Exact analytical solution of a polariton model: Undetermined coefficient approach

G. Qin,^{1,2} K. L. Wang,¹ and Z. D. Wang^{2,3}

¹Department of Astronomy and Applied Physics, University of Science and Technology of China, Hefei, People's Republic of China

²Department of Physics, University of Hong Kong, Pokfulam Road, Hong Kong, People's Republic of China

³Department of Materials Science and Engineering, University of Science and Technology of China, Hefei, People's Republic of China

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Using a concise approach with undetermined coefficients, instead of the conventional diagonalization method, we obtain rigorously the energies and analytical wave functions of the ground state and excited states of a polariton model. The results indicate that our method is not only equivalent to the conventional one, but also has its own advantage. We also study several interesting properties of the polariton ground state.

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Polaritons [1] are collective excitations (phonons, excitons, magnons, etc.) of a crystal generated from a coherent linear interaction between a polar material mode and the electromagnetic field. Since several pieces of pioneering work published half a century ago [2-4], polaritons have been extensively studied both theoretically and experimentally for the bulk, layer, as well as interface systems. Artoni and Birman [5] developed a quantum-mechanical Hamiltonian formulation to treat the exciton polariton in the framework of quantum optics. They studied the conventional Hopfield Hamiltonian and a more general one, demonstrating that the polaritons are squeezed with respect to states of an intrinsic, nonpolaritonic, mixed photon-exciton boson. Ghoshal and Chatterjee [6,7] discussed two quantummechanical models of phonon polaritons. Their results showed that both the photon and phonon subsystems can exhibit nonclassical behaviors. In these investigations the canonical Bogoliubov transformation is used to diagonalize the definite positive Hamiltonian with the creation and annihilation operators in bilinear form [8-10], where the corresponding eigenstates are the general multimode squeezed states related to the original free states by a unitary operator [10-12].

On the other hand, Wang *et al.* [13] solved the model in Ref. [7] by a concise approach, where the wave function of the ground state is *a priori* taken as a squeezed form. The ground energy and the parameters of the squeezed form can be solved by comparing the coefficients of each independent term of both sides of the Schrödinger equation. We refer to this concise approach as the undetermined coefficient approach (UCA).

In the framework of the conventional diagonalization method (CDM), the canonical transformation between the new and old operators is first solved as the eigenvectors of the Hamiltonian matrix, and the polariton energies are just the corresponding eigenvalues. Then the polariton wave functions are derived using the theory of multimode squeezed states [5,10]. In this Brief Report, we solve a polariton model using the UCA. We first obtain the energy and wave function of the ground state, based on which we derive the canonical transformation, and consequently the energies and wave functions of the excited states. As a comparison with the results in Refs. [5–7], we also study several interesting properties of the ground state.

The polariton model has been reviewed in several textbooks, such as in Ref. [14]. When only linear effects are taken into account for the dielectric medium interacting with a photon field, the Hamiltonian of the system reads [15]

$$\hat{H} = \sum_{\mathbf{k}\alpha} \left[E_{1\mathbf{k}} \left(c_{1\mathbf{k}\alpha}^{\dagger} c_{1\mathbf{k}\alpha} + \frac{1}{2} \right) + E_{2\mathbf{k}} \left(c_{2\mathbf{k}\alpha}^{\dagger} c_{2\mathbf{k}\alpha} + \frac{1}{2} \right) \right. \\ \left. + E_{3\mathbf{k}} \left(c_{1\mathbf{k}\alpha}^{\dagger} c_{2\mathbf{k}\alpha} - c_{1\mathbf{k}\alpha} c_{2\mathbf{k}\alpha}^{\dagger} - c_{1\mathbf{k}\alpha} c_{2-\mathbf{k}\alpha}^{\dagger} \right. \\ \left. + c_{1-\mathbf{k}\alpha}^{\dagger} c_{2\mathbf{k}\alpha}^{\dagger} \right], \tag{1}$$

