

Quantum Fisher information and polaron picture for identification of transition coupling in quantum Rabi model

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The quantum Rabi model (QRM) is a fundamental model for light-matter interactions. A fascinating feature of the QRM is that it manifests a quantum phase transition which is applicable for critical quantum metrology (CQM). Effective application for CQM needs the exact location of the transition point, however the conventional expression for the transition coupling is only valid in the extreme limit of low frequency, while apart from zero frequency an accurate location is still lacking. In the present work we conversely use the quantum Fisher information (QFI) in the CQM to identify the transition coupling, which finds out that transition coupling indeed much deviates from the conventional one once a finite frequency is turned on. Polaron picture is applied to analytically reproduce the numeric QFI. An accurate expression for the transition coupling is obtained by the inspiration from the fractional-power-law effect of polaron frequency renormalization. From the QFI in the polaron picture we find that the transition occurs around a point where the effective velocity and the susceptibility of the single-photon absorption rate reach maximum. Our result provides an accurate reference of transition couplings for quantum metrology at non-zero frequencies. The formulation of the QFI in the polaron picture also prepares an analytic method with an accurate compensation for the parameter regime difficult to access for the numerics. Besides the integer/fractional power law analysis to extract the underlying physics of transition, the QFI/velocity relation may also add some insight in bridging the QFI and transition observables.

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I. INTRODUCTION

In the modern research trends of light-matter interactions induced by both theoretical [1–4] and experimental [5, 6] progresses, few-body quantum phase transitions [4, 7–21] and topological phase transitions [15–19, 22] have recently arisen as a special focus. Applications for critical quantum metrology [23–27] have been proposed, with a great potential to become practical ultra-high-precision quantum technology in the contemporary era of ultra-strong coupling [5, 6, 28–41] and even deep-strong coupling [41–43].

A most fundamental prototype of light-matter interaction is the quantum Rabi model (QRM) [44–46] which contains both the rotating-wave terms [47, 48] and counter-rotating terms. In the ultra-strong coupling regime, it has been experimentally found that the counter-rotating terms are playing an indispensable role [33, 49], which brings more attention to the QRM. Theoretically, the milestone work [1] revealing the integrability of the QRM has inspired a massive dialogue [2] between mathematics and physics in light-matter interactions [1–26, 39, 44, 48–81, 84–101]. A fascinating feature of the QRM is that as a few-body system it possesses [4, 7–18, 20] a quantum phase transition (QPT) [102] which traditionally lies in condensed matter, despite that it might be a matter of taste to term the

transition quantum or not by considering the negligible quantum fluctuations in the photon vacuum state [11]. Indeed, the QPT in the QRM can be bridged to the thermodynamical limit via the universality of the critical exponent [12]. Moreover, extended versions of the QRM with anisotropy [12, 15–18, 49, 81–83] and Stark nonlinear coupling [17, 19, 56–58] also manifest single-qubit topological phase transitions [15–18], including both conventional ones [15–18] and unconventional ones [16–18], analogously to those in condensed matter [103–116]. The conventional topological phase transitions occur with gap closing, while the unconventional ones emerge unexpectedly in gapped situations either in level anti-crossing [18, 19] or completely without any tendency of gap closing [16, 17]. At this point it may be worthwhile to mention that finite-size QPTs can also occur with level crossing in other fields, e.g. in pairing-depairing models [117–119] and coupled fermion-boson models [120–122] where one also encounters transitions of topological structure in the energy spectrum [117–119] and the real space [117]. As a matter of fact, the finite system in lighter-matter interaction forms a mini-world of phase transitions [16]. The abundant physics in such a mini-world also brings conceptional renovations, e.g., universality and diversity as antagonists by nature can counter-intuitively support each other [16, 17]; it is also found that the conventionally incompatible symmetry-breaking Landau class of transitions [123] and symmetry-protected topological class of transitions [109–114] can coexist in a same system and even occur simultaneously [17, 19]. Favorably for practical applications the topological features

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are robust against the non-Hermiticity induced by decay rates and dissipation [22].

Unlike the topological phase transitions which emerge at finite frequencies [15–18], the QPT of the QRM occurs at low frequencies [4, 7–9, 11–17, 20]. The conventional expression for the QPT of the QRM was obtained in semi-classical approximation [7, 13, 14] which is valid only in the extreme limit of low frequency. However, in reality one always has a finite frequency in the practical systems. It has been found that the transition will shift away from the conventional transition coupling once one goes away from zero frequency and an improved scale of transition coupling was proposed [8]. Although the new scale of transition coupling can qualitatively better capture the transition coupling, a quantitatively accurate expression for the transition coupling is still lacking. On the other hand, the QPT of the QRM has been applied for critical quantum metrology [23–26] to achieve high precision bound of experimental measurements represented by the quantum Fisher information (QFI) [124–126, 128, 129]. Actually such applications depend on the knowledge of the exact location of the transition coupling beforehand, which in turn raises the requirement to know the accurate location of transition coupling. In such a situation, an accurate expression for the frequency dependence of the transition coupling of the QRM is highly desirable.

In the present work we conversely use the QFI in the quantum metrology to identify the transition coupling of the QRM. The result from the QFI shows that the transition couplings of the QRM indeed much deviate from the conventional expression of the transition coupling once a finite frequency is turned on. Besides the numerics by the exact diagonalization on the QFI, we also formulate the QFI in the variational polaron picture[8] to analytically reproduce the numeric results of the QFI. An accurate expression for the transition coupling is obtained by the inspiration from the fractional-power-law effect of polaron frequency renormalization. From the QFI in the polaron picture we find that the transition occurs around a point where the effective polaron velocity and the susceptibility of the single-photon absorption rate reach their maxima. Our results provide an accurate reference of transition couplings for quantum metrology at non-zero frequencies. The QFI in the polaron picture also provides an accurate compensation for the parameter regime where the exact diagonalization can not access due to demanding requirement of large basis cutoff. Our analysis may also add some insight for the bridge of the QFI and the transition properties.

The paper is organized as follows. Section II introduces the QRM. Section III shows the deviation of the conventional transition coupling at non-zero frequencies. Section IV presents the QFI with numerical identification and analytical expressions for accurate transition coupling. Section V is devoted for formulation of the QFI in the polaron picture. The general expression of the QFI is simplified by a finding of a vanishing term. Maximum effective velocity is shown around the tran-

sition identified by the QFI. Section VII demonstrates the transition coincidence with the maximum susceptibility of single-photon absorption rate. Finally Section VII gives a summary of conclusions.

II. MODEL AND SYMMETRY

The QRM [44–46] takes the following form

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

which describes the coupling between a bosonic mode with frequency ω and a qubit represented by the Pauli matrices $\sigma_{x,y,z}$. Here we have adopted the spin notation as in Ref.[55], in which $\sigma_z = \pm$ conveniently represents the two flux states in the flux-qubit circuit system[132], while superconducting circuit systems can realize ultra-strong coupling [5, 6, 28–38, 41] and even deep-strong coupling [41, 42], respectively with coupling strength g beyond 0.1ω and 1.0ω . The operator $a^\dagger$ (a) creates (annihilates) a boson and $a^\dagger a$ is the boson (photon) number. In the conventional spin notation Ω is the level splitting. One can retrieve the conventional notation by a spin rotation $\{\sigma_x, \sigma_y, \sigma_z\} \rightarrow \{\sigma_z, -\sigma_y, \sigma_x\}$ around the axis $\vec{x} + \vec{z}$.

By transformation $a^\dagger = (\hat{x} - i\hat{p})/\sqrt{2}$, $a = (\hat{x} + i\hat{p})/\sqrt{2}$, where x and $\hat{p} = -i\frac{\partial}{\partial x}$ are the effective position and momentum, we can rewrite the Hamiltonian in position space

$$H = \sum_{\sigma_z = \pm} h_{\sigma_z} |\sigma_z\rangle \langle \sigma_z| + \frac{\Omega}{2} \sum_{\sigma_z = \pm} |\sigma_z\rangle \langle \bar{\sigma}_z| \quad (2)$$

where $\sigma_z = -\bar{\sigma}_z = \pm$ represents the spin state in z direction. Here $h_{\sigma_z} = \frac{\omega}{2} \hat{p}^2 + v_{\sigma_z}(x)$ is effective single-particle Hamiltonian in the spin-dependent potential $v_{\sigma_z}(x) = \omega(x + \tilde{g}\sigma_z)^2/2 + \varepsilon_0^z$ with a constant energy $\varepsilon_0^z = -\frac{1}{2}[\tilde{g}^2 + 1]\omega$. Indeed x and p can be represented by the flux and charge of Josephson junctions in circuit systems [132, 133]. In such a representation the coupling plays a role to separate the potential in opposite directions with a displacement denoted by the rescaled coupling $\tilde{g} = \sqrt{2}g/\omega$. The Ω term now acts as spin flipping in σ_z space or tunneling in position space [8, 55].

