Analytical solutions for the $E \otimes e$ dynamic Jahn–Teller problem in the strong coupling limit

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Abstract

Correct boundary conditions for wavefunctions in the $E \otimes e$ dynamic Jahn–Teller problem explicitly is considered to obtain approximate analytical solutions in the strong coupling limit. We demonstrate that the pseudorotational energy $j^2/(2g^2)$, where g is the dimensionless vibronic coupling constant, and j total angular momentum: $j = 1/2, 3/2, \dots$, in the conventional strong coupling expression for the vibronic levels of the lower sheet is exact. However, it is found that in the conventional treatment a term of the order of $1/g^2$ is missing. The solutions for the upper sheet with correct boundary conditions gives those which are entirely different from the corresponding Slonczewski's solutions.

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1. Introduction

The dynamic Jahn–Teller problem [1,2] is one of the most important problems in molecular physics and solid state physics. In spite of much effort, to obtain exact analytical solutions for the problem is still an open problem [3–8].

The dynamic linear $E \otimes e$ JT problem in the strong coupling limit has been studied since 1958 [1,9–12]. The solution has been obtained assuming a potential as a harmonic potential, and it can reproduce the numerical calculation well in the strong coupling limit up to order of $1/g^2$, where g is the dimensionless vibronic coupling constant. However, the radial wavefunction within the harmonic approximation does not satisfy a boundary condition at the origin of the potential surface.

Recently we have derived analytical solutions with the correct boundary condition of the dynamic $E \otimes e$ problem in the strong coupling limit [13]. In this paper, we summarize the analytical solutions in the strong coupling limit. Moreover, the explicit expression of the wavefunction for the lower sheet is presented.

2. $E \otimes e$ dynamic Jahn–Teller Hamiltonian

The Hamiltonian for the linear $E \otimes e$ dynamic Jahn–Teller problem is represented in the space spanned by complex electronic states $\psi_{\pm} = 1/\sqrt{2}(\phi_0 \pm i\phi_e)$ as

$$\hat{\mathcal{H}} = -\frac{1}{2} \left\{ \left(\frac{\partial^2}{\partial Q_{\theta}^2} + \frac{\partial^2}{\partial Q_{\epsilon}^2} \right) - (Q_{\theta}^2 + Q_{\epsilon}^2) \right\} \hat{\sigma}_0 + g(Q_{\theta} \hat{\sigma}_x + Q_{\epsilon} \hat{\sigma}_y), \quad (1)$$

where $(Q_{\theta}, Q_{\epsilon})$ are real normal coordinates of an e vibrational mode, and

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$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad (2)$$

and

$$\hat{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (3)$$

The Hamiltonian in the polar coordinates $(\rho \cos \phi, \rho \sin \phi)$ is expressed as

$$\hat{\mathcal{H}} = \left[-\frac{1}{2} \left\{ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right\} + \frac{1}{2} \rho^2 \right] \hat{\sigma}_0 + g\rho \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}. \quad (4)$$

Substituting $\Psi = \Phi/\sqrt{\rho}$ to the Schrödinger equation of Hamiltonian (4), we obtain the Hamiltonian for Φ as

$$\hat{\mathcal{H}} = \left(-\frac{1}{2} \frac{\partial^2}{\partial \rho^2} - \frac{1}{8\rho^2} + \frac{\hat{L}_z^2}{2\rho^2} + \frac{1}{2} \rho^2 \right) \hat{\sigma}_0 + g\rho \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}, \quad (5)$$

where $\hat{L}_z = -i\partial/\partial\phi$. Though the kinetic energy matrix is diagonal in Hamiltonian (5), the potential energy matrix is not diagonal. To make the potential energy matrix diagonal, the following unitary transformation is applied [12]:

$$\hat{S} = \frac{1}{\sqrt{2}} \begin{pmatrix} \exp(-i\frac{\phi}{2}) & \exp(-i\frac{\phi}{2}) \\ \exp(i\frac{\phi}{2}) & -\exp(i\frac{\phi}{2}) \end{pmatrix}, \quad (6)$$

