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## HAMILTONIAN APPROACH TO EXCITON-POLARITON LUMINESCENCE SPECTRUM CALCULATION

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### Abstract

The Hamiltonian approach provides a comprehensive theoretical framework for calculating exciton-polariton luminescence spectra in semiconductor microcavities. This study presents the fundamental theoretical foundations and methodological advances in applying Hamiltonian formulations to describe the optical emission properties of strongly coupled exciton-photon systems. We derive the key mathematical expressions for polariton eigenstates, analyze the spectral characteristics through master equation techniques, and demonstrate how the Hamiltonian approach enables accurate prediction of luminescence line shapes, intensities, and polarization dependencies. The theoretical framework encompasses both equilibrium and non-equilibrium polariton dynamics, providing essential tools for understanding cavity-mediated light-matter interactions in modern photonic devices. Our analysis reveals that proper treatment of the interaction Hamiltonian is crucial for capturing the rich physics of polariton emission, including coherence properties, nonlinear effects, and quantum statistical behavior.

### Introduction

Semiconductor microcavities operating in the strong coupling regime between quantum well excitons and confined photons have emerged as fascinating systems for studying fundamental light-matter interactions [1]. In these structures, the strong coupling leads to the formation of new eigenstates known as exciton-polaritons—hybrid quasi-particles that inherit properties from both their excitonic and photonic constituents [2]. The optical emission from these polariton states exhibits rich spectral features that reflect the underlying quantum mechanical nature of the light-matter hybridization.



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The theoretical description of polariton luminescence spectra requires sophisticated quantum mechanical approaches that can capture both the coherent dynamics of the strongly coupled system and the incoherent processes that lead to luminescence [3]. Among the various theoretical frameworks developed for this purpose, the Hamiltonian approach has proven to be particularly powerful, providing a systematic method for calculating emission spectra while maintaining physical transparency [4].

The Hamiltonian formulation begins with the identification of the relevant degrees of freedom in the microcavity system: the excitonic transitions in the quantum well and the confined photonic modes of the cavity [5]. The interaction between these subsystems, characterized by the vacuum Rabi coupling, leads to the formation of upper and lower polariton branches with characteristic energy dispersions. The calculation of luminescence spectra then involves determining how these polariton eigenstates decay through various dissipative channels and how their populations are established under optical excitation.

Recent advances in experimental techniques have enabled precise measurement of polariton emission spectra with high energy and angular resolution, providing detailed tests of theoretical predictions [6]. These developments have highlighted the importance of accurate theoretical modeling that can account for the complex interplay between coherent polariton dynamics and dissipative processes. The Hamiltonian approach, when combined with master equation techniques and quantum regression methods, provides a comprehensive framework for such calculations.

**Theoretical framework: basic hamiltonian description of exciton-polariton interactions.** The theoretical description of exciton-polariton systems begins with the construction of an appropriate Hamiltonian that captures the essential physics of light-matter coupling in microcavities. The total Hamiltonian can be written as [7]:

$$\hat{H} = \hat{H}_{\text{ex}} + \hat{H}_{\text{ph}} + \hat{H}_{\text{int}}$$

where  $\hat{H}_{\text{ex}}$  represents the excitonic Hamiltonian,  $\hat{H}_{\text{ph}}$  describes the confined photonic modes, and  $\hat{H}_{\text{int}}$  accounts for the exciton-photon interaction.

The excitonic Hamiltonian for a quantum well system is given by:

$$\hat{H}_{\text{ex}} = \sum_{\mathbf{k}} E_{\text{ex}}(\mathbf{k}) \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}$$

where  $E_{\text{ex}}(\mathbf{k})$  is the exciton dispersion relation, and  $\hat{b}_{\mathbf{k}}^{\dagger}$  and  $\hat{b}_{\mathbf{k}}$  are the creation and annihilation operators for excitons with in-plane wave vector  $\mathbf{k}$ .

The photonic Hamiltonian for a planar microcavity is expressed as:

$$\hat{H}_{\text{ph}} = \sum_{\mathbf{k}} E_{\text{ph}}(\mathbf{k}) \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}}$$

where  $E_{\text{ph}}(\mathbf{k}) = \hbar c \sqrt{k^2 + (m\pi/L_{\text{eff}})^2} / n_{\text{eff}}$  is the cavity photon dispersion, with  $L_{\text{eff}}$  being the effective cavity length and  $n_{\text{eff}}$  the effective refractive index.

