main contribution to the band gaps (the Bragg gaps) arises from the mixing of these two states by the potential $U$. The solving of the two linear algebraic equations (14) results in the energy spectrum of dressed electrons near borders of the Brillouin zones, which is plotted in Fig. 1a. Correspondingly, the Bragg gaps in the energy spectrum (12) read as

$$\Delta \tilde{\varepsilon}_n = 2 \left| J_0 \left( \frac{\varepsilon E_0 g_n}{m \omega^2} \right) U_{g_n} \right|. \quad (16)$$

The argument of the Bessel function in Eq. (16) is the parameter describing the interaction between an electron and a dressing field. If the field is absent ($E_0 = 0$), the gaps (16) exactly coincide with the Bragg gaps in spectra of bare electrons, $\Delta \varepsilon_n = 2 \left| U_{g_n} \right|$. If the field is strong, the Bessel function leads to the oscillating behavior of the gaps (16) and can turn the gaps into zero (see Fig. 1b). Generally, the collapse of the Bragg gaps in periodical structures corresponds to the zeros of the renormalized periodical potential (11), which are defined by the condition

$$J_0 \left( \frac{\varepsilon E_0 g}{m \omega^2} \right) = 0. \quad (17)$$

Since the condition (17) does not depend on concrete form of the periodical potential, the discussed effect is of universal physical nature and can take place in various periodical structures, including both natural crystalline solids and artificial superlattices.

From the physical point of view, the collapse of the Bragg gap (17) means that a dressing field suppresses the Bragg reflection of electron waves. In order to describe this phenomenon accurately, let us assume that an electron is in the state (2) with the wave vector $k = g_n/2$ at the time $t = 0$. Then the coefficients in the electron wave function (14) are $a_k(0) = 0$. Substituting the expansion (14) into the Schrödinger equation (3) and considering the periodical potential $U(r)$ in the equation as a scattering perturbation, we obtain the expression

$$a_k(t) = -i \frac{U_{k-k'}}{\hbar} \int_0^t e^{i(\varepsilon_{k'} - \varepsilon_k)t'/\hbar} e^{i f_{k-k'} \sin \omega t'} dt'. \quad (18)$$

which describes the amplitude of electron scattering from the initial state $k = g_n/2$ to the final state $k'$ in the first order of the conventional perturbation theory. Applying the Jacoby-Anger expansion to transform the exponent in the right side of Eq. (18), we arrive from the scattering amplitude (18) to the scattering probability,

$$|a_k(t)|^2 = \frac{\left| U_{k-k'} \right|^2}{\hbar^2} \sum_{n = -\infty}^{\infty} J_n \left( f_{k-k'} \right) e^{i(\varepsilon_{k'} - \varepsilon_k + n \hbar \omega) t/2 \hbar} \times \int_{-t/2}^{t/2} e^{i(\varepsilon_{k'} - \varepsilon_k + n \hbar \omega) t'/\hbar} dt' \right|^2. \quad (19)$$

For long time $t \to \infty$, the integrals in the right side of Eq. (19) turn into the delta functions, $\delta(\varepsilon_{k'} - \varepsilon_k + n \hbar \omega)$. Therefore, the scattering probability (19) reads as

$$|a_k(t)|^2 = 4 \pi^2 \left| U_{k-k'} \right|^2 \sum_{n = -\infty}^{\infty} J_n^2 \left( f_{k-k'} \right) \times \delta^2(\varepsilon_{k'} - \varepsilon_k + n \hbar \omega). \quad (20)$$

In the considered case of nonresonant dressing field, the terms with $n \neq 0$ in Eq. (20) are turned into zero with the
delta functions. Transforming the remaining square delta function, \( \delta^2(\varepsilon_k - \varepsilon_k') \), with the conventional procedure,

\[
\delta^2(\varepsilon) = \delta(\varepsilon)\delta(0) = \frac{\delta(\varepsilon)}{2\pi\hbar} \lim_{t \to \infty} \int_{-t/2}^{t/2} e^{i\varepsilon t'\hbar} dt' = \frac{\delta(\varepsilon)t}{2\pi\hbar},
\]

the probability (21) can be rewritten as

\[
w_{k'k} = \frac{d|a_{k_0}(t)|^2}{dt} = \frac{2\pi\hbar}{|U_{g_n}|^2} \left( \frac{e^{0}\delta_{k_0}g_n}{\omega n^2} \right) \delta(\varepsilon_{k'} - \varepsilon_k). \tag{21}
\]

The nonzero delta function in Eq. (21) corresponds physically to the case of the Bragg reflection, \( k' = -k \). Therefore, Eq. (21) describes the probability of the Bragg reflection per unit time. As expected, the probability (21) turns into zero under the condition (17). This means that a periodical structure can be almost transparent for electrons in the presence of a strong high-frequency field.

