

Editor's Suggestion

Solutions and quantum dynamics of the quantum Rabi model with A-square terms

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Received 23 November 2024, revised 4 December 2024

Accepted for publication 4 December 2024

Published 30 January 2025



Abstract

It is well known that the A-square term must be considered in both cavity and circuit quantum electrodynamics systems, because it arises in the derivation from the minimal coupling Hamiltonian at any finite coupling strength. In this paper, we study the quantum Rabi model with A-square terms using the Bogoliubov operator approach. After a unitary transformation, the A-square terms can be eliminated, resulting in a modified quantum Rabi model with renormalized parameters. A transcendental function responsible for the exact solution is then derived. The presence of the A-square terms is found to significantly alter the energy spectrum. The dynamics are also studied using the obtained exact wave function, which is sensitive to the strength of the A-square terms at strong coupling. We believe that these results could be observed in future light–matter interaction systems in the ultra-strong and deep strong coupling regimes.

Supplementary material for this article is available [online](#)

Keywords: light–matter interaction, quantum Rabi model, A-square terms, ultra-strong strong coupling, dynamics

1. Introduction

Recent advancements in solid-state quantum platforms and quantum simulations, including superconducting circuit QED [1–3], trapped ions [4, 5], and cold atoms [6], have led to light-matter interactions reaching the ultra-strong and even deep strong coupling regimes. This progress has stimulated numerous theoretical studies on light-matter interaction models in quantum systems. Specifically, several intriguing features of the ultra-strong and deep strong coupling regimes have been explored within the quantum Rabi model (QRM) [7, 8], the anisotropic QRM [9–11], and the quantum Rabi triangle [12].

In cavity QED, Rzaeskimo *et al* argued that the A-square term, derived from the minimal coupling Hamiltonian, must be considered at any finite coupling strength in the Dicke model if

the Thomas–Reich–Kahn (TRK) sum rule for atoms is properly accounted for [13]. These A-square terms are also applicable to the QRM [8]. In the effective model of circuit QED, Nataf and Ciuti proposed that the TRK sum rule in cavity QED could be violated [14]. Viehmann *et al* questioned that even within a complete microscopic treatment, the A-square term still applies to the circuit QED [15]. These arguments revolve around the applicability of the TRK sum rule in different light-matter interaction systems [15, 16] and the controversy over whether the A-square term can be engineered in superconducting qubit circuits [17–20]. On the other hand, the validity of the two-level approximation is crucial for constructing the Dicke model in various solid-state devices. The applicability of Coulomb and electric dipole gauges, as well as different experimental schemes leading to distinct A-square terms, has also been widely

discussed in the literature (see [21–23] and references therein). So far, no consensus has been reached yet.

Since the \mathbf{A} -square term also appears in many cavity and circuit QED systems, where the QRM is commonly used to describe their physical features [8], it is of significant interest to consider the \mathbf{A} -square term in this model theoretically. In the literature, \mathbf{A} -square terms are extensively studied in the Dicke and Rabi models to explore superradiant phase transitions [8, 24–26], as they occur in the deep strong coupling regime. Prior to the phase transition, while the system remains in the ultra-strong and deep strong coupling regimes, a central issue is how the \mathbf{A} -square terms affects the energy spectrum and dynamics of the model. In this paper, we will exactly solve the QRM with arbitrary \mathbf{A} -square terms. Using these exact solutions, we will address these issues in this work.

The paper is organized as follows: in section 2, we provide a brief introduction to the QRM with the \mathbf{A} -square term. In section 3, using the Bogoliubov transformation, we exactly solve the QRM with the \mathbf{A} -square term within a derived mathematically well-defined transcendental function. We then obtain the energy spectra from the zeros of this function and explore the dynamics in section 4. Finally, we present the conclusions in section 5.

2. Model

The QRM with \mathbf{A} -square term can be described as follows

$$H = \omega a^\dagger a + \frac{\Delta}{2} \sigma_z + g(a + a^\dagger) \sigma_x + D(a + a^\dagger)^2, \quad (1)$$

where the operator a (a^\dagger) creates (annihilates) a photon of the electromagnetic mode with frequency ω , Δ is the qubit energy splitting, σ_i ($i = x, y, z$) represents the Pauli matrices, g is the coupling strength, and D is the strength of the \mathbf{A} -square term. The QRM with the \mathbf{A} -square term (1) possesses the same \mathbb{Z}_2 symmetry as the QRM, with the parity operator $P = -\sigma_z e^{i\pi a^\dagger a}$.