The model possesses the parity symmetry $\hat{P} = \sigma_x(-1)^{a^\dagger a}$ which commutes with the Hamiltonian. The parity symmetry leads to an antisymmetric ground-state wave function under exchange of spin and inversion of position simultaneously, which will simplify our formulation.

III. CONVENTIONAL TRANSITION COUPLING AND DEVIATIONS AT NON-ZERO FREQUENCIES

The QRM manifests a quantum phase transition[4, 7–18, 20] at a critical point which has a conventional loca-

tion at

$$g_{c0} = \frac{\sqrt{\omega\Omega}}{2}. \quad (3)$$

Note here that g_{c0} is frequency-dependent. However, in reality this expression of g_{c0} is exact only in the extreme limit of low frequency. It has been found that the transition will shift away from g_{c0} at finite frequencies and a new scale of transition coupling was proposed as [8]

$$g_{c1} = \sqrt{\omega^2 + \sqrt{\omega^4 + g_{c0}^4}} \quad (4)$$

which better captures the transition at finite frequencies.

Figures 1(a) and 1(b) compare the frequency dependence of g_{c0} (orange dotted line) and g_{c1} (green (light gray) solid line) in linear scale and logarithmic scale of the frequency ratio ω/Ω . From Fig. 1(b) one sees that g_{c0} and g_{c1} coincide at $\omega/\Omega = 0$, while they depart from each other immediately once the frequency is turned on to any finite value. This indicates that g_{c0} may be inaccurate even at the very low frequencies except right at zero frequency, which turns out to be true as in comparison with the result of the QFI (dots, later addressed in next section). In practice, the bosonic mode in the light-matter interaction has a non-zero frequency, the inaccuracy of g_{c0} at non-zero frequencies would hinder the application, especially when high precision is the goal of quantum metrology which in turn requires the knowledge of accurate location of the transition coupling. On the other hand, although g_{c1} yields a qualitative improvement in scale estimation of the transition coupling, a quantitatively more accurate transition coupling is still lacking. We shall obtain an accurate transition coupling g_{c2} by a combination of the QFI and the polaron picture in the following section.

IV. QUANTUM FISHER INFORMATION (QFI) AND ACCURATE FREQUENCY DEPENDENCE OF TRANSITION COUPLING

A. QFI for quantum phase transition

In measurements the precision of any experimental estimation of the parameter λ in the Hamiltonian is bounded by $F_Q^{1/2}$ [124]. Here F_Q is the QFI [124–126] which takes the following form for pure states

$$F_Q = 4 \left[\langle \psi'(\lambda) | \psi'(\lambda) \rangle - \langle \psi'(\lambda) | \psi(\lambda) \rangle \langle \psi(\lambda) | \psi'(\lambda) \rangle \right], \quad (5)$$

where $'$ denotes the derivative of the ground state $|\psi(\lambda)\rangle$ of H with respect to λ . So the QFI is the precision criteria quantity in quantum metrology, with higher QFI meaning higher measurement precision. Around a QPT the ground-state wave function is varying quickly, which provides a sensitivity resource for the so-called critical quantum metrology [23–26], with the a maximum QFI

(thus a maximum measurement precision) available at the QPT.

On the other hand, actually $\chi_F = F_Q/4$ is the susceptibility of the fidelity [129–131]

$$F = |\langle \psi(\lambda) | \psi(\lambda + \delta\lambda) \rangle| = 1 - \frac{\delta\lambda^2}{2} \chi_F \quad (6)$$

in an infinitesimal variation $\delta\lambda$ of the parameter λ . The fidelity can be a basic quantity to characterize the QPT [127–131], with a peak of the fidelity susceptibility being a transition signal.

B. QFI of the QRM

From both points of view of the critical quantum metrology and the fidelity theory of the QPT, we can utilize the QFI F_Q to identify the QPT in the QRM. Here the coupling g is taken as the parameter for λ . Figure 2 shows the evolution of F_Q , numerically obtained by the method of exact diagonalization (ED) [14, 18], in the variation of the coupling g . Here in panel (a) of the figure F_Q is scaled by its maximum $F_Q^{\max}$ at each fixed frequency ratio ω/Ω . We see that F_Q indeed has a peak, which is located at g_{c0} in the extreme limit of low frequency $\omega/\Omega \rightarrow 0$ but moves to larger relative coupling $\bar{g} = g/g_{c0}$ once the frequency is raised from zero. We denote as g_{cF} for the transition coupling identified by the location of $F_Q^{\max}$. The result confirms the inaccuracy of g_{c0} and the shift of the transition away from g_{c0} for any finite frequency. The evolutions of the peak position and the peak value $F_Q^{\max}$ can be seen more clearly from the black dots in Fig. 2b where F_Q is un-rescaled. Here the logarithmic plot of F_Q indicates the large values of the QFI around $F_Q^{\max}$, which is favorable for the quantum metrology.

C. Accurate transition coupling of the QRM

As afore-mentioned in Sec. III, the frequency dependence of the conventional transition coupling g_{c0} has large deviations from the beginning in going away from zero frequency and the improved one g_{c1} is not either accurate enough even at low frequencies. Actually g_{c0} can be equivalently obtained by a semiclassical approximation which assumes a mass of point as the classical particle in the effective field for the spatial part while keeping quantum character for the spin part [13, 14]. It is the classical treatment in the spatial part that leads to the deviation, since in full quantum mechanical picture the particle should appear as a wave packet for spatial distribution instead of a point of mass. As an improvement g_{c1} considers the spatial wave packet in the polaron picture, however as an analytical simplification the frequency renormalization of the polarons has not been included [8].

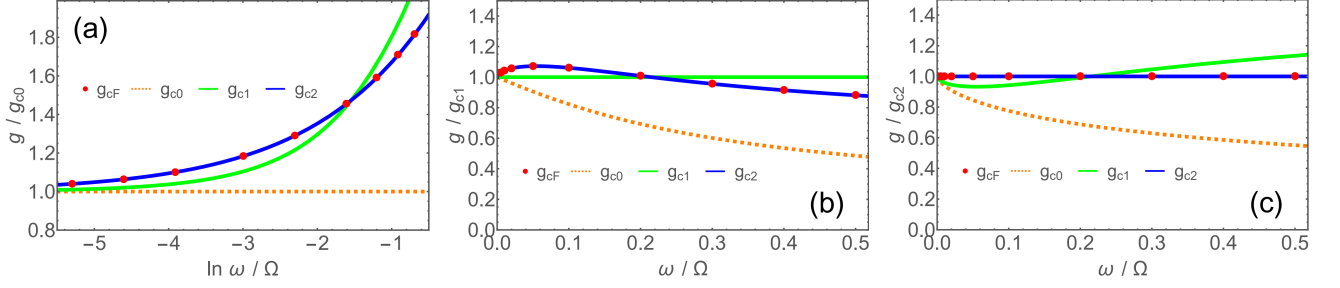


FIG. 1. Frequency dependence of transition coupling g_c in different expressions. (a) g_c scaled by g_{c0} in natural logarithm of frequency ratio ω/Ω . (b) g_c scaled by g_{c1} versus ω/Ω . (c) g_c scaled by g_{c2} . Here g_{cF} (black dots) as the reference of accurate transition coupling is numerically extracted from position of $F_Q^{\max}$, while g_{c0} (orange dotted line) is the conventional transition coupling in (3), g_{c1} (green (light gray) solid line) is the transition coupling in polaron picture in (4), and finally g_{c2} (blue (dark gray) solid line) is the analytical transition coupling obtained from $F_Q^{\max}$ in (7).

