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Eigenvalue Spectra of Rabi Models with Infinite Matrix Representations

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Abstract: We investigate the relationship between confluent Heun functions and the eigenvalue spectra of infinite matrices related to the semi-classical and quantum Rabi models, revealing distinct connections in each case. In the semi-classical model, the eigenvalues are explicitly expressed through confluent Heun functions, whereas in the quantum Rabi model, they are determined by zeros of a condition involving confluent Heun functions. Our findings establish a unified framework for solving the eigenvalue problem of infinite-dimensional unbounded matrices related to the Rabi models. We derive some new identities for confluent Heun functions, enabling simplifications and broader applications in mathematics and physics. The explicit eigenvalue expressions in the semi-classical case align with approximate results from earlier studies, while the derived conditions for the quantum model provide a concise and unified form, encompassing special cases that are typically treated as exceptions. We also discuss the energy spectrum of the quantum Rabi model, uncovering intriguing phenomena and patterns. Our results deepen the understanding of Rabi models and extend their potential applications in quantum optics and quantum information.

Keywords: Rabi model; confluent Heun function; infinite matrix; quantum optics; eigenvalue problem

MSC: 81Q05; 81Q80; 35Q40; 35Q41; 81Q93

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1. Introduction

The Rabi model, initially proposed by Isidor I Rabi in 1936 [1,2], describes the interaction between a two-level atom and a classical oscillating magnetic field. It is one of the simplest and most fundamental models for studying matter–light interactions and has served as a basis for various areas in quantum physics [3–7], including quantum optics, quantum information, and condensed matter physics. A widely used approximation, the Jaynes–Cummings model applies when the coupling between the two-level system and the oscillator is weak, allowing certain terms in the Hamiltonian to be neglected, which is the rotating wave approximation (RWA) [8–14]. In recent years, advancements in experimental techniques have allowed the exploration of regimes beyond the applicability of the Jaynes–Cummings model, particularly the ultra-strong and deep-strong coupling regimes. In these regimes, the RWA fails, and the full regimes of the Rabi model must be used to accurately describe the system.

Two typical classifications are the semi-classical Rabi model and the quantum Rabi model [14–24].

Definition 1. *A semi-classical Rabi model [1,2] is usually defined as* $H = \frac{\beta}{2}\sigma_z + \frac{g}{2}\cos(\omega t)\sigma_x$*, where* $\sigma_x, \sigma_y, \sigma_z$ *are Pauli matrices and* β *is the transition frequency of the two-level system. The parameters* ω *and* g *are the frequency and amplitude of harmonic driving. A quantum Rabi model [8,14] has the Hamiltonian as* $H = \omega a^\dagger a + \mu\sigma_z + \lambda\sigma_x(a^\dagger + a)$*, where* a $(a^\dagger)$ *is the destruction (creation) operator,* 2μ *is the qubit frequency,* ω *is the mode frequency, and* λ *is the coupling strength of the light–matter interaction.*

The semi-classical Rabi model can be regarded as the classical version of the effective Hamiltonian of the quantum Rabi model in the interaction picture. Recent theoretical developments, including analytical solutions for the quantum Rabi model, have further increased interest in the Rabi model. Braak's analytic solution [15] provided a basis for determining the full energy spectrum of the model, sparking ongoing research on various extensions, such as multi-photon, two-mode, and multi-atom Rabi models. The quantum Rabi model is focused on its eigenvalues, while the semi-classical Rabi model is focused on its evolution since its eigenvalue is trivial [21–24]. Both kinds of model can be transformed into an infinite matrix, to solve the above problem, although by different methods. Those matrices are unbound operators, and are often difficult to solve in mathematics.

In this paper, we present a new theoretical approach to obtain the eigenvalues and eigenvectors of certain types of infinite matrices, by establishing a link with the corresponding physical Rabi models. By solving this specific physical model problem, we actually also address the related mathematical problem of determining the eigenvalues of infinite unbounded matrices. The interesting thing is that confluent Heun functions appear in both the semi-classical and quantum Rabi models. We find that the eigenvalue of the matrix with the semi-classical Rabi model is determined by the confluent Heun functions, while the eigenvalue spectra of the quantum Rabi model are the roots of the equation defined by the confluent Heun functions. The analytical solution for the regular energy spectrum of the quantum Rabi model was first presented by Braak [15]. The results of Zhong [17] and Maciejewski [18] combine the regular energy spectrum with the other two special cases. The advantage of our approach lies in its ability to unify the regular case with the other two special cases. Additionally, we examine the energy spectrum of the quantum Rabi model, revealing intriguing phenomena and patterns. Our results enhance the understanding of Rabi models, broaden their potential applications in quantum optics and quantum information [3–7], and offer a framework for further exploration of confluent Heun functions in related fields.

We introduce the solvable infinite matrix generated by the semi-classical Rabi model in Section 2, while the infinite matrix for the quantum Rabi model is discussed in Section 3. Our discussions and conclusions are presented in Section 4 and Section 5, respectively.

2. Solvable Infinite Matrix Generated by Semi-Classical Rabi Models

2.1. The Infinite Matrix

We consider an infinite-dimensional Hermitian matrix $H_{\mathcal{F}}$, related to the semi-classical Rabi model under Fourier transform. Floquet theory can solve this so-called Floquet Hamiltonian $H_{\mathcal{F}}$, and here, we can continue to obtain the analytical expression of the eigenvalues q_i of $H_{\mathcal{F}}$ by solving the semi-classical Rabi model. Let us observe the expression of the infinite matrix $H_{\mathcal{F}}$, which can be divided into 2×2 block matrices as $H_{\mathcal{F}}^{m,n} = H_{\mathcal{F}}^{n,m} = \boldsymbol{h}_{m-n}\cdot\hat{\boldsymbol{\sigma}} + \delta_{mn}n\omega\mathcal{I}$, where $\mathcal{I}$ is the identity matrix, $\boldsymbol{h}_i = (x_i, y_i, z_i)^\top$, $\hat{\boldsymbol{\sigma}} = (\sigma_x, \sigma_y, \sigma_z)$, and $\sigma_x, \sigma_y, \sigma_z$ are Pauli matrices. Then, through the inverse Fourier transform, we can obtain the expression of the corresponding Hamiltonian as $H_f = \sum_{n=-\infty}^{\infty} \cos(n\omega t)\boldsymbol{h}_n \cdot \hat{\boldsymbol{\sigma}}$. Since $H_{\mathcal{F}}$ is Hermitian, the coefficient $\boldsymbol{h}_i$ must be symmetric as $\boldsymbol{h}_i = \boldsymbol{h}_{-i}$. We rewrite the Hamiltonian as $H_f = \boldsymbol{h} \cdot \hat{\boldsymbol{\sigma}}$, where $\boldsymbol{h} = \boldsymbol{h}_0 + 2\sum_{n=1}^{\infty} \boldsymbol{h}_n \cos(n\omega t)$.

For simplicity, we choose the semi-classical Rabi model as $H = \frac{\beta}{2}\sigma_z + \frac{g}{2}\cos(\omega t)\sigma_x$. The corresponding coefficients are $\boldsymbol{h}_0 = (0, 0, \beta/2)^{\mathsf{T}}$, $\boldsymbol{h}_1 = (g/4, 0, 0)^{\mathsf{T}}$, and $\boldsymbol{h}_{i\geq 2} = 0$. Then, the Floquet Hamiltonian $H_{\mathcal{F}}$ has the following infinite matrix representation in Floquet states

$$
\begin{pmatrix}
\ddots & \cdots & & & & & & & & \\
\vdots & s_{-2}^{-} & g/4 & 0 & 0 & 0 & 0 & 0 & 0 & \\
 & g/4 & s_{-1}^{+} & 0 & 0 & g/4 & 0 & 0 & 0 & \\
 & 0 & 0 & s_{-1}^{-} & g/4 & 0 & 0 & 0 & 0 & \\
 & 0 & 0 & g/4 & s_{0}^{+} & 0 & 0 & g/4 & 0 & \\
 & 0 & g/4 & 0 & 0 & s_{0}^{-} & g/4 & 0 & 0 & \\
 & 0 & 0 & 0 & 0 & g/4 & s_{1}^{+} & 0 & 0 & \\
 & 0 & 0 & 0 & g/4 & 0 & 0 & s_{1}^{-} & g/4 & \\
 & 0 & 0 & 0 & 0 & 0 & 0 & g/4 & s_{2}^{+} & \vdots \\
 & & & & & & & & \cdots & \ddots
\end{pmatrix}, \tag{1}
$$

where $s_n^{\pm} = n\omega \pm \beta/2$. To solve the eigenvalue of the infinite matrix $H_{\mathcal{F}}$ is in principle to solve $\det(H_{\mathcal{F}} - \lambda\mathcal{I}) = 0$. It is easy to check that, if λ is the eigenvalue of $H_{\mathcal{F}}$, $\lambda + n\omega$ is also an eigenvalue for any integer n. According to Floquet theory, the time evolution operator of the Hamiltonian H_f can be expressed as $U(t; t_0) = F(t)F^{-1}(t_0)$, and $F(t)$ has the form [25–28]

$$F(t) = M(t)\mathrm{e}^{-\mathrm{i}Qt}, \tag{2}$$

where $M(t)$ is a periodic matrix of t and the constant Q is the characteristic diagonal matrix as $Q = \mathrm{diag}(q_\alpha, q_\beta)$. Since we consider a two-level system here, the number of the characteristic eigenvalue is two, and the relation $q_\alpha + q_\beta = \mathrm{Tr}H_f = 0$ makes only one characteristic exponent independent. Thus, the characteristic matrix Q can be written as $Q = q_\alpha\sigma_z$.