In this paper, we define the strength of the \mathbf{A} -square term as $D = \kappa D_0$, where κ is a nonnegative constant and $D_0 = g^2/\Delta$. For $\kappa = 1$, this corresponds to the minimum strength of the \mathbf{A} -square term as required by the TRK sum rule for the atom. In the original light-matter interaction platform, consisting of a real atom coupled to the photonic mode, the \mathbf{A} -square term originates from $(\mathbf{p} - q\mathbf{A})^2/2m$ in the minimal coupling Hamiltonian, where \mathbf{p} (electron momentum operator), q (charge), and \mathbf{A} (electromagnetic vector potential) are defined. Theoretically, this \mathbf{A} -square term is often neglected in the literature, even in the strong coupling regime, leading to extensive studies of the QRM for $\kappa = 0$. Since this \mathbf{A} -square term can be non-negligible in both cavity and circuit QEDs, its strength can be adjusted to arbitrary values to accommodate a wide range of applications.

3. Exact solutions

To facilitate the analytical study, we first eliminate the \mathbf{A} -square term by introducing the following new bosonic operators, based on the Bogoliubov transformation of the

original operators.

$$b = \mu a + \nu a^\dagger, \quad (2)$$

$$b^\dagger = \mu a^\dagger + \nu a. \quad (3)$$

To ensure the bosonic nature of the new operators, the coefficients must satisfy the constraint $\mu^2 - \nu^2 = 1$. If $D(\mu - \nu)^2 - \omega\mu\nu = 0$ holds, the original Hamiltonian can be transformed into the following form without \mathbf{A} -square terms,

$$H = \omega' b^\dagger b + \frac{\Delta}{2} \sigma_z + g'(b + b^\dagger) \sigma_x + C, \quad (4)$$

where $\omega' = (\mu + \nu)^2 \omega$, $g' = g(\mu - \nu)$, and the constant $C = \omega\nu^2 - D(\mu - \nu)^2$. For later reference, we list the two constraints on μ and ν

$$\mu = \frac{1}{\sqrt{2}} \sqrt{\left(1 + \frac{2D}{\omega}\right) / \sqrt{1 + \frac{4D}{\omega}}}, \quad (5)$$

$$\nu = \frac{\sqrt{2}D}{\omega} / \left\{ \sqrt{\left(1 + \frac{4D}{\omega}\right) (1 + 2\mu^2)} \right\}. \quad (6)$$

Since $\mu > \nu$, it follows that $g' > 0$. Finally, we obtain the modified version of the QRM with a modified cavity frequency and qubit-cavity coupling.

The exact solution to the QRM using the Bogoliubov transformation was proposed by one of the present authors and collaborators in [27]. Here we briefly outline the main steps for exact solutions for completeness on the one hand, and provide the wavefunction on the other hand. Introducing the following two Bogoliubov transformations for the operators b (b^\dagger),

$$B = b + g'/\omega', \quad B^\dagger = b^\dagger + g'/\omega', \quad (7)$$

the wavefunction can be expressed as a series expansion of the Fock space in the B -space.

$$|\Psi\rangle = \left(\begin{array}{c} \sum_{n=0}^{\infty} e_n \sqrt{n!} |n\rangle_B \\ \sum_{n=0}^{\infty} f_n \sqrt{n!} |n\rangle_B \end{array} \right), \quad (8)$$

where $|n\rangle_B$ represents the Fock state of B (B^\dagger), which can be expanded as $|n\rangle_B = \frac{(B^\dagger)^n}{\sqrt{n!}} |0\rangle_B$. The vacuum state $|0\rangle_B$ is a coherent state of b (b^\dagger) and is given by $|0\rangle_B = e^{-g^2/\omega^2(b^\dagger - b)} |0\rangle$, where $|0\rangle$ is the original vacuum state. From the Schrodinger equation $H|\Psi\rangle = E|\Psi\rangle$, one can obtain the coefficients.

$$e_m = \frac{\frac{\Delta}{2} f_m}{\omega' m + \alpha - E}, \quad (9)$$

$$f_m = \frac{-(g' + \omega'\lambda)[f_{m-1} + (m+1)f_{m+1}] + \frac{\Delta}{2} e_m}{\omega m + \beta - E}, \quad (10)$$

where $\alpha = g'^2/\omega'^2$ and $\beta = 3g'^2/\omega'^2$. So coefficient f_m can be defined recursively as

$$\Omega(m) = \frac{mf_m}{2g'} = \frac{\Omega(m-1)f_{m-1} - f_{m-2}}{\left[(\omega' m + \beta - E) - \frac{\Delta^2}{4(\omega' m - \alpha - E)} \right]}. \quad (11)$$