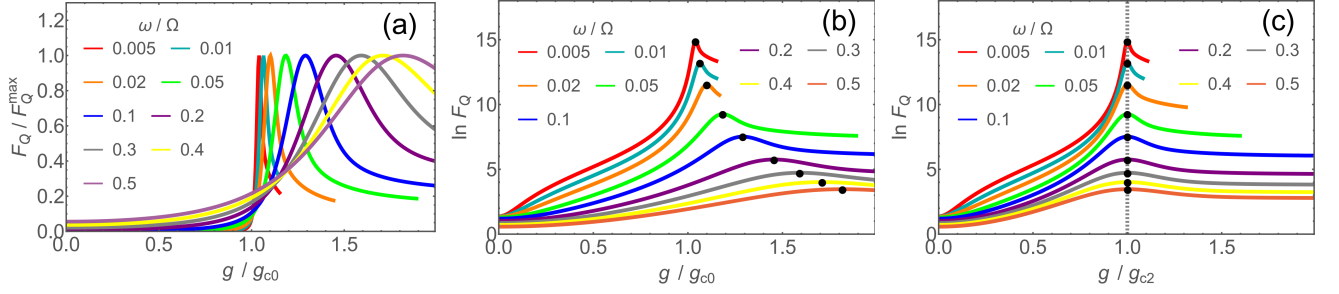


FIG. 2. Quantum Fisher information F_Q with respect to coupling g at different frequency ratios ω/Ω . (a) F_Q renormalized by its maximum (peak value) $F_Q^{\max}$. (b) F_Q with maximum $F_Q^{\max}$ (black dots) in natural logarithm. (c) F_Q with maximum positions (black dots) re-aligned in a vertical line in a scaling g/g_{c2} by the accurate transition coupling g_{c2} in (7). Here F_Q is numerically obtained by exact diagonalization (ED) for $\omega/\Omega = 0.005, 0.01, 0.02, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5$ from left to right in (a) and from upper to lower in (b).

Indeed, as demonstrated in Appendix A, when the frequency renormalization of the polarons is picked up one gets a correct direction for further improvement of the transition coupling as $g_{c\xi}$. It turns out that the frequency renormalization effect enters in the improvement of the transition coupling in a form of fractional power low $\omega^{2n/3}$ of the frequency as in (A11).

Although $g_{c\xi}$ is still not accurate enough due to the analytical simplification, it inspires us to propose accurate expressions with adjusted coefficients from $g_{c\xi}$. To the second order we find

$$g_{c2} = g_{c0} \left[1 + \frac{1}{100\alpha_{\text{FS}}} \left(\frac{\omega}{\Omega} \right)^{2/3} - \frac{1}{8} \left(\frac{\omega}{\Omega} \right)^{4/3} \right], \quad (7)$$

where $\alpha_{\text{FS}} = 1/137$ by coincidence is the fundamental fine-structure constant in quantum mechanics, works very accurately in $\omega/\Omega \in [0, 0.5]$ regime by comparison with the numerical g_{cF} , as one sees in Fig. 1(a-c) and Fig. 2(c). Another second-order expression

$$g_{c2} = g_{c0} \left[1 + \frac{4}{3} \left(\frac{\omega}{\Omega} \right)^{2/3} - \frac{3}{40} \left(\frac{\omega}{\Omega} \right)^{4/3} \right], \quad (8)$$

can extend the validity up to $\omega/\Omega = 3.0$ with a small price of larger error than (7) in order 10^{-3} in $\omega/\Omega \in$

$[0, 0.5]$. These expressions are extracted by coefficient fractionization in second-order least-squares fitting. If one keeps decimalized coefficients, a fitting expression in the third order

$$g_{c2}^{\text{fitting}} = g_{c0} \left[1 + c_1 \left(\frac{\omega}{\Omega} \right)^{2/3} + c_2 \left(\frac{\omega}{\Omega} \right)^{4/3} + c_3 \left(\frac{\omega}{\Omega} \right)^{6/3} \right], \quad (9)$$

with $c_1 = 1.3715$, $c_2 = -0.1311$, $c_3 = 0.0184$ can capture the maximum point of F_Q accurately in the entire frequency regime up to $\omega/\Omega = 3.0$, though the transition becomes a crossover in high frequencies. A comparison with the ED result in low-frequency regime and high-frequency regime is provided in Appendix B. Despite that g_{c2}^{fitting} has a wider range for accuracy of the position of $F_Q^{\max}$, the expression g_{c2} in (7) and (8) is easier to remember with the fractionized coefficients (rather than decimalized) and it has the same accuracy as g_{c2}^{fitting} in the low-frequency regime where the transition makes more sense.

At this point one might speculate that a Fourier expansion with integer powers of the frequency $(\omega/\Omega)^n$ should also work without need of the fractional-power form. However, as demonstrated in Appendix A5, such a Fourier-expansion fitting is very inefficient while fractional-power fitting already reaches a good conver-

gence with only a couple of orders, without mentioning that such a Fourier expansion does not provide any physical insight if it were not coinciding with integer-power-series law of g_{c1} as in Eq. (A13). This indicates that the integer-power law in the Fourier expansion does not capture the physical essence of frequency renormalization around the transition in the QRM.

The accurate transition coupling g_{c2} should be useful in applications of the quantum metrology as in practice the frequency is non-zero. Even if the transition becomes more broadened at a higher frequency, g_{c2} still can provide an accurate location for the maximum QFI where one can find relatively the highest measurement precision in variation of the coupling despite that one does not achieve an ideal divergence.

V. POLARON PICTURE FOR QFI

As afore-mentioned, the above result of the QFI at finite frequencies is numerically obtained by the method of ED [14, 18] which needs a cutoff of the basis number. In the presence of a large coupling at low frequencies such a basis number might be divergently large, which might lead to a heavy computation cost and even goes beyond the numerical access limit. In such a situation an analytical form for the QFI would be desirable. The variational method of polaron picture (PP) [8] provides such a possibility with high accuracy over the entire coupling regime including the transition area. The validity of the PP is not limited by the frequency and it often facilitates the understanding of underlying physics in light-matter interactions [4, 8, 13–17, 69, 70]. In this section we shall formulate the QFI of the QRM in the PP.

A. Formulation of QFI in polaron picture

The eigen wave function of the QRM has two spin components

$$|\psi(\bar{g})\rangle = \frac{1}{\sqrt{2}} \sum_{\sigma_z=\pm} \psi_{\sigma_z}(\bar{g}) |\sigma_z\rangle \quad (10)$$

subject to the normalization condition

$$\langle\psi(\bar{g})|\psi(\bar{g})\rangle = \frac{1}{2} \sum_{\sigma_z=\pm} \langle\psi_{\sigma_z}(\bar{g})|\psi_{\sigma_z}(\bar{g})\rangle = 1. \quad (11)$$

Equivalently $\langle\psi_{\sigma_z}(\bar{g})|\psi_{\sigma_z}(\bar{g})\rangle = 1$ and the inner product can be written in integral form $\langle\psi_{\sigma_z}(\bar{g})|\psi_{\sigma_z}(\bar{g})\rangle = \int dx \psi_{\sigma_z}^*(\bar{g}, x) \psi_{\sigma_z}(\bar{g}, x)$ in the position space. Here we have defined the scaled coupling $\bar{g} = g/g_{c0}$, while the QFI with respect to g simply differs by a factor

$$F_Q(g) = F_Q(\bar{g}) \left(\frac{d\bar{g}}{dg} \right)^2 = \frac{1}{g_{c0}^2} F_Q(\bar{g}). \quad (12)$$

In the following we formulate the QFI $F_Q(\bar{g})$ with respect to $\bar{g}$ in the PP.

In the variational PP each spin component of the wave function can be decomposed into a linear combination of polarons represented by φ_i

$$\psi_+(\bar{g}, x) = \sum_{i=\alpha, \beta} w_i(\bar{g}) \varphi_i(\bar{g}, x) \quad (13)$$

$$\psi_-(\bar{g}, x) = P\psi_+(\bar{g}, -x) \quad (14)$$

where $P = -1$ is the negative parity for the ground state. Explicitly the polaron in the ground state takes the form of Gaussian wave packet

$$\varphi_i(\bar{g}, x) = (\xi_i/\pi)^{1/4} \exp \left[-\xi_i (x + x_i)^2 / 2 \right] \quad (15)$$

with polaron displacement $x_i = \zeta_i g'$, as renormalized from the potential displacement g' by ζ_i , and the frequency renormalization factor ξ_i [8]. The frequency renormalization gives a more compact representation of polarons than the coherent state expansion[86] and in Appendix A we also see that the frequency renormalization yields an correct direction for improvement of the transition coupling.

Here we have adopted the two-polaron decomposition [8] for the ground state of the QRM with the weights

$$w_\alpha(\bar{g}) = \alpha, \quad w_\beta(\bar{g}) = \beta. \quad (16)$$

The two-polaron decomposition with frequency renormalization is already accurate enough for our discussion and convenient for physical descriptions, although extension to multi-polaron representation is direct and might gives some small quantitative improvements[69].

