Quantum Gap Solitons and Many-Polariton–Atom Bound States in Dispersive Medium and Photonic Band Gap

Valery I. Rupasov* and M. Singh
Centre for Chemical Physics and Department of Physics, University of Western Ontario, London, Ontario, Canada N6A 3K7
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A system of polaritons interacting with a two-level atom placed within a frequency dispersive medium is proven to be integrable and diagonalized exactly by the Bethe ansatz method, despite a nonlocal effective polariton-polariton coupling. Its spectrum consists of bound many-polariton complexes (quantum solitons) and exhibits unusual features due to the existence of the polaritonic gap. Only solitons containing an even number of polaritons ("even" solitons) propagate within the gap, while an "odd" soliton is pinned to the atom and forms a many-polariton–atom bound state. [S0031-9007(96)00570-4]

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In the present paper we study a quantum three-dimensional system of polaritons interacting with a two-level atom placed within a frequency dispersive medium (DM). In contrast to photonic-band-gap (PBG) materials [1], a frequency gap in a DM is caused by photon coupling to a medium excitation, e.g., an exciton, optical phonon, etc. [2]. But the model Hamiltonian under consideration [see Eq. (3)] has quite a general structure and can also be derived in the case of PBG materials. The information about the polariton spectrum is contained in the atomic form factor $z(\epsilon)$ and the integration contour C. The obtained results are valid for arbitrary $z(\epsilon)$ and C; therefore, they can also be applied to the case of PBG materials. In other words, we study here quantum electrodynamics of a two-level atom placed within a medium whose spectrum of elementary electromagnetic excitations exhibits essential deviations from the linear vacuum law in the vicinity of the atomic transition frequency.

In empty space, the standard Dicke and Bloch-Maxwell models [3] describing a photons + atoms system are integrable and diagonalized exactly [4] by means of the Bethe ansatz technique [5]. In a dispersive medium a polariton-atom coupling is *nonlocal* and leads to an effective *nonlocal* polariton-polariton coupling. Therefore, integrability of a polaritons + atom system is very questionable and requires a thorough analysis.

To diagonalize the model Hamiltonian, we introduce *auxiliary* particles and show that the many-particle scattering process is factorized into two-particle ones. The two-polariton factorization of a many-polariton scattering is *hidden* and manifested only in the limit of large interpolariton separations. Imposing the periodic boundary conditions on the many-polariton wave function, we derive the Bethe ansatz equations, which completely determine the spectrum of the system. Their "string" solutions (bound many-polariton complexes or quantum solitons) exhibit some nontrivial features due to the existence of the gap in the one-polariton spectrum. Only solitons containing an even number of polaritons ("even" solitons) propagate within the gap. A soliton with an odd number of polaritons ("odd" soliton) is pinned to the atom and forms a many-polariton–atom bound state, in which the radiation and the medium polarization are localized in the vicinity of the atom.

The Hamiltonian of the field + medium + atom system has the form

$$\begin{aligned} H = {} & \omega_{12}\left(\sigma^z + \frac{1}{2}\right) \\ & + \int d\mathbf{r}\left\{\frac{1}{8\pi}[\mathbf{E}^2(\mathbf{r}) + \mathbf{H}^2(\mathbf{r})] \right. \\ & \left. + \frac{1}{2m_0}[\mathbf{P}^2(\mathbf{r}) + m_0^2\Omega^2\mathbf{Q}^2(\mathbf{r})]\right\} \\ & + e\sqrt{n}\int d\mathbf{r}\,\mathbf{Q}(\mathbf{r})\cdot\mathbf{E}(\mathbf{r}) - \mathbf{d}\cdot\mathbf{E}(0), \end{aligned} \tag{1}$$

