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THE BERRY PHASE OF AN E ⊗ϵ SYSTEM

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Abstract. In this paper, we consider an E⊗ϵ-type Jahn–Teller system described by a two-mode Hamiltonian. The Berry phase method enables the calculation of the probabilities of non-adiabatic transitions. We have calculated the Berry phase for an E⊗ϵ Jahn–Teller system. The results are two types of transitions, one modifying j and the other one leaving j constant.

Key words: Jahn–Teller system, Berry phase, quantum transitions.

1. INTRODUCTION

The E⊗ϵ Jahn–Teller system represents a model which permits complete calculations and which has been extensively studied [1–5].

The Berry phase method has a wide field of application: coherent states [6–8] and the Jahn–Teller effect [1,9]. The method permits the calculation of the evolution of states in time.

In this paper the Berry phase method is illustrated applied to an E⊗ϵ system.

2. THE E ⊗ϵ MODEL OF THE JAHN–TELLER EFFECT

Let us consider a Jahn–Teller system of a type E ⊗ϵ, using the Reik model [5] which consists of a two-level system, the levels being separated by $1+4\delta$, with the aid of a Rabi Hamiltonian representing a bosons system with two modes:

$$H = a_1^\dagger a_1 + a_2^\dagger a_2 + \left(\frac{1}{2}+2\delta\right)\sigma_z + 2k[(a_1 + a_2^\dagger)\sigma_+ + (a_1^\dagger + a_2)\sigma_-], \quad (1)$$

where $a_i^\dagger$, a_i represents the creation – annihilation operators of the ith mode. This model corresponds to a Schwinger representation [9, 10]. The operators obey the commutation relations:

$$[a_1, a_1^\dagger] = [a_2, a_2^\dagger] = 1,$$

$$[a_1, a_2] = [a_1^\dagger, a_2^\dagger] = [a_1, a_2^\dagger] = [a_2, a_1^\dagger] = 0, \tag{2}$$

and for the Pauli matrices:

$$[\sigma_+, \sigma_-] = 2\sigma_z,$$
$$[\sigma_z, \sigma_+] = \sigma_+, \tag{3}$$
$$[\sigma_z, \sigma_-] = -\sigma_- .$$

The eigenstates of this Hamiltonian can be expressed by using the eigenstates $|\uparrow>, |\downarrow>$ for the σ_z operator. Denoting the vacuum state for a two-boson system by $|00>$, we can write the eigenstates for (1) as

$$|j + \frac{1}{2} >= a_1^{\dagger j+1} \Phi(a_1^\dagger, a_2^\dagger)|00> |\uparrow> + a_2^{\dagger j+1} f(a_1^\dagger, a_2^\dagger)|00> |\downarrow> . \tag{4}$$

The Hamiltonian can be expressed as a function of the momentum operator J and the operator h_+, defined as

$$J = a_1^\dagger a_1 - a_2^\dagger a_2 + \frac{1}{2}\sigma_z,$$

$$h_+ = a_2^\dagger a_2 + \delta\sigma_z + k[(a_1 + a_2^\dagger)\sigma_+ + (a_1^\dagger + a_2)\sigma_-].$$

Hamiltonian (1) can be expressed as follows:

$$H = J + 1 + 2h_+.$$

The eigenvalues for the Hamiltonian are

$$\lambda = j + \frac{3}{2} + 2\epsilon, \tag{5}$$

where ϵ represents the eigenvalues for h_+:

$$h_+|j + \frac{1}{2} >= \epsilon|j + \frac{1}{2} >; \tag{6}$$

ϵ can be expressed as a function of Judd's parameter v:

$$\epsilon = \frac{v}{2} - \frac{j}{2} - \frac{1}{2} - k^2.$$

The rising and lowering operators for the $|j + \frac{1}{2} >$ state are the $J_\pm$ operators defined as

$$J_{\pm} = J_x \pm i J_y. \tag{7}$$

The action of the operator J is:

$$J \left| j + \frac{1}{2} \right> = \left(j + \frac{1}{2} \right) \left| j + \frac{1}{2} \right> . \tag{8}$$

The operators $a_i, a_i^{\dagger}$ can be expressed in the variables ξ, η:

$$a_1^{\dagger} = \xi, \quad a_1 = \frac{\partial}{\partial \xi}, \quad a_2^{\dagger} = \eta, \quad a_2 = \frac{\partial}{\partial \eta}. \tag{9}$$

In these variables:

$$J = \xi \frac{\partial}{\partial \xi} - \eta \frac{\partial}{\partial \eta} + \frac{1}{2} \sigma_z,$$

$$h_+ = \eta \frac{\partial}{\partial \eta} + \delta \sigma_z + k \left(\frac{\partial}{\partial \xi} + \eta \right) \sigma_+ + k \left(\frac{\partial}{\partial \eta} + \xi \right) \sigma_-, \tag{10}$$

$$|j + \frac{1}{2}> = \xi^{j+1} \Phi(z) | \uparrow> |00> + \eta^{j+1} f(z) | \downarrow> |00> ,$$

where $z = \xi \eta$.