The two terms in F_Q are then obtained by

$$\begin{aligned} & \langle\psi'(\bar{g})|\psi(\bar{g})\rangle \\ &= \sum_{i,j} [w_i(\bar{g}) w_j(\bar{g}) \langle\varphi'_i|\varphi_j\rangle + w'_i(\bar{g}) w_j(\bar{g}) \langle\varphi_i|\varphi_j\rangle] \end{aligned} \quad (17)$$

and

$$\begin{aligned} & \langle\psi'(\bar{g})|\psi'(\bar{g})\rangle \\ &= \sum_{i,j} [w_i(\bar{g}) w_j(\bar{g}) \langle\varphi'_i|\varphi'_j\rangle + w'_i(\bar{g}) w'_j(\bar{g}) \langle\varphi_i|\varphi_j\rangle] \\ &+ \sum_{i,j} [w_i(\bar{g}) w'_j(\bar{g}) \langle\varphi'_i|\varphi_j\rangle + w'_i(\bar{g}) w_j(\bar{g}) \langle\varphi_i|\varphi'_j\rangle] \end{aligned} \quad (18)$$

The first-order derivative terms of the inter products include the variations of displacement and frequency renormalization with respect to the coupling

$$\langle\varphi'_i|\varphi_j\rangle = \left\langle \frac{\partial\varphi_i}{\partial x_i} \middle| \varphi_j \right\rangle \frac{dx_i}{d\bar{g}} + \left\langle \frac{\partial\varphi_i}{\partial \xi_i} \middle| \varphi_j \right\rangle \frac{d\xi_i}{d\bar{g}}. \quad (19)$$

and the second-order derivative terms collect their quadratic mixture

$$\begin{aligned} \langle\varphi'_i|\varphi'_j\rangle &= \left\langle \frac{\partial\varphi_i}{\partial x_i} \middle| \frac{\partial\varphi_j}{\partial x_j} \right\rangle \frac{dx_i}{d\bar{g}} \frac{dx_j}{d\bar{g}} + \left\langle \frac{\partial\varphi_i}{\partial x_i} \middle| \frac{\partial\varphi_j}{\partial \xi_j} \right\rangle \frac{dx_i}{d\bar{g}} \frac{d\xi_j}{d\bar{g}} \\ &+ \left\langle \frac{\partial\varphi_i}{\partial \xi_i} \middle| \frac{\partial\varphi_j}{\partial x_j} \right\rangle \frac{d\xi_i}{d\bar{g}} \frac{dx_j}{d\bar{g}} + \left\langle \frac{\partial\varphi_i}{\partial \xi_i} \middle| \frac{\partial\varphi_j}{\partial \xi_j} \right\rangle \frac{d\xi_i}{d\bar{g}} \frac{d\xi_j}{d\bar{g}} \end{aligned} \quad (20)$$

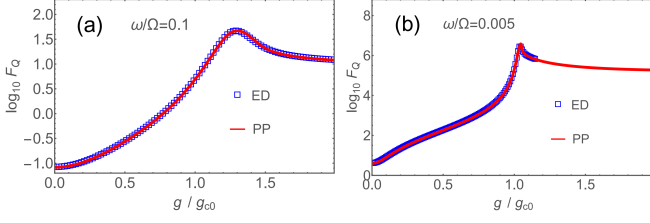


FIG. 3. Comparison of F_Q for the ED (symbols) and the variational method of polaron picture (PP) (solid lines). (a) $\omega/\Omega = 0.1$. (b) $\omega/\Omega = 0.005$. The missing data in (b) indicates the numerical difficulty for the ED in low frequencies and large couplings, while it is readily accessible and compensated by the variational PP.

The expressions for $\langle \varphi'_i | \varphi_j \rangle$, $\langle \varphi'_i | \varphi'_j \rangle$, $dx_i/d\bar{g}$ and $d\xi_i/d\bar{g}$ are explicitly available as provided in Appendix C.

B. Accuracy of QFI in polaron picture and compensation for ED

The result of the QFI in the PP is quite accurate and also provides a compensation for the ED in case that the ED leads to an overload of computation cost due to the need of large cutoff of basis number. Indeed, as illustrated by Fig.3, the PP (solid lines) basically reproduces the ED results (circles) of the QFI in the entire regime of coupling. Note here the ED can go deep into the large coupling regime beyond the transition for the frequency $\omega/\Omega = 0.1$ in Fig.3(a), while access to large couplings by the ED might become difficult at low frequencies as indicated by the missing data at $\omega/\Omega = 0.05$ in Fig.3(b). Nevertheless, with the accuracy guaranteed, as checked in the ED-accessible regime, the missing data in the inaccessible regime for the ED can be readily compensated by the result of the PP as demonstrated by the extended solid line in Fig.3(b). Thus, the formulation of the QFI in the PP provides an accurate and convenient tool without heavy cost of computation to cover the entire parameter regime.

C. Vanishing $\langle \psi'(\lambda) | \psi(\lambda) \rangle$ term

From the convenient analysis in the PP we come across the vanishing of the first derivative term in the QFI

$$\langle \psi'(\bar{g}) | \psi(\bar{g}) \rangle = 0. \quad (21)$$

We find this consequence stems from the non-degeneracy of the eigenstate of the QRM. Actually we can prove more generally for a parameter λ that the vanishing relation

$$\langle \psi'(\lambda) | \psi(\lambda) \rangle = 0 \quad (22)$$

holds for a general non-degenerate state $\psi(\lambda)$. Indeed, we can always choose the general $\psi(\lambda)$ to be real

$$\psi^*(\lambda, x) = \psi(\lambda, x) \quad (23)$$

at any position x , up to an irrelevant total phase, since otherwise supposed linear-independent real part and imaginary part of a complex wave function would yield degenerate eigenstates contradictorily to the non-degenerate assumption. Thus, with the real wave function, we have

$$\begin{aligned} \frac{d}{d\lambda} \langle \psi(\lambda) | \psi(\lambda) \rangle &= \langle \psi'(\lambda) | \psi(\lambda) \rangle + \langle \psi(\lambda) | \psi'(\lambda) \rangle \\ &= 2\langle \psi'(\lambda) | \psi(\lambda) \rangle. \end{aligned} \quad (24)$$

On the other hand, from the normalization condition $\langle \psi(\lambda) | \psi(\lambda) \rangle = 1$ we have $\frac{d}{d\lambda} \langle \psi(\lambda) | \psi(\lambda) \rangle = 0$, which leads to $\langle \psi'(\lambda) | \psi(\lambda) \rangle = 0$ in combination with Eq. (24). As a result, we can simplify the QFI with respect to a single parameter λ as

$$F_Q = 4\langle \psi'(\lambda) | \psi'(\lambda) \rangle \quad (25)$$

for non-degenerate eigen states.

D. Maximum effective velocity around transition

The transition coupling identified by the QFI is then determined by the peak position

$$\frac{dF_Q(\bar{g})}{d\bar{g}} = 4 \frac{d\langle \psi'(\bar{g}) | \psi'(\bar{g}) \rangle}{d\bar{g}} = 0, \quad (26)$$

where we have taken Eq. (22) into account to use (25).

In the polaron picture essentially the process of the transition in the ground state of the QRM is the splitting or separating of the polarons under the competition of the tunneling energy and the potential energy. The tunneling energy between the two spin components is negative in the negative parity, while the potentials $v_{\sigma_z}(x)$ in (2) have different values for the two spin components as they are separated by the effective coupling $\tilde{g}$. When the tunneling energy is dominant the polarons tend to stay around the origin $x = 0$ to gain a maximum negative tunneling energy, otherwise when the potential cost is too high to stay around the origin the polarons leave the origin and the transition occurs. Such a picture of transition agrees with the ED result in Figure 4(b).