2.2. Solution to the Characteristic Exponent

The solution to the characteristic exponent q_α is related to the time evolution operator $U(t; t_0)$ of a two-level system $H = \frac{\beta}{2}\sigma_z + \frac{g}{2}\cos(\omega t)\sigma_x$, which has been previously discussed [21–23]. Here, we recall the time evolution operator $U(t; t_0)$ in a more concise way. After a rotation $R = \mathrm{e}^{-\mathrm{i}\frac{\pi}{2}\sigma_x}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}\sigma_y}$, the efficient Hamiltonian takes a new form as $H_1 = RHR^\dagger = \frac{\beta}{2}\sigma_x + \frac{g}{2}\cos(\omega t)\sigma_z$, leaving the structure of the energy spectrum unchanged. The parameter ω can be regarded as a scaling parameter [23,29]. We choose a transform as $\tau = \omega t - \frac{\pi}{2}$; then, the Hamiltonian can be obtained as $H' = \frac{\beta'}{2}\sigma_x + \frac{g'}{2}\sin(\tau)\sigma_z$, where $\beta' = \beta/\omega$ and $g' = g/\omega$. For simplicity, we assume $\omega = 1$ and denote the Hamiltonian as $H = \frac{\beta}{2}\sigma_x + \frac{g}{2}\sin(t)\sigma_z$. The time period remains $T = 2\pi/\omega = 2\pi$. The Schrödinger equation is

$$\mathrm{i}\partial_t|\psi\rangle = H(t)|\psi\rangle = \left(\frac{\beta}{2}\sigma_x + \frac{g}{2}\sin(t)\sigma_z\right)|\psi\rangle, \tag{3}$$

where $|\psi\rangle = (c_1, c_2)^{\mathsf{T}}$ is the normalized wave function of the two-level system and $\hbar$ is set to 1. Then, after removing c_2 (or c_1), we obtain a second-order differential equation for c_1 (or c_2), as

$$\partial_t^2 c_1 + (\mathrm{i}\frac{g}{2}\cos t + \frac{g^2}{4}\sin^2 t + \frac{\beta^2}{4})c_1 = 0. \tag{4}$$

Next, applying the change in the variable from t to $z = \frac{1}{2}(1 - \cos t)$ and another transform $c_1 = \mathrm{e}^{\mathrm{i}gz} f$, we can obtain the differential equation as

$$z(z-1)\frac{\partial^2 f}{\partial z^2} + \left[\frac{1}{2}(z-1) + \frac{1}{2}z - 2\mathrm{i}gz(z-1)\right]\frac{\partial f}{\partial z} + (-\frac{\beta^2}{4})f = 0. \tag{5}$$

Compared to the standard confluent Heun equation

$$z(z-1)y'' + [\gamma(z-1) + \delta z + z(z-1)\epsilon]y' + (\alpha z - q)y = 0, \tag{6}$$

we can obtain the coefficients $q = \frac{\beta^2}{4}$, $\alpha = 0$, $\gamma = \frac{1}{2}$, $\delta = \frac{1}{2}$, $\epsilon = -2\mathrm{i}g$. The solution that satisfies the confluent Heun equation is the confluent Heun function $\mathrm{HC}(q, \alpha; \gamma, \delta, \epsilon; z)$, with the initial condition $\mathrm{HC}(q, \alpha; \gamma, \delta, \epsilon; 0) = 1$ [30–32]. The confluent Heun function can be expressed as a standard power-series expansion around $z = 0$ as $\mathrm{HC}(q, \alpha; \gamma, \delta, \epsilon; z) = \sum_{n=0}^{\infty} b_n z^n$. The coefficients b_n are determined by the three-term recurrence relation $R_n b_n + Q_{n-1} b_{n-1} + P_{n-2} b_{n-2} = 0$ with the initial conditions $b_{-2} = b_{-1} = 0$ and $b_0 = 1$. Here, $R_n = n(n - 1 + \gamma)$, $Q_n = q - n(n - 1 + \gamma + \delta - \epsilon)$, and $P_n = -\alpha - \epsilon n$. Therefore, the solution to Equation (4) is

$$c_1(t) = \mathrm{e}^{-\mathrm{i}gz}\mathrm{HC}\left(\frac{\beta^2}{4}, 0; \frac{1}{2}, \frac{1}{2}, -2\mathrm{i}g; z\right) := \mathrm{e}^{-\mathrm{i}gz}\mathrm{HC}(a_1; z), \tag{7}$$

where parameters $a_1 := \left(\frac{\beta^2}{4}, 0; \frac{1}{2}, \frac{1}{2}, -2\mathrm{i}g\right)$, and $z = \sin^2 \frac{t}{2}$. Here, we choose the initial condition $c_1(t = 0) = 1, c_2(t = 0) = 0$.

From the symmetry of the two functions c_1 and c_2, we can observe that, apart from g changing sign to $-g$, c_1 and c_2 satisfy differential equations of the same form. Then, according to the initial condition $c_2(t = 0) = 0$, we know that c_2 is the other linearly independent solution $z^{1-\gamma}\mathrm{HC}(q + (1-\gamma)(\epsilon - \delta), \alpha + (1-\gamma)\epsilon, 2 - \gamma, \delta, \epsilon, z)$, which is

$$c_2(t) = \mathrm{i}^{\eta}\beta \sin\frac{t}{2}\mathrm{e}^{\mathrm{i}gz}\mathrm{HC}\left(\frac{\beta^2 - 1}{4} + \mathrm{i}g, \mathrm{i}g; \frac{3}{2}, \frac{1}{2}, 2\mathrm{i}g; z\right) := \mathrm{i}^{\eta}\beta \sin\frac{t}{2}\mathrm{e}^{\mathrm{i}gz}\mathrm{HC}(a_2; z), \tag{8}$$

where parameters $a_2 := \left(\frac{\beta^2-1}{4} + \mathrm{i}g, \mathrm{i}g; \frac{3}{2}, \frac{1}{2}, 2\mathrm{i}g\right)$, $z = \sin^2 \frac{t}{2}$, and $\eta = 1 + 2\lfloor \frac{t-\pi}{T} \rfloor$ with the floor function $\lfloor x \rfloor$. The parameter η can be treated as a constant within each continuous period $t \in [(2n-1)\pi, (2n+1)\pi)$. Then, we can construct the time evolution operator as

$$U_1(t) = \begin{pmatrix} c_1(t) & -c_2(t)^* \\ c_2(t) & c_1(t)^* \end{pmatrix}. \tag{9}$$

According to the symmetry $H(t) = \sigma_x H(t - \frac{T}{2})\sigma_x$, we derive $U_2(t) = \sigma_x U_1(t - \frac{T}{2})\sigma_x$. Consequently, the total time evolution operator can be expressed (see Appendix B) as

$$U(t, 0) = U_2(t - NT)U_2^{\dagger}(0)\mathrm{e}^{\mathrm{i}2N\Theta\sigma_{\boldsymbol{n}}/2}, \tag{10}$$

where $N = \lfloor \frac{t}{T} \rfloor$, $\Theta = 2\arcsin|c_2(\frac{T}{2}^-)|$, and $\sigma_{\boldsymbol{n}} = \sin\Phi\sigma_x + \cos\Phi\sigma_y$ with $\Phi = \arg[c_1^*(\frac{T}{2}^-)c_2(\frac{T}{2}^-)]$. For simplicity, some notations (e.g., $f(t^-)$) are defined in Appendix A.

The continuity of the functions $c_1(t)$ and $c_2(t)$ in Equations (7) and (8) is worth mentioning. If the reader has no concerns about continuity, this section can be skipped. It should be noted that the two functions $c_1(t)$ and $c_2(t)$ are discontinuous at the periodic points $t = (2n+1)\pi$, $n \in \mathrm{Z}$. As a result, they only satisfy the differential Equation (3) within a single period. The parameter η indicates that the solution $c_2(t)$ differs by a negative sign between adjacent periodic intervals. Thus, we use $U_1(t)$ and $U_2(t)$ to construct the total time evolution operator $U(t,0)$, ensuring that $U(t,0)$ remains continuous at all times. This approach guarantees that $U(t,0)$ depends solely on the complete evolution during the first period. For example, we can obtain the continuity at $t = T$, as $N = 0$ and $U(T^-,0) = U_2(T^-)U_2^\dagger(0) = \mathrm{e}^{\mathrm{i}2\Theta\sigma_{\boldsymbol{n}}/2} = U_2(0)U_2^\dagger(0)\mathrm{e}^{\mathrm{i}2\Theta\sigma_{\boldsymbol{n}}/2} = U(T,0) = U(T^+,0)$.