where $c_{1\mathbf{k}\alpha}$ ($c_{1\mathbf{k}\alpha}^{\dagger}$) is the annihilation (creation) operator for a photon with wave vector **k** and polarization α , $c_{2\mathbf{k}\alpha}$ ($c_{2\mathbf{k}\alpha}^{\dagger}$) represents the corresponding operator for a polarization quantum, and $E_{1\mathbf{k}}=\hbar ck$, $E_{2\mathbf{k}}$ $=\sqrt{\epsilon}\hbar\omega_0$, $E_{3\mathbf{k}}=i\hbar[(\epsilon-1)ck\omega_0/4\sqrt{\epsilon}]^{1/2}$, with $k=|\mathbf{k}|$, cthe light speed, \hbar the reduced Plank constant, ϵ the dielectric constant, and ω_0 the eigenfrequency of the free oscillators standing for the medium. For simplicity, we shall use the index **k** for the combination of the summation indices. Physically, the first and second terms represent the energy spectra of the free photon field and the free polarization field, respectively, and the third term describes the interaction between the two fields.

Since coupling exists only between a photon and polarization quantum with the same or opposite wave vector and the same polarization, we shall pay attention only to the polariton states with specific $\pm \mathbf{k}$. Correspondingly, the simplified Hamiltonian is

$$\hat{H} = \sum_{i=1,2} \left[E_i (c_{i+}^{\dagger} c_{i+} + c_{i-}^{\dagger} c_{i-} + 1) \right] \\ + E_3 \left[(c_{1+}^{\dagger} - c_{1-}) (c_{2-}^{\dagger} + c_{2+}) \right] \\ + (c_{1-}^{\dagger} - c_{1+}) (c_{2+}^{\dagger} + c_{2-}) \right].$$
(2)

Also, for simplicity, we here use the index + (-) to denote the index **k** (-**k**).

Assuming the polariton ground state to take the form

$$|0\rangle_{p} = N_{c} \exp[\rho_{1}c_{1+}^{\dagger}c_{1-}^{\dagger} + \rho_{2}c_{2+}^{\dagger}c_{2-}^{\dagger} + \rho_{3}(c_{1+}^{\dagger}c_{2-}^{\dagger} + c_{1-}^{\dagger}c_{2+}^{\dagger})]|0\rangle, \qquad (3)$$

where $|0\rangle$ is the vacuum state for the free photon and polarization field, and N_c is the normalization constant, we can prove that (see the Appendix)

$$|N_{c}|^{2} = (1 - |\rho_{1}|^{2} - |\rho_{3}|^{2})(1 - |\rho_{2}|^{2} - |\rho_{3}|^{2}) - |\rho_{1}\rho_{3}^{*} + \rho_{2}^{*}\rho_{3}|^{2},$$
(4)

where the ρ_i 's are constrained by the following relations:

$$2 \pm (\rho_1 - \rho_2) > 0, \quad 1 \pm (\rho_1 - \rho_2) - \rho_1 \rho_2 + \rho_3^2 > 0.$$
 (5)

Substituting Eqs. (2) and (3) into the Schrödinger equation for the ground state

$$\hat{H}|0\rangle_p = E|0\rangle_p, \qquad (6)$$

and reducing it by the identity $c_{1+}|0\rangle_p = \rho_1 c_{1-}^{\dagger}$ + $\rho_3 c_{2-}^{\dagger}|0\rangle_p$, $c_{2+}|0\rangle_p = \rho_2 c_{2-}^{\dagger} + \rho_3 c_{1-}^{\dagger}|0\rangle_p$, we obtain an expanded form of Eq. (6). Then by comparing the coefficients of the terms $|0\rangle_p$, $c_{1+}^{\dagger}c_{1-}^{\dagger}|0\rangle_p$, $c_{2+}^{\dagger}c_{2-}^{\dagger}|0\rangle_p$, and $(c_{1+}^{\dagger}c_{2-}^{\dagger} + c_{1-}^{\dagger}c_{2+}^{\dagger})|0\rangle_p$ of the two sides of this equation, we have

$$E_1 + E_2 - 2E_3\rho_3 = E, (7)$$

$$E_1 \rho_1 + E_3 \rho_3 (1 - \rho_1) = 0, \tag{8}$$

$$E_2 \rho_2 - E_3 \rho_3 (1 + \rho_2) = 0, \tag{9}$$

$$(E_1 + E_2)\rho_3 + E_3[(1 - \rho_1)(1 + \rho_2) - \rho_3^2] = 0.$$
(10)

