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Semiconductor cavity QED: Band gap induced by vacuum fluctuationsT. Espinosa-Ortega,¹ O. Kyriienko,^{1,2} O. V. Kibis,^{1,3} and I. A. Shelykh^{1,2}¹*Division of Physics and Applied Physics, Nanyang Technological University 637371, Singapore*²*Science Institute, University of Iceland, Dunhagi-3, IS-107, Reykjavik, Iceland*³*Department of Applied and Theoretical Physics, Novosibirsk State Technical University,**Karl Marx Avenue 20, 630073 Novosibirsk, Russia*

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We consider theoretically a semiconductor nanostructure embedded in one-dimensional microcavity and study the modification of its electron energy spectrum by the vacuum fluctuations of the electromagnetic field. To solve the problem, a nonperturbative diagrammatic approach based on the Green's function formalism is developed. It is shown that the interaction of the system with the vacuum fluctuations of the optical cavity opens gaps within the valence band of the semiconductor. The approach is verified for the case of large photon occupation numbers, proving the validity of the model by comparing to previous studies of the semiconductor system excited by a classical electromagnetic field. The developed theory is of general character and allows for unification of quantum and classical descriptions of the strong light-matter interaction in semiconductor structures.

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I. INTRODUCTION

The interaction between light and matter is an important part of modern physics, interesting from both a fundamental and an applied point of view. The investigation of the regime of strong light-matter coupling, where the interaction between photons and material excitations cannot be treated perturbatively, is of special interest. One of the fundamental phenomena in this domain is the dynamic (AC) Stark effect [1] associated with the stationary energy shift of electron energy levels under the influence of an electromagnetic wave and taking place in both atomic systems and solids [2–10]. Particularly, the dynamic Stark effect opens stationary band gaps in semiconductor systems, which take place in resonant points of the Brillouin zone satisfying the condition where the photon energy is equal to the energy interval between electron bands of the semiconductor. This gap can manifest itself in various physical effects [8–10].

Phenomena similar to the dynamic Stark effect can take place not only for electrons interacting with strong classical electromagnetic waves, but for electrons interacting with vacuum fluctuations of the electromagnetic field as well. In the latter case, the accounting for the corrections given by quantum electrodynamics (QED) becomes crucial. Their study has begun with experimental observation and theoretical explanation of the Lamb shift [11,12] and the Casimir effect [13,14]. In the domain of cavity QED, vacuum field fluctuations were shown to induce vacuum Rabi oscillations which leads to the shift of atomic energy levels [15], the generation of correlated photonic pairs [16], and persistent currents in a quantum ring [17].

Though the dynamic Stark effect has been known longer than half a century, for solids the previous studies were either focused on the case of strong (“classical”) electromagnetic wave, where the quasiclassical description of the field is valid (see, e.g., Refs. [6,7]), or the electron interaction with photons can be treated using a perturbation theory [17,18]. As to a consistent nonperturbative quantum theory of the effect, it was unknown before. In order to fill this gap in the theory, in the given paper we develop a nonperturbative

approach which is applied to study the dynamic Stark effect in one-dimensional (1D) cavities. Conceptually, the approach is based on summation of an infinite series of Feynman diagrams describing emissions and absorptions of cavity photons [19–21]. Using the Dyson equation for renormalized electron Green's functions, we calculate the electron dispersion and reveal the appearance of photon-induced band gaps in the density of electron states. We show that our theory reconfirms previous results in the classical limit of strong electromagnetic wave [6,7] and allows for correct calculation of the vacuum-induced band gaps. Such a merging of the concepts of vacuum-induced corrections to electron energy spectra and strong light-matter coupling in microcavities opens an interdisciplinary area of research, lying in the boundary between quantum electrodynamics and condensed-matter physics.

II. MODEL

We analyze a semiconductor quantum wire embedded in the antinode of a cavity, as shown in Fig. 1. Let us consider the physically relevant case where the valence band is filled by electrons and the conduction band is initially empty. We account for a single waveguiding mode of the 1D cavity and a single subband in the conduction and valence band of the wire. These assumptions allow us to simplify the consideration and get analytical results. The generalization for the multimode case is straightforward.