Lemma 1. *Compared to the Floquet theory [25–28], an additional rotation is required, which is* $R_s = \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}\sigma_x}\mathrm{e}^{-\mathrm{i}\frac{\Phi}{2}\sigma_z}$*. Then, we can obtain the Floquet operator* $F(t)$ *as*

$$F(t) = R_s U R_s^\dagger = R_s U_2(t-NT)U_2^\dagger(0)R_s^\dagger \mathrm{e}^{\mathrm{i}N\Theta\sigma_z}. \tag{11}$$

Proof of Lemma 1. Following Equations (3)–(10), the total time evolution operator $U(t,0)$ is given by (for a more detailed derivation, see Appendix B)

$$U = U(t,0) = U_2(t-NT)U_2^\dagger(0)\mathrm{e}^{\mathrm{i}2N\Theta\sigma_{\boldsymbol{n}}/2}. \tag{12}$$

Since the direction of the spin in Equation (2) is σ_z, we need a rotation R_s to modify the direction $\sigma_{\boldsymbol{n}}$, which is $\sigma_{\boldsymbol{n}'} = R_s\sigma_{\boldsymbol{n}}R_s^\dagger = \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}\sigma_x}\mathrm{e}^{-\mathrm{i}\frac{\Phi}{2}\sigma_z}(\sin\Phi\sigma_x + \cos\Phi\sigma_y)\mathrm{e}^{\mathrm{i}\frac{\Phi}{2}\sigma_z}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}\sigma_x} = \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}\sigma_x}\sigma_y\mathrm{e}^{\mathrm{i}\frac{\pi}{4}\sigma_x} = \sigma_z$. Then, we can obtain the Floquet Operator as $F(t) = R_sUR_s^\dagger = R_sU_2(t-NT)U_2^\dagger(0)R_s^\dagger R_s\mathrm{e}^{\mathrm{i}2N\Theta\sigma_{\boldsymbol{n}}/2}R_s^\dagger = R_sU_2(t-NT)U_2^\dagger(0)R_s^\dagger\mathrm{e}^{\mathrm{i}N\Theta\sigma_z}$. □

Theorem 1. *The characteristic value* q_α *is*

$$q_\alpha = \frac{\Theta}{T} = \frac{2\arcsin|c_2(\frac{T}{2}^-)|}{2\pi} \tag{13}$$

$$= \frac{1}{\pi}\arcsin\left(\sqrt{2}\beta\mathrm{Re}[\mathrm{e}^{\mathrm{i}g}\mathrm{HC}(a_1^*;\frac{1}{2})\mathrm{HC}(a_2;\frac{1}{2})]\right) \tag{14}$$

Proof of Theorem 1. Equation (11) is a little different from the standard Floquet operator (2). Thus, we modify Equation (11) as

$$\begin{aligned} F(t) &= R_sU_2(t-NT)U_2^\dagger(0)R_s^\dagger\mathrm{e}^{\mathrm{i}N\Theta\sigma_z} && (15)\\ &= R_sU_2(t-NT)U_2^\dagger(0)R_s^\dagger\mathrm{e}^{-\mathrm{i}(t-NT)\frac{\Theta}{T}\sigma_z}\mathrm{e}^{\mathrm{i}(t-NT)\frac{\Theta}{T}\sigma_z}\mathrm{e}^{\mathrm{i}NT\frac{\Theta}{T}\sigma_z} && (16)\\ &= R_sU_2(t-NT)U_2^\dagger(0)R_s^\dagger\mathrm{e}^{-\mathrm{i}(t-NT)\frac{\Theta}{T}\sigma_z}\mathrm{e}^{\mathrm{i}t\frac{\Theta}{T}\sigma_z} && (17)\\ &\equiv M(t)\mathrm{e}^{-\mathrm{i}Qt}, && (18)\end{aligned}$$

where $M(t) = R_sU_2(t-NT)U_2^\dagger(0)R_s^\dagger\mathrm{e}^{-\mathrm{i}(t-NT)\frac{\Theta}{T}\sigma_z}$ and $Q = \frac{\Theta}{T}\sigma_z$. Then, compared with $Q = q_\alpha\sigma_z$, we can obtain $q_\alpha = \frac{\Theta}{T} = \arcsin|c_2(\frac{T}{2}^-)|/\pi$. □

2.3. Comparison with Previous Results

The approximate result for $\beta \ll 1$ was well studied in Refs. [5,27–29,33–39], and the one proposed earliest among them is [29]. The approximate result for β is $q_\alpha^{\mathrm{app}} \approx \frac{\sqrt{2}\beta}{\pi}\mathrm{Re}[\mathrm{e}^{\mathrm{i}g}\mathrm{HC}(a_1^*|_{\beta=0};\frac{1}{2})\mathrm{HC}(a_2|_{\beta=0};\frac{1}{2})] \equiv \frac{\beta}{2}J_0(g)$. These transformations, $\tau = \omega t - \pi/2$ and $\cos(\omega t) = \sin\tau$, introduce a bias of $1/2$ to the characteristic value q_α, which should be noted when comparing with the previous work [29].

When $g \ll 1$, the approximate result [29] is

$$q_\alpha^{\mathrm{app}} \approx \frac{\beta}{2} - \frac{\beta}{8(1-\beta^2)}g^2 + \frac{\beta(3\beta^2+1)}{128(1-\beta^2)^3}g^4 + \dots, \tag{19}$$

which can also be obtained by a perturbation expansion. Figure 1 shows the micro difference between the approximate and exact results when $g \ll 1$. If we compare the Taylor expansions of the two results, we will find some identities about the confluent Heun function, which are

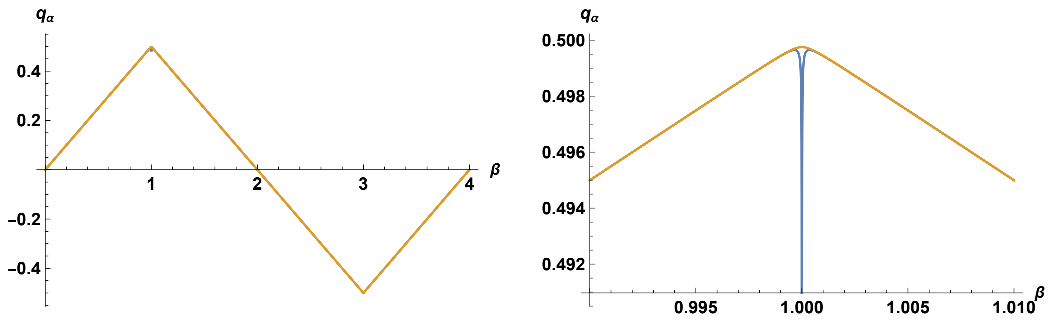

Figure 1. The difference between the exact and approximate characteristic value q_α with $g = 0.01$. The yellow line is the exact value q_α, while the blue line is the approximate value q_α^{app} . The right panel is an enlarged view near $\beta = 1$.

$$\left.\frac{\partial q_\alpha}{\partial g}\right|_{g=0} = 0, \left.\frac{\partial^2 q_\alpha}{\partial g^2}\right|_{g=0} = (-1)^{\lfloor\frac{\beta-1}{2}\rfloor}\frac{\beta}{4(1-\beta^2)}. \tag{20}$$

When β is large ($\beta \gg 1$), the approximate result [29] is

$$q_\alpha^{\text{app}} \approx \frac{1}{2} + \frac{g}{\pi x}\mathrm{E}(x), \tag{21}$$

where $x^2 = \frac{g^2}{g^2+(1-\beta)^2}$ and $\mathrm{E}(x)$ is the complete elliptic integral. As shown in Figure 2, the difference becomes very small when β is large.

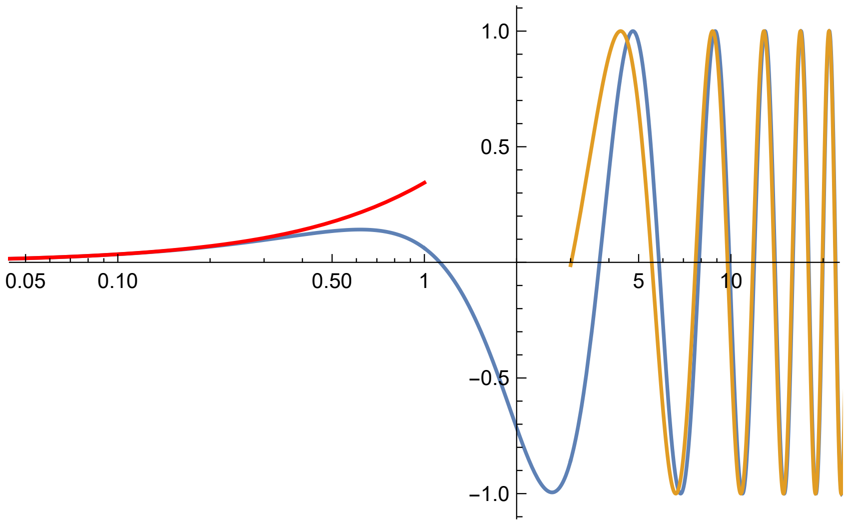

Figure 2. Comparison of the exact and approximate values of the characteristic value q_α when β is small or large. The continuous blue line is $\sin[q_\alpha \pi]$. The yellow line is $\sin\left[\frac{g}{x}\mathrm{E}(x)\right]$, $\mathrm{E}(x)$ is the average of the first and second kinds of the complete elliptic integral. The red line is $\sin\left[\frac{\beta}{2}J_0(g)\pi\right]$, where $J_0(g)$ is the first kind of the Bessel function of 0-order.

