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利用「等效漢彌頓」法解雙振盪的隧道效應
Solution of Double Oscillatory Tunneling by Effective Hamiltonian Method

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ABSTRACT — A double oscillatory potential which is found to be useful in modeling the problem of atomic rate transition is analysed by effective hamiltonian method. The result is the same as rigorous analysis. A back tunneling of the particle due to the accumulation effect on final local state must be taken into account in this double oscillatory case, suggesting that the golden rule of transition is a rough approximation and is not applicable to bound state tunneling.

I. Introduction

In many cases of rate determinations such as interstitial and vacancy diffusions [1], reorientation [2,3], molecular inversion [4] and the others at low temperature, mainly by tunneling, there requires an one-dimension-double-oscillator potential model as shown in Fig. 1 to count for the transition rate of a particle hopping from one equilibrium position to the other. Although, in general, the barrier tip is rounded-up, it nevertheless does not lose the main picture of a true potential shape.

While the exact quantum solution of the double oscillatory potential [5] has its wavefunctions spreaded out in two troughs (r and ℓ) there is no tunneling jump can be observed from these wavefunctions directly. But by suitably linear combination of a symmetric wavefunction and an antisymmetric wavefunction of about the same energy a localized picture will be obtained, and one observes this wavefunction which represents the location of a classical particle swings back and forth between these two troughs with a frequency $\omega'=\Delta E/2\hbar$ where ΔE is the difference of the eigen-energies between the two exact wavefunctions.

It has been shown [6] that the energy difference $\Delta E=(2\hbar^2/M)\psi_r$

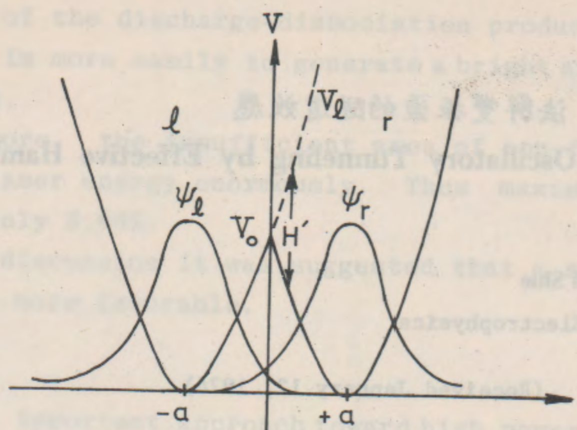

Fig. 1

$V_\ell = \frac{1}{2}M\omega^2\,(x+a)^2$, the effective potential at left.
$V = \frac{1}{2}M\omega^2\,(|x|-a)^2$, the total potential of a double oscillator.
H' the effective perturbation to left state and is equivalent to $H-H_\ell$

(x=0) ψ_r' (x=0), and for ground state tunneling it reads

$$\omega' = \omega\sqrt{\frac{2V_o}{\hbar\omega\pi}}\,\exp\left(-\frac{2V_o}{\hbar\omega}\right) \qquad (1)$$

We have repeated the problem by using the effective hamiltonian method. It is found that an exact result can be obtained when we correctly count the accumulation effect of the back tunneling. It turns out that the golden rule of transition probability is a very rough approximation and is not applicable here as it is used in the case of square barrier tunneling [7,8].

II. The Effective Hamiltonian Method

Consider a quesi-particle subjects to a potential V as shown in Fig. 1, and makes transition adiabatically between two troughs, that is between two equivalent states. Let the effective hamiltonian on the left region, H_ℓ, has an effective potential denoted by dotted line in the figure, so that its wavefunctions can be solved exactly by equation

$$H_\ell\psi_\ell = E_\ell\psi_\ell \qquad (2)$$

with

$$H = H_\ell + H' \qquad (3)$$

The same argument can be applied to the right region and one has

$$H_r \psi_r = E_r \psi_r \quad (4)$$

Both the oscillator wavefunctions are good solutions to their effective hamiltonian and represent the two localized quesi-particle states respectively, but they are not good solutions to the total hamiltonian H. The good solution should be the linear combination of the two, that is

$$\psi = a(t)\psi_\ell\, e^{-\frac{iE_\ell}{\hbar}t} + b(t)\psi_r\, e^{-\frac{iE_r}{\hbar}t} \quad (5)$$

