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Coherent–incoherent transition in the spin–boson model with a super-ohmic bath*

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The temperature effect on tunnelling splitting in the spin–boson model with a super-ohmic bath is studied by the small polaron theory. The coherent–incoherent transition temperature is calculated and its dependence on dissipation strength and bare tunnelling splitting is analysed. In additional to the traditional transition point described in textbooks, a new kind of transition is found in the low dissipation region, showing different temperature dependence in the transition. The relation to the corresponding transition in the polaron–phonon system is also discussed.

Keywords: the spin–boson model, coherent–incoherent transition, polaron–phonon system
PACC: 7340G, 7335C, 6630J

1. Introduction

Quantum tunnelling has been an interesting subject in both theoretical and experimental research since the so-called 'Leggett program' was proposed.[1−3] Roughly speaking, there are two kinds of tunnelling event; the first kind of tunnelling can lead to a 'directly observable' effect and is always considered as the candidate of the 'qubit', a basic unit in quantum computation.[1,4] One example is the tunnelling in a single-molecular-magnet (SMM), which can lead to relaxation of the magnetization which is directly measurable in experiments.[5,6] Other well-known examples are the Josephson charge qubit and the Josephson flux qubit.[4] The second kind of tunnelling is not observed directly but can only be inferred from spectroscopic data (like the Mössbauer effect or microwave absorption).[7−10] The best-known example is 'ammonia inversion', the first observed tunnelling states in solids.[1,7] Historically, tunnelling of defects in solids was an interesting subject long before the SQUID was built,[7] while in recent years, thanks to the quick development of quantum information research, the main interest has turned to the qubit. However, recent experimental progress on atomic tunnelling in the so-called stoichiometric clathrate compound has raised new interest in tunnelling in solids.[8−10] In fact, the four equivalent sites of magnetic europium in clathrate $Eu_8Ga_{16}Ge_{30}$ represent the best toy-model in quantum tunnelling.[8] One important issue in the study of quantum tunnelling is the dissipation effect from the environment. Theoretically the best-known model of quantum dissipation is the spin–boson model,[1−3] while the difference between the two kinds of tunnelling mentioned above stems from the spectral function of the environment. For the first kind of tunnelling, the physical environment is represented by the ohmic bath,[1] while for the second kind of tunnelling, it is the super-ohmic bath.[11]

The temperature effect on quantum tunnelling is an important issue since all real systems are at finite temperatures. For those systems with so-called double-linear coupling to a phonon bath, like the spin–boson model and the polaron–phonon (or exciton–phonon) system,[12] the small polaron theory provides a good way to trace the temperature effect.[13,14] However, since the diagonal contribution by the adiabatic approximation (i.e., the usual Debye–Waller factor) in the spin–boson model with an ohmic bath is null, the temperature effect on the first kind of tunnelling cannot be quantitatively found by the small polaron theory.[15] Theoretically the temperature effect on the second kind of tunnelling can be traced by the small polaron theory and this point was mentioned in the review article by Leggett *et al.*[1] Nevertheless, a detailed calculation on this subject has not been found in the literature and this is the main interest of the present paper. In this paper, we use the small polaron theory to study the coherent–incoherent transition in the

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spin–boson model with a super-ohmic bath. The rest of the paper is organized as follows. The model and the explanation are given in the next section, calculations of both the diagonal and non-diagonal transition rate and the analysis of coherent–incoherent transition are provided in Section 3. A conclusion and discussion are given in the last section.

2. The model and the explanation

The Hamiltonian of the spin–boson model is given by (setting $\hbar = 1$)[1,3]

$$\hat{H} = -\frac{\Delta_0}{2}\hat{\sigma}_x + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \hat{\sigma}_z \sum_k g_k(\hat{b}_k^\dagger + \hat{b}_k), \quad (1)$$

where Δ_0 is the bare tunnelling splitting, $\hat{\sigma}_i$ ($i = x, y, z$) is the Pauli matrix, $\hat{b}_k(\hat{b}_k^\dagger)$ is the annihilation (creation) operator of the kth phonon mode with energy ω_k and g_k is the coupling parameter. The first and second terms of the above Hamiltonian represent the unbiased two-state-system (TSS) and the phonon bath respectively, while the final term is the double-linear coupling term. The above model can be used to describe quantum tunnelling between two levels in resonance or the atomic tunnelling in solids under the influence of the phonon bath; it can also represent the 'two-site' problem in the polaron–phonon (or exciton–phonon) system.[12]