The solutions of Eqs. (7)-(10) are

$$E = \pm \sqrt{E_1^2 + E_2^2} \pm 2\sqrt{E_1^2 E_2^2 + 4E_1 E_2 E_3^2}, \qquad (11)$$

$$\rho_1 = \frac{E_1 + E_2 - E}{E_2 - E_1 - E}, \quad \rho_2 = \frac{E_1 + E_2 - E}{E_2 - E_1 + E}, \quad \rho_3 = \frac{E_1 + E_2 - E}{2E_3}.$$
(12)

We can prove that only the largest value of E in Eq. (11) satisfies the constraint (5). As a result, the polariton ground state energy is

$$E = \sqrt{E_1^2 + E_2^2 + 2\sqrt{E_1^2 E_2^2 + 4E_1 E_2 E_3^2}},$$
 (13)

and the corresponding wave function is given by Eqs. (3) and (12).

Having obtained the wave function of the polariton ground state, we are able to find the canonical transformation from the free photon operators and polarization quantum operators to the polariton operators. The Hamiltonian in the polariton operators is a diagonalized one:

$$\hat{H} = \sum_{i=1,2} \Omega_i (g_i^{\dagger} g_i + g_{i-}^{\dagger} g_{i-} + 1), \qquad (14)$$

where Ω is the quantized energy for the upper or lower branch polariton, and $g(g^{\dagger})$ are the annihilation (creation) operators for the polariton. The indices 1 and 2 correspond to the upper and the lower branch polariton, respectively; while the indices + and - represent different combinations of the $\pm \mathbf{k}$ photons and the $\pm \mathbf{k}$ polarization quanta, which can be seen clearly from the transformation in a matrix form as

$$\begin{bmatrix} g_+ \\ g_-^* \end{bmatrix} = \begin{bmatrix} u & v \\ v^* & u^* \end{bmatrix} \begin{bmatrix} c_+ \\ c_-^* \end{bmatrix},$$
 (15)

where c_+ (c_-^{\dagger}) is short for $[c_{1+} c_{2+}]^T ([c_{1-}^{\dagger} c_{2-}^{\dagger}]^T)$, g_+ (g_-^{\dagger}) for $[g_{1-} g_{2-}]^T ([g_{1-}^{\dagger} g_{2-}^{\dagger}]^T)$. Here, both *u* and *v* are 2×2 matrices, and the indices *T* and * denote the transpose and the complex conjugate of a matrix, respectively.

From the well-known commutation rules $[g_{i+}, g_{j+}^{\dagger}] = \delta_{ij}, [g_{i+}, g_{j-}] = 0, i, j = 1, 2$, we have

$$uu^{\dagger} - vv^{\dagger} = 1, \quad uv^{T} = vu^{T}.$$
(16)

The inverse form of the transformation is then found to be

$$\begin{bmatrix} c_+\\ c_-^{\dagger} \end{bmatrix} = \begin{bmatrix} u^{\dagger} & -v^T\\ -v^{\dagger} & u^T \end{bmatrix} \begin{bmatrix} g_+\\ g_-^{\dagger} \end{bmatrix}.$$
 (17)

For the polariton ground state $|0\rangle_p$,

$$g_{1+}|0\rangle_p = g_{2+}|0\rangle_p = 0.$$
 (18)

Substituting Eqs. (3) and (15) into Eq. (18), it is found that

$$v = -u\rho, \tag{19}$$

where
$$\rho = \begin{bmatrix} \rho_1 & \rho_3 \\ \rho_3 & \rho_2 \end{bmatrix}$$
. (20)

Therefore only u is the independent matrix to be determined.