Stimulated by vacuum electromagnetic fluctuations, an electron in the valence band [with energy $E_v(k)$ and wave vector k along the wire] can absorb a vacuum photon with energy ν and wave vector q , and make a transition to an empty state in the conduction band with energy $E_c(k+q)$. Consequently, it can emit the same photon and return to the initial state in the valence band. The process we described is called resonant (see the discussion of the Jaynes-Cummings model in Ref. [22]), and it makes the main contribution to the electron-photon interaction in the case of classically strong electromagnetic field [6,7,9]. However, in the case of vacuum fluctuations, we have to take into account also other—antiresonant—processes in which an electron, being

FIG. 1. (Color online) Sketch of the system. The one-dimensional cavity with a semiconductor structure embedded in the antinode. Since the cavity dimensions satisfy the condition $L \gg L_0$, the cavity photon mode is confined along the y, z axes and can propagate with the wave vector $\mathbf{q} = (q, 0, 0)$ only along the x axis. The same is assumed to be true for electrons and holes in the structure.

initially in the valence band, gets excited to the conduction band with energy $E_c(k - q)$, and simultaneously emits a vacuum photon with energy ν and wave vector q . Later the electron returns to its initial state in the valence band, with the absorption of the same photon. The aforementioned processes can take place many times, leading to hybridization of the electron and photon states that are typically referred to as electron state “dressed” by vacuum fluctuations. The antiresonant processes can play a significant role in a variety of physical situations. In particular, they lead to the transition to ultrastrong [16,23,24] and deep strong [25] coupling regimes, quantum phase transition from a normal to superradiant state in the Dicke model [26–29], dynamical Casimir effect [16,30], and others.

In what follows, we will show that these vacuum-induced interband electron transitions can lead to the intraband gap opening in the same way as the transitions induced by a classical field [6,7,9]. We specially stress that the one-dimensional geometry of the photonic cavity is crucial for the effect. Physically, this is a consequence of the van Hove singularity in the photonic density of states at the point $q = 0$. Indeed, the photonic dispersion can be estimated as $E(q) = c\hbar\sqrt{q^2 + 2\pi^2/L_0^2}$, where L_0 is the lateral size of the cavity, and thus the photonic density of states diverges as $\sim 1/q$ at $q \rightarrow 0$. As a result, vertical transitions with virtual photons become predominant, and the band gap is opened as discussed below. We have checked that the effect is absent in planar microcavities, where the photonic density of states is regular.

Formally, the accounting for all possible repetitions of resonant and antiresonant vacuum-induced transitions can be done using the Feynman diagrams which describe multiple absorptions and reemissions of vacuum photons (see Fig. 2). The process corresponding to an electron being in the conduction band dressed by the vacuum fluctuations can be represented in a diagrammatic form by the series given in Fig. 2(a). The analogous case for a dressed electron being initially in the valence band is presented in Fig. 2(b). Using the diagrammatic representation, it is possible to account for electron-photon interaction up to infinite order by solving the

FIG. 2. Dyson equations for renormalized electron Green's functions corresponding to the conduction band (a) and the valence band (b). The self-energy operators responsible for the light-induced dressing of the conduction band (c) and the valence band (d). The dashed line corresponds to a virtual cavity photon and g denotes the electron-photon coupling constant.

corresponding Dyson equation for the Green's function of the electrons dressed by electromagnetic field.