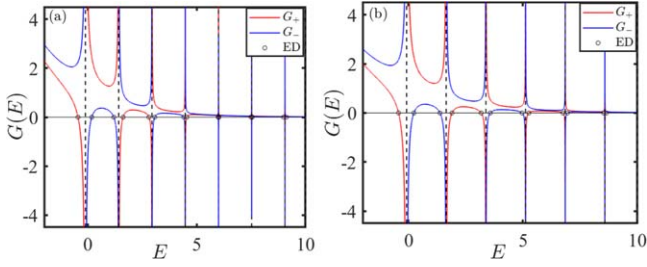


Figure 1. The curves from equation (12) for $\kappa = 1$ (a) and $\kappa = 1.5$ (b), with parameters $\Delta = 0.75$, $\omega = 1$, and $g = 0.5$. Open circles represent the eigenenergies obtained from numerical exact diagonalizations. Vertical dashed lines indicate the pole energy of the G function. Red and black lines represent the G -curves with positive and negative parity.

Utilizing the conserved parity, one can obtain a transcendental function for the QRM with \mathbf{A} -square terms [27],

$$G_{\pm}(E) = \sum_{n=0}^{\infty} f_n \left(1 \pm \frac{\Delta/2}{\omega' n - \left(\frac{g'^2}{\omega'^2} + E\right)} \right) \left(\frac{g'}{\omega'} \right)^n, \quad (12)$$

where \pm represents the positive and negative parity of the eigenfunction, respectively. The eigenvalues E of the system can be obtained from the solutions of the equation $G_{\pm}(E) = 0$. Given the energy E , the wavefunction can be obtained using equation (8). The coefficients f_n can be determined from the three-term recurrence relation, starting with $f_0 = 1$, $f_{-1} = 0$.

To visualize the solution of the equation, we plot the function $G(E)$ as a function of E in figure 1. We choose the parameters $\Delta = 0.75$, $\omega = 1$ for $\kappa = 1$ and $\kappa = 1.5$. The zeros of $G(E)$ agree perfectly with the numerical results obtained through exact diagonalization (ED).

To fully illustrate the accuracy of the G function, the low-energy spectrum obtained from equation (12) as a function of coupling strength g is shown in figure 2. We choose typical parameters $\Delta = 0.75$ and $\kappa = 1, 1.5$. Note that the parameters $\kappa \geq 1$ satisfy the TRK sum rule. It is shown that our results, obtained from the solution of equation (12), agree excellently with the numerical ED results. The coupling strength ranges from zero to deep strong coupling ($g = 2$). Since the variable D controls the \mathbf{A} -square terms, which are also influenced by the coupling strength, the energy spectrum exhibits an upward trend as the coupling strength increases. Figure 2 shows that, as the energy increases, the energy spectrum becomes denser. In the original QRM $\kappa = 0$, the energy level goes as $n - g^2$ (n is an inter) in the strong coupling regime, it is immediately evident that the presence of the \mathbf{A} -square terms drastically alters the energy spectrum.

4. Dynamics

Due to the inevitable interaction with the environment, decoherence is unavoidable in the long-time regime. Consequently, understanding the dynamical evolution prior to the loss of coherence is critical for elucidating various physical properties. In this section, we investigate the early-time

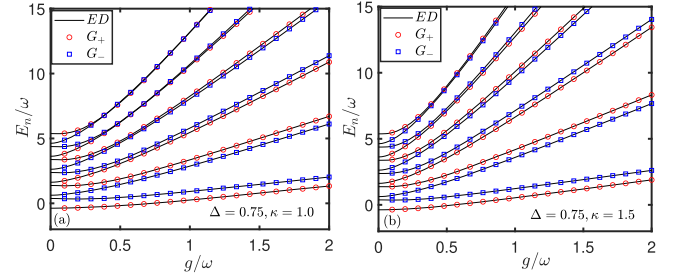


Figure 2. The energy levels as a function of g/ω for $\kappa = 1$ (a) and $\kappa = 1.5$ (b), with parameters $\Delta = 0.75$ and $\omega = 1$. Open symbols represent the zeros of equation (12), while solid curves show the results from numerical exact diagonalizations. Red (blue) indicates positive (negative) parity.

dynamics of the QRM with \mathbf{A} -square terms. The accuracy of different approaches is crucial for determining the dynamics. The transition frequency Δ , defined by the energy difference of the qubits, determines the peak position of the Fourier transform of the real-time evolution, while the amplitude of the dynamics is governed by the corresponding eigenfunctions.