Substituting Eq. (15) into the commutation relation $[g_{i+}, \hat{H}] = \Omega_i g_{i+}$, and then comparing the coefficients of terms c_{1+} and c_{2+} as well as eliminating v by Eq. (19), we obtain the secular equation

$$\begin{bmatrix} E_1 - \rho_3 E_3 & -(1 + \rho_2) E_3 \\ (1 - \rho_1) E_3 & E_2 - \rho_3 E_3 \end{bmatrix} u^T = u^T \begin{bmatrix} \Omega_1 & 0 \\ 0 & \Omega_2 \end{bmatrix}.$$
 (21)

From Eq. (21), we find

$$\Omega_{1,2} = \left[\frac{E_1^2 + E_2^2 \pm \sqrt{(E_1^2 - E_2^2)^2 - 16E_1E_2E_3^2}}{2}\right]^{1/2}, \quad (22)$$

which is the same as the result obtained by the CDM [14]. Moreover, combining Eq. (19) and the first equation of (16), we obtain

$$u = \sqrt{\frac{-E_3^2}{\Omega_1^2 - \Omega_2^2}} \begin{bmatrix} \sqrt{\frac{E_2(\Omega_1 + E_1)}{\Omega_1(\Omega_1 - E_1)}} & i\sqrt{\frac{E_1(\Omega_1 + E_2)}{\Omega_1(\Omega_1 - E_2)}} \\ i\sqrt{\frac{E_2(\Omega_2 + E_1)}{\Omega_2(E_1 - \Omega_2)}} & \sqrt{\frac{E_1(\Omega_2 + E_2)}{\Omega_2(E_2 - \Omega_2)}} \end{bmatrix},$$
(23)

$$v = \sqrt{\frac{-E_3^2}{\Omega_1^2 - \Omega_2^2}} \begin{bmatrix} -\sqrt{\frac{E_2(\Omega_1 - E_1)}{\Omega_1(\Omega_1 + E_1)}} & i\sqrt{\frac{E_1(\Omega_1 - E_2)}{\Omega_1(\Omega_1 + E_2)}} \\ i\sqrt{\frac{E_2(E_1 - \Omega_2)}{\Omega_2(\Omega_2 + E_1)}} & -\sqrt{\frac{E_1(E_2 - \Omega_2)}{\Omega_2(\Omega_2 + E_2)}} \end{bmatrix}.$$
 (24)

It is straightforward to check that the original Hamiltonian (2) is simplified to the diagonalized form (14) if we substitute Eqs. (17), (23), and (24) into it. Furthermore, from Eqs. (14) and (22), the polariton ground energy is

$$E_p(0) = \Omega_1 + \Omega_2$$

= $\sqrt{E_1^2 + E_2^2 + 2\sqrt{E_1^2 E_2^2 + 4E_1 E_2 E_3^2}},$ (25)

recovering Eq. (13) and implying self-consistency of our method.

We also checked that all the above results can be retrieved by using the CMD, so the UCA and the CMD are actually equivalent. The advantages of our approach appear to be that, on one hand, we can obtain the energy and wave function of the ground state without the knowledge of the canonical transformation; on the other hand, the derivation of the canonical transformation is actually an eigenvalue problem of a 2×2 matrix, much simpler than the eigenvalue problem of a 4×4 matrix obtained by using the CMD (for an *n*-mode polariton system, the eigenvalue problems solved by the UCA and the CDM are connected to $n \times n$ and $2n \times 2n$ matrices, respectively).

The energy of the excited state is

$$E_p(n_{1+}, n_{2+}, n_{1-}, n_{2-})$$

= $(n_{1+} + n_{1-} + 1)\Omega_1 + (n_{2+} + n_{2-} + 1)\Omega_2$
(26)

from Eq. (14), where $n_{1\pm}$ $(n_{2\pm})$ is the quantum number of the upper (lower) branch polariton corresponding to $g_{1\pm}$ $(g_{2\pm})$. The corresponding wave function can be derived as [10]