Master Equation Approach for Luminescence Calculations The exciton-photon interaction is described by the Hamiltonian [8]:

$$\hat{H}_{\text{int}} = \sum_{\mathbf{k}} \hbar g(\mathbf{k}) (\hat{a}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + \hat{a}_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger})$$

where  $g(\mathbf{k})$  is the coupling strength. For a quantum well of width  $L_w$  embedded in a cavity, the coupling strength is given by:

$$\hbar g = \hbar \Omega_R \sqrt{\frac{\Gamma_0 L_w}{2L_{\text{eff}}}}$$

where  $\Omega_R$  is the Rabi frequency and  $\Gamma_0$  represents the radiative broadening.

In the strong coupling regime, where  $2g > |\gamma_{\text{ex}} - \gamma_{\text{ph}}|$ , the system exhibits characteristic avoided crossing behavior. The polariton eigenstates are found by diagonalizing the coupled system Hamiltonian, yielding the upper polariton (UP) and lower polariton (LP) energies:

$$E_{\text{UP/LP}}(\mathbf{k}) = \frac{E_{\text{ex}}(\mathbf{k}) + E_{\text{ph}}(\mathbf{k})}{2} \pm \frac{1}{2} \sqrt{4\hbar^2 g^2 + [E_{\text{ex}}(\mathbf{k}) - E_{\text{ph}}(\mathbf{k})]^2}$$

The polariton eigenstates can be expressed in terms of the excitonic and photonic basis states using Hopfield coefficients:

$$|\text{LP}, \mathbf{k}\rangle = X_{\mathbf{k}} |1_{\text{ex}}, 0_{\text{ph}}\rangle + C_{\mathbf{k}} |0_{\text{ex}}, 1_{\text{ph}}\rangle$$

where  $|X_{\mathbf{k}}|^2 + |C_{\mathbf{k}}|^2 = 1$ , and the Hopfield coefficients are determined by the diagonalization procedure.

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**Master equation approach for luminescence calculations.** The calculation of polariton luminescence spectra requires accounting for dissipative processes that cannot be described by the coherent Hamiltonian evolution alone. The master equation approach provides a systematic framework for including these effects [9]. The dynamics of the system density matrix  $\hat{\rho}$  is governed by the master equation:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \mathcal{L}_{\text{diss}}[\hat{\rho}]$$

where  $\mathcal{L}_{\text{diss}}[\hat{\rho}]$  represents the dissipative superoperator accounting for polariton decay, dephasing, and pumping processes.

For polariton systems, the dissipative contributions typically include:

1. Cavity photon leakage: This process is described by the Lindblad operator:

$$\mathcal{L}_{\text{ph}}[\hat{\rho}] = \sum_{\mathbf{k}} \gamma_{\text{ph}} \left( \hat{a}_{\mathbf{k}} \hat{\rho} \hat{a}_{\mathbf{k}}^{\dagger} - \frac{1}{2} \{ \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}}, \hat{\rho} \} \right)$$

2. Excitonic dephasing: Represented by:

$$\mathcal{L}_{\text{ex}}[\hat{\rho}] = \sum_{\mathbf{k}} \gamma_{\text{ex}} \left( \hat{b}_{\mathbf{k}} \hat{\rho} \hat{b}_{\mathbf{k}}^{\dagger} - \frac{1}{2} \{ \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}, \hat{\rho} \} \right)$$

3. Incoherent pumping: Modeled as:

$$\mathcal{L}_{\text{pump}}[\hat{\rho}] = \sum_{\mathbf{k}} P(\mathbf{k}) \left( \hat{b}_{\mathbf{k}}^{\dagger} \hat{\rho} \hat{b}_{\mathbf{k}} - \frac{1}{2} \{ \hat{b}_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger}, \hat{\rho} \} \right)$$

**Quantum regression theorem and spectral calculations.** The luminescence spectrum is calculated using the quantum regression theorem, which relates the two-time correlation functions of system operators to single-time expectation values [10]. The emission spectrum at frequency  $\omega$  and wave vector  $\mathbf{k}$  is given by:

$$S(\omega, \mathbf{k}) = \text{Re} \int_0^{\infty} dt e^{i\omega t} \langle \hat{a}_{\mathbf{k}}^{\dagger}(t) \hat{a}_{\mathbf{k}}(0) \rangle_{\text{ss}}$$

where the subscript "ss" denotes the steady-state expectation value.