3. Solvable Infinite Matrix Generated by Quantum Rabi Models

3.1. The Quantum Rabi Model

The Hamiltonian of the quantum Rabi model [15–20] is described by

$$H = \omega a^\dagger a + \mu\sigma_z + \lambda\sigma_x\left(a^\dagger + a\right), \tag{22}$$

where a ($a^\dagger$) is the destruction (creation) operator, and $\sigma_{x,z}$ are Pauli matrices. The energy difference between the two levels is 2μ, and λ denotes the coupling strength between the two-level system and the bosonic mode. We set the frequency $\omega = 1$ for simplicity, without loss of generality. The eigenvalue equation $H|\psi\rangle = E|\psi\rangle$ can be regarded as a matrix equation $H_M|\psi\rangle = E|\psi\rangle$, where H_M is an infinite matrix and $|\psi\rangle$ is the eigenvector corresponding to eigenvalue E. The eigenstates $|\psi\rangle$ for the model can be written

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle|\uparrow\rangle + d_n|n\rangle|\downarrow\rangle, \tag{23}$$

where $|n\rangle$ is the Fock state for the bosonic mode, and $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of σ_z with eigenvalues 1 and -1, respectively.

The infinite matrix H_M can be divided into 2×2 block matrices as $H_M^{m,n} = \boldsymbol{h}_{m,n} \cdot \hat{\boldsymbol{\sigma}} + \delta_{mn} n\mathcal{I}$, for $m, n \geq 0$. Here, $\boldsymbol{h}_{n,n} = (0, 0, \mu)^\mathsf{T}$, $\boldsymbol{h}_{m,n} = \sqrt{(m+n+1)/2}(\lambda, 0, 0)^\mathsf{T}$ for $|m-n| = 1$ and $\boldsymbol{h}_{m,n} = 0$ for $|m-n| \geq 2$. These terms for $|m-n| \geq 2$ arise when considering multi-photon interactions, which are not addressed in this paper. Then, the Hamiltonian $H_{\mathcal{M}}$ has the following infinite matrix representation

$$\begin{pmatrix} \mu & 0 & 0 & \lambda & 0 & 0 & 0 & \\ 0 & -\mu & \lambda & 0 & 0 & 0 & 0 & \\ 0 & \lambda & 1+\mu & 0 & 0 & \lambda\sqrt{2} & 0 & \\ \lambda & 0 & 0 & 1-\mu+ & \lambda\sqrt{2} & 0 & & \\ 0 & 0 & 0 & \lambda\sqrt{2} & 2+\mu & 0 & 0 & \\ 0 & 0 & \lambda\sqrt{2} & 0 & 0 & 2-\mu & \lambda\sqrt{3} & \\ 0 & 0 & 0 & 0 & 0 & \lambda\sqrt{3} & 3+\mu & \\ & & & & & & \cdots & . \end{pmatrix}. \tag{24}$$

From the structure of the matrix, we can see that the solution space is naturally divided into two subspaces (odd and even), which can also be derived from the conditions (Equation (45)) formed by the confluent Heun functions later. Actually, it is very difficult to directly obtain the eigenvalue spectrum for this infinite matrix, as it is an unbounded operator. From an analytical perspective, the spectrum of unbounded operators may contain various components (e.g., point spectrum, continuous spectrum, and residual spectrum), whereas truncation methods struggle to handle the continuous and residual spectra. Numerically, the matrix elements of unbounded operators may grow rapidly as the row or column indices increase. When truncated to finite-dimensional matrices, issues such as truncation errors and convergence problems may arise, sometimes even introducing spurious eigenvalues unrelated to the original operator. However, its eigenvalue spectrum can be determined by connecting it to the physically relevant quantum Rabi model, which can be solved using creation and annihilation operators. This functional method yields Heun functions as exact solutions in a power series form. Even when considering finite truncations of these power series, the numerical precision can be controlled to any desired level of accuracy.

3.2. Conditions for Eigenvalues

There are several approaches to derive the conditions that the eigenvalues should satisfy. The earliest was the G-function form of the recurrence coefficient type given by Braak [15]. Next, Chen proposed a more physical way using Bogoliubov transformations [16]. Then, Zhong introduced a concise form by using the confluent Heun functions [17]. Here, we will follow some of Zhong's steps to solve the eigenvalues, then provide a more direct and concise expression for the conditions. We use analytical functions $\psi_{1,2}$ of the creation operator $a^\dagger$ to rewrite the eigenstates $|\psi\rangle$ in Equation (23) as

$$|\psi\rangle = \psi_1\left(a^\dagger\right)|0\rangle|\uparrow\rangle + \psi_2\left(a^\dagger\right)|0\rangle|\downarrow\rangle, \tag{25}$$

where $|0\rangle$ is the vacuum state for the bosonic mode.

From the eigenvalue equation $H|\psi\rangle = E|\psi\rangle$, the operator functions $\psi_{1,2}$ are found to satisfy the differential equations [17,40–42] as

$$z\frac{\mathrm{d}\psi_1}{\mathrm{d}z} + \lambda\left(\frac{\mathrm{d}\psi_2}{\mathrm{d}z} + z\psi_2\right) + \mu\psi_1 = E\psi_1, \tag{26}$$

$$z\frac{\mathrm{d}\psi_2}{\mathrm{d}z} + \lambda\left(\frac{\mathrm{d}\psi_1}{\mathrm{d}z} + z\psi_1\right) - \mu\psi_2 = E\psi_2, \tag{27}$$

where $z = a^\dagger$ can be formally regarded as a complex number. Using the linear combinations $f = \psi_1 + \psi_2$ and $g = \psi_1 - \psi_2$, the above equations can be transformed into a second-order differential equation for $f(z)$ or $g(z)$, which is

$$\frac{\mathrm{d}^2 f}{\mathrm{d}z^2} + p(z)\frac{\mathrm{d}f}{\mathrm{d}z} + q(z)f = 0 \tag{28}$$

with $p(z) = [(1-2E-2\lambda^2)z - \lambda]/[z^2-\lambda^2]$, $q(z) = [\lambda z - \lambda^2(z^2+1) + E^2 - \mu^2]/[z^2-\lambda^2]$.

We can transform the above equation into the standard confluent Heun equation by the two transformations as $f_1(z) = \mathrm{e}^{-\lambda z}\phi_1(x_1)$ and $f_2(z) = \mathrm{e}^{\lambda z}\phi_2(x_2)$, where $x_1 = \frac{\lambda - z}{2\lambda}$ and $x_2 = \frac{\lambda+z}{2\lambda}$. Firstly, we use the transformation $x_1 = \frac{\lambda-z}{2\lambda}$, and Equation (28) becomes

$$x_1(x_1-1)\phi_1'' + [\gamma(x_1-1) + \delta x_1 + x_1(x_1-1)\epsilon]\phi_1' + (\alpha x_1 - q)\phi_1 = 0, \tag{29}$$

where $q = \mu^2 - (E+\lambda^2)^2$, $\alpha = -4\lambda^2(E+\lambda^2)$, $\gamma = -(E+\lambda^2)$, $\delta = -(E+\lambda^2)+1$, $\epsilon = 4\lambda^2$. From the form of Equation (29), we can naturally express the eigenvalue E in terms of a new variable as $k = E + \lambda^2$. Here, k can be regarded as a quasi-energy value of a modified Hamiltonian $H' = H + \lambda^2$, which makes this formulation convenient for subsequent discussions. The parameters in the confluent Heun Equation (29) can be re-expressed as $q = \mu^2 - k^2$, $\alpha = -4k\lambda^2$, $\gamma = -k$, $\delta = 1-k$, $\epsilon = 4\lambda^2$. Therefore, the solution to Equation (28) is

$$f_1(z) = \mathrm{e}^{-\lambda z}\mathrm{HC}\left(\mu^2 - k^2, -4k\lambda^2; -k, 1-k, 4\lambda^2; x_1\right) := \mathrm{e}^{-\lambda z}\mathrm{HC}(a_3; x_1), \tag{30}$$

with the parameter $a_3 := \left(\mu^2 - k^2, -4k\lambda^2; -k, 1-k, 4\lambda^2\right)$. The other linearly independent solution of the Heun confluent function is $x_1^{1-\gamma}\mathrm{HC}(q + (1-\gamma)(\epsilon-\delta), \alpha + (1-\gamma)\epsilon; 2-\gamma, \delta, \epsilon; x_1)$, which requires separate discussion only when $1-\gamma \in \mathbb{N}$, due to the physical meaning of $z = a^\dagger$. Since $a^{\dagger n}|0\rangle = \sqrt{n!}|n\rangle$ in the Bargmann space, the analytical functions $\psi_{1,2}$ do not always correspond to valid states as they may not be normalized. Under certain conditions, the coefficients b_n in Heun confluent function $\mathrm{HC}(q, \alpha; \gamma, \delta, \epsilon; x)$ may satisfy $b_n/b_{n-1} \simeq -\epsilon/n$ for large n, where the analytical functions $\psi_{1,2}$ can be normalized and are thus valid. However, these conditions are not explicitly provided in the confluent Heun functions and are often related to the convergence at the singular point $x = 1$. Therefore, we use an alternative approach to determine the conditions for the eigenvalues, employing the next transformation and an additional solution.