$$\begin{aligned} |n_{1+}, n_{2+}, n_{1-}, n_{2-}\rangle_{p} \\ &= \frac{(g_{1+}^{\dagger})^{n_{1+}}}{\sqrt{n_{1+}!}} \frac{(g_{2+}^{\dagger})^{n_{2+}}}{\sqrt{n_{2+}!}} \frac{(g_{1-}^{\dagger})^{n_{1-}}}{\sqrt{n_{1-}!}} \frac{(g_{2-}^{\dagger})^{n_{2-}}}{\sqrt{n_{2-}!}} |0\rangle_{p} \\ &= \prod_{i=1,2} \frac{d^{n_{i+}+n_{i-}}}{dp_{i}^{n_{i+}} dq_{i}^{n_{i-}}} \frac{e^{p^{T}v^{*}u^{-1}q + p^{T}u^{-T}c_{+}^{\dagger} + q^{T}u^{-T}c_{-}^{\dagger}}}{\sqrt{n_{i+}!n_{i-}!}} \Big|_{p_{i}=q_{i}=0} |0\rangle_{p} . \end{aligned}$$

$$(27)$$

For example, $|0,1,0,0\rangle_p = (u^{-T}c^{\dagger}_+)_2|0\rangle_p$, and $|0,2,0,1\rangle_p$ = $(1/\sqrt{2})[(u^{-T}c^{\dagger}_+)_2^2(u^{-T}c^{\dagger}_-)_2 + 2(v^*u^{-1})_{22}(u^{-T}c^{\dagger}_+)_2]|0\rangle_p$.

Now we pay more attention to the properties of the polariton ground state. We introduce the quadrature operators [16] $X_i = (c_{i+} + c_{i-} + c_{i+}^{\dagger} + c_{i-}^{\dagger})/2\sqrt{2}$, $Y_i = (c_{i+} + c_{i-} - c_{i+}^{\dagger} - c_{i-}^{\dagger})/2\sqrt{2}i$. For the polariton ground state $|0\rangle_p$, the uncertainties of the photon coordinate and momentum quadratures are given by

$$\Delta X_1^2 = \frac{x+1}{4\sqrt{x^2 + 2x + \varepsilon}} < \frac{1}{4},$$
(28)

$$\Delta Y_1^2 = \frac{x+\varepsilon}{4\sqrt{x^2+2x+\varepsilon}} > \frac{1}{4},\tag{29}$$

where $x = ck/\omega_0$. Clearly the polariton ground state is always squeezed in the photon coordinate quadrature. In fact, it is also squeezed in the polarization quantum momentum quadrature for

$$\Delta X_2^2 = \sqrt{\varepsilon} \Delta X_1^2 > \frac{1}{4}, \quad \Delta Y_2^2 = \frac{1}{\sqrt{\varepsilon}} \Delta Y_1^2 < \frac{1}{4}.$$
(30)

Since $\Delta X_i^2 \Delta Y_i^2 > 1/16$ (*i*=1,2), it is never the minimum uncertainty state.

The uncertainty relations of the photon and polarization quantum numbers for the polariton ground state are found to be

$$\Delta N_1^2 = \frac{(\varepsilon - 1)(4x + \varepsilon - 1)}{16(x^2 + 2x + \varepsilon)} > \langle N_1 \rangle, \qquad (31)$$

$$\Delta N_2^2 = \frac{(\varepsilon - 1)x[(\varepsilon - 1)x + 4\varepsilon]}{16\varepsilon(x^2 + 2x + \varepsilon)} > \langle N_2 \rangle, \qquad (32)$$

where $\langle N_1 \rangle$ ($\langle N_2 \rangle$) is the average number of photons (polarization quanta) in the ground state,

$$\langle N_1 \rangle = \frac{2x + \varepsilon + 1}{4\sqrt{x^2 + 2x + \varepsilon}} - \frac{1}{2},\tag{33}$$

$$\langle N_2 \rangle = \frac{(\varepsilon+1)x + 2\varepsilon}{4\sqrt{\varepsilon}\sqrt{x^2 + 2x + \varepsilon}} - \frac{1}{2}.$$
 (34)

Therefore both photon and polarization quantum subsystems of the ground state exhibit super-Poissonian statistics.

All the above statistical properties are qualitatively consistent with the results presented in Refs. [5-7].