For a system described by the master equation, the two-time correlation function satisfies:

$$\frac{d}{dt} \langle \hat{a}_{\mathbf{k}}^{\dagger}(t) \hat{a}_{\mathbf{k}}(0) \rangle = \langle \mathcal{L}^{\dagger}[\hat{a}_{\mathbf{k}}^{\dagger}](t) \hat{a}_{\mathbf{k}}(0) \rangle$$

where  $\mathcal{L}^{\dagger}$  is the adjoint of the Liouvillian superoperator.



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### **Results and analysis: polariton energy dispersion and spectral characteristics.**

The energy dispersion of polaritons exhibits the characteristic avoided crossing behavior that is the hallmark of strong coupling. The energy splitting at resonance ( $\mathbf{k} = 0$  for typical cavity geometries) gives the vacuum Rabi splitting  $\hbar\Omega_R = 2\hbar g$ . This splitting is directly observable in luminescence spectra as two distinct emission peaks corresponding to the upper and lower polariton branches.

The luminescence intensity from each polariton branch depends on the respective Hopfield coefficients. The lower polariton branch, which typically has stronger photonic character at small wave vectors, exhibits more efficient light extraction and therefore dominates the emission spectrum in this regime. Conversely, at larger wave vectors where the lower polariton acquires more excitonic character, the emission becomes less efficient due to reduced coupling to the leaky cavity modes. Temperature and excitation density effects. The Hamiltonian approach allows for systematic investigation of temperature and excitation density effects on the luminescence spectra. At low temperatures and excitation densities, the polariton populations follow Boltzmann statistics, leading to predominantly lower polariton emission. As the temperature or excitation density increases, thermal population of the upper polariton branch becomes significant, resulting in dual-peak emission spectra.

The linewidths of the emission peaks provide information about the various broadening mechanisms. Homogeneous broadening arises from the finite polariton lifetimes, while inhomogeneous broadening results from disorder in the quantum well and cavity structure. The Hamiltonian approach, combined with appropriate averaging over disorder distributions, can account for both contributions.

Nonlinear effects and polariton interactions. At high excitation densities, nonlinear effects become important due to polariton-polariton interactions. These interactions can be incorporated into the Hamiltonian formalism through additional terms:

$$\hat{H}_{nl} = \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \hat{\psi}_{\mathbf{k}+\mathbf{q}}^\dagger \hat{\psi}_{\mathbf{k}'-\mathbf{q}}^\dagger \hat{\psi}_{\mathbf{k}'} \hat{\psi}_{\mathbf{k}}$$

where  $\hat{\psi}_{\mathbf{k}}$  represents the polariton field operators and  $V_{\mathbf{k}, \mathbf{k}', \mathbf{q}}$  is the interaction matrix element.



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These nonlinear terms lead to phenomena such as polariton condensation, parametric oscillation, and the appearance of additional spectral features in the luminescence. The theoretical treatment of these effects within the Hamiltonian framework provides insights into the rich nonlinear dynamics of polariton systems.

The application of external magnetic fields provides an additional control parameter for polariton systems and introduces new spectral features [11]. In the presence of a magnetic field  $\mathbf{B} = B\hat{z}$ , the Hamiltonian acquires additional terms:

$$\hat{H}_{\text{mag}} = \sum_{\mathbf{k}} \mu_B g_{\text{eff}} B \hat{\sigma}_z \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}$$

where  $\mu_B$  is the Bohr magneton,  $g_{\text{eff}}$  is the effective g-factor, and  $\hat{\sigma}_z$  is the Pauli spin matrix.

The magnetic field lifts the spin degeneracy of the excitonic states, leading to circularly polarized polariton modes. The luminescence spectrum then exhibits additional structure with distinct peaks for each spin state. The magnetic field also modifies the oscillator strength through changes in the exciton wave function, providing another mechanism for controlling the emission properties.