To find the tunneling rate between the two localized states one must follow the standard time-dependent perturbation procedures, as suggested by the effective hamiltonian method, with H' as a perturbation. That is, one puts equation (5) into time-dependent schrodinger equation

$$H\psi = i\hbar \frac{\partial}{\partial t}\psi \quad (6)$$

and solves for a(t) and b(t) with conditions of normalizations and orthogonalization, namely

$$\int \psi_r^* \psi_r \, dx = 1 \quad (7a)$$

$$\int \psi_\ell^* \psi_\ell \, dx = 1 \quad (7b)$$

and

$$\int \psi_r^* \psi_\ell \, dx \cong 0 \quad (7c)$$

The results at any time t are given by

$$\dot{a}(t) \cong -\frac{1}{\hbar} H'_{r\ell}\, b(t) \quad (8)$$

and

$$\dot{b}(t) \cong -\frac{1}{\hbar} H'_{\ell r}\, a(t) \quad (9)$$

here H'_{ij} are the effective transition matrix elements. Solving equations (8) and (9) simultaneouly one obtains

$$\ddot{a}(t) + \frac{|H'_{r\ell}|^2}{\hbar^2}\, a(t) = 0 \quad (10)$$

$$\ddot{b}(t)+\frac{|H_{r\ell}'|^2}{\hbar^2}\, b(t)=0 \tag{11}$$

Obviously,

$$a(t)=A\cos\left(\frac{|H_{r\ell}'|}{\hbar}t\right)+iA'\sin\left(\frac{|H_{r\ell}'|}{\hbar}t\right) \tag{12}$$

$$b(t)=B\cos\left(\frac{|H_{r\ell}'|}{\hbar}t\right)+iB'\sin\left(\frac{|H_{r\ell}|}{\hbar}t\right) \tag{13}$$

and if one puts the initial conditions a(0)=1 and b(0)=0 with normalization conditions (7a) and (7b) into equations (12) and (13) one obtains

$$\psi=\cos\left(\frac{|H_{r\ell}'|}{\hbar}t\right)\psi_\ell+i\sin\left(\frac{|H_{r\ell}'|}{\hbar}t\right)\psi_r \tag{14}$$

It is readily shown by the effective hamiltonian method that the transition matrix element

$$H_{r\ell}' = -i\hbar j_{r\ell}(x=0)$$

$$= -\frac{\hbar^2}{2M}\left(\psi_r^* \frac{d\psi_\ell}{dx} - \psi_\ell \frac{d\psi_r^*}{dx}\right)_{x=0} \tag{15}$$

where $j_{r\ell}$ is the current operator. With linear oscillator wavefunctions put into equation (15), one can find that it equals to $\hbar\omega'$ as indicated in equation (1). Therefore, effective hamiltonian method gives the correct answer to the double oscillator tunneling rate.

III. Conclusion

Some remarks can be summarized as following:

(1) The golden rule of transition probability can not be applied to this case. For if it is true, the transition probability, $W_{r\ell}$, would read

$$W_{r\ell}=\frac{2\pi}{\hbar}|H_{r\ell}'|^2$$

which means, for ground state tunneling,

$$W_{r\ell} \propto e^{-\frac{4V_o}{\hbar\omega}}$$

which is obviously not correct. The reason is that unlike square well tunneling where a particle, after tunneling through a barrier, runs forever away from the barrier and never exerts a "back pressure", however, in the present case the particle is accumulated at the right region and back tunneling has to be taken into account, resulting in an oscillatory jumping.

(2) The effective hamiltonian is quite a good approximation in counting the transition rate as long as the over-lapping of the two wavefunctions is negligible, that is $v_o >> \frac{1}{2}\hbar\omega$.

(3) The most distinguishing advantage of the present method is that it can be applied to the more general problems such as unsymmetric double oscillatory potential, multioscillatory potential as well as the radiative transition and other external perturbation cases. To these problems, the effective hamiltonian method probably can be offered as a most intuitive tool without introducing new difficults.

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