Note tunneling energy is proportional to the overlap of the polarons, while the frequency renormalization can extend the polaron wavepackets to increase the overlap. Around the transition the polaron frequency nearly reaches the maximum renormalization to keep the remnant tunneling energy as much as possible, with $\xi'_i(\bar{g}) \approx 0$ around the transition [8]. On the other hand, around and beyond the transition the overlap between the separated polarons becomes exponentially small. As an approximation we can neglect the effect of weight variation in the polaron splitting due to the insight that the weight lost in one polaron would go to the other polaron, which may not much affect the variation of the total contribution of the wave function to the QFI. As another simplification

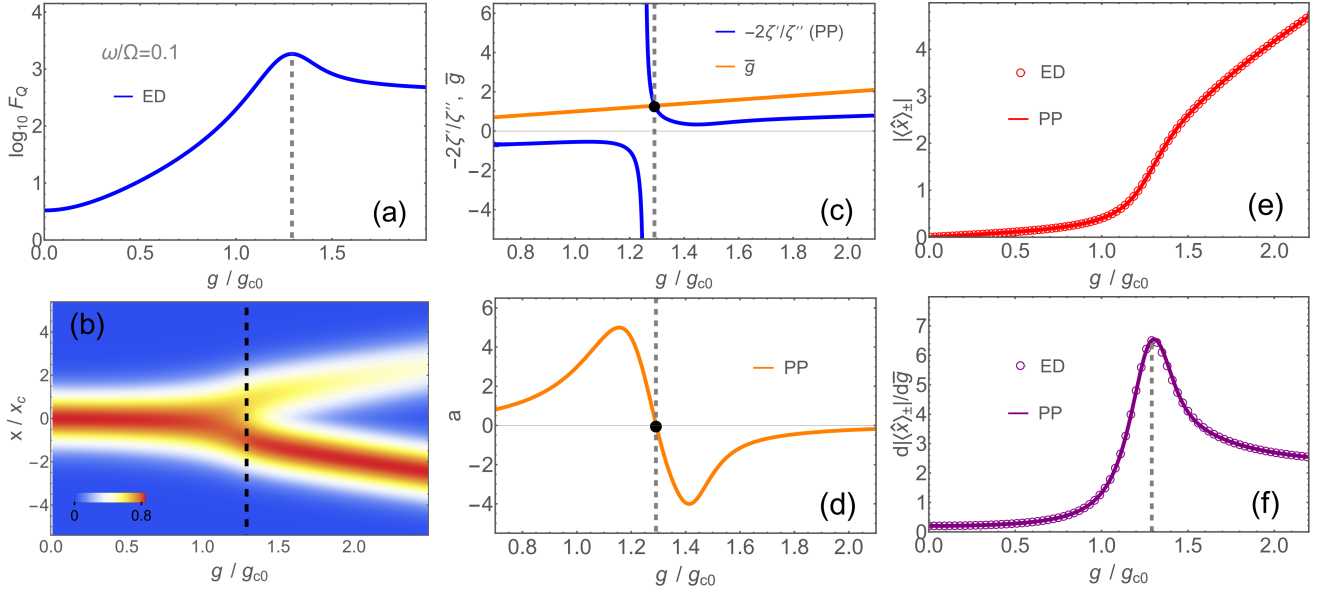


FIG. 4. Bridge of the QFI and transition property around the transition. (a) The transition position in F_Q (solid line). (b) The distribution probability in spin-up component. (c) Transition coupling by crossing point (black dot) of g (orange (light gray) solid line) and $-2\zeta'/\zeta''$ in (28). (d) Polaron acceleration a versus g . (e) The spin-component displacement expectation $\langle \hat{x} \rangle_{\pm}$. The PP (solid line) yields a same result as the ED (circles). (f) The spin-component displacement velocity $d\langle \hat{x} \rangle_{\pm}/dg$. Here $\omega/\Omega = 0.1$ and the vertical dashed lines in all panels mark the transition coupling at $F_Q^{\max}$. The $a = 0$ point (black dot) in (d) indicates the maximum polaron velocity at transition similarly to the expectation in (f).

we assume the same frequency renormalization ξ and displacement renormalization magnitude ζ for the separating polarons. Under all these considerations, the QFI around the transition is simplified to be

$$F_Q(\bar{g}) \approx \frac{\Omega}{\omega} [\zeta'(\bar{g})\bar{g} + \zeta(\bar{g})]^2 \xi(\bar{g}) \quad (27)$$

in the leading order. Then from Eq. (26) we find the transition coupling in the PP

$$\bar{g}_{cF}^{PP} = \frac{2\zeta'(\bar{g})}{-\zeta''(\bar{g})}. \quad (28)$$

Here we have defined the derivatives $\zeta'(\bar{g}) = \frac{d}{d\bar{g}}\zeta(\bar{g})$ and $\zeta''(\bar{g}) = \frac{d^2}{d\bar{g}^2}\zeta(\bar{g})$.

The solution (28) can be re-arranged to be

$$\frac{d^2}{d\bar{g}^2}(\zeta\bar{g}) = 0. \quad (29)$$

Note $\tilde{g} = \sqrt{2}g/\omega$ is the potential position and $x_p = \zeta\tilde{g}$ is the polaron displacement, thus it is also equivalent to

$$a \equiv \frac{d^2}{dg^2}x_p = 0. \quad (30)$$

If we vary g with a uniform speed, a is actually the effective acceleration of the polaron in the increase of the coupling up to a square factor of the increasing speed of the coupling. In such a sense, the transition condition

(30) means a vanishing polaron acceleration or the maximum polaron velocity (the first derivative dx_p/dg with respect to the increase of the coupling).

In turn, when we recall the relation (27), the FQI around the transition is then endowed a more physical connotation to be a renormalized effective kinetic energy

$$F_Q(\bar{g}) \approx \frac{1}{2}m_F\bar{v}_p^2 \quad (31)$$

with renormalized mass, position and velocity $m_F, \bar{x}_p, \bar{v}_p$:

$$m_F = 2\frac{\Omega}{\omega}\xi(\bar{g}), \quad \bar{v}_p = \frac{d\bar{x}_p}{d\bar{g}}, \quad \bar{x}_p = \zeta\bar{g}. \quad (32)$$

Figure 4 illustrates an example at $\omega/\Omega = 0.1$ to show the validity of the relations (28) and (30). Here in the figure panel (a) shows the QFI in logarithm numerically calculated by the ED, with the vertical dashed line marking the transition coupling g_{cF} . Panel (b) shows the distribution probability by the ED, one sees that the wave packet stays around the origin $x = 0$ before the transition while it splits into two wave packets and depart from each other after the transition. The wave packets represent the polarons. Panel (c) shows the crossing point (black dot) of the $\bar{g}$ line and the curve of $2\zeta'(\bar{g})/[-\zeta''(\bar{g})]$ in (28) by the main polaron with a larger weight α , which is the solution for $\bar{g}_{cF}^{PP}$. We see that $\bar{g}_{cF}^{PP}$ is in good agreement with the accurate g_{cF} (vertical dashed line). Panel (d) tracks the corresponding evolution of the polaron acceleration a , the zero point (black dot) also matches well with the transition coupling g_{cF} .

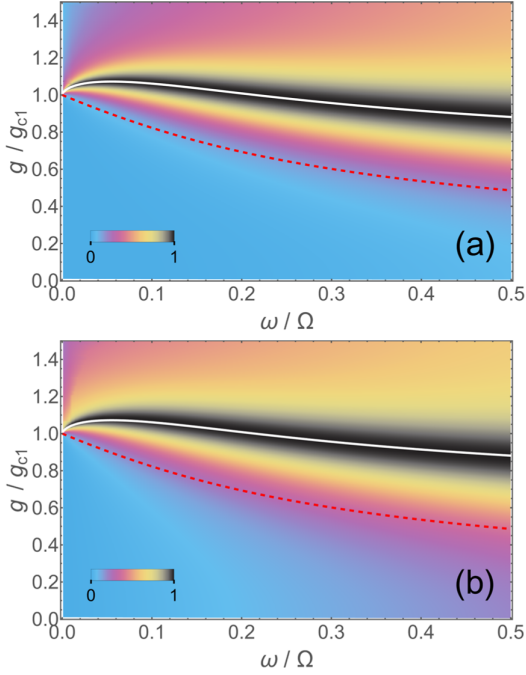


FIG. 5. Density plots of the QFI F_Q (a) and the susceptibility of single-photon absorption rate $d|\langle\hat{x}\rangle_{\pm}|/dg$ (b), both renormalized by their maxima at fixed frequencies. Their maxima coincide with each other, which is well captured by g_{c2} in Eq.(7) (white solid line) but missed by the conventional g_{c0} (red dashed line).