We apply the second transformation $x_2 = \frac{\lambda+z}{2\lambda}$, and through a similar sequence of steps, we obtain another solution to Equation (28) as

$$f_2(z) = \mathrm{e}^{\lambda z}\mathrm{HC}(a_4; x_2) := \mathrm{e}^{\lambda z}\mathrm{HC}\left(\mu^2 - k^2 + 4\lambda^2, 4(1-k)\lambda^2; 1-k, -k, 4\lambda^2; x_2\right), \tag{31}$$

with the parameter $a_4 := (\mu^2 - k^2 + 4\lambda^2, 4(1-k)\lambda^2; 1-k, -k; 4\lambda^2)$. When E is an eigenvalue of the quantum Rabi model, the two forms of the solution $f(z)$ must coincide within the common domain of definition (up to a multiplicative constant), which implies that the Wronskian determinant vanishes. Noticing $x_1 + x_2 = 1$, we can obtain the Wronskian determinant [18,20] as

$$W(k,\lambda,\mu;y) = f_1\partial_z f_2 - f_2\partial_z f_1 \tag{32}$$

$$= \frac{1}{2\lambda}[4\lambda^2 \mathrm{H}_3(y)\mathrm{H}_4(1-y) + \mathrm{H}_3'(y)\mathrm{H}_4(1-y) + \mathrm{H}_3(y)\mathrm{H}_4'(1-y)], \tag{33}$$

where $y = x_1$, $\mathrm{H}_i(y) := \mathrm{HC}(a_i; y)$, and $\mathrm{H}_i'(y_0) := \partial_y \mathrm{HC}(a_i; y)|_{y=y_0}$.

Lemma 2. *The Wronskian can be expressed without explicitly involving derivatives, which is*

$$W(k,\lambda,\mu;y) = k^2\mathrm{H}_3(y)\mathrm{H}_3(1-y) - \mu^2\mathrm{H}_4(y)\mathrm{H}_4(1-y), \tag{34}$$

where a parameter $2k\lambda(y-1)$ is multiplied.

Theorem 2. *The Wronskian Equation (34) must vanish in the intersection of domains of solutions. By choosing $y = 1/2$, we can obtain a more concise form as*

$$w(k,\lambda,\mu) := W(k,\lambda,\mu; y = 1/2) = k^2\mathrm{H}_3^2(1/2) - \mu^2\mathrm{H}_4^2(1/2) \tag{35}$$

$$= [k\mathrm{H}_3(1/2) - \mu\mathrm{H}_4(1/2)][k\mathrm{H}_3(1/2) + \mu\mathrm{H}_4(1/2)], \tag{36}$$

where $\mathrm{H}_i(1/2) := \mathrm{HC}(a_i; 1/2)$. From the above equation, we can see that the condition can be divided into two parts $k\mathrm{H}_3(1/2) - \mu\mathrm{H}_4(1/2) = 0$ and $k\mathrm{H}_3(1/2) + \mu\mathrm{H}_4(1/2) = 0$, and those conditions are more concise than previous results [15–19].

Proof of Lemma 2 and Theorem 2. After applying the identity Equations (52) and (53), we can simplify Equation (33) as

$$\begin{aligned} W(k,\lambda,\mu;y) &= \frac{1}{2\lambda}[4\lambda^2\mathrm{H}_3(y)\mathrm{H}_4(1-y) + \frac{\mu^2\mathrm{H}_4(y) - k^2\mathrm{H}_3(y)}{k(1-y)}\mathrm{H}_4(1-y) \\ &\quad + \mathrm{H}_3(y)\frac{(k - 4\lambda^2(1-y))\mathrm{H}_4(1-y) - k\mathrm{H}_3(1-y)}{1-y}] \end{aligned} \tag{37}$$

$$\begin{aligned} &= \frac{1}{2k\lambda(1-y)}[4k\lambda^2(1-y)\mathrm{H}_3(y)\mathrm{H}_4(1-y) + (\mu^2\mathrm{H}_4(y) - k^2\mathrm{H}_3(y))\mathrm{H}_4(1-y) \\ &\quad + k\mathrm{H}_3(y)\Big((k - 4\lambda^2(1-y))\mathrm{H}_4(1-y) - k\mathrm{H}_3(1-y)\Big)] \end{aligned} \tag{38}$$

$$\begin{aligned} &= \frac{1}{2k\lambda(1-y)}[\mathrm{H}_3(y)\mathrm{H}_4(1-y)(4k\lambda^2(1-y) - k^2 + k(k - 4\lambda^2(1-y))) \\ &\quad - k^2\mathrm{H}_3(y)\mathrm{H}_3(1-y) + \mu^2\mathrm{H}_4(y)\mathrm{H}_4(1-y)] \end{aligned} \tag{39}$$

$$= \frac{1}{2k\lambda(y-1)}\Big[k^2\mathrm{H}_3(y)\mathrm{H}_3(1-y) - \mu^2\mathrm{H}_4(y)\mathrm{H}_4(1-y)\Big]. \tag{40}$$

When $y = 1/2$, we can obtain

$$w(k,\lambda,\mu) = 2k\lambda(y-1) * W(k,\lambda,\mu;y) \tag{41}$$

$$= k^2\mathrm{H}_3(1/2)\mathrm{H}_3(1-1/2) - \mu^2\mathrm{H}_4(1/2)\mathrm{H}_4(1-1/2) \tag{42}$$

$$= k^2\mathrm{H}_3^2(1/2) - \mu^2\mathrm{H}_4^2(1/2) \tag{43}$$

□

3.3. The Energy Spectrum of Quantum Rabi Model

We have now derived the conditions that the energy $E = k - \lambda^2$ needs to satisfy. These conditions are explicitly restated as

$$k\mathrm{HC}(a_3; 1/2) \pm \mu \mathrm{HC}(a_4; 1/2) = 0, \tag{44}$$

where $a_3 := (\mu^2 - k^2, -4k\lambda^2; -k, 1-k, 4\lambda^2)$ and $a_4 := (\mu^2 - k^2 + 4\lambda^2, 4(1-k)\lambda^2; 1-k, -k; 4\lambda^2)$. When the energy $E = k - \lambda^2$ satisfies Expression (44) above, we can reconstruct a physical eigenstate with the corresponding eigenvalue of E that can be normalized. If we look at the above equation from the perspective of parameter k, we will find that it has poles at $k \in \mathrm{Z}^+$. A new method is to multiply the condition expressions by a constant, the Gamma function $\Gamma(1-k)$, so that they no longer diverge at these poles. The use of Gamma functions to eliminate poles in the equivalent of G-functions for the asymmetric quantum Rabi model was also proposed theoretically in Refs. [43–45].

Remark 1. *The Wronskian condition* (44) *becomes* $l_\mp(k) = 0$, *where*

$$l_\mp(k) := \mathrm{HC}(a_3; 1/2)/\Gamma(-k) \mp \mu \mathrm{HC}(a_4; 1/2)/\Gamma(1-k). \tag{45}$$

Figure 3 shows the above functions $l_\mp$ and their zeros, which are consistent with the previous results [15–19]. Since these functions $l_\mp$ have no poles, we can observe their zero distributions more clearly.

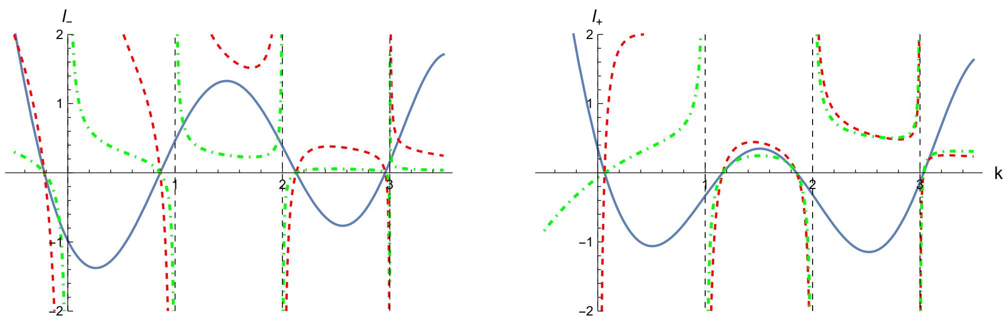

Figure 3. Comparison with previous results for $\mu = 0.4, \lambda = 0.7, \omega = 1$. The zeros of $G_\mp$ in Ref. [15], $G^+_{1(4)}|_{z=0}$ in Ref. [17], and $l_\mp$ in this paper are consistent. (**Left panel**): G_- (red dash lines), G^+_1 (green dot-dash lines), and l_- (blue solid lines). (**Right panel**): G_+ (red dash lines), G^+_4 (green dot-dash lines), and l_+ (blue solid lines). To enhance clarity, the values of the $l_\mp$ functions have been rescaled by a constant factor of 5.

The structure of the energy spectrum $E = k - \lambda^2$ is shown in Figure 4. The energies of the blue solid (red dashed) lines belong to the odd (even) subspace and satisfy the energy condition $l_- = 0$ ($l_+ = 0$). We can see that the non-trivial crossings occur only at $k \in \mathrm{Z}^+$ and there are trivial crossings when μ and k are half-integers, and $\lambda = 0$. The non-trivial crossings of the spectral lines occur only between lines of different colors or shapes, indicating that non-trivial energy degeneracy does not occur within the same subspace. We can then use the ordering of energies within the corresponding subspace to label the energy levels ($-$ for odd subspace and $+$ for even subspace), as illustrated in Figure 4. As λ approaches infinity, the quasi-energy value k converges to the corresponding marked level n. This type of marking indicates that non-trivial crossings occur only when the energies are at the same marked level, while trivial crossings occur between adjacent marked levels. This result has been verified using numerical methods; however, a theoretical proof would require a deeper understanding of confluent Heun functions and the quantum Rabi model, and is therefore not provided here. Numerical calculations show that when k is a half-integer, approximate crossing points appear. The lower right corner of the right panel in Figure 4 provides a magnified view of this situation.