As is known, the solution of this model depends on the so-called bath spectral function (density) which is defined as[1,3] $J(\omega) = \pi \sum_k g_k^2 \delta(\omega - \omega_k)$. For frequencies below a high-energy cutoff ω_c, the spectral function has the power law form,

$$J(\omega) = \frac{\pi}{2}\alpha\omega^s/\omega_{\rm c}^{s-1}, \qquad 0 < \omega \leq \omega_{\rm c}, \quad (2)$$

where α is a dimensionless coupling strength which characterizes the dissipation strength and the parameter s characterizes the property of the bath, i.e., $0 < s < 1$, $s = 1$, and $s > 1$ represent the sub-ohmic, ohmic, and super-ohmic cases, respectively. If the TSS is a qubit, the physical environment is an ohmic bath(i.e., $s = 1$), while if the TSS represents the tunnelling state in solids, the physical environment is the super-ohmic bath, i.e., $s = 3$ or $s = 5$.[11] The main interest of the present work is the latter one.

In the following section, the small polaron theory will be employed to study the temperature effect on tunnelling and we shall concentrate on the coherent–incoherent transition as temperature rises.

3. Coherent–incoherent transition

According to the small polaron theory,[13,14] there are mainly two kinds of contribution to quantum tunnelling, say, the diagonal and non-diagonal transitions. The diagonal transitions make the main contribution to the tunnelling splitting at the beginning of the low temperature regions, where the expectation value of the phonon number is small. The diagonal transition rate can be found in the following way given in Refs.[13] and [14]. Firstly, a canonical transformation is applied to the Hamiltonian in Eq.(1), i.e.,

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^{-1} = \hat{\mathcal{H}}_0 + \hat{V}, \quad (3)$$

where $\hat{U} = \exp\{\hat{\sigma}_z \sum_k (g_k/\omega_k)(\hat{b}_k^\dagger - \hat{b}_k)\}$,

$$\hat{\mathcal{H}}_0 = \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k - \sigma_z^2 \sum_k g_k/\omega_k^2, \quad (4)$$

$$\hat{V} = \frac{\Delta_0}{4}(\hat{\sigma}_+ e^{\hat{\Theta}} + \hat{\sigma}_- e^{-\hat{\Theta}}), \quad (5)$$

and $\hat{\Theta} = \sum_k (g_k/\omega_k)(\hat{b}_k - \hat{b}_k^\dagger)$. The diagonal transition rate is given by[13,14]

$$w_{\rm d}(T) = {\rm Tr}_{\rm bath}\langle i|\hat{V}|i\rangle = \frac{\Delta_0}{2}{\rm e}^{-S_T}, \quad (6)$$

where

$$S_T = 2\sum_k (g_k/\omega_k)^2(2n_k + 1), \quad n_k = ({\rm e}^{\beta\omega_k} - 1)^{-1}, \quad (7)$$

and $\beta = 1/(k_{\rm B}T)$. It is easy to see that, $(2n_k + 1) = \coth(\beta\omega_k/2)$, which is a monotonic-increasing function of temperature; accordingly ${\rm d}S_T/{\rm d}T > 0$ and hence $w_{\rm d}(T)$ will decrease with increasing temperature.

To find out the non-diagonal transition rate, one needs to calculate the following correlation function[13,14]

$$W(t) = {\rm Tr}_{\rm bath}[\langle i|\hat{V}(t)\hat{V}(0)|i\rangle - |\langle i|\hat{V}|i\rangle|^2] \quad (8)$$

with $\hat{V}(t) = {\rm e}^{{\rm i}\,\hat{\mathcal{H}}_0 t}\hat{V}{\rm e}^{-{\rm i}\,\hat{\mathcal{H}}_0 t}$. In the thermodynamic limit, one can find that[13]

$$W(t) = (\Delta_0/2)^2 {\rm e}^{-2S_T}[{\rm e}^{\varphi(t)} - 1], \quad (9)$$

where

$$\varphi(t) = \sum_k (2g_k/\omega_k)^2[(n_k + 1){\rm e}^{-{\rm i}\,\omega_k t} + n_k {\rm e}^{{\rm i}\,\omega_k t}]. \quad (10)$$