Realizing the aforementioned theoretical scheme, we restrict our consideration to the valence band, but the proper generalization for the conduction band can be easily made. Generally, a dressed electron in the valence band with energy ε and wave vector k can be described by the Dyson equation shown in Fig. 2(b), which can be written in the algebraic form as

$$G_v(\varepsilon, k) = \frac{G_v^0(\varepsilon, k)}{1 - \Sigma_v(\varepsilon, k)G_v^0(\varepsilon, k)}, \quad (1)$$

where $G_v^0(\varepsilon, k)$ is the bare Green's function for the electron in the valence band and $\Sigma_v(\varepsilon, k)$ is the self-energy operator depicted in Fig. 2(d). The self-energy accounts for interband transitions, where a photon with energy ν and wave vector q is absorbed and emitted (or conversely). It is given by

$$i\Sigma_v(\varepsilon, k) = -g^2 L \int_{\nu} \int_q \frac{d\nu dq}{(2\pi)^2} D^0(\nu, q) G_c^0(\varepsilon - \nu, k - q), \quad (2)$$

where $G_c^0(\varepsilon, k)$ is the bare conduction electron Green's function, $D^0(\nu, q)$ is the bare photon Green's function, and the integration is performed over all photon energies ν and photon wave vectors q . Here the matrix element of the operator of the electron-photon interaction, being the electron-photon coupling constant, reads $g = |d_{cv}| \sqrt{\omega_0(0)/2\epsilon\epsilon_0 S L}$ [31,32], where d_{cv} is the dipole matrix element of interband transition, $\omega_0(q)$ is the energy of the cavity photon, ϵ is the material permittivity, ϵ_0 is the vacuum permittivity, $S = L_0^2$ is the cross-section area of the cavity, and L is the cavity length. The expressions for the bare Green's functions have the form

$$D^0(\nu, q) = \frac{2\omega_0(q)}{[\nu - \omega_0(q) + i\delta][\nu + \omega_0(q) - i\delta]}, \quad (3)$$

$$G_v^0(\varepsilon, k) = [\varepsilon - E_v(k) + i\delta]^{-1}, \quad (4)$$

$$G_c^0(\varepsilon, k) = [\varepsilon - E_c(k) - i\delta]^{-1}, \quad (5)$$

where δ is the infinitesimally small shift arising from the causality principle, the electron energy spectrum for the conduction band and the valence band are $E_c(k) = \hbar^2 k^2 / 2m_e + E_g/2$ and $E_v(k) = -\hbar^2 k^2 / 2m_e - E_g/2$, the semiconductor band gap is E_g , and m_e is the effective electron mass in the semiconductor. The energy spectrum of the principal cavity photon mode, $\omega_0(q)$, is given by

$$\omega_0(q) = \frac{\hbar c}{n_0} \sqrt{q^2 + q_y^2 + q_z^2} \approx \omega_0 + \frac{\hbar^2 q^2}{2m_0}, \quad (6)$$

where n_0 is the refractive index of the medium, $q_y = q_z = \pi/L_0$ are the quantized components of the photon wave vector in the one-dimensional cavity, $\omega_0 = \hbar c \pi \sqrt{2}/n_0 L_0$ is the cavity photon rest energy, and $m_0 = \hbar n_0 \pi / \sqrt{2} L_0 c$ is the cavity photon effective mass.

It should be stressed that the dashed lines representing the photon propagators have no preferable direction (see diagrams shown in Fig. 2). This comes from the fact that the photon Green's function $D^0(v, q)$ has two poles in Eq. (3). As a consequence, it leads to the simultaneous accounting of both resonant and antiresonant processes. Evidently, the treatment of these quantum processes is impossible within conventional models based on classical (or perturbative) descriptions of electron-field interaction (see, e.g., Refs. [6,7]). Therefore, there is a substantial improvement of the discussed diagrammatic approach to describe the vacuum-induced processes in semiconductor structures as compared to other methods used before.