where the first three terms represent the Hamiltonians of the atom, the radiation, and the medium, while the fourth and fifth terms represent the medium-field and atom-field couplings, respectively. The operators $\mathbf{E}$ and $\mathbf{H}$ describe the radiation field. The operators $\mathbf{Q}(\mathbf{r})$ and $\mathbf{P}(\mathbf{r})$ are the operators of the displacement and the momentum of the medium, respectively. The medium is treated here as a continuous set of charge harmonic oscillators, each with frequency Ω, charge e, and mass m_0. Here n is the density of the number of oscillators, and $\mathbf{d} = d\mathbf{e}(\sigma^+ + \sigma^-)$ is the atomic dipole operator, where d is the matrix element of the dipole operator, $\mathbf{e}$ is the unit vector along z axis, and $\sigma^i = (\sigma^x, \sigma^y, \sigma^z)$; $\sigma^\pm = \sigma^x \pm i\sigma^y$ are the spin operators. For the sake of simplicity, we do not account here for a possible degeneration of atomic levels, and we treat the atom as a quantum two-level system [3] with the transition frequency ω_{12}.

Because of the spherical symmetry of the problem, the Hamiltonian (1) can be reduced to a one-dimensional form [4,5]. Indeed, let us choose the system of coordinates with the origin at the point of the atom's position and expand

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field and medium variables in terms of spherical harmonic vectors [6]. In the electrodipole approximation only the electrodipole harmonic of the radiation field is coupled to the atom. Therefore, omitting all the higher harmonics uncoupled to the atom, we arrive at the following one-dimensional form of the model Hamiltonian:

$$H = \omega_{12}\left(\sigma^z + \frac{1}{2}\right) + \int_0^\infty \frac{dk}{2\pi}\{kc^+(k)c(k) + \Omega b^+(k)b(k) + \sqrt{k\Delta}[c^+(k)b(k) + b^+(k)c(k)] - \sqrt{\gamma(k)}[c(k)\sigma^+ + \sigma^- c^+(k)]\}, \tag{2}$$

where $\Delta = \pi e^2 n/m_0\Omega$, $\gamma(k) = 4k^3d^2/3$, while the Bose operators $c(k)$ and $b(k)$ describe the field and medium electrodipole harmonics, respectively. The terms c^+b^+ (cb), which create (annihilate) both field and medium excitations simultaneously, as well as the analogous terms $(c^+\sigma^+$ and $c\sigma^-)$ in the atom-field coupling operator, are omitted in accordance with the Heitler-London [2] and the resonance [3] approximations.

The field-medium part of the Hamiltonian is diagonalized in terms of polariton operators $p_a(k)$ corresponding to the lower $(a = -)$ and upper $(a = +)$ polariton branches, respectively [2,7]. For our purposes, it is more convenient to introduce the energy variable ϵ, $k = \epsilon(\Omega - \epsilon)/(\Omega - \Delta - \epsilon)$, and the polariton operators $p(\epsilon)$ on the "energy scale," $p(\epsilon_a(k)) = \{[\epsilon_+(k) - \epsilon_-(k)]/[|\Omega - \Delta - \epsilon_a(k)|]\}^{1/2}p_a(k)$, where $\epsilon_\pm(k) = (1/2)[(\Omega + k) \pm \sqrt{(\Omega - k)^2 + 4k\Delta}]$ are the polariton spectra. Then, the model Hamiltonian finally takes the form

$$H = \omega_{12}\left(\sigma^z + \frac{1}{2}\right) + \int_C \frac{d\epsilon}{2\pi}\{\epsilon\, p^+(\epsilon)p(\epsilon) - \sqrt{\gamma}\, z(\epsilon)[p(\epsilon)\sigma^+ + \sigma^- p^+(\epsilon)]\}, \tag{3}$$

where the atomic form factor $z(\epsilon) = (\Omega - \epsilon)^2/[(\Omega - \Delta - \epsilon)^2 + \kappa^2]$ reflects the growth of the polariton-atom coupling and the density of polariton states near the upper edge of the lower polariton branch. The constant κ is introduced to account for relaxation processes in the medium. In accordance with the resonance approximation we extended the integration over the energy ϵ in the lower limit to $-\infty$. Because of the existence of the gap the integration contour in Eq. (3) consists of two semi-infinite intervals, $C = (-\infty, \Omega - \Delta]\bigcup[\Omega, \infty)$.