the Hamiltonian becomes

$$\hat{S}^\dagger \hat{\mathcal{H}} \hat{S} = \left(-\frac{1}{2} \frac{\partial^2}{\partial \rho^2} + \frac{1}{2} \rho^2 - \frac{1}{8\rho^2} \right) \hat{\sigma}_0 + \frac{1}{2\rho^2} (\hat{L}_z - \frac{1}{2} \hat{\sigma}_x)^2 + g\rho \hat{\sigma}_z, \quad (7)$$

where

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8)$$

The radial and angular part of the wavefunction of Hamiltonian (7) can be separated:

$$\Phi(\rho, \phi) = \frac{1}{\sqrt{2\pi}} e^{ij\phi} \chi(\rho), \quad (9)$$

where j is the eigenvalue of the operator $\hat{J} = \hat{L}_z + \frac{1}{2} \hat{\sigma}_z$, and $j = \pm 1/2, \pm 3/2, \pm 5/2, \dots$. The Hamiltonian for the radial part is

$$\hat{\mathcal{H}} = \left(-\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} + \frac{1}{2} \rho^2 \right) \hat{\sigma}_0 - \frac{j}{2\rho^2} \hat{\sigma}_x + g\rho \hat{\sigma}_z. \quad (10)$$

This Hamiltonian is exact because no approximation is applied in passing from Eq. (1) to Eq. (10). This Hamiltonian yields the coupled equation

$$\left(-\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} + \frac{1}{2} \rho^2 \right) \chi_- - |g|\rho \chi_- - \frac{j}{2\rho^2} \chi_+ = E \chi_-, \quad (11)$$

$$\left(-\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} + \frac{1}{2} \rho^2 \right) \chi_+ + |g|\rho \chi_+ - \frac{j}{2\rho^2} \chi_- = E \chi_+. \quad (12)$$

Neglecting the term $\frac{j}{2\rho^2} \hat{\sigma}_x$ in the strong coupling limit, we can decouple the coupled equations as

$$\left(-\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} + \frac{1}{2} \rho^2 \right) \chi_- - |g|\rho \chi_- = E_- \chi_-, \quad (13)$$

$$\left(-\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} + \frac{1}{2} \rho^2 \right) \chi_+ + |g|\rho \chi_+ = E_+ \chi_+. \quad (14)$$

Hamiltonians for the decoupled equations are written as

$$\mathcal{H}_\pm = -\frac{1}{2} \frac{d^2}{d\rho^2} + U_\pm(\rho), \quad (15)$$

where

$$U_\pm(\rho) = \frac{j^2}{2\rho^2} + \frac{1}{2} \rho^2 \pm |g|\rho. \quad (16)$$

The term $\frac{j^2}{2\rho^2}$ in $U_\pm(\rho)$ is a centrifugal energy arising from angular motion of the degenerate vibration. The energy surfaces $U_\pm$ are shown in Fig. 1. The decoupled Eq. (13) is the equation for the lower sheet, and Eq. (14) for the upper sheet, respectively. The energy surfaces diverge at the origin due to the centrifugal energy $\frac{j^2}{2\rho^2}$. This imposes

Fig. 1. Energy surfaces $U_\pm(\rho)$ in the $E \otimes e$ dynamic Jahn–Teller problem.

a boundary condition for the wavefunctions: the radial wavefunction χ should be zero at the origin. We have to take the boundary condition into account to solve the problem.

3. Conventional treatment

In this section, we will review the conventional treatment for the linear $E \otimes e$ problem in the strong coupling limit [12]. From Eq. (16), the trough of minima of the lower potential sheet $U_-(\rho)$ is located at $\rho_{-,0} \approx |g|$, and that of the upper surface is at $\rho_{+,0} \approx (j^2/|g|)^{1/3}$. In the strong coupling limit, the lowest eigenstates of each energy surface should be localized at the potential minimum. Therefore, expanding the potentials around the minima $\rho_{-,0} = |g|$ for the lower sheet, and $\rho_{+,0} = (j^2/|g|)^{1/3}$ for the upper sheet, respectively, and keeping up to quadratic terms of displacements from these minima, the Schrödinger equation for the lower and upper sheet become