III. RESULTS AND DISCUSSION

The energy spectrum of emergent electron-photon quasiparticles, $\varepsilon(k)$, can be obtained by finding poles of the electron Green's function given by Eq. (1). With this goal in mind, let us calculate the self-energy operator $\Sigma_v(\varepsilon, k)$. Substituting the bare Green's functions (3) and (5) into Eq. (2) and performing the integration over the photon energy v , we find three poles located at energies $v_1 = \omega_0(q) - i\delta$, $v_2 = -\omega_0(q) + i\delta$, and $v_3 = \varepsilon - E_c(k - q) - i\delta$. The contour integration can be made over the positive half-plane, enclosing the pole v_2 . Then, using Eq. (6) and applying the residue theorem, we can write Eq. (2) as

$$\Sigma_v(\varepsilon, k) = \int_{-\infty}^{\infty} \frac{g^2 L dq}{2\pi [\omega_0(q) + \varepsilon - E_c(k - q) - i2\delta]}. \quad (7)$$

Performing the integration in Eq. (7), we arrive at the expression

$$\Sigma_v(\varepsilon, k) = \frac{\mu g^2 L}{\hbar^2 \sqrt{\alpha(\varepsilon, k)}} \frac{\alpha(\varepsilon, k)}{|\alpha(\varepsilon, k)|}, \quad (8)$$

where

$$\alpha(\varepsilon, k) = \frac{2\mu}{\hbar^2} \left[\varepsilon + \omega_0 - \frac{E_g}{2} - \frac{\hbar^2 k^2}{2m} (1 + \mu/m) \right] \quad (9)$$

and $\mu = m_0 m_e (m_e - m_0)^{-1}$. The poles of the renormalized Green's function (1) are given by

$$1 - \Sigma_v(\varepsilon, k) G_v^0(\varepsilon, k) = 0. \quad (10)$$

FIG. 3. (Color online) Gapped electron energy spectrum in a semiconductor induced by vacuum fluctuations of electromagnetic field in a one-dimensional microcavity.

Substituting Eqs. (4) and (8) into Eq. (10) and solving this equation, we can find the energy spectrum of electrons dressed by vacuum fluctuations, $\varepsilon(k)$, which is shown schematically in Fig. 3. The remarkable feature of this spectrum consists in the vacuum-induced gap $\Delta\varepsilon$, which takes place at the electron wave vector where the difference of energy between the conduction band and the valence band is equal to the energy of the photons with $q = 0$. It follows from Eq. (10) that in the physically relevant case $\mu \approx m_0$ this gap appears at the electron wave vectors $k_0 = \pm \sqrt{m_e(\omega_0 - E_g)/\hbar}$, and its value is

$$\Delta\varepsilon = \left(\frac{m_0^{1/2} g^2 L}{\sqrt{2}\hbar} \right)^{2/3}. \quad (11)$$

It should be noted that both the parameter describing the strength of electron-photon interaction in the cavity, $g^2 L = |d_{cv}|^2 \omega_0 / (2\epsilon \epsilon_0 S)$, and the gap Eq. (11) do not depend on the cavity length L and, therefore, the developed theory is consistent in the limit $L \rightarrow \infty$.

The calculation of the vacuum-induced gap (11) for various semiconductor materials is presented in Table I. It can be seen from Table I that the band gap can be macroscopically large. Therefore, the discussed gap opening can be observable in the current experiments.

As we previously mentioned, the discussed effect strongly depends on the cavity geometry. Namely, the gap opening occurs only in a one-dimensional resonator where photon cavity modes are confined along the y, z axes (see Fig. 1).

TABLE I. Vacuum-induced band gap $\Delta\varepsilon$ in different semiconductor materials and cavities.

Semiconductor	CdTe	ZnO	GaN	GaAs
L_0 (nm)	224	132	100	160
$\Delta\varepsilon$ (meV)	0.03	0.04	0.06	0.07

Physically, this follows from the singularity of the photon density of states, which takes place in one-dimensional photonic systems at the photon wave vector $q = 0$. As a result of the singularity, interband electron transitions induced by virtual photons with $q = 0$ (vertical transitions) prevail over other possible transitions. Therefore, the gap is opened at the electron wave vector k_0 , where the interband distance is equal to the energy $\omega(0)$ (see Fig. 3). On the contrary, in conventional planar (2D) photonic cavities there is no singularity in the photon density of states. Therefore, virtual photons with different wave vectors q and energies $\omega(q)$ shift different electron energy levels equivalently and the gap $\Delta\varepsilon$ is absent in this case.