It is interesting to compare the energy of the polariton vacuum with that of the free vacuum. From Eq. (25), $E_p(0) < E_1 + E_2 = E(0)$, where E(0) is the energy of the free vacuum. Thus the energy of the polariton vacuum is always lower than that of the corresponding free vacuum, as expected, which was also discussed in Refs. [10,13]. Hence it is the polariton vacuum rather than the free vacuum that exists in the dielectric, even if there is no photon at all.

To conclude, we have rigorously derived analytical energies and wave functions of the ground state and excited states for a simple polariton model using an undetermined coefficient approach instead of the conventional diagonalization method. Our method is not only equivalent to the conventional one, but also has its own advantages in obtaining the energy and wave function of the ground state and solving the eigenvalue problem to get the canonical transformation. We proved that the polariton ground state is always squeezed in the photon coordinate quadratures and polarization quantum momentum quadratures. We also found that both the photon and polarization quantum subsystems of the ground state always exhibit super-Poissonian statistics. Finally, we indicate that the polariton vacuum is stable in the dielectric.

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APPENDIX: NORMALIZATION AND CONSTRAINT ON COEFFICIENTS OF THE POLARITON GROUND STATE

Inserting the overcompleteness relation of the coherent state

$$\prod_{i=1,2} \int \frac{d\alpha_{i+} d\alpha_{i+}^*}{2\pi i} \frac{d\alpha_{i-} d\alpha_{i-}^*}{2\pi i} |\alpha_{i+}, \alpha_{i-}\rangle \langle \alpha_{i+}, \alpha_{-i}| = 1$$
(A1)

between the bra and the ket of the normalization relation ${}_{p}\langle 0|0\rangle_{p}=1$ for the polariton ground state (3), and with the help of the relation $c_{i\pm}|\alpha_{i+},\alpha_{i-}\rangle = \alpha_{i\pm}|\alpha_{i+},\alpha_{i-}\rangle$, we have

$$|N_{c}|^{-2} = \prod_{i=1,2} \int \frac{d\alpha_{i+} d\alpha_{i+}^{*}}{2\pi i} \frac{d\alpha_{i-} d\alpha_{i-}^{*}}{2\pi i} e^{-V^{T}_{A}V/2} = |A|^{-1/2},$$
(A2)

where $V = [\alpha_{1+}^* \alpha_{2+}^* \alpha_{1-}^* \alpha_{2-}^* \alpha_{1+} \alpha_{2+} \alpha_{1-} \alpha_{2-}]^T$, and

$$A = \begin{bmatrix} I_2 & 0 & 0 & \rho \\ 0 & I_2 & \rho & 0 \\ 0 & \rho^* & I_2 & 0 \\ \rho^* & 0 & 0 & I_2 \end{bmatrix}.$$
 (A3)

Equation (A2) can be simplified to

$$|N_c|^2 = |I_2 - \rho^* \rho|.$$
 (A4)

Substituting Eq. (20) into Eq. (A4), we obtain Eq. (4).

The constraint on the coefficients stems from the convergence of the integral expression (A2), which requires all the real parts of the eigenvalues of the 8×8 matrix A to be positive. An eigenvalue λ satisfies the determinant equation $|A - \lambda| = 0$, i.e., $|(I_2 - \lambda)^2 - \rho^* \rho| = 0$, which is simplified to be

$$(1-\lambda)^{4} - (|\rho_{1}|^{2} + |\rho_{2}|^{2} + 2|\rho_{3}|^{2})(1-\lambda)^{2} + |\rho_{1}\rho_{2} - \rho_{3}^{2}|^{2} = 0$$
(A5)

by substituting Eq. (20) into it. From Eq. (12), we know that $\rho_{1,2}$ is real and ρ_3 is purely imaginary, so Eq. (A5) is reduced to

$$\lambda^{2} - [2 \pm (\rho_{1} - \rho_{2})]\lambda + 1 \pm (\rho_{1} - \rho_{2}) - \rho_{1}\rho_{2} + \rho_{3}^{2} = 0,$$
(A6)

from which the constraint (5) is necessary to ensure that the real part of λ is positive.

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