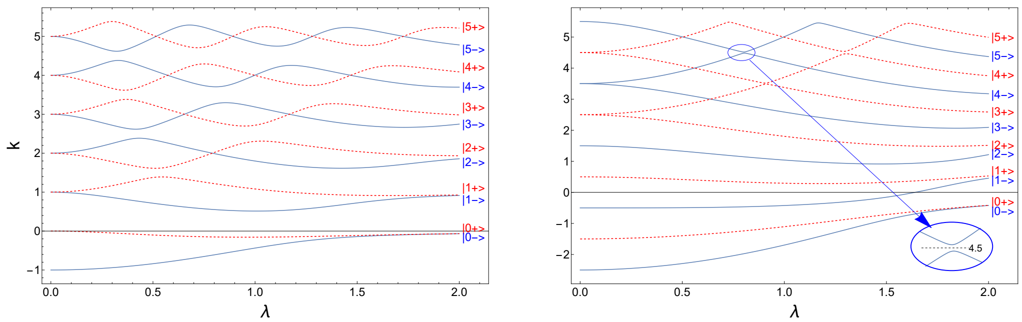

Figure 4. Quasi-energy spectrum ($k = E + \lambda^2$) of quantum Rabi models for $\mu = 1$ (**left panel**) and $\mu = 2.5$ (**right panel**). The energies of the blue solid lines belong to the odd subspace and satisfy the energy condition $l_- = 0$. The energies of the red dashed lines belong to the even subspace and satisfy the energy condition $l_+ = 0$.

When a non-trivial crossing occurs at $k_z \in \mathrm{Z}^+$, the two condition functions $l_\mp$ also intersect at k_z, where the eigenstates degenerate into the Jude states [46–48] (polynomial states). We find that the number m of non-trivial crossings at $k_z \in \mathrm{Z}^+$ is given by $m(\mu, k_z) = \lfloor \max(0, k_z + 1 - |\mu|) \rfloor$, where $\lfloor x \rfloor$ represents the floor function and $|x|$ represents the absolute value function; this result has also been verified by numerical methods. The result m represents the number of Juddian isolated exact solutions [45–47] and is consistent with the findings in Ref. [48] for the case $|\mu| < 1$. Another situation is that only one of the condition functions, l_- or l_+, equals zero at k_z. This situation implies that the limiting values of the two functions $\mathrm{H}_3(1/2)/\Gamma(-k)$ and $\mu \mathrm{H}_4(1/2)/\Gamma(1-k)$ at the pole k_z are either identical or opposite, corresponding to the odd or even subspace, respectively. Figure 5 shows these two situations, and we can regard these two special cases $k \in \mathrm{Z}^+$ as the limiting situations at the poles, from the perspective of the criterion $l_\mp(k) = 0$. Our method unifies the conditions into a single consistent formula, whether k is a pole or not, indicating that we do not need to treat the poles as special cases. For both the regular and exceptional spectra, this consistent formula provides a clear understanding of the roots of conditional Equation (45).

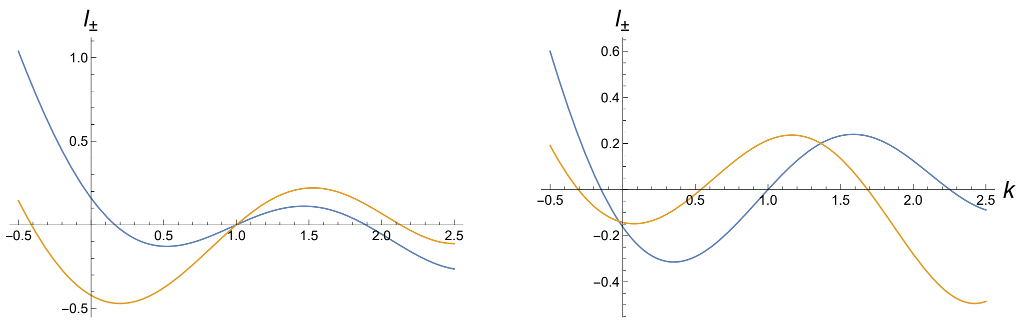

Figure 5. Exceptional quasi-energy $k = 1$ with the $l_\mp$ functions (yellow line for l_- and blue line for l_+). The **left** panel represents the degenerate case with $\mu = 1/2, \lambda = \sqrt{3}/4$, and the **right** panel represents the non-degenerate case with $\mu = 1, \lambda = 1.1647879$.

Although we have obtained the exact conditions for the eigenvalues of the quantum Rabi model, the explicit expressions for a specific energy level remain unclear, as the exact forms of the roots involving the confluent Heun functions are difficult to obtain. Here, we obtain the upper and lower bounds for the energy E_0, which is the ground state energy of the quantum Rabi model.

Remark 2. *The ground state energy is the lowest root of the odd parity condition $l_- = 0$, for which we obtain a lower bound, denoted as*

$$E_0 + \lambda^2 \geq e_g = -\mu + \frac{\mu}{1 + \lambda^{-2}(\mu + 1/2)}, \tag{46}$$

where we consider $\mu > 0$. When λ is small or large, we can obtain two more concise upper bounds $E_0 + \lambda^2 \leq \min(e^s_{\text{up}}, e^l_{\text{up}})$ as

$$e^s_{\text{up}} = -\mu + \frac{\mu}{\frac{1/4}{\mu+1/2} + \lambda^{-2}(\mu + 1/2)}, \; e^l_{\text{up}} = -\mu + \frac{\mu}{1 + \lambda^{-2}(\mu/4)}. \tag{47}$$

Figure 6 illustrates the differences between the three bounds and the exact ground quasi-energy k, which are negligible when λ is either small or large. This expression for small λ can be derived using perturbation theory (see Appendix C), while numerical checks are employed for other regions.

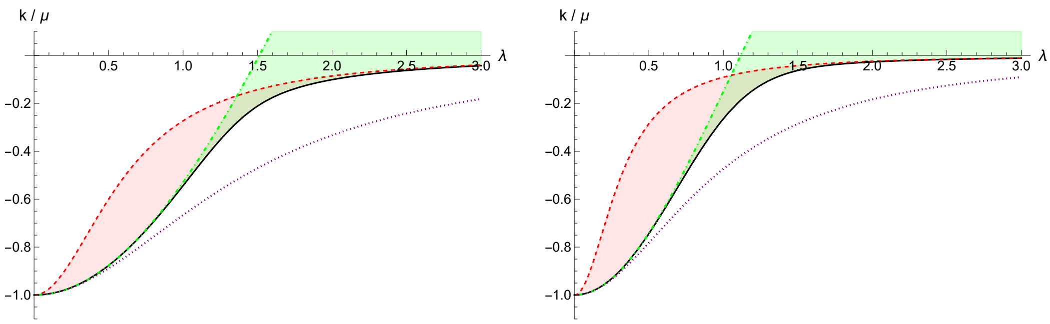

Figure 6. The upper and lower bound for the ground states with $\mu = 1.5$ (**left panel**) and $\mu = 0.4$ (**right panel**). The black solid lines are the exact quasi-energy of the ground states. The two upper bounds are e^l_{up} (red dashed line) and e^s_{up} (green dot-dash line), while the lower bound is e_g (purple dotted line) at the bottom right corner.

4. Discussion

The confluent Heun functions are used in both the semi-classical and quantum Rabi models, which is an interesting and noteworthy phenomenon. However, in these two cases, the relationship between the confluent Heun functions and the eigenvalue spectrum differs. In the semi-classical Rabi model, the eigenvalues q_α are expressed directly in terms of the confluent Heun functions as

$$q_\alpha = \frac{1}{\pi} \arcsin\left(\sqrt{2}\beta \text{Re}[\text{e}^{\text{i}g}\text{HC}(a_1^*; \frac{1}{2})\text{HC}(a_2; \frac{1}{2})] \right), \tag{48}$$

whereas in the quantum Rabi model, the eigenvalues $E = k - \lambda^2$ are determined as the zeros of a condition defined by the confluent Heun functions as

$$0 = \text{HC}(a_3; 1/2)/\Gamma(-k) \mp \mu\text{HC}(a_4; 1/2)/\Gamma(1-k). \tag{49}$$

In both cases, the special point $x = 1/2$ in confluent Heun functions $\text{HC}(a_i; x)$ is utilized, suggesting that this specific value $x = 1/2$ warrants further investigation. And we find that they are both related to the convergence at the singularity $x = 1$. In the semi-classical Rabi model, we ensure that the confluent Heun functions converge at $x = 1$ and take the value as

$$\text{HC}(a_1; x = 1) = \text{HC}^2(a_1; 1/2) - \frac{\beta^2}{2}\text{e}^{2\text{i}g}\text{HC}^2(a_2; 1/2). \tag{50}$$

In the quantum Rabi model, we find that the convergence of the confluent Heun function at $x = 1$ is a necessary condition for the energy E to be an eigenvalue. It should be clarified that the confluent Heun functions can also converge at $x = 1$ when E is not an eigenvalue. There are two modes of convergence. One mode in the semi-classical case is that $\mathrm{Re}(\delta) < 1$ ensures the convergence of the Heun confluent function. The other mode, relevant to the eigenvalue spectrum of the quantum Rabi model, requires the convergence to occur more rapidly, as the coefficients satisfy $b_n/b_{n-1} \sim -\epsilon/n$.