The non-diagonal transition rate can be found by using the so-called saddle-point integration

$$w_n(T) = \int_{-\infty}^{\infty} W(t){\rm d}t \simeq (\Delta_0/2)^2(\pi/\gamma)^{1/2}{\rm e}^{-2S_T + \varphi(0)}, \quad (11)$$

where $\gamma = \sum_k g_k^2[n_k(n_k+1)]^{1/2}$ and

$$\varphi(0) = 2\sum_k (g_k/\omega_k)^2[n_k(n_k+1)]^{1/2}. \quad (12)$$

Using the spectral function given in Eq.(2), one can find that

$$S_T = \frac{2}{\pi}\int_0^{\omega_c} \frac{J(\omega)}{\omega^2}\coth(\beta\omega/2)\mathrm{d}\omega, \quad (13)$$

$$\varphi(0) = \frac{1}{2\pi}\int_0^{\omega_c} \frac{J(\omega)}{\omega^2\sinh^2(\beta\omega/2)}\mathrm{d}\omega, \quad (14)$$

and

$$\gamma = \frac{1}{2\pi}\int_0^{\omega_c} \frac{J(\omega)}{\sinh^2(\beta\omega/2)}\mathrm{d}\omega. \quad (15)$$

Here one can see that, for both ohmic and sub-ohmic baths (i.e., $0 < s \leq 1$), we have $S_T \to \infty$, and accordingly $w_\mathrm{d}(T) = 0$, which makes quantitative analysis impossible. Nevertheless, the difficulty does not exist for a super-ohmic bath.

In the small polaron theory,[13,14] the main contribution to tunnelling splitting at the beginning of the low temperature region is the diagonal transition which decreases with increasing temperature. On the other hand, the non-diagonal transition is thermally activated and hence increases with temperature. This point is usually explained by the expansion of $w_n(T)$ in the high temperature region.[13,14] For $\omega_c/(k_\mathrm{B}T) \ll 1$ (or $n_k \gg 1$), one can find that

$$w_n(T) \simeq \Delta_0^2\sqrt{\frac{\pi}{BT}}\mathrm{e}^{-B/T}, \quad B = \frac{1}{k_\mathrm{B}}\sum_k \frac{g_k^2}{\omega_k} \quad (16)$$

from which one can see that $w_n(T)$ increases with temperature. As the temperature increases, the main contribution to tunnelling splitting will change from diagonal transition to non-diagonal transition. Since the diagonal transition is a coherent tunnelling process while the non-diagonal transition is considered as an incoherent tunnelling process, a coherent–incoherent transition point is defined as[14,16]

$$w_n(T_c) = w_\mathrm{d}(T_c), \quad (17)$$

or

$$\frac{\Delta_0}{2}(\pi/\gamma)^{1/2}\mathrm{e}^{\varphi(0)-S_T}\Big|_{T=T_c} = 1. \quad (18)$$

Here we shall firstly present some explanation on the determination of the transition temperature T_c. It is important to note that T_c can be safely found through Eq.(17), i.e., by making plots of both $w_n(T)$