VI. BRIDGING QFT TO TRANSITION OBSERVABLE: TRANSITION COINCIDENCE WITH MAXIMUM SUSCEPTIBILITY OF SINGLE-PHOTON ABSORPTION RATE

The above discussion with the transition equation (30) obtained from the QFI inspires us to bridge the QFI to a transition observable. The effective velocity and acceleration in Sec.VD is defined on a polaron. We can also check the position expectation $\langle\hat{x}\rangle_{\pm}$ for the spin components which is polaron-picture independent and are available both in the ED and in the PP. In the PP we have

$$\langle\hat{x}\rangle_{+} = \alpha^2\langle\varphi_{\alpha}|\hat{x}|\varphi_{\alpha}\rangle + \beta^2\langle\varphi_{\beta}|\hat{x}|\varphi_{\beta}\rangle + 2\alpha\beta\langle\varphi_{\alpha}|\hat{x}|\varphi_{\beta}\rangle \quad (33)$$

subject to the normalization condition $\alpha^2 + \beta^2 + 2\alpha\beta\langle\varphi_{\alpha}|\varphi_{\beta}\rangle = 1$. The spin-down component has the opposite sign, $\langle\hat{x}\rangle_{-} = -\langle\hat{x}\rangle_{+}$, due to the parity symmetry. In the ED

$$\langle\hat{x}\rangle_{\pm} = \langle\psi_{\pm}|\hat{x}|\psi_{\pm}\rangle = \langle\psi_{\pm}|\frac{a^{\dagger} + a}{\sqrt{2}}|\psi_{\pm}\rangle = \sqrt{2}\langle\psi_{\pm}|a|\psi_{\pm}\rangle \quad (34)$$

is defined directly on the ED eigenstate $|\psi_{\pm}\rangle$ expanded on the Fock states.

We plot the amplitude $|\langle\hat{x}\rangle_{\pm}|$ in Fig. 4(e,f) where in panel (e) one sees that the results by the PP (solid line) and the ED (circles) completely coincide with each other. Similarly to the introduced velocity dx/dg in the PP, in

panel (f) we also present the evolution of $d|\langle\hat{x}\rangle_{\pm}|/dg$ which, if getting out of the PP language, is actually the susceptibility of the displacement or the single-photon absorption rate, as indicated by Eq. (34), in response to the coupling variation. Corresponding to the zero velocity (maximum acceleration) in the PP, we see that $d|\langle\hat{x}\rangle_{\pm}|/dg$ really reaches the maximum around the transition (vertical dashed line).

Density plots in the ω - g plane for the QFI and the susceptibility of single-photon absorption rate $d|\langle\hat{x}\rangle_{\pm}|/dg$ are provided in Fig. 5. We see that the maxima (black) of the QFI and $d|\langle\hat{x}\rangle_{\pm}|/dg$ coincide with each other in the wide frequency regime, as indicated by their simultaneous agreements with g_{c2} in (7) (white solid line). In contrast, the coinciding maxima are missed by the conventional transition coupling g_{c0} (red dashed line).

Thus, via the transition we bridge the QFI maximum point, the maximum polaron velocity and the maximum susceptibility of the single-photon absorption rate.

VII. CONCLUSIONS

We have combined the quantum Fisher information (QFI) and the variational polaron picture (PP) to identify and extract the accurate transition couplings for the quantum phase transition of the quantum Rabi model (QRM). With the combined QFI-PP analysis we also gain some implication and insight for the underlying physics of transition in the QRM.

The continuing interest on the QRM is only lying in the fact that it is a fundamental model for light-matter interactions but also is attracted by the quantum phase transition it possesses which can be applied for the critical quantum metrology. In quantum metrology, the square root of the QFI represents the precision bound of experimental measurement. In the present work we have conversely used the peak location of the QFI to identify the transition couplings in the QRM. By the QFI result from exact diagonalization (ED) we have demonstrated that transition couplings at finite frequencies much deviate from the conventional one which is exact actually only right at zero frequency. Inspired by the fractional-power-law behavior in the influence of polaron frequency renormalization on the expression improvement for the transition coupling, we have obtained an accurate expression of the transition coupling which coincides with the numeric transition couplings by the QFI in the variation of frequency. Besides the implication acquired from the integer/fractional power law analysis for a deeper understanding of the essence of transition, the transition coupling can provide an accurate reference in the practical applications of the quantum phase transition in the quantum metrology, since in practice the bosonic mode always has a non-zero frequency which invalidates the frequency-dependence of the conventional transition coupling.

We have also formulated the QFI in the PP. The PP is capable of analytically reproducing the numeric QFI by

ED, without a heavy computation cost as in the ED. On the other hand, the QFI in the PP can compensate for the missing data of the ED in the regime where the ED cannot access due to the demanding need of large basis number. Such a situation emerges in the large coupling regime, especially at low frequencies where the phase transition is sharp and provides the best sensitivity resource for raising the measurement precision. Therefore, the formulation of the QFI in the PP prepares an accurate and convenient tool to get the precision bound in covering the entire parameter regime, which may also be helpful in applications of quantum metrology.

From the QFI in the PP we have also come across the vanishing of the first-derivative term in the QFI in the QRM. We find this vanishing consequence comes from the non-degeneracy of the eigenstate. The conclusion has been extended for general non-degenerate pure states, which simplifies the expression of the QFI.

Finally from the QFI in the PP we see that the transition occurs with a zero polaron acceleration or maximum polaron velocity. Correspondingly the susceptibility of single-photon absorption rate reaches the maximum around the transition. This finding might add some insight in bridging the QFI and the physical properties at the transition.

As a closing remark, it is worthwhile to mention that, besides the transition in the QRM addressed in this work, similar transitions [4, 12–17, 26] also occur at low frequencies in other forms of light-matter interactions, such as the anisotropic coupling [12, 15–18, 49, 81], the mixture with nonlinear two-photon coupling [13, 14, 26] and the Stark nonlinear coupling [17, 19, 56–58]. On the other hand, although the two-polaron description in the PP has reached a very high accuracy, extension to the multi-polaron representation[69] is direct if even higher accuracy is needed. Our treatment addressed in the present work concerning the QFI and the transition coupling can be readily applied to these systems, which we shall leave for some future works.

ACKNOWLEDGEMENTS

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Appendix A: Inspiration for the transition coupling from frequency renormalization effect of polarons

From Fig. 4 in the main text, one may realize that the transition is essentially the splitting of the wave packet, which can be well described by the separation of the two polaron represented by $\varphi_i(\bar{g}, x) = (\xi_i/\pi)^{1/4} \exp[-\xi_i(x+x_i)^2/2]$ in (15). Here $x_\alpha = \zeta_\alpha \tilde{g}$

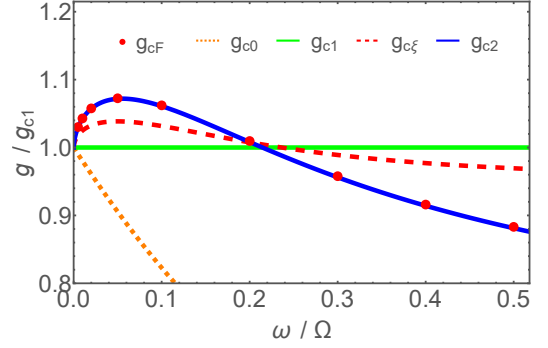


FIG. 6. Inspiration from the transition coupling $g_{c\xi}$ by including frequency renormalization. $g_{c\xi}$ (red dashed line) in (A9) has some improvements over g_{c0} (orange dashed) and g_{c1} (green (light gray) solid line). Although $g_{c\xi}$ is still not accurate in comparison with g_{cF} (red dots), it has the right direction of improvement and provides inspiration for formulation of g_{c2} (blue (dark gray) solid line).

and $x_\alpha = \zeta_\beta \tilde{g}$ with $\tilde{g} = \sqrt{2}g/\omega$. As a simplification we can assume two same polarons by setting

$$\zeta_\alpha = -\zeta_\beta = \zeta, \quad \xi_\alpha = \xi_\beta = \xi. \quad (\text{A1})$$

Here the minus sign of ζ_β denotes the displacement direction opposite to the other polaron α . Thus the distance of the two polarons is $2\zeta\tilde{g}$. The overlap of the two polarons is decreasing exponentially in the separation. The overlapping degree is decided by the crossing point of the two polaron wave packets which is moving away from the peak by a distance d . One can regard the separation to be basically complete when d reaches some point d_c where the polaron overlap becomes small enough to complete the transition. The distance relation around the transition is then given by

$$2\zeta\tilde{g} = 2d_c. \quad (\text{A2})$$

Note that in the low-frequency limit we have the explicit displacement renormalization factor [7, 8, 13]

$$\zeta \approx \sqrt{1 - \frac{g_{c0}^4}{g^4}} \quad (\text{A3})$$

starting from the transition, which can be applied to obtain improved expressions of the transition coupling.