In order to verify the developed diagrammatic approach, let us apply it to a semiconductor system excited by a strong laser-generated electromagnetic field. This system can be described using the methods of classical electrodynamics, and the theory of the gap opening induced by a laser has been elaborated in details [6,7,9,10]. Therefore, it is instructive to compare this well-known theory with results obtained from the discussed diagrammatic approach in the limit of large photon occupation numbers. For the sake of comparison, we will consider the physical situation where a cavity is absent and a semiconductor structure is irradiated by a strong laser beam. In contrast to the previously considered case of vacuum fluctuations, the wave vector of laser-emitted photon q_l is fixed. To account for this fact in the self-energy (2), we do not need to perform the integration over q , but account for the macroscopic population of the mode. The photon propagator under this assumption is given by the expression

$$D^0(\nu) = \frac{2N_l\omega_l}{(\nu - \omega_l + i\delta)(\nu + \omega_l - i\delta)}, \quad (12)$$

where ω_l is the energy of the laser-emitted photon and N_l is the photon occupation number of the laser mode. Substituting the propagator (12) into Eq. (2) and performing the integration over the photon energy ν , we arrive at the self-energy

$$\Sigma_v(\varepsilon, k) = \frac{g^2 N_l}{\omega_l + \varepsilon - E_c(k)}. \quad (13)$$

Solving Eq. (10) with the usage of Eq. (13), we can write the energy spectrum of electrons dressed by the laser field, ε , as

$$\varepsilon(k) = \frac{E_c(k) + E_v(k)}{2} - \frac{\omega_l}{2} + \frac{k_l - k}{2|k_l - k|} \times \sqrt{(\hbar\Omega_R)^2 + [\omega_l - E_c(k) + E_v(k)]^2}, \quad (14)$$

where $k_l = \sqrt{m_e(\omega_l - E_g)}/\hbar$, and $\Omega_R = 2g\sqrt{N_l}/\hbar$ is the Rabi frequency of interband laser-induced electron transitions. The eigenenergies (14) describe the energy spectrum of electrons in the valence band dressed by the laser field. It follows from Eq. (14) that the field-induced gaps within

the valence band, $\Delta\varepsilon = \hbar\Omega_R$, take place at electron wave vector $k_l = \pm\sqrt{m_e(\omega_l - E_g)}/\hbar$, which satisfies the condition of interband electron transitions, $E_c(k_l) - E_v(k_l) = \omega_l$. As expected, this gapped spectrum exactly coincides with the energy spectrum of dressed electrons obtained before from the classical consideration of electromagnetic field [10]. This can serve as a confirmation for the consistency of the developed theory.

Finally, it is worth discussing dissipation processes that are not accounted for in our model. The most important among them includes the finite lifetime of the cavity photons provided by nonideal structure of the cavity and the phonon scattering. The role of the phonon scattering can be reduced by lowering the temperature. The characteristic value of the gap of $50 \mu\text{eV}$ corresponds to the temperature of 0.5 K, which is freely accessible in up-to-date experiments. As to the quality of the cavity, $50 \mu\text{eV}$ corresponds to photon lifetime of about 10 ps. Modern technology allows the fabrication of planar microcavities with lifetimes of up to 100 ps [33]. By the other side, 3D cavities of very high quality allowing one to detect the vacuum Rabi splitting in individual quantum dots of the same order of magnitude were also reported in recent experiments [34]. Therefore, we believe that the predicted effect can be experimentally observed at the modern stage of technology.

IV. CONCLUSIONS

We developed a nonperturbative diagrammatic approach based on the Green's function formalism, which is applied to describe the renormalization of the electron energy spectrum of a one-dimensional system consisting of quantum wire and cavity. The van Hove singularity in the photonic density of states enables a band-gap opening in the electron energy spectrum induced by vacuum fluctuations in the cavity. The approach is verified by comparison with well-known results obtained before within classical electrodynamics in the regime of strong electromagnetic field. The elaborated theory is of general character: it allows for unification of quantum and classical descriptions of the strong light-matter interaction in various semiconductor systems.

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