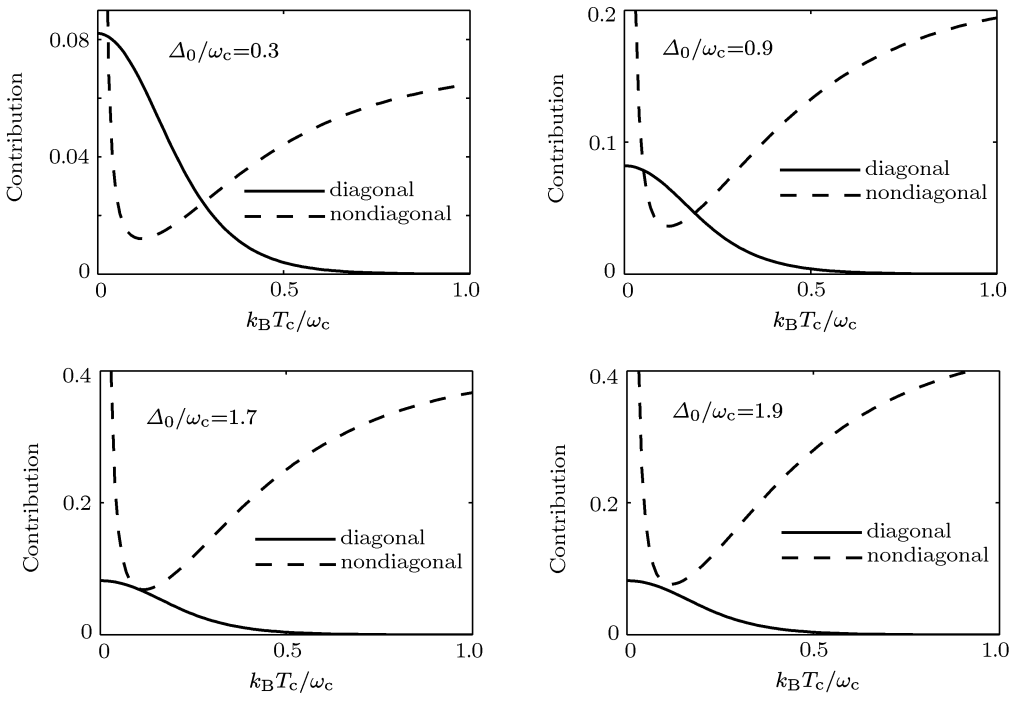


Fig.1. Variation of both $w_\mathrm{d}(T)$ and $w_n(T)$ with temperature in the case of $s = 3$ and $\alpha = 5$. The unexpected 'up-turn' of $w_n(T)$ comes from the divergence of factor $\gamma^{-1/2}$, which leads to the additional fake solution. It is seen that no cross-point can be found when Δ_0/ω_c increases to some critical value.

and $w_{\rm d}(T)$ against T and finding the cross-point, otherwise a direct solution of Eq.(18) can lead to fake solutions. It is usually found that Eq.(18) has two solutions, making the determination of $T_{\rm c}$ impossible. Figure 1 shows the variation of both $w_{\rm d}(T)$ and $w_n(T)$ with temperature for some specified parameters. One can see that the non-diagonal transition rate $w_n(T)$ has an divergent 'up-turn' as $T \to 0$. From Eqs.(11) and (15), it is seen that the 'up-turn' comes from the factor $\gamma^{-1/2}$ which tends to diverge as $T \to 0$. Such an 'up-turn' leads to an additional cross-point, which is obviously a fake solution. Since the divergent behaviour of $\gamma^{-1/2}$ is independent of spectral function, such a fake solution exists for both the $s = 3$ and $s = 5$ cases.

Numerical analysis shows there are two kinds of transition points. The first kind of transition point is the traditional one as described in the literature,[13,14,16] i.e., $w_{\rm d}(T)$ decreases while $w_n(T)$ increases with increasing T respectively, and a cross-point can be found at $T = T_{\rm c}$. An illustration is shown in Fig.2, which is similar to that found by Holstein.[16] For this kind of transition, tunnelling splitting will firstly decrease with increasing temperature and then, as the transition point is reached, the temperature dependence will reverse. In other words, such a transition can be directly known by observing the temperature dependence of tunnelling splitting and hence is termed the observable transition.

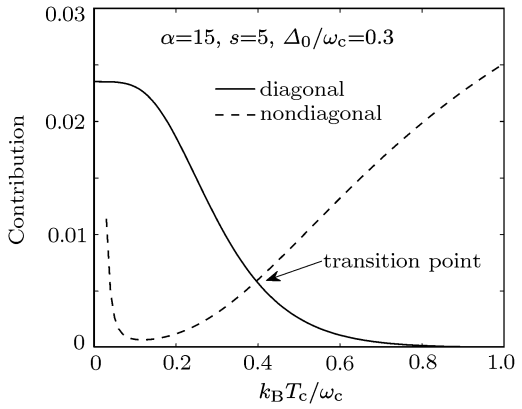


Fig.2. Illustration of the first kind of transition point for some specified parameters. Here $w_{\rm d}(T)$ increases while $w_n(T)$ decreases with increasing temperature respectively. As the transition point is reached, the main contribution to tunnelling splitting changes from $w_{\rm d}(T)$ to $w_n(T)$ and hence the temperature dependence on tunnelling splitting reverses.

In additional to the traditional transition point, we have another kind of transition point. For this case, both $w_{\rm d}(T)$ and $w_n(T)$ decrease with increasing temperature and the former has a faster decreasing rate than the later. As the transition point is reached, the main contribution to tunnelling splitting changes from $w_{\rm d}(T)$ to $w_n(T)$ as usual, but the temperature dependence on tunnelling splitting does not change. An illustration of the second kind of transition point is given in Fig.3. Obviously such a transition cannot be directly detected by observing the temperature dependence on tunnelling splitting and hence is termed the unobservable transition point.