1. g_{c0} by classical mass point

To mark the difference from the polaron frequency renormalization we set $d_c = d_{c1}/\sqrt{\xi}$ where d_{c1} is the transition distance in the absence of frequency renormalization. If the polaron wave packet is regarded as a classical mass point, then the separation process is immediately complete at $d_c = 0$, substitution of which in (A2)

retrieves the conventional transition coupling

$$g_c = g_{c0} = \frac{\sqrt{\omega\Omega}}{2} \quad (\text{A4})$$

as in (3).

2. g_{c1} by neglecting polaron frequency renormalization

However, in quantum mechanics the mass point should be replaced by the wave packet and d_c is finite. As a first order of improvement with finite d_c , we can neglect the polaron frequency renormalization by setting $\xi = 1$. We can judge the transition by a point where the wave function φ_i at the crossing point decays to an exponentially small value by the ratio $\varphi_i/\varphi_i^{\text{peak}} = e^{-2}$ which occurs at $d_c = 2$. Then Eq. (A2) becomes

$$\sqrt{1 - \frac{g_{c0}^4}{g_c^4}} \frac{\sqrt{2}g_c}{\omega} = 2 \quad (\text{A5})$$

which yields

$$g_c = g_{c1} = \sqrt{\omega^2 + \sqrt{\omega^4 + g_{c0}^4}} \quad (\text{A6})$$

in (4) as an improved transition coupling over g_{c0} .

3. $g_{c\xi}$ by including polaron frequency renormalization

We now pick up the polaron frequency renormalization and notice the frequency-displacement relation $\xi/\zeta \approx 1$ starting from the transition in the low frequency limit, i.e. [8]

$$\xi \approx \zeta \approx \sqrt{1 - \frac{g_{c0}^4}{g_c^4}}. \quad (\text{A7})$$

In such a consideration Eq. (A2) becomes much more nonlinear

$$\sqrt{1 - \frac{g_{c0}^4}{g_c^4}} \frac{\sqrt{2}g_c}{\omega} = \frac{d_{c1}}{\sqrt{\xi}} = \frac{d_{c1}}{\left(1 - \frac{g_{c0}^4}{g_c^4}\right)^{1/4}}. \quad (\text{A8})$$

Nevertheless, Equation (A8) still can be analytically solved, with the explicit solution being

$$g_c = g_{c\xi} = \sqrt[4]{g_{c0}^4 + \frac{\omega_{c1}^4}{12} (f^4 + 1 + f^{-4} + 24f^{-4}\tilde{g}_{c0}^4)}, \quad (\text{A9})$$

where we have defined $\omega_{c1} = d_{c1}\omega$, $\tilde{g}_{c0} = \frac{g_{c0}}{\omega_{c1}}$, and

$$f = \sqrt[12]{1 + 36\tilde{g}_{c0}^4 + 216\tilde{g}_{c0}^8 + 24\sqrt{3}\tilde{g}_{c0}^6\sqrt{27\tilde{g}_{c0}^4 + 1}}. \quad (\text{A10})$$

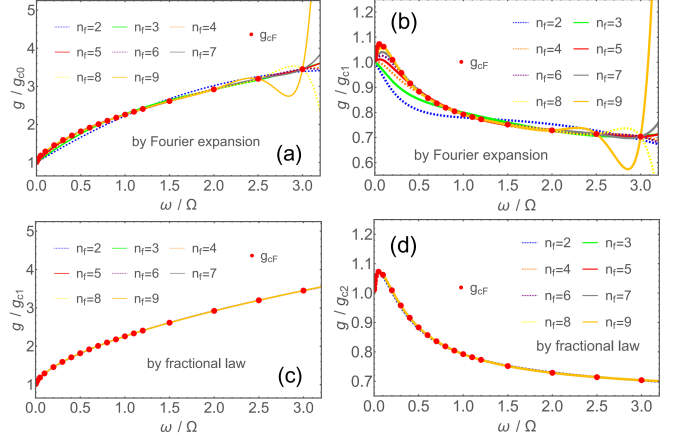


FIG. 7. Comparison of fitting of the transition coupling g_{cF} by Fourier expansion (a,b) and by fractional-power law (c,d) with different expansion order n_f . (a,c) g scaled by g_{c0} (b,d) g scaled by g_{c1} .

4. Inspiration of fractional-power-law expansion for g_{c2}

In Fig. 6 we give a comparison for g_{c0} (dotted line), g_{c1} (green (light-gray) solid line) and $g_{c\xi}$ (red dashed line) with $d_{c1} = 1.9$. Compared with g_{cF} (dots), g_{c1} is qualitatively better but quantitatively still not accurate enough, as also mentioned in the main text. By taking into the effect of the polaron frequency renormalization, $g_{c\xi}$ yields some more improvements over g_{c1} , especially in the low-frequency tendency. Although $g_{c\xi}$ does not achieve a perfect accuracy due to the simplifications we have introduced in the above discussion, e.g. in (A1) and (A7), the improvements added by the polaron frequency renormalization is in the correct direction. Note here the frequency renormalization effect manifests itself a behavior of fractional-power-series law in low frequencies

$$\begin{aligned} g_{c\xi} &= g_{c0} \left[1 + \left(\frac{d_{c1}}{2}\right)^{\frac{4}{3}} \left(\frac{\omega}{\Omega}\right)^{\frac{2}{3}} + \frac{7}{6} \left(\frac{d_{c1}}{2}\right)^{\frac{8}{3}} \left(\frac{\omega}{\Omega}\right)^{\frac{4}{3}} + \dots \right] \\ &= g_{c0} \left[1 + \sum_{n=1}^{\infty} c_n^{\xi} \left(\frac{\omega}{\Omega}\right)^{n\frac{2}{3}} \right], \end{aligned} \quad (\text{A11})$$

which inspires us to propose the expressions g_{c2} and g_{c2}^{fitting} in (7) and (9) for the transition coupling. It turns out that g_{c2} and g_{c2}^{fitting} are very accurate with only a couple of terms in the fractional power law expansion.

5. Unfavorable mathematical expansion by Fourier Series

It should be stressed that accuracy and efficiency of the fractional-power form of g_{c2} and g_{c2}^{fitting} in (7) and (9) are based on the physical analysis from frequency renormalization effect of polarons, as addressed in last sections.

One might speculate that a mathematical expansion by Fourier Series

$$g_c^{\text{Fourier}} = g_{c0} \left[1 + \sum_{n=1}^{n_f} c_n^{\text{Fourier}} \left(\frac{\omega}{\Omega} \right)^n \right] \quad (\text{A12})$$

would also work without need of the fractional-power form. It is true that a Fourier expansion can mathematically make a fitting finally, however such a Fourier-series fitting is much more inefficient, without mentioning that it does not provide any physical insight. We show some orders of the Fourier-expansion fitting in Fig. 7 via the least-squares fit. One sees in panel (a) by the coupling scale g_{c0} that $n_f = 2$ (blue dotted most-deviated line) in Fourier expansion does not fit well at all, the qualitative deviations can be seen more clearly in panel (b) by the coupling scale g_{c1} . Higher orders up to $n_f = 9$ approach to some convergence at low frequencies but large oscillations appear at high frequencies due to sparser reference data of g_{cF} (red dots). In a sharp contrast, fitting by the fractional law in (A11) already reaches a good convergence even at $n_f = 2$. Moreover, larger n_f converge well without the oscillation problem as the Fourier expansion even in the same sparse reference data.

In fact, the expression (A6) obtained by neglecting polaron frequency renormalization, if expanded, has an integer-power-series law as g_c^{Fourier}

$$\begin{aligned} g_{c1} &= g_{c0} \left(1 + \frac{2\omega}{\Omega} + \frac{2\omega^2}{\Omega^2} - \frac{4\omega^3}{\Omega^3} - \frac{10\omega^4}{\Omega^4} + \dots \right) \\ &= g_{c0} \left[1 + \sum_{n=1}^{\infty} c_{n1} \left(\frac{\omega}{\Omega} \right)^n \right]. \end{aligned} \quad (\text{A13})$$

Both the inefficiency of fitting convergence and the coincidence of integer-power-series law with g_{c1} indicate that the Fourier-series fitting g_c^{Fourier} does not capture the physical essence of frequency renormalization effect around the transition in the QRM.