It results in the eigenvalue equations for Φ, f expressed in z:

$$z \frac{d\Phi}{dz} - \left(\frac{v}{2} - \frac{j}{2} - \frac{1}{2} - \delta - k^2 \right) \Phi + k \left[z \frac{df}{dz} + (j + 1 + z) f \right] = 0,$$

$$k \left[\left(\frac{d\Phi}{dz} \right) + \Phi(z) \right] + \left[z \frac{df}{dz} - \left(\frac{v}{2} - \frac{j}{2} - \frac{1}{2} + \delta - k^2 \right) f \right] = 0.$$

The Rabi Hamiltonian can be obtained from a particular condition of a single mode:

$$H = a^{\dagger} a + \frac{1}{2} + \left(\frac{1}{2} + 2\delta \right) \sigma_z + \sqrt{k} (a^{\dagger} + a)(\sigma_+ + \sigma_-) .$$

3. THE BERRY PHASE

We consider a Hamiltonian $H(\alpha)$ which depends on a parameter α of a space D. We assume that we know the states of this system, ($|n(\alpha)>$), which depend on the parameter α. These states satisfy [1]:

$$H(\alpha)|n(\alpha)> = E(\alpha)|n(\alpha)> . \tag{11}$$

The parameter α can be of a vector form.

If the system has a temporal evolution from the moment t_0 to t along a smooth path $\alpha(t)$, we can write:

$$|\Psi(t)>=|n(\alpha(t))>\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}E_n(\alpha(t'))dt'\right].$$

In the adiabatic approximation we have [1]

$$<n(\alpha(t))|\frac{\partial}{\partial t}|n(\alpha(t))>=0. \quad (12)$$

For a non-adiabatic transition between the initial state $|n_i>$ and the final state $|n_f>$ there exists a relation

$$|n_f>=e^{i\gamma_n(C)}|n_i>. \quad (13)$$

It can be seen that the two states are linked by a phase factor $\gamma_n(C)$, called the Berry phase.

This phase factor corresponds to the transport of the state $|n>$ along the curve C, the factor being defined as

$$\gamma_n(C)=-\oint_C <n|dn>. \quad (14)$$

One can also define a generalized vector potential:

$$\vec{A}=<n_\alpha|\nabla_\alpha|n_\alpha>, \quad (15)$$

where ∇_α represents a gradient-type potential, defined in the space of the parameter $\vec{\alpha}$. As a result

$$\gamma(C)=\oint_C \vec{A}d\vec{\alpha}. \quad (16)$$

If this factor is non-zero, then between the initial and final states there exists relation (13) and the transition is possible.

For the parameter $\vec{\alpha}$ of the dimension n

$$\gamma_n(C)=-\text{Im}\sum_{i=1}^{n}\oint<n(\alpha_i)|\frac{\partial n(\alpha_i)}{\partial\alpha_i}>d\alpha_i. \quad (17)$$

4. THE BERRY PHASE FOR THE E $\otimes\epsilon$ SYSTEM

The generators which leave the eigenstates of E $\otimes\epsilon$ unchanged are σ_z and the operators

$$J=a_1^\dagger a_1-a_2^\dagger a_2+\frac{1}{2}\sigma_z,$$

$$N_2=a_2^\dagger a_2$$

or $a_1^\dagger a_1$, $a_2^\dagger a_2$, and σ_z.