**Advanced theoretical developments: Bogoliubov theory for polariton condensates.** When polariton systems undergo Bose-Einstein condensation, the Hamiltonian approach must be extended to include the macroscopic occupation of the ground state. The Bogoliubov theory provides a systematic method for treating quantum fluctuations around the condensate [12]:

$$\hat{\psi}_{\mathbf{k}} = \delta_{\mathbf{k},0} \sqrt{N_0} + u_{\mathbf{k}} \hat{a}_{\mathbf{k}} - v_{\mathbf{k}} \hat{a}_{-\mathbf{k}}^{\dagger}$$

where  $N_0$  is the condensate population, and  $u_{\mathbf{k}}$  and  $v_{\mathbf{k}}$  are the Bogoliubov coefficients.

The elementary excitations of the condensate have energies:

$$E_{\mathbf{k}}^{\text{Bog}} = \sqrt{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}} + 2gN_0)}$$

where  $\epsilon_{\mathbf{k}}$  is the single-particle dispersion and  $g$  is the interaction strength.

Non-equilibrium Green's functions. For systems far from thermal equilibrium, the non-equilibrium Green's function approach provides a powerful extension of the Hamiltonian method [13]. The retarded Green's function is defined as:

$$G_{\mathbf{k}}^R(\omega) = \langle\langle \hat{\psi}_{\mathbf{k}}; \hat{\psi}_{\mathbf{k}}^{\dagger} \rangle\rangle_{\omega}$$



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The spectral function, which is directly related to the luminescence spectrum, is given by:

$$A(\mathbf{k}, \omega) = -2\text{Im}[G_{\mathbf{k}}^R(\omega)]$$

This approach is particularly useful for treating systems with strong driving, complex dissipation mechanisms, or multiple coupled degrees of freedom.

**Computational methods and numerical implementation.** The numerical solution of the master equation for realistic polariton systems requires sophisticated computational techniques. The Hilbert space dimension grows exponentially with the number of modes considered, necessitating approximation schemes such as:

1. Truncated Fock space: Limiting the maximum occupation number for each mode
2. Mean-field approximations: Factorizing higher-order correlation functions
3. Quantum trajectory methods: Using stochastic simulations to solve the master equation
4. Matrix product state techniques: Exploiting entanglement structure for efficient computation

The choice of numerical method depends on the specific system parameters and the physical quantities of interest. For weak to moderate excitation, truncated Fock space approaches are often sufficient. For strongly driven systems or those with significant quantum correlations, more sophisticated methods may be required.

**Experimental validation, applications, and future directions.** The theoretical predictions derived from the Hamiltonian approach have been thoroughly validated through experimental measurements. Key experimental observables that are computed and compared include angle-resolved photoluminescence spectra, which provide insights into polariton dispersion and lifetime; time-resolved emission, revealing polariton dynamics and relaxation processes; polarization-resolved spectroscopy, probing spin and orbital degrees of freedom; and nonlinear optical response, testing the predictions related to polariton interactions. The overall agreement between theory and experimental data has been exceptional, reinforcing the validity of the Hamiltonian approach and increasing confidence in theoretical predictions for new systems and parameter regimes.



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The Hamiltonian approach has found applications in a variety of fields, including the optimization of cavity designs for polariton lasers to achieve efficient lasing operation; exploring polaritons as qubits or quantum memories for quantum information processing; designing systems for frequency conversion and parametric processes in nonlinear optics; investigating exotic phases and edge states in topological polaritons; and understanding the modification of chemical reactions in cavities through polariton chemistry.

Looking forward, future developments are expected to focus on employing machine learning techniques, such as neural networks, to tackle complex many-body problems; advancing multiscale modeling to bridge microscopic Hamiltonians and device-level properties; improving the treatment of environmental effects and decoherence in open quantum systems; and utilizing polaritons for quantum simulation of other quantum many-body systems.

### Conclusion

The Hamiltonian approach offers a clear and systematic framework for calculating exciton-polariton luminescence spectra, combining quantum mechanical light-matter coupling with treatments of dissipation and many-body effects. This approach allows for accurate spectral predictions across diverse system parameters and conditions.

Its strengths lie in its systematic structure, physical transparency, and flexibility to incorporate various effects, with the master equation formalism naturally handling dissipative processes. The quantum regression theorem enables the direct calculation of observable quantities such as emission spectra.

Recent computational advancements have expanded the approach's applicability to more complex systems, and the excellent agreement between theory and experiment reinforces its reliability. Moving forward, further development of this approach, alongside improvements in experimental and computational techniques, will enhance our understanding of polariton physics and foster new applications in photonics, quantum technology, and fundamental physics.



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