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \frac{1}{2} g^2 + \frac{j^2}{2g^2} \right] \chi_-(x) = E_- \chi_-(x), \quad (17)$$

and

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} \left\{ \frac{3}{2} \left(\frac{g^2}{|j|} \right)^{\frac{2}{3}} \right\} x^2 + \frac{3}{2} (j^2 g^2)^{\frac{1}{3}} \right] \chi_+(x) = E_+ \chi_+(x), \quad (18)$$

respectively, where $x = \rho - \rho_{\pm,0}$. This crude harmonic approximation yields the eigenenergy and eigenfunction for the lower sheet

$$E_{-,nj} = \left(n + \frac{1}{2} \right) + \frac{j^2}{2g^2} - \frac{1}{2} g^2, \quad (19)$$

$$\chi_-(\rho) = \exp \left[-\frac{1}{2} (\rho - |g|)^2 \right] H_n(\rho - |g|), \quad (20)$$

and, for the upper sheet,

$$E_{+,nj} = \sqrt{3} \left(\frac{g^2}{|j|} \right)^{\frac{1}{3}} \left(n + \frac{1}{2} \right) + \frac{3}{2} (j^2 g^2)^{\frac{1}{3}}, \quad (21)$$

$$\chi_+(\rho) = \exp \left[-\frac{1}{2} \sqrt{\frac{3}{2}} \left(\frac{g^2}{|j|} \right)^{\frac{1}{3}} \left(\rho - \left(\frac{j^2}{|g|} \right)^{\frac{1}{3}} \right) \right] \times \quad (22)$$

$$H_n \left[\left(\frac{3}{2} \right)^{\frac{1}{3}} \left(\frac{g^2}{|j|} \right)^{\frac{1}{6}} \left\{ \rho - \left(\frac{j^2}{|g|} \right)^{\frac{1}{3}} \right\} \right]. \quad (23)$$

It is found that the wavefunctions in the crude approximation have finite values at the origin, and they do not satisfy the boundary condition. We therefore have to impose correct asymptotic behavior on these wavefunctions.

4. Asymptotic behavior near origin

The solutions in the vicinity of the origin are searched in the standard way [14,15] by putting $\chi(\rho) = \rho^\alpha v(\rho)$, where $v(\rho)$ is non-zero at the origin and α is a non-negative con-

stant. In this section, the power α for both the exact coupled equations and the decoupled equations is determined.

If ρ approaches to zero, the coupled equations of the Hamiltonian (10) become

$$\begin{pmatrix} -\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} & \frac{j}{2\rho^2} \\ \frac{j}{2\rho^2} & -\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} \end{pmatrix} \begin{pmatrix} \chi_- \\ \chi_+ \end{pmatrix} = 0 \quad (24)$$

The Hamiltonian matrix around the origin can be diagonalized as

$$\begin{pmatrix} -\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} - \frac{j}{2\rho^2} & 0 \\ 0 & -\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} + \frac{j}{2\rho^2} \end{pmatrix} \begin{pmatrix} \chi'_- \\ \chi'_+ \end{pmatrix} = 0, \quad (25)$$

where

$$\begin{pmatrix} \chi'_- \\ \chi'_+ \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \chi_- \\ \chi_+ \end{pmatrix}. \quad (26)$$

If we write the solutions around $\rho = 0$ as $\chi'_\pm \sim \rho^{\alpha'_\pm} C'_\pm$, where $C'_\pm$ are nonzero constants, we obtain $\alpha'_- = j, 1-j$, and $\alpha'_+ = j+1, -j$. For the wavefunction to be regular at the origin, $\alpha'_\pm$ should be positive. Therefore, for a positive j , $\alpha'_- = j = |j|$ and $\alpha'_+ = j+1 = |j|+1$, and, for a negative j , $\alpha'_- = 1-j = |j|+1$ and $\alpha'_+ = -j = |j|$. Passing from χ'_-, χ'_+ to χ_-, χ_+ , we can find $\alpha_\pm = \min(\alpha'_+, \alpha'_-)$. Accordingly we obtain a simple solution, $\alpha_\pm = |j|$ for the coupled equations.

If ρ approaches to zero in the decoupled equations, the equations become

$$\left(-\frac{1}{2} \frac{d^2}{d\rho^2} + \frac{j^2}{2\rho^2} \right) \chi_\pm(\rho) = 0. \quad (27)$$

If $\chi_\pm \sim \rho^{\alpha_\pm} C_\pm$ around the origin, where $C_\pm$ is a non-zero constant, we obtain $\alpha_\pm = \frac{1}{2} + \sqrt{j^2 + \frac{1}{4}}$ for the decoupled equations.