To show the dynamical effect of the \mathbf{A} -square terms, we begin with the Hamiltonian of equation (4) in the σ_x space. The time-dependent Schrödinger equation reads

$$i \frac{\partial |\Psi\rangle}{\partial t} = H |\Psi\rangle. \quad (13)$$

We assume the initial state at the atomic up state and photonic vacuum state in the B -space of equation (8), which can be written as

$$|\Psi_0\rangle = \begin{pmatrix} |0\rangle_B \\ 0 \end{pmatrix}, \quad (14)$$

where $|0\rangle_B = e^{g'/\omega'(b^\dagger - b)} |0\rangle$ and $|0\rangle$ is the vacuum state of b -space. The evolution of $|\psi(t)\rangle$ can be written as

$$|\Psi(t)\rangle = \sum_{n=0}^{\infty} c_n e^{-iE_n t} |\psi_n\rangle, \quad (15)$$

with $c_n = \langle \Psi_0 | \psi_n \rangle$ and $E_n, |\psi_n\rangle$ are the eigenvalue and eigenstate of Hamiltonian (4).

We investigate the dynamic behavior of the atom population $\langle \sigma_z(t) \rangle$ for $g = 0.1, 0.2, 0.5, \text{ and } 1.0$ for $\kappa = 0, 1, 1.5$. The results are presented in figure 3. The atomic frequency is set to resonance, with $\Delta = \omega = 1.0$. For small coupling strength ($g = 0.1$), the evolution for different values of κ is almost identical over the time range $t = 0 \sim 100$. However, as the coupling strength increases, the evolution remains similar over a short time, but significant differences emerge over longer times. Particularly in the deep strong coupling regime, the evolution of the system with and without the \mathbf{A} -square terms.

To investigate the dynamics influenced by the atomic frequency Δ , we study the evolution of $\langle \sigma_z \rangle$ for $\Delta = 1.0, 1.5, 2, 5.0$ at the fixed coupling strength of $g = 0.5$. When Δ is small, for instance, $\Delta = 1.0$, the dynamical behavior varies significantly with different values of κ , as

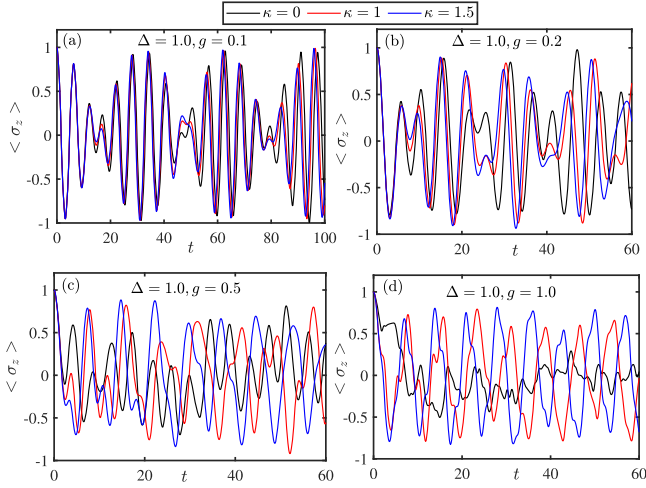


Figure 3. Evolution of $\langle \sigma_z \rangle$ at resonance ($\Delta = 1$) for different coupling strengths: $g = 0.1$ (a), 0.2 (b), 0.5 (c), and 1.0 (d). The values of κ are 0 (black), 1 (red), and 1.5 (blue).