**Discussion and conclusions.**— The expressions (16) and (21) are derived in the first-order (main) approximation of the Bragg problem, which corresponds to the direct Bragg scattering of electron waves between the two states, \( k_{\pm} = \pm g_n/2 \). In many periodical structures, this approximation is enough to describe electronic properties adequately. However, the suppression of the direct Bragg scattering requires to take into account the Bragg scattering through intermediate electron states. Just this indirect scattering process is responsible for the remnant Bragg gap when the first-order gap (10) is zero. In order to estimate values of the remnant gaps, let us consider a meander-like one-dimensional periodical potential with the Fourier components \( U_{g_n} = (V_0/n\pi) \sin(n\pi/2) \), which is commonly used to describe the potential relief of semiconductor superlattices [20]. Substituting the Fourier components into Eq. (11) and assuming the condition (17) to be satisfied, one can calculate the remnant band gaps, \( \delta\varepsilon_n \). In the case of typical superlattice parameters \( \Delta\varepsilon_n \sim 10 \text{ meV} \) and \( d \sim 10^{-9} \text{ m} \), the remnant gaps should be estimated as negligibly small, \( \delta\varepsilon_n/\Delta\varepsilon_n \sim 10^{-6} \). Thus, a high-frequency field can collapse the Bragg gaps effectively.

It should be noted that the Bragg reflection of electrons can be suppressed in full for the special case of harmonic periodical potential, \( U(x) = V_0 \cos(2\pi x/d) \), which can be realized, particularly, in solids with using an acoustic wave [27]. Formally, this follows from the fact that the harmonic potential has only nonzero Fourier component, \( U_{g_1} = V_0/2 \). Turning the sole renormalized Fourier component, \( \tilde{U}_{g_1} \), into zero with the condition (17), we turn the renormalized periodical potential (12) into zero as a whole. Generally, one can conclude that the renormalized periodical potential (12) can be effectively controlled by a high-frequency field. This creates physical prerequisites for the band engineering with the field.

In order to collapse the band gaps, the condition (20) should be satisfied for the electron wave vector at the border of the Brillouin zone, \( k = g/2 \). Substituting the energy spectrum (15) into the inequality (20) and keeping in mind that the unperturbed Bragg gap is \( \Delta\varepsilon \approx 2|U_{g}| \), one can rewrite the condition (10) for this wave vector in the well-behaved form, \( \Delta\varepsilon/\hbar \omega \ll 1 \). Thus, we have to satisfy both this high-frequency condition and the gap-closing condition (17). Since the condition (17) can be easily satisfied for low-frequencies \( \omega \), periodical structures with small band gaps are most appropriate from experimental viewpoint. Particularly, the narrow-gap semiconductor superlattices dressed by an infra-red irradiation seem to be most promising. Let us assume that the field frequency lies in the infra-red range, \( \hbar \omega \sim 10 \text{ meV} \), the period of the superlattice is \( d \sim 10^{-9} \text{ m} \), and the effective electron mass in the semiconductor material is \( m \sim 10^{-29} \text{ g} \). Then the condition (17) can be satisfied for a dressing field with the amplitude \( E_0 \sim 10^3 \text{ V/cm} \). Correspondingly, this relatively weak dressing field can collapse the band gaps of meV scale. It order to collapse greater band gaps, the irradiation intensity should be increased. However, the increasing of stationary irradiation can fluidize a condensed-matter periodical structure. To avoid the fluidizing, it is reasonable to use narrow pulses of irradiation which dress the periodical structure and narrow pulses of a weak probing field which detect collapsing band gaps. This pump-and-probe methodology has been elaborated long ago and is commonly used to observe various dressing-field effects — particularly, modifications of energy spectrum of dressed electrons arisen from the optical Stark effect — in semiconductor structures [4, 28, 30]. Since giant dressing fields (up to \( \text{GW/cm}^2 \)) can be applied to semiconductor structures within this approach, wide band gaps can be collapsed with the pulsing fields.

Finalizing the discussion, it should be noted that the present effect is conceptually opposite to the effect of dynamic localization [18–21]. Formally, the both effects take place in periodical structures driven by an alternating (ac) field. However, the first effect collapses the electron band gaps, \( \Delta\varepsilon \), and turns a periodical structure to be transparent for electron waves, whereas the second one collapses the allowed electron bands and leads to the localization of electron wave packets. To avoid misunderstandings, it should be stressed that these two different effects take place in the two different frequency ranges of the ac-field: The dynamic localization takes place at low frequencies of the ac-field, \( \omega \), which satisfy the condition \( \Delta\varepsilon/\hbar \omega \gg 1 [19] \), whereas the present effect takes place at high-frequencies satisfying the opposite condition \( \Delta\varepsilon/\hbar \omega \ll 1 \). Thus, the low-frequency and high-frequency ac-fields lead to the substantially different electronic phenomena in periodical structures.

Summarizing the aforesaid, one can conclude that a nonresonant electromagnetic field can collapse band gaps in electron energy spectra of periodical structures. Physically, the collapse of the band gaps is caused by the field-
induced suppression of the Bragg reflection of electron waves. Therefore, periodical structures can be almost transparent for electrons strongly coupled to the field. Since the discussed effects are of universal nature, they can take place in various periodical structures. Superlattices seem to be most promising to observe these novel quantum phenomena.

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