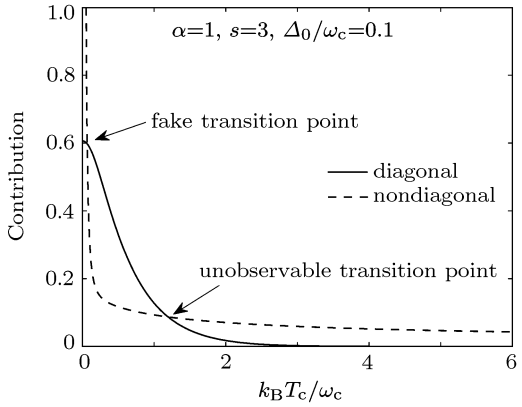


Fig.3. Illustration of the second kind of transition point for some specified parameters. Here both $w_{\rm d}(T)$ and $w_n(T)$ decrease with increasing temperature; as the transition is reached, the main contribution to tunnelling splitting changes from $w_{\rm d}(T)$ to $w_n(T)$ but the temperature dependence on tunnelling splitting does not change.

Our analysis shows that two kinds of transition can be found for both the $s = 3$ and $s = 5$ cases. For a given $\Delta_0/\omega_{\rm c}$, one can only find the second kind of transition in the low dissipation region, and the first kind of transition takes place when the dissipation strength exceeds some threshold $\alpha_{\rm c}$. Figure 4 shows the boundary lines for those two kinds of transition for both the $s = 3$ and $s = 5$ cases. The boundary lines shown in Fig.4 seem to suggest that the threshold is independent of $\Delta_0/\omega_{\rm c}$, nevertheless, it is found that the threshold increases slightly with $\Delta_0/\omega_{\rm c}$. For example, in the case of $s = 5$, $\alpha_{\rm c}$ varies approximately from 3.5933 to 3.5943 when $\Delta_0/\omega_{\rm c}$ changes from 1 to 10. Such a tiny variation is hard to see on the scale shown in Fig.4.

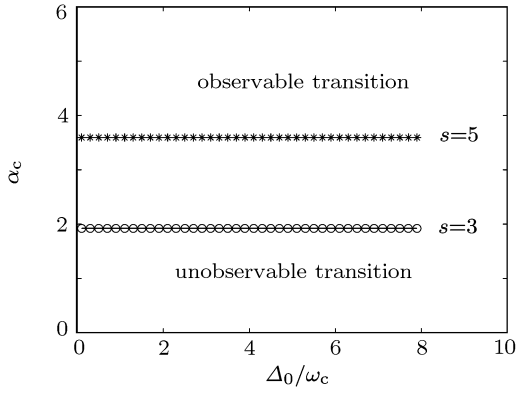


Fig.4. The boundary lines for two kinds of transition in the cases of $s = 3$ and $s = 5$. In both cases, the threshold α_c increases slightly with Δ_0/ω_c.

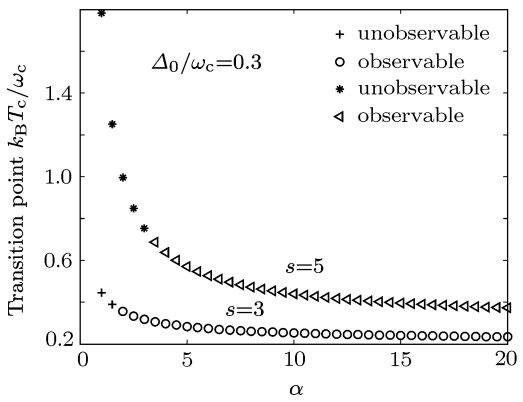


Fig.5. The dependence of the transition temperature on the dissipation strength α in the case of $\Delta_0/\omega_c = 0.3$. For both $s = 3$ and $s = 5$, the transition temperature decreases with increasing α at the beginning, then when α increases to some value, the transition temperature becomes insensitive to α and tends to a fixed value.