One-particle eigenstates of the model,

$$|\lambda\rangle = \left[g(\lambda)\sigma^+ + \int_C \frac{d\epsilon}{2\pi} f(\epsilon|\lambda)p^+(\epsilon)\right]|0\rangle, \tag{4}$$

are found from the Schrödinger equation

$$(\epsilon - \lambda)f(\epsilon|\lambda) - \sqrt{\gamma}\, z(\epsilon)g(\lambda) = 0,$$

$$(\lambda - \omega_{12})g(\lambda) + \sqrt{\gamma}\int_C \frac{d\epsilon}{2\pi} z(\epsilon)f(\epsilon|\lambda) = 0\,.$$

Their full spectrum consists of both the continuous spectrum with eigenenergy λ lying outside the gap, $f(\epsilon|\lambda) = 2\pi z(\lambda)\delta(\epsilon - \lambda) + \sqrt{\gamma}\, z(\epsilon)g(\lambda)/(\epsilon - \lambda - i0)$, $g(\lambda) = \sqrt{\gamma}\, z^2(\lambda)/[\omega_{12} - \lambda - \Sigma(\lambda)]$, $\Sigma(\lambda) = \gamma\int_C(d\epsilon/2\pi)z^2(\epsilon)/(\epsilon - \lambda - i0)$, and the discrete mode, $f_d(\epsilon|\Lambda) = \sqrt{\gamma}\, z(\epsilon)g_d(\Lambda)/(\epsilon - \Lambda)$, $\Sigma_d(\Lambda) = \gamma\int_C(d\epsilon/2\pi)z^2(\epsilon)/(\epsilon - \Lambda)$. The eigenenergy Λ lying within the gap is found as a root of the equation $\Lambda - \omega_{12} + \Sigma_d(\Lambda) = 0$. The value $g_d(\Lambda)$ is determined from the normalization condition $\langle\Lambda|\Lambda\rangle = 1$. The discrete mode corresponds to the polariton-atom bound state predicted in the case of PBG materials in Ref. [8]. The existence of the bound state, in which the polariton field is localized in the vicinity of the atom, leads to a significant suppression of the spontaneous emission.

For what follows it is convenient to rewrite Eq. (4) in terms of the Fourier transform of polariton operators and wave functions,

$$|\lambda\rangle = \left[g(\lambda)\sigma^+ + \int_{-\infty}^\infty d\tau\, \psi(\tau|\lambda)p^+(\tau)\right]|0\rangle,$$

$$\psi(\tau|\lambda) = \int_C \frac{d\epsilon}{2\pi} f(\epsilon|\lambda)e^{i\epsilon\tau}.$$

The polariton wave function in the auxiliary τ space $\psi(\tau)$ is not equal to the Fourier image of the function $f(\epsilon)$ due to the existence of the gap. Therefore, we introduce the auxiliary function $\phi(\epsilon|\lambda) = z^{-1}(\epsilon)f(\epsilon|\lambda)$, and represent $\psi(\tau)$ in its terms,

$$\psi(\tau|\lambda) = \int_{-\infty}^\infty dt\, u(\tau - t)\phi(t|\lambda),$$

where $u(\tau) = \int_C(d\epsilon/2\pi)z(\epsilon)\exp(i\epsilon\tau)$. In the auxiliary space, the Schrödinger equation,

$$(-i\partial_\tau - \lambda)\phi(\tau|\lambda) = \sqrt{\gamma}\, g(\lambda)\delta(\tau),$$

describes an auxiliary particle scattering on the pointlike potential. Its solution corresponding to the continuous spectrum is given by

$$\phi(\tau|\lambda) = \frac{h(\lambda) - (i/2)\mathrm{sgn}(\tau)}{h(\lambda) + i/2}e^{i\lambda\tau}, \qquad h(\lambda) = \frac{\lambda - \omega_{12} + \Sigma'(\lambda)}{\gamma z^2(\lambda)}, \tag{5}$$

where $\mathrm{sgn}(\tau) = (-1, \tau < 0; 0, \tau = 0; 1, \tau > 0)$, $\Sigma'(\lambda) = \mathrm{Re}\,\Sigma(\lambda)$.