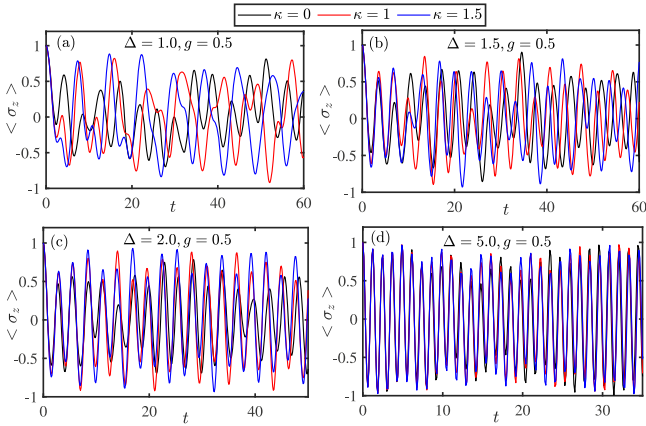


Figure 4. Evolution of $\langle \sigma_z \rangle$ at ultra-strong coupling strength ($g = 0.5$) for different qubit energy splitting: $\Delta = 1.0$ (a), 1.5 (b), 2.0 (c), and 5.0 (d). The values of κ are 0 (black), 1 (red), and 1.5 (blue).

demonstrated in figure 4. As Δ increases, the differences in the dynamical behavior for different values of κ gradually diminish. When $\Delta = 5.0$, the dynamical behavior for $\kappa = 0, 1, 1.5$ becomes almost identical, as shown in figure 4(d). Physically, an increase in Δ enlarges the gap of the energy levels, making tunneling between the atomic energy levels more difficult. When Δ is sufficiently large, such as $\Delta = 5$ in figure 4(d), even under ultra-strong coupling, the tunneling difficulty remains unchanged by the dynamics for different values of $\kappa = 0, 0.1, 0.2, 0.5$, leading to identical dynamical evolutions.

By performing a Fourier transform on the dynamics of $\langle \sigma_z \rangle(t)$, we analyze the frequency spectrum, as shown in figure 5, revealing the frequency structure of different dynamical behaviors. Here, we use data from a much longer time period than those shown in figure 3. When the coupling strength is small, e.g., $g = 0.1$, as seen in shown in figure 5(a), for the same κ , the time evolution of $\langle \sigma_z \rangle(t)$

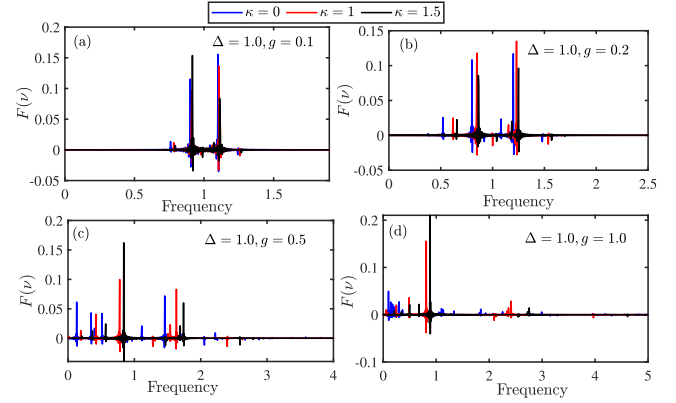


Figure 5. The Fourier transform of $\langle \sigma_z \rangle(t)$ at resonance ($\Delta = 1$) for different coupling strengths: $g = 0.1$ (a), 0.2 (b), 0.5 (c), and 1.0 (d). The values of κ are 0 (black), 1 (red), and 1.5 (blue).

exhibits two dominant frequencies. As the coupling strength increases, the number of dominant frequencies decreases. When the coupling strength reaches $g = 1$, only one dominant frequency is observed.

5. Conclusion

In this paper, we apply the Bogoliubov transformation method to calculate the energy spectrum of the QRM with **A**-square terms exactly. Our results are in excellent agreement with numerical methods. We find that the **A**-square terms significantly alter the spectrum of the original QRM. We also investigate the effect of the **A**-square terms on the dynamical behavior of the qubits and demonstrate that, when the TRK condition is satisfied, their presence leads to a significant difference in dynamics compared to the QRM without the **A**-square terms in the ultra-strong coupling regime. However, increasing the atomic frequency eliminates the effect of **A**-square terms on the dynamics, resulting in consistent dynamical behavior. Our frequency spectrum analysis shows that, at lower coupling strengths, the dynamics are driven by two main frequencies. As the coupling strength increases and enters the deep strong coupling regime, the dynamics are dominated by a single main frequency. We believe that these newly predicted dynamical behaviors could be observed in both cavity and circuit QED systems if the ultra-strong and deep strong coupling regimes are reached, where the effect of the **A**-square terms cannot be ignored.

Acknowledgments

This work is supported by the National Science Foundation of China under Grant Nos. 12305009 (XYC) and 11834005 (QHC), and the China Postdoctoral Science Foundation under Grant No. 2022M720387 (XYC).

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