Now we turn to the dependence of the transition temperature on the dissipation strength α. A typical result is shown in Fig.5 for the case of $\Delta_0/\omega_c = 0.3$. It is seen that, at the beginning of the low dissipation region, the transition temperature decreases with increasing dissipation strength, and the $s = 5$ case has a faster decreasing rate than $s = 3$. When the dissipation strength increases to some value which depends on both s and Δ_0/ω_c, the transition temperature becomes insensitive to the dissipation strength and tends to a fixed value. It is interesting to see that the transition temperature does not tend to zero as the dissipation strength increases. Our analysis shows that, in the case of the super-ohmic bath, localization is impossible for any finite dissipation strengths, and therefore the diagonal transition always has a non-zero contribution as the dissipation strength increases, leading to a finite transition temperature. It should be noted that the present result is in accord with the exact solution of the single-mode case.[17] In the single-mode case, it was found that, for both low and high frequency modes, the coherent–incoherent transition point becomes insensitive to the coupling strength provided that the coupling strength is strong enough.[17] According to the influence-functional theory,[18] the present case is just a weighted integration of the single-mode result. Consequently, the transition temperature becomes insensitive to the dissipation strength in the strong dissipation regions.

For a given dissipation strength α, the transition temperature depends on Δ_0/ω_c. A typical result for the case of $\alpha = 5$ is shown in Fig.6. One can see that the transition temperature decreases with increasing Δ_0/ω_c, and the larger the s, the faster the decreasing rate. For both the $s = 3$ and $s = 5$ cases, the present analysis cannot help to find the transition point when Δ_0/ω_c increases to a large number as illustrated in Fig.1. The result we found is qualitatively in agreement with but obviously different from the result found by Holstein in the high temperature region by ignoring the dispersion, where the transition point was found to be remarkably insensitive to Δ_0.[13,16] This indicates the difference between the case of dispersive phonons and the case of ignoring the dispersion. As a matter of fact, Holstein's calculation can be considered as the case of the Einstein model and hence corresponds to the single-mode case. In the single-mode case,[17] it is found that the transition point varies approximately from 0.6 to $0.4\Delta_0/k_B$ as Δ_0/ω_c changes from 1/3 to 3. This result is in accord with Holstein's calculation. The exact solution of the single-mode case shows that the transition temperature increases with decreasing Δ_0/ω, i.e., for a given Δ_0, the higher the frequency, the higher the transition temperature.[17] In the present model, the quality Δ_0/ω_c sets the population of the high and low frequency, namely, the larger Δ_0/ω_c, the larger the population of the low frequency modes with $\Delta_0/\omega < 1$ in the bath, leading to a lower transition temperature.

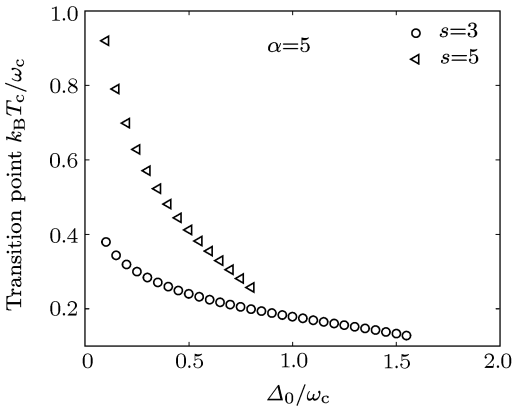


Fig.6. The dependence of the transition temperature on Δ_0/ω_c in the case of $\alpha = 5$. For both $s = 3$ and $s = 5$, the transition temperature decreases with increasing Δ_0/ω_c, and the larger the s, the faster the decreasing rate.

4. Conclusion and discussion

In this paper, coherent–incoherent transition in the spin–boson model with a super-ohmic bath is studied by the small polaron theory. The transition temperature is calculated for both the $s = 3$ and $s = 5$ cases and its dependence on both the dissipation strength α and the bare tunnelling splitting Δ_0 is also analysed. The result we found is in agreement with the exact solution of the single-mode case. In additional to the traditional transition point as described in the textbook, there is another kind of transition which takes place in the weak dissipation region. As the transition point is reached, the temperature dependence on tunnelling splitting will keep decreasing, in contrast to the traditional one. The coherent–incoherent transition picture in the weak dissipation regions is enriched by the finding of this transition. Coherent–incoherent transition in the polaron–phonon system is a well-known concept and has been observed in some experimental systems like TiO_2. We hope that the coherent–incoherent transition discussed here can be found in the newly-developed stoichiometric clathrate compounds, like $Eu_8Ga_{16}Ge_{30}$. Physically the transition can be found by observing the temperature dependence of tunnelling splitting. However, tunnelling splitting in the system mentioned above is not directly observable but can only be inferred from the Mössbauer-effect and microwave absorption. This situation is more complicated than the polaron–phonon system. Further analysis is needed to find out the observable effect of the transition on the Mössbauer-effect and microwave absorption.

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