Now we look for N-particle eigenstates in the form

$$|\Psi_N\rangle = \left[\int_{-\infty}^\infty \Psi(\tau_1, \ldots, \tau_N)\prod_{j=1}^N p^+(\tau_j)\,d\tau_j + \int_{-\infty}^\infty J(\tau_1, \ldots, \tau_{N-1})\sigma^+\prod_{j=1}^{N-1} \times p^+(\tau_j)d\tau_j\right]|0\rangle,$$

where the N-polariton wave functions are also expressed in terms of auxiliary functions,

$$\Psi(\tau_1,\ldots,\tau_N) = \int_{-\infty}^{\infty} \Phi(t_1,\ldots,t_N) \prod_j u(\tau_j - t_j)\, dt_j,$$

$$J(\tau_1,\ldots,\tau_{N-1}) = \int_{-\infty}^{\infty} G(t_1,\ldots,t_{N-1}) \prod_j u(\tau_j - t_j)\, dt_j.$$

In the two-particle case, the auxiliary functions obey the Schrödinger equation

$$(-i\partial_{\tau_1} - i\partial_{\tau_2} - E)[\Phi(\tau_1,\tau_2) + \Phi(\tau_2,\tau_1)] = \sqrt{\gamma}\,[\delta(\tau_1)G(\tau_2) + G(\tau_1)\delta(\tau_2)], \qquad (6a)$$

$$(-i\partial_\tau + \omega_{12} - E)G(\tau) = \sqrt{\gamma}\int_{-\infty}^{\infty} d\tau'\, v(\tau')\,[\Phi(\tau,\tau') + \Phi(\tau',\tau)], \qquad (6b)$$

where $v(\tau) = \int_C (d\epsilon/2\pi) z^2(\epsilon)\exp(-i\epsilon\tau)$. We look for the solution of Eqs. (6) in the form $\Phi(\tau_1,\tau_2) = A(\tau_1,\tau_2|\lambda_1,\lambda_2)\phi(\tau_1|\lambda_1)\phi(\tau_2|\lambda_2)$, where $E = \lambda_1 + \lambda_2$ is the eigenenergy. An unknown function $A(\tau_1 - \tau_2)$ depending only on the difference of the particle coordinates is introduced to describe the effective particle-particle coupling caused by the particle-atom scattering. Putting this expression into Eq. (6a), we find that $G(\tau|\lambda_1,\lambda_2) = A(\tau)\phi(\tau|\lambda_1)g(\lambda_2) + A(-\tau)g(\lambda_1)\phi(\tau|\lambda_2)$. Substituting now the expressions for Φ and G into Eq. (6b), we obtain the following equation for the function $A(\tau)$:

$$\phi(\tau|\lambda_1)g(\lambda_2)\left[-i\frac{d}{d\tau}A(\tau)\right] + \phi(\tau|\lambda_2)g(\lambda_1)\left[-i\frac{d}{d\tau}A(-\tau)\right] + \sqrt{\gamma}\,g(\lambda_1)g(\lambda_2)[A(\tau) + A(-\tau)]\delta(\tau)$$
$$+\sqrt{\gamma}\,\phi(\tau|\lambda_1)\int_{-\infty}^{\infty} d\tau'\, v(\tau')\phi(\tau'|\lambda_2)[A(\tau) - A(\tau - \tau')] + \sqrt{\gamma}\,\phi(\tau|\lambda_2)\int_{-\infty}^{\infty}$$
$$\times d\tau'\, v(\tau')\phi(\tau'|\lambda_1)[A(-\tau) - A(-\tau + \tau')] = 0\,. \qquad (7)$$