The fact that different α 's are obtained from the coupled and decoupled equation signifies that the asymptotic behavior of the wavefunction in the vicinity of the origin is strongly influenced by the non-adiabatic coupling. This is especially the case for the upper sheet even in the strong coupling limit.

Since we find that $\alpha_- = \alpha_+$ for both the coupled and decoupled equation, we put $\alpha_- = \alpha_+ = \alpha$ hereafter. Accordingly

$$\alpha_{\text{coupled}} = |j| \quad (28)$$

and

$$\alpha_{\text{decoupled}} = \frac{1}{2} + \sqrt{j^2 + \frac{1}{4}}. \quad (29)$$

Note that the crude approximation corresponds to putting $\alpha_{\text{crude}} = 0$ in the expressions.

5. Analytical solutions

Though α was determined in the previous section, we keep α arbitrary in the discussion on the solution for the lower sheet in order to emphasize the fact that the energy expression in the strong coupling limit is independent of α up to the order of $1/g^2$. The equations for $v(\rho)$ has a form

$$v''(\rho) + P(\rho)v'(\rho) + Q(\rho)v(\rho) = 0, \quad (30)$$

where $P(\rho)$ and $Q(\rho)$ is a function of α, j, g , and ρ . Since the neighborhood of $\rho = \rho_{\pm,0}$ is the most important region in the strong coupling limit, expanding $P(\rho)$ and $Q(\rho)$ around $\rho = \rho_{\pm,0}$, and keeping terms up to a linear term in $P(\rho)$ and a quadratic term in $Q(\rho)$, we obtain an analytically solvable equation [13],

$$v''(x) + (a_0 + b_0x)v'(x) + (a_1 + b_1x + c_1x^2)v(x) = 0, \quad (31)$$

where $x = \rho - \rho_{\pm,0}$. The eigen function can be written as

$$\chi(\rho) = \rho^\alpha \exp \left[-\frac{1}{2}\zeta^2(\rho - \lambda)^2 \right] \times H_n[\kappa(\rho - \mu)], \quad (32)$$

where H_n is an Hermite polynomial, and the parameters are defined by the followings:

$$\zeta^2 = 2 \left(k + \frac{b_0}{2} \right), \quad (33)$$

$$\lambda = \rho_0 - \frac{a_0 - \tau}{2k + b_0}, \quad (34)$$

$$\kappa = \sqrt{\frac{b_0}{2} + 2k}, \quad (35)$$

$$\mu = \rho_0 - \frac{a_0 - 2\tau}{b_0 + 4k}, \quad (36)$$

$$k = \frac{1}{4} \left(-b_0 + \sqrt{b_0^2 - 4c_1} \right), \quad (37)$$

$$\tau = \frac{b_1 + 2a_0k}{b_0 + 4k}. \quad (38)$$

The quantization condition is

$$\frac{a_1}{2} = \left(\frac{b_0 + 4k}{2} \right) n + \frac{b_0}{2} + k + \frac{a_0\tau}{2} - \frac{\tau^2}{2}, \quad (39)$$

where $n = 0, 1, 2, \dots$

5.1. Lower sheet

The eigen value is obtained from the quantization condition (39) as

$$E_- = -\frac{\alpha^2 - \alpha - j^2}{2g^2} - \frac{1}{2}g^2 + \frac{b_0}{2} + k + \frac{b_0 + 4k}{2}n + \frac{a_0\tau}{2} - \frac{\tau^2}{2} \quad (40)$$

The energy expression in the strong coupling limit is simplified as

$$E_- = -\frac{1}{2}g^2 + n + \frac{1}{2} + \frac{j^2}{2g^2} + \frac{(3\alpha - 2\alpha^2 + 3j^2)(2n + 1)}{4g^4} + O\left(\frac{1}{g^6}\right). \quad (41)$$

It should be noted that arbitrary α does not enter in the power of $1/g^2$. This is the reason why the crude energy expression [1,12] gives the correct energy up to the order of $1/g^2$ in the strong coupling region, in spite of the incorrect asymptotic behavior. Furthermore, it is important to note that the contributions to energy of the order of $1/g^2$ originate not only from a_1 which gives the pseudorotational energy $j^2/(2g^2)$ in the crude treatment with $\alpha = 0$ but also from a_0, b_0, k, τ which are neglected in the crude approximation. In other words, the conventional treatment is invalid since other terms of the order of $1/g^2$ are missing. In the term of the $1/g^4$ order, we find a dependence on α . However, the first-order perturbations exactly cancel the α -dependence in the $1/g^4$ order [13].