We will define the operators as follows:

$$T_1 = \exp[-i\alpha\sigma_z],$$
$$T_2 = \exp[-i\theta a_1^\dagger a_1], \tag{18}$$
$$T_3 = \exp[-i\beta a_2^\dagger a_2] \ .$$

After the application of these operators the Hamiltonian is

$$H_1 = T_1^\dagger H T_1 = H_0 + 2k[(a_1 + a_2^\dagger)T_1^\dagger \sigma_+ T_1 + (a_2 + a_1^\dagger)T_1^\dagger \sigma_- T_1],$$

where

$$H_0 = a_1^\dagger a_1 + a_2^\dagger a_2 + 1 + \left(\frac{1}{2} + \delta\right)\sigma_z \ .$$

It can be verified that

$$\exp[i\alpha\sigma_z]\sigma_+ \exp[-i\alpha\sigma_z] = \sigma_+ \exp[i\alpha],$$
$$\exp[i\alpha\sigma_z]\sigma_- \exp[-i\alpha\sigma_z] = \sigma_- \exp[-i\alpha] \ .$$

As a result the Hamiltonian is as follows:

$$H_1 = H_0 + 2k[(a_1 + a_2^\dagger)\sigma_+ \exp[i\alpha] + (a_2 + a_1^\dagger)\sigma_- \exp[-i\alpha]] \ .$$

It can be seen that

$$\exp[i\theta a_1^\dagger a_1]a_1 \exp[-i\theta a_1^\dagger a_1] = a_1 \exp[-i\theta],$$
$$\exp[i\theta a_1^\dagger a_1]a_1^\dagger \exp[-i\theta a_1^\dagger a_1] = a_1^\dagger \exp[i\theta],$$
$$\exp[i\beta a_2^\dagger a_2]a_2 \exp[-i\beta a_2^\dagger a_2] = a_2 \exp[-i\beta],$$
$$\exp[i\beta a_2^\dagger a_2]a_2^\dagger \exp[-i\beta a_2^\dagger a_2] = a_2^\dagger \exp[i\beta].$$

Applying successively the transformations T_2 and T_3 to the Hamiltonian H_1, we obtain:

$$H_2 = T_2^\dagger H_1 T_2 = H_0 + 2k[(a_1 \exp[-i\theta] + a_2^\dagger)\sigma_+ \exp[i\alpha] +$$
$$+ (a_1^\dagger \exp[i\theta] + a_2)\sigma_- \exp[-i\alpha]],$$

$$H_3 = T_3^\dagger H_2 T_3 = H_0 + 2k[(a_1 \exp[-i\theta] + a_2^\dagger \exp[i\beta])\sigma_+ \exp[i\alpha] +$$

$$+(a_1^\dagger \exp[i\theta] + a_2 \exp[-i\beta])\sigma_- \exp[-i\alpha]]. \quad (19)$$

As a result, the Berry phase can be calculated from the interaction term of the transformed Hamiltonian:

$$\gamma(C) = 2k \oint_C \mathrm{Im}\Big[< j' + \frac{1}{2}|a_1\sigma_+|j + \frac{1}{2} > \exp[i(\alpha - \theta)] +$$

$$+ < j'+\frac{1}{2}|a_2^\dagger\sigma_+|j+\frac{1}{2} > \exp[i(\alpha+\beta)] < j'+\frac{1}{2}|a_1^\dagger\sigma_-|j+\frac{1}{2} > \exp[i(-\alpha+\theta)]+$$

$$+ < j' + \frac{1}{2}|a_2\sigma_-|j + \frac{1}{2} > \exp[i(-\alpha - \beta)]\Big] ds. \quad (20)$$

5. CONCLUSION

By taking the domain contour (and the parameter's domain) in an adequate way, we obtain for the Berry phase non-zero integrals with the terms varying the total quantum number (corresponding to $a^\dagger\sigma_+$ and $a\sigma_-$) and the terms which do not affect j (corresponding to $a\sigma_+$ and $a^\dagger\sigma_-$).

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(E $\otimes\epsilon$)-SÜSTEEMI BERRY FAAS

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On vaadeldud (E $\otimes\epsilon$)-tüüpi Jahni–Telleri süsteemi, mida kirjeldab kahemoodiline hamiltoniaan. Berry faasi meetod võimaldab arvutada mitteadiabaatiliste siirete tõenäosusi. Töös on arvutatud Berry faas nimetatud süsteemi jaoks. Tulemuseks on kahte liiki siirded, millest üks muudab kvantarvu j ja teine jätab selle konstantseks.

ФАЗА БЕРРИ ДЛЯ (E ⊗ ϵ)-СИСТЕМЫ

Георге Е. ДРАГАНЕСКУ, Николаэ М. АВРАМ

В работе рассматривается ян–теллеровская система типа E ⊗ ϵ, описываемая двухмодовым гамильтонианом. Метод фазы Берри позволяет вычислить вероятности неадиабатических переходов; в работе вычислена фаза Берри для рассматриваемой системы. Результатом являются переходы двух типов, один из них меняет квантовое число *j*, другой оставляет *j* постоянным.