In empty space, $v(\tau) \to \delta(\tau)$, and the integral terms in Eq. (7) vanish. That immediately leads to the solution, in which the function $A(\tau)$ has only a discontinuous jump at the point $\tau = 0$ [4]. In the case of a dispersive medium, we could expect a more complicated behavior of the function $A(\tau)$, therefore, we look for a solution of Eq. (7) in the form

$$A(\tau|\lambda_1,\lambda_2) = B(\lambda_1,\lambda_2) + iC(\lambda_1,\lambda_2)\mathrm{sgn}(\tau) + D(\tau|\lambda_1,\lambda_2),$$

where $D(\tau = 0) = 0$. Equation (7) gives both the relationship between the parameters B and C,

$$C(\lambda_1,\lambda_2)[\phi(0|\lambda_1)g(\lambda_2) - \phi(0|\lambda_2)g(\lambda_1)] + \sqrt{\gamma}\,g(\lambda_1)g(\lambda_2)B(\lambda_1,\lambda_2) = 0\,, \qquad (8a)$$

and the equation for $D(\tau)$,

$$\phi(\tau|\lambda_1)g(\lambda_2)\left[-i\frac{d}{d\tau}D(\tau|\lambda_1,\lambda_2)\right] + \phi(\tau|\lambda_2)g(\lambda_1)\left[-i\frac{d}{d\tau}D(-\tau|\lambda_1,\lambda_2)\right] + \sqrt{\gamma}\,\phi(\tau|\lambda_1)\int_{-\infty}^{\infty} d\tau'\, v(\tau')\phi(\tau'|\lambda_2)$$
$$\times [D(\tau|\lambda_1,\lambda_2) - D(\tau - \tau'|\lambda_1,\lambda_2)] + \sqrt{\gamma}\,\phi(\tau|\lambda_2)\int_{-\infty}^{\infty} d\tau'\, v(\tau')\phi(\tau'|\lambda_1)[D(-\tau|\lambda_1,\lambda_2) - D(-\tau + \tau'|\lambda_1,\lambda_2)]$$
$$= -i\sqrt{\gamma}\,C(\lambda_1,\lambda_2)\int_{-\infty}^{\infty} d\tau'\, v(\tau')[\phi(\tau|\lambda_1)\phi(\tau'|\lambda_2) - \phi(\tau|\lambda_2)\phi(\tau'|\lambda_1)][\mathrm{sgn}(\tau) - \mathrm{sgn}(\tau - \tau')]. \qquad (8b)$$

The right-hand side of Eq. (8b) vanishes for any τ, and hence, $D(\tau) \equiv 0$. Indeed, if τ and τ' have the same sign, the term in the first brackets vanishes, while if they have different signs, the term in the second brackets equals zero. Choosing $B = 1$, we finally find

$$A(\tau_1,\tau_2|\lambda_1,\lambda_2) = 1 + \frac{i}{h(\lambda_1) - h(\lambda_2)}\,\mathrm{sgn}(\tau_1 - \tau_2). \qquad (9)$$

The two-particle scattering matrix, $S(\lambda_1,\lambda_2) = [h(\lambda_1) - h(\lambda_2) - i]/[h(\lambda_1) - h(\lambda_2) + i]$, is the obvious solution of the Yang-Baxter equations [5]. Hence, a many-particle scattering process of auxiliary particles is factorized into two-particle ones, and the N-particle auxiliary function has the following Bethe ansatz form:

$$\Phi(\tau_1,\ldots,\tau_N) = \prod_{j<l} A(\tau_j,\tau_l|\lambda_j,\lambda_l)\prod_{j=1}^{N}\phi(\tau_j|\lambda_j). \qquad (10)$$

The two-polariton factorization of the many-polariton scattering and the Bethe ansatz construction of the many-polariton wave function are hidden due to the nonlocal coupling in the polariton system and become visible only in the limit of large interpolariton separations.