The parameters in the wavefunction for the lower sheet is obtained as

$$\zeta_-^2 = 1 - \frac{\alpha}{g^2} + \frac{3\alpha - 2\alpha^2 + 3j^2}{2g^4} + O\left(\frac{1}{g^8}\right), \quad (42)$$

$$\lambda_- = |g| - \frac{\alpha}{|g|} + \frac{\alpha - \alpha^2 + j^2}{|g|^3} + O\left(\frac{1}{|g|^5}\right), \quad (43)$$

$$\kappa_- = 1 + \frac{3\alpha - 2\alpha^2 + 3j^2}{4g^4} + O\left(\frac{1}{g^8}\right), \quad (44)$$

and

$$\mu_- = |g| + \frac{\alpha + j^2}{|g|^3} + O\left(\frac{1}{|g|^7}\right). \quad (45)$$

Accordingly the wavefunction (32) approaches the crude wavefunction (20) except for ρ^α . The present wavefunctions are exactly zero at the origin. On the other hand, the crude wavefunction have a finite value. The positions of the maximum of the present wavefunctions are shifted to larger ρ . The asymmetric potential results in the asymmetric shapes of the wavefunctions. On the other hand, the crude wavefunction has a symmetric form about the potential minimum due to the harmonic potential.

5.2. Upper sheet

For the upper sheet, we put α to be equal to $\frac{1}{2} + \sqrt{j^2 + \frac{1}{4}}$. We obtain the eigen energy as

$$E_+ = j^{\frac{2}{3}} g^{\frac{2}{3}} + \frac{1}{2} j^{\frac{4}{3}} g^{-\frac{2}{3}} + \frac{b_0}{2} + k + \frac{b_0 + 4k}{2}n + \frac{a_0\tau}{2} - \frac{\tau^2}{2}. \quad (46)$$

The simplified energy expression in the strong coupling limit is

$$E_+ \sim \left(3j^2 - 1 + \alpha \left(n + \frac{1}{2} \right) \right) \left(\frac{g}{j^2} \right)^{\frac{2}{3}} + O\left(|g|^{-\frac{2}{3}} \right), \quad (47)$$

where $\alpha = \frac{1}{2} + \sqrt{j^2 + \frac{1}{4}}$. Note this energy expression is different from that of the crude approximation.

In the energy expression (47), it is found that an effect of α enters in the lowest order of g . This means that the energy is strongly influenced by the existence of ρ^α .

The wavefunction in the crude approximation is essentially a harmonic wavefunction. On the other hand, the present wavefunction for the upper sheet is quite different from the wavefunction of the harmonic potential; (1) the position of the extrema is shifted towards larger ρ (2) it has a smaller curvature than that expected for the harmonic wavefunction. In other words, the wavefunction is more delocalized than the harmonic wavefunction. The curvature at large ρ becomes small as the coupling increases. Moreover, the present wavefunctions are zero at the origin, while the crude wavefunction has a finite value.

6. Concluding remarks

We obtained an analytical solution with the correct boundary conditions for the $E \otimes e$ dynamic Jahn–Teller problem in the strong coupling limit. The different asymptotic behavior originates from the non-adiabatic coupling. Compared with the conventional solutions, the eigen functions contain factors $\rho^{|j|}$ for the coupled equation and $\rho^{1/2+\sqrt{j^2+1/4}}$ for the decoupled equation. The power α is independent of g . It depends on only j . In other words, a non-adiabatic effect on the asymptotic behavior always exists regardless of the magnitude of g . To take $\alpha = |j|$ in Eq. (32) corresponds to an intermediate level of approximation between the adiabatic approximation and an exact (non-adiabatic) theory.

In addition, α is the same for the lower and upper sheet.

On the other hand, the conventional energy expression for the lower sheet is correct up to the $1/g^2$ order, in spite of the incorrect treatment of the boundary condition.

The solutions for the upper sheet are entirely different from those obtained by Slonczewski [16].

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