Within the convergence range of the function, we derive several useful identities. Among them, some have been obtained previously, while others are new and useful. In the semi-classical case, we obtain the following identity equation

$$e^{\epsilon x}\mathrm{HC}(q, \alpha; \gamma, \delta, \epsilon; x) = \mathrm{HC}(q - \gamma\epsilon, \alpha - \epsilon(\gamma + \delta); \gamma, \delta, -\epsilon; x), \tag{51}$$

which has also been presented in previous work [49]. In the quantum case, we obtain two identities as

$$k(1 - x)\mathrm{HC}'(a_3; x) = \mu^2\mathrm{HC}(a_4; x) - k^2\mathrm{HC}(a_3; x), \tag{52}$$

$$x\mathrm{HC}'(a_4; x) = (k - 4\lambda^2 x)\mathrm{HC}(a_4; x) - k\mathrm{HC}(a_3; x), \tag{53}$$

where $\mathrm{HC}'(a_i; x)$ represents the x-derivative of $\mathrm{HC}(a_i; x)$. Equations (52) and (53) above are identities involving the derivatives of the confluent Heun functions and have been used to simplify the Wronskian (33).

Our method can be generalized to handle more general cases. In the classical model, it can be extended to incorporate higher-order trigonometric functions, such as $\sin n\omega t$ and $\cos n\omega t$. From a theoretical perspective, based on the Fourier transform, such a series approximation can be applied to approximate any given function. Although this introduces additional complexity, it remains a feasible approach. In the quantum model, we can introduce multi-photon interactions, thereby enabling the expansion of our formalized matrix (24). Naturally, after such a modification, the resulting solution is no longer a Heun function; instead, it may correspond to the solution to a more complex equation. With a deeper understanding of the confluent Heun function, we hope to obtain explicit forms of eigenvalues in the future, which will require further research.

5. Conclusions

In conclusion, we establish the relationship between infinite-dimensional matrices and the Rabi model, and applying the confluent Heun functions, we present a unified approach to derive the eigenvalue spectrum of these unbounded matrices. For the first kind of matrix related to the semi-classical Rabi model, we obtain the explicit form of the eigenvalues, which is consistent with the previous approximate results. For the second kind of matrix related to the quantum Rabi model, we derive an explicit condition that the eigenvalue must satisfy. This condition is more concise than the previous results, and is valid to all situations. We have discussed the degeneracy of the energy spectrum, which aligns with the findings of previous studies. We obtain numerical upper and lower bounds in explicit forms for the eigenvalue, which fit well in the regimes where the interaction strength is either small or large.

The relationship between mathematics and physics is complementary since our approach actually solves the eigenvalue problem of infinite-dimensional unbounded matrices. We derive some identities involving the confluent Heun functions, which can not only be applied in the situation of this paper but also in many other related fields of mathematics and physics. The eigenvalues in the Rabi models are related to the special values of the confluent Heun functions and their convergence at the singular point $x = 1$. Our results enhance the understanding and potential applications of the Rabi model in quantum optics, quantum information, and condensed matter physics.

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Appendix A. Notations in This Paper

x^* represents the complex conjugate of x. $\mathrm{Re}[x]$ represents the real part of x, while $\mathrm{Im}[x]$ represents the imaginary part of x. The function $\arg(x)$ represents the argument of the complex number x. $\lfloor x \rfloor$ represents the floor function as $\lfloor x \rfloor = \max\{m \in \mathbb{Z} | m \leq x\}$. $J_0(x)$ is the first kind of the Bessel function of 0-order and $j_0(n)$ represents the n-th zero point of the Bessel function $J_0(x)$. $f(x_0^\pm)$ represents $f(x_0^\pm) \equiv \lim_{x \to x_0 + 0^\pm} f(x)$.

Appendix B. Key Derivations in the Semi-Classical Rabi Model

The Schrödinger equation is

$$\mathrm{i}\partial_t |\psi\rangle = H(t)|\psi\rangle = \left(\frac{\beta}{2}\sigma_x + \frac{g}{2}\sin(t)\sigma_z\right)|\psi\rangle, \tag{A1}$$

where $|\psi\rangle = (c_1, c_2)^{\mathrm{T}}$ is the normalized wave function. The Schrödinger equation can be written into two equations as

$$\mathrm{i}\frac{\partial c_1}{\partial t} - \frac{g}{2}c_1 \sin t = \frac{\beta}{2}c_2 \tag{A2}$$

$$\mathrm{i}\frac{\partial c_2}{\partial t} + \frac{g}{2}c_2 \sin t = \frac{\beta}{2}c_1 \tag{A3}$$

Then, after removing c_2 (or c_1), we obtain a second-order differential equation for c_1 (or c_2), as

$$\frac{\partial^2 c_1}{\partial t^2} + (\mathrm{i}\frac{g}{2}\cos t + \frac{g^2}{4}\sin^2 t + \frac{\beta^2}{4})c_1 = 0. \tag{A4}$$

Applying the change in the variable from t to $z = \frac{1}{2}(1 - \cos t) = \sin^2 \frac{t}{2}$, we can obtain (for $0 \leq t \leq \pi/2$)

$$\begin{aligned}
\cos t &= 1 - 2z && \text{(A5)}\\
|\sin t| &= \sin t = 2\sqrt{z(1-z)} && \text{(A6)}\\
\frac{\partial z}{\partial t} &= \frac{1}{2}\sin t = \sqrt{z(1-z)} && \text{(A7)}\\
0 &= z(1-z)\frac{\partial^2 c_1}{\partial z^2} + (\frac{1}{2} - z)\frac{\partial c_1}{\partial z} + (\mathrm{i}g(\frac{1}{2} - z) + g^2 z(1-z) + \frac{\beta^2}{4})c_1. && \text{(A8)}
\end{aligned}$$

By applying another transform $c_1 = \mathrm{e}^{-\mathrm{i}gz} f$, we can obtain

$$\frac{\partial c_1}{\partial z} = \frac{\partial}{\partial z}(\mathrm{e}^{-\mathrm{i}gz} f) = \mathrm{e}^{-\mathrm{i}gz}(\frac{\partial f}{\partial z} - \mathrm{i}gf) \tag{A9}$$

$$\frac{\partial^2 c_1}{\partial z^2} = \frac{\partial}{\partial z}\left(\mathrm{e}^{-\mathrm{i}gz}(\frac{\partial f}{\partial z} - \mathrm{i}gf)\right) = \mathrm{e}^{-\mathrm{i}gz}\left(-g^2 f - 2\mathrm{i}g\frac{\partial f}{\partial z} + \frac{\partial^2 f}{\partial z^2}\right) \tag{A10}$$

$$z(1-z)\left(-g^2 f - 2\mathrm{i}g\frac{\partial f}{\partial z} + \frac{\partial^2 f}{\partial z^2}\right)+ \\ (\frac{1}{2} - z)(\frac{\partial f}{\partial z} - \mathrm{i}gf) + +(\mathrm{i}g(\frac{1}{2} - z) + g^2 z(1-z) + \frac{\beta^2}{4})f = 0 \tag{A11}$$

$$z(1-z)\frac{\partial^2 f}{\partial z^2} + \left[(\frac{1}{2} - z) - 2\mathrm{i}gz(1-z)\right]\frac{\partial f}{\partial z} + (\mathrm{i}g(\frac{1}{2} - z) + \frac{\beta^2}{4} - (\frac{1}{2} - z)\mathrm{i}g)f = 0 \tag{A12}$$

$$z(z-1)\frac{\partial^2 f}{\partial z^2} + \left[-2\mathrm{i}gz(z-1) + (z - \frac{1}{2})\right]\frac{\partial f}{\partial z} + (-\frac{\beta^2}{4})f = 0. \tag{A13}$$

Then, we can obtain the differential equation as

$$z(z-1)\frac{\partial^2 f}{\partial z^2} + \left[\frac{1}{2}(z-1) + \frac{1}{2}z - 2\mathrm{i}gz(z-1)\right]\frac{\partial f}{\partial z} + (-\frac{\beta^2}{4})f = 0. \tag{A14}$$

Compared to the standard confluent Heun equation

$$z(z-1)y'' + [\gamma(z-1) + \delta z + z(z-1)\epsilon]y' + (\alpha z - q)y = 0, \tag{A15}$$

we obtain the coefficients $q = \frac{\beta^2}{4}$, $\alpha = 0$, $\gamma = \frac{1}{2}$, $\delta = \frac{1}{2}$, $\epsilon = -2\mathrm{i}g$. The solution that satisfies the confluent Heun equation is the confluent Heun function $H_C(q, \alpha; \gamma, \delta, \epsilon; z)$, with the initial condition $H_C(q, \alpha; \gamma, \delta, \epsilon; 0) = 1$ [30–32]. The confluent Heun function can be expressed as a standard power-series expansion around $z = 0$ as $\mathrm{HC}(q, \alpha; \gamma, \delta, \epsilon; z) = \sum_{n=0}^{\infty} b_n z^n$. The coefficients b_n are determined by the three-term recurrence relation $R_n b_n + Q_{n-1} b_{n-1} + P_{n-2} b_{n-2} = 0$ with the initial conditions $b_{-2} = b_{-1} = 0$ and $b_0 = 1$. Here, $R_n = n(n-1+\gamma)$, $Q_n = q - n(n-1+\gamma+\delta-\epsilon)$, and $P_n = -\alpha - \epsilon n$. Thus, the solution to Equation (A4) is

$$c_1(t) = \mathrm{e}^{-\mathrm{i}gz}\mathrm{HC}\left(\frac{\beta^2}{4}, 0; \frac{1}{2}, \frac{1}{2}, -2\mathrm{i}g; z\right) := \mathrm{e}^{-\mathrm{i}gz}\mathrm{HC}(a_1; z), \tag{A16}$$

where parameters $a_1 := \left(\frac{\beta^2}{4}, 0; \frac{1}{2}, \frac{1}{2}, -2\mathrm{i}g\right)$, and $z = \sin^2\frac{t}{2}$. Here, we choose the initial condition $c_1(t=0) = 1, c_2(t=0) = 0$.