Appendix B: Comparison of g_{c2} in different coefficient choices

In Sec. IV C we provide different expressions of the transition coupling (7)-(9). Here we make a comparison for their difference. Figure 8 shows g_{c2} in Eq. (7) with $\alpha_{\text{FS}} = 1/137$ (thin blue dashed line), g_{c2} in Eq. (8) with $c_1 = 4/3$ (thin black dashed line) and g_{c2}^{fitting} in (9) with $c_1 = 1.3715$, $c_2 = 0.1311$, $c_3 = 0.0184$ (green long-dashed line) in comparison with the g_{cF} data (red dots) numerically extracted from the peak locations of the QFI. As shown in Fig. 8(a), the expression (7) with $\alpha_{\text{FS}} = 1/137$ is very accurate and is actually producing g_{cF} in the low frequency regime $\omega/\Omega < 0.5$. Although considerable deviations appear in the high frequency regime $1 < \omega/\Omega < 3$ in Fig. 8(b), the transition loses the sense there as it becomes much broadened. Nevertheless, the QFI always has a peak value, an expression

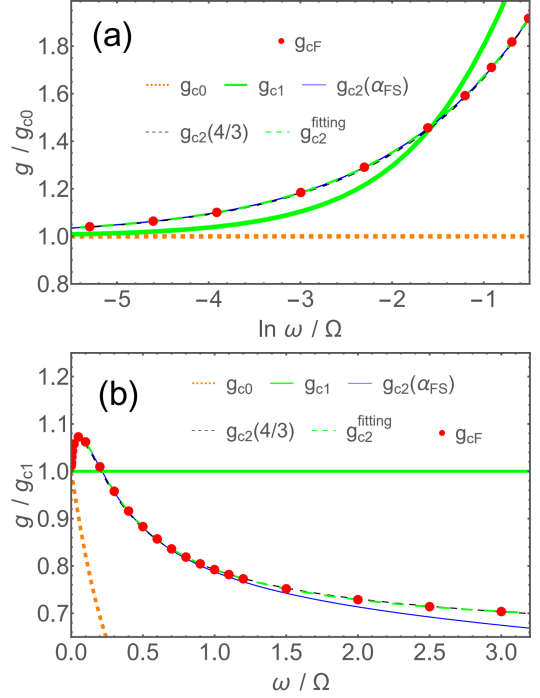


FIG. 8. Comparison of g_{c2} with different coefficients in low-frequency regime (a) and high-frequency regime (b): g_{c2} in Eq. (7) with $\alpha_{\text{FS}} = 1/137$ (thin blue dashed line), g_{c2} in Eq. (8) with $c_1 = 4/3$ (thin black dashed line) and g_{c2}^{fitting} in (9) with $c_1 = 1.3715$, $c_2 = 0.1311$, $c_3 = 0.0184$ (green long-dashed line). The result of g_{cF} (red dots) is the accuracy reference. g_{c0} (thick orange dotted line) and g_{c1} (thick green solid line) are taken as the coupling scale in (a) and (b).

valid for the entire parameter regime would be a perfect goal. In this need, the expression (8) with $c_1 = 4/3$ is accurate up to $\omega/\Omega = 3$, despite it is slightly less accurate in the low frequency regime with an error of the order 10^{-3} larger than (7). Finally g_{c2}^{fitting} is very accurate really in the entire frequency regime up to $\omega/\Omega = 3$. Note g_{c2} in (7) and (8) is in the second order of $(\omega/\Omega)^{2n/3}$ power law, while g_{c2}^{fitting} is in the third order, which already reaches the convergence as shown by Fig. 7(c,d) in Appendix A 5.

Appendix C: Explicit expressions for the QFI in the variational polaron picture

Explicitly, by the wave function of the polaron in Eq. (15) for the non-derivative terms we have

$$\langle \varphi_\alpha | \varphi_\alpha \rangle = \langle \varphi_\beta | \varphi_\beta \rangle = 1, \quad (\text{C1})$$

$$\langle \varphi_\alpha | \varphi_\beta \rangle = \frac{\sqrt{2} \xi_\alpha^{1/4} \xi_\beta^{1/4}}{\sqrt{\xi_\alpha + \xi_\beta}} \exp \left[-\frac{(x_\alpha - x_\beta)^2 \xi_\alpha \xi_\beta}{2(\xi_\alpha + \xi_\beta)} \right], \quad (\text{C2})$$

For the polaron-derivative terms in (19) we get

$$\langle \frac{\partial \varphi_i}{\partial x_i} | \varphi_j \rangle = \frac{\sqrt{2} \xi_i^{5/4} \xi_j^{5/4} (x_j - x_i)}{(\xi_i + \xi_j)^{3/2} f_E}, \quad (C3)$$

$$\langle \varphi_j | \frac{\partial \varphi_j}{\partial x_j} \rangle = \frac{\sqrt{2} \xi_i^{5/4} \xi_j^{5/4} (x_i - x_j)}{(\xi_i + \xi_j)^{3/2} f_E}, \quad (C4)$$

$$\langle \frac{\partial \varphi_i}{\partial \xi_i} | \varphi_j \rangle = \frac{\sqrt{2} \xi_j^{1/4} \{\xi_i^2 + \xi_j^2 [2\xi_i (x_i - x_j)^2 - 1]\}}{\xi_i^{3/4} (\xi_i + \xi_j)^{5/2} f_E} \quad (C5)$$

$$\langle \varphi_i | \frac{\partial \varphi_j}{\partial \xi_j} \rangle = \frac{\sqrt{2} \xi_i^{1/4} \{\xi_j^2 + \xi_i^2 [2\xi_j (x_i - x_j)^2 - 1]\}}{\xi_j^{3/4} (\xi_i + \xi_j)^{5/2} f_E} \quad (C6)$$

and in (20) the explicit expressions read

$$\langle \frac{\partial \varphi_i}{\partial x_i} | \frac{\partial \varphi_j}{\partial x_j} \rangle = \frac{\sqrt{2} \{\xi_i + \xi_j - \xi_i \xi_j (x_i - x_j)^2\}}{(\xi_i + \xi_j)^{5/2} \xi_i^{-5/4} \xi_j^{-5/4} f_E}, \quad (C7)$$

$$\langle \frac{\partial \varphi_i}{\partial x_i} | \frac{\partial \varphi_j}{\partial \xi_j} \rangle = \frac{\{\xi_j^2 + \xi_i^2 [2\xi_j (x_i - x_j)^2 - 5] - 4\xi_i \xi_j\}}{2\sqrt{2} (\xi_i + \xi_j)^{7/2} \xi_i^{-5/4} \xi_j^{-1/4} (x_i - x_j)^{-1} f_E}, \quad (C8)$$

$$\langle \frac{\partial \varphi_i}{\partial \xi_i} | \frac{\partial \varphi_j}{\partial x_j} \rangle = \frac{\{\xi_i^2 + \xi_j^2 [2\xi_i (x_i - x_j)^2 - 5] - 4\xi_i \xi_j\}}{2\sqrt{2} (\xi_i + \xi_j)^{7/2} \xi_j^{-5/4} \xi_i^{-1/4} (x_j - x_i)^{-1} f_E}, \quad (C9)$$

$$\langle \frac{\partial \varphi_i}{\partial \xi_i} | \frac{\partial \varphi_j}{\partial \xi_j} \rangle = \frac{4\xi_i^3 \xi_j^3 x_{ij}^4 + \xi_{ij}^+ (2\xi_i \xi_j x_{ij}^2 - \xi_{ij}^+) (\xi_i^2 + \xi_j^2 - 10\xi_i \xi_j)}{8\sqrt{2} (\xi_i + \xi_j)^{9/2} \xi_i^{3/4} \xi_j^{3/4} f_E}, \quad (C10)$$

where we have defined $\xi_{ij}^+ = (\xi_i + \xi_j)$, $x_{ij} = (x_i - x_j)$ and $f_E = \exp\{(x_i - x_j)^2 \xi_i \xi_j / [2(\xi_i + \xi_j)]\}$. The displacement-derivative factor is

$$\frac{dx_i}{d\bar{g}} = \frac{d\zeta_i}{d\bar{g}} \bar{g} \sqrt{\frac{\Omega}{2\omega}} + \zeta_i \sqrt{\frac{\Omega}{2\omega}}, \quad (C11)$$

explicitly.

The variational parameters $\{w_i, \zeta_i, \xi_j\}$ for the ground state are determined by minimization of the energy subject to normalization condition (11) of the wave function [8].

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