To find the spectrum of the system we have to put the system in a finite "box" of size L and to impose the periodic boundary conditions on the polariton wave function. Then, we find the Bethe ansatz equations

$$e^{ik(\lambda_j)L}\frac{h(\lambda_j)-i/2}{h(\lambda_j)+i/2} = -\prod_{l=1}^{N}\frac{h(\lambda_j)-h(\lambda_l)-i}{h(\lambda_j)-h(\lambda_l)+i}, \quad E = \sum_{j=1}^{N}\lambda_j, \tag{11}$$

where $k(\lambda) = \lambda(\Omega - \lambda)/(\Omega - \Delta - \lambda)$ is the polariton wave vector describing the spatial behavior of the wave functions. If one of the polaritons is bound to the atom, its "rapidity" $h_d(\Lambda) = 0$.

As $L \to \infty$, Eqs. (11), apart from real solutions, admit complex ones, in which "rapidities" $h_j \equiv h(\lambda_j)$ are grouped into "strings,"

$$h_j = h_0 + \frac{i}{2}(n + 1 - 2j), \qquad j = 1, \ldots, n, \tag{12}$$

where h_0 is a common real part, and n is the order of a string. The parameters λ_j, corresponding to rapidities h_j can be found from Eq. (12) and the analytical continuation of Eq. (5) in the complex λ plane,

$$h(\lambda) = \begin{cases} [\gamma z^2(\lambda)]^{-1}[\lambda - \omega_{12} + \Sigma(\lambda) - (i\gamma/2)z^2(\lambda)], & \mathrm{Im}\ \lambda > 0, \\ [\gamma z^2(\lambda)]^{-1}[\lambda - \omega_{12} + \Sigma(\lambda) + (i\gamma/2)z^2(\lambda)], & \mathrm{Im}\ \lambda 0. \end{cases}$$

For h_j lying far from the real axis, one gets $h_j \sim (\lambda_j - \omega_{12})/\gamma$, and the parameters λ_j are also grouped into a string structure similar to Eq. (12), $\lambda_j \sim \lambda_0 + i(\gamma/2)(n + 1 - 2j)$.

Even strings ($n = 2k$) are obvious to exist for arbitrary magnitude of h_0. In an odd string ($n = 2k + 1$) one of the rapidities lies on the real axis, $h(\mu) = h_0$. Therefore, the corresponding one-particle function $\phi(\tau|\mu)$ and, hence, the many-particle function vanish for μ lying within the gap. The only exception is $\mu = \Lambda$, where Λ is the eigenenergy of the discrete one-particle mode. In this case, one can build an odd string

$$h_j = \frac{i}{2}(n + 1 - 2j), \quad n = 2k + 1, \tag{13}$$

which is pinned to the atom and can be treated as a many-polariton generalization of the polariton-atom bound state.

The generalization of the obtained results to the case of many atoms located in a small volume within a dispersive medium (the Dicke model) is given by the replacement

$$\phi(\tau|\lambda) \Rightarrow \phi_D(\tau|\lambda) = \frac{h_D(\lambda) - i(M/2)\mathrm{sgn}(\tau)}{h_D(\lambda) + iM/2}, \tag{14}$$

where $h_D(\lambda) = [\lambda - \omega_{12} + M\Sigma'(\lambda)]/\gamma z^2(\lambda)$, and M is the number of atoms. The integrability of an extended atomic system (the Bloch-Maxwell model) placed within a dispersive medium is not so obvious and requires a special study.

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*On leave from Landau Institute for Theoretical Physics and the Institute of Spectroscopy, Russian Academy of Sciences. Electronic address (internet): vrupasov@julian.uwo.ca and msingh@uwovax.uwo.ca

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