From the symmetry of the Equations (A2) and (A3), we can see that except for g becoming $-g$, c_1 and c_2 have differential equations of the same form. Then, according to the initial condition $c_2(t=0) = 0$, we know that c_2 is the other linearly independent solution $z^{1-\gamma}\mathrm{HC}(q + (1-\gamma)(\epsilon - \delta), \alpha + (1-\gamma)\epsilon, 2-\gamma, \delta, \epsilon, z)$, which is

$$c_2(t) = \mathrm{i}^{\eta}\beta z^{1/2}\mathrm{e}^{\mathrm{i}gz}\mathrm{HC}\left(\frac{\beta^2 - 1}{4} + \mathrm{i}g, \mathrm{i}g; \frac{3}{2}, \frac{1}{2}, 2\mathrm{i}g; z\right) := \mathrm{i}^{\eta}\beta\sin\frac{t}{2}\mathrm{e}^{\mathrm{i}gz}\mathrm{HC}(a_2; z), \tag{A17}$$

where parameters $a_2 := \left(\frac{\beta^2-1}{4} + \mathrm{i}g, \mathrm{i}g; \frac{3}{2}, \frac{1}{2}, 2\mathrm{i}g\right)$, $z = \sin^2\frac{t}{2}$, and $\eta = 1 + 2\lfloor\frac{t-\pi}{T}\rfloor$ with the floor function $\lfloor x \rfloor$. Then, we can construct the time evolution operator as

$$U_1(t) = \begin{pmatrix} c_1(t) & -c_2(t)^* \\ c_2(t) & c_1(t)^* \end{pmatrix}. \tag{A18}$$

The question is whether U_1 or c_2 is discontinuous at the points $t = (2k+1)\frac{T}{2}, k \in \mathbb{Z}$. Hence, an alternative form of the evolution operator U_2 is required to ensure continuity at these junctures. According to the symmetry $H(t) = \sigma_x H(t - \frac{T}{2})\sigma_x$, we derive $U_2(t) = \sigma_x U_1(t - \frac{T}{2})\sigma_x$. By combining U_1 and U_2, the evolution of half a period is attainable as $U_{\frac{T}{2}} \equiv U(\frac{T}{2}, 0) = U_2^\dagger(\frac{T}{4})U_1(\frac{T}{4})$. We need three parameter functions as follows: $\phi_1 = \arg(c_1^* c_2)$, $\theta_1 = 2\arcsin|c_2|$, and $\gamma_1 = -\arg(c_1 c_2)$. Now, we can obtain the evolution over a complete period as $U_T = U_2(T^-)U_2^\dagger(0) = e^{i2\Theta\sigma_{\boldsymbol{n}}/2}$, where $\sigma_{\boldsymbol{n}} = \sin\Phi\sigma_x + \cos\Phi\sigma_y$, $\Phi = \phi_1(\frac{T}{2}^-)$, and $\Theta = \theta_1(\frac{T}{2}^-)$. This U_T represents a clockwise rotation by an angle 2Θ in the $\boldsymbol{n}$-direction. Consequently, the total time evolution operator can be expressed as

$$U(t, 0) = U_2(t - NT)U_2^\dagger(0)\mathrm{e}^{\mathrm{i}2N\Theta\sigma_{\boldsymbol{n}}/2}, \tag{A19}$$

where $N = \lfloor \frac{t}{T} \rfloor$ and $U_2^\dagger(0) = U_{\frac{T}{2}}$. Here, $U_{\frac{T}{2}}$ as $U_{\frac{T}{2}} = \mathrm{e}^{-\frac{1}{2}\mathrm{i}\Phi\sigma_z}\mathrm{e}^{-\frac{1}{2}\mathrm{i}\Theta\sigma_y}\mathrm{e}^{-\frac{1}{2}\mathrm{i}\Gamma\sigma_z}$, where $\Phi = \phi_1(\frac{T}{2}^-)$, $\Theta = \theta_1(\frac{T}{2}^-)$ and $\Gamma = \gamma_1(\frac{T}{2}^-)$ with the notation $f(x_0^\pm) \equiv \lim_{x \to x_0 + 0^\pm} f(x)$.

As compared to Floquet theory [25–28], there is one more rotation needed, which is $R_s = \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}\sigma_x}\mathrm{e}^{-\mathrm{i}\frac{\Phi}{2}\sigma_z}$. Then, we can obtain the operator $F(t)$ as

$$F(t) = R_s U R_s^\dagger = R_s U_2(t - NT)U_2^\dagger(0)R_s^\dagger \mathrm{e}^{\mathrm{i}N\Theta\sigma_z}. \tag{A20}$$

As we all can see, the characteristic value q_α should be

$$q_\alpha = \frac{\Theta}{T} = \frac{2\arcsin|c_2(\frac{T}{2}^-)|}{2\pi} \tag{A21}$$

$$= \frac{2}{\pi}\arcsin\left(\sqrt{2}\beta\mathrm{Re}[\mathrm{e}^{\mathrm{i}g}\mathrm{HC}^*(a_1; \frac{1}{2})\mathrm{HC}(a_2; \frac{1}{2})]\right) \tag{A22}$$

Appendix C. Perturbation Theory for the Ground State Energy

We use the perturbation theory to derive the explicit form for a small interaction strength λ. The Hamiltonian H of the system can be written as the sum of a solvable part H_0 (the unperturbed Hamiltonian) and a small perturbation V (the perturbing Hamiltonian):

$$H = H_0 + \lambda V, \tag{A23}$$

where λ is a small parameter controlling the strength of the interaction, $H_0 = a^\dagger a + \mu\sigma_z$, $V = \sigma_x(a^\dagger + a)$. The spectrum of the unperturbed Hamiltonian H_0 is $E^{(0)}_{n,\pm 1} = n \pm \mu$. Consider the odd subspace. The spectrum becomes $e_n^{(0)} = E_{n,(-1)^{n+1}} = n + (-1)^{n+1}\mu$, while the corresponding eigenstates are denoted as $|n\rangle$. In the representation of $|n\rangle$, the perturbation Hamiltonian V and the transformation matrix U can be expressed as

$$V_{i,j} = \langle i|V|j\rangle,\ U_{i,j} = \langle i|U|j\rangle. \tag{A24}$$

The transformation matrix U can also be expressed in the power series of λ as $U = \sum_{i=0}^{\infty} \lambda^i U^i$. The first-order perturbation term for the energy is shown as

$$e_n^{(1)} = \langle n|V|n\rangle = 0. \tag{A25}$$

and the second-order perturbation term for the energy is shown as

$$e_n^{(2)} = \sum_{l \neq n} \frac{V_{n,l}V_{l,n}}{e_n^{(0)} - e_l^{(0)}} = \frac{2\mu(-1)^n(2n-1)+1}{4\mu^2 - 1}. \tag{A26}$$

We observe that the odd-order perturbation of the energy is always zero. Here, we are concerned with the ground state, so we obtain the perturbation term of the ground energy with the sixth-order as

$$e_0^{(0)} = -\mu,\ e_0^{(2)} = -\frac{1}{1+2\mu},\ e_0^{(4)} = -\frac{2\mu}{(2\mu+1)^3},\ e_0^{(6)} = -\frac{4\mu\left(4\mu^2+4\mu-1\right)}{(2\mu+1)^5(2\mu+3)}. \tag{A27}$$

Then, we expand the equations in (46) and (47) when λ is small, which are

$$e_g = -\mu+\lambda^2-\frac{\lambda^2}{1+2\mu}-\frac{4\mu\lambda^4}{(2\mu+1)^2}+\frac{8\mu\lambda^6}{(2\mu+1)^3}+\mathrm{O}\left(\lambda^7\right), \tag{A28}$$

$$e_{\mathrm{up}}^s = -\mu+\lambda^2-\frac{\lambda^2}{1+2\mu}-\frac{2\mu\lambda^4}{(2\mu+1)^3}+\frac{2\mu\lambda^6}{(2\mu+1)^5}+\mathrm{O}\left(\lambda^7\right). \tag{A29}$$

Since $-\frac{4\mu\left(4\mu^2+4\mu-1\right)}{(2\mu+1)^5(2\mu+3)} < \frac{2\mu}{(2\mu+1)^5}$ when $\mu > 0$, we deduce that $e_g < E_0 + \lambda^2 < e_{\mathrm{up}}^s$ for small λ.

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