EFFECT OF INTRINSIC DEGREES OF FREEDOM ON THE QUANTUM TUNNELLING OF A COLLECTIVE VARIABLE

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The motivation to set up a theory to treat the multidimensional quantum tunneling problem need not be restricted to nuclear physics. The problem of vacuum tunneling in gauge field theories as well as the tunneling of magnetic flux in solids have been treated within the framework of the path integral formalism. One advantage of this formalism is that the explicit introduction of wave function can be avoided. In nuclear physics there are mainly two problems for which quantum tunneling is important: spontaneous fission and subbarrier fusion. In the first case, one could use the path integral formalism to describe the decay width of the fissioning state, but for the second, the explicit introduction of the wave function is unavoidable, as well as for any scattering problem.

We propose a method to obtain a multidimensional WKB like wave function (1), which is less general than the method of Gervais and Sakita (2), but better adapted for physical applications.

The presentation of the theory as well as its application to the tunneling problem will be developed below, as well as some preliminary results on the modification of the transmission coefficient of a parabolic barrier due to the presence of other degrees of freedom. The details of the derivations and the justification of approximations are given in (1).

II. Presentation of the Method

In this section, we aim at finding an approximate solution to the time independent Schrödinger equation associated with the following hamiltonian

$$H = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial q^2} + V(q) + h(x_\alpha, q)$$

$$h(x_\alpha, q) = \sum_\alpha \left\{ -\frac{\hbar^2}{2m_\alpha}\frac{\partial^2}{\partial x_\alpha^2} + \frac{1}{2} m_\alpha \omega_\alpha^2 x_\alpha^2 + c_\alpha x_\alpha q \right\} \qquad \text{(II-1)}$$

The coupling could have a more general form

$$\sum_\alpha c_\alpha q x_\alpha \longrightarrow \sum_\alpha f_\alpha(q)\, x_\alpha$$

without changing the argument.

We write the wave function of our problem as

$$\Psi(x_\alpha, q) = \phi(x_\alpha, q)\, \exp\left(i\epsilon W(q)/\hbar\right) \qquad \text{(II-2)}$$

where $\epsilon = \pm 1$ in a classically allowed region and $\epsilon = \pm i$ in a classically forbidden region. The wave function (II-2) satisfies the Schrödinger equation $H\Psi = E\Psi$ if W and ϕ satisfy

$$-\frac{\epsilon^2}{2M}\left(\frac{dW}{dq}\right)^2 + V(q) = E_0 \qquad \text{(II-3)}$$

$$-\frac{\hbar^2}{2M}\left\{ \frac{i\epsilon\phi}{\hbar}\frac{d^2W}{dq^2} + \frac{2i\epsilon}{\hbar}\frac{\partial\phi}{\partial q}\frac{dW}{dq} + \frac{\partial^2\phi}{\partial q^2} \right\} + h(x_\alpha, q)\phi = E_\perp \phi \qquad \text{(II-4)}$$

where (II-5)

$$E = E_0 + E_\perp$$

In a more general trial wave function, W would depend on x_α as well as on q. We prefer the form (II-2) because it leads to simple results and a transparent physical interpretation.

The solution of eq. (II-3) is

$$W(q) = \int \sqrt{2M|E_o - V(q)|}\, dq \tag{II-6}$$

The next step to simplify eq. (II-4) is to introduce a new variable ζ, which replaces the variable q in the following way

$$\frac{dq}{d\zeta} = \frac{1}{M}\frac{dW}{dq} = \sqrt{2|E_o - V(q)|/M} \tag{II-7}$$

so that

$$\frac{\partial}{\partial \zeta} = \frac{1}{M}\frac{dW}{dq}\frac{\partial}{\partial q}$$

We also put $\phi = \chi / \sqrt{dW/dq}$ (II-9)

and then eq. (II-4) can be rewritten as

$$-i\hbar\epsilon\frac{\partial \chi}{\partial \zeta} + h(x_\alpha, q(\zeta))\chi - E_1\chi = \underbrace{\frac{\hbar^2}{2M}\sqrt{\frac{dW}{dq}}\frac{\partial^2\phi}{\partial q^2}}_{\simeq 0} \tag{II-10}$$

The term proportional to $\partial^2\phi/\partial q^2$ has been neglected, this is the approximation m de in our method. Its conditions of validity are discussed in section 6 of (1).

III. *The Tunneling Problem*

Let us assume (with no loss of generality) that the collective coordinate q is coupled to one coordinate χ. Furthermore if one takes the potential to be of the form

$$V(q) = \frac{1}{2} M\omega_o^2 q^2 (1 - q/q_o) \tag{III-1}$$

and take it to be $V(q) = \frac{1}{2} M\omega_o^2 q^2$ for $q = 0$, one can then write the wave function of the lowest stationary state in the potential pocket as $(0 < q < q_o)$

$$\phi(q,x) = \frac{N}{N_0}\phi_0(q)\exp\left\{\frac{-1}{2b^2}(x - \bar{x}(\zeta))^2 + \frac{1}{2}G(\zeta)\right\} \tag{III-2}$$

whe

$$\frac{N^2}{N_0^2} = \sqrt{1 - \frac{c^2}{2mM}\frac{2\omega + \omega_0}{\omega_o^2\omega(\omega+\omega_0)^2}}$$

$$N_0 = \frac{1}{\pi b b_0} \qquad b = \sqrt{\frac{\hbar}{m\omega}} \qquad b_0 = \sqrt{\frac{\hbar}{M\omega s}},$$

$$\bar{x}(\zeta) = -\frac{cb^2}{h} I(\zeta) \tag{III-3}$$

$$G(\zeta) = \frac{c^2}{m\hbar}\left(\frac{1}{\omega}I^2(\zeta) + \int_{-\infty}^{\zeta} I^2(\zeta')d\zeta'\right) \tag{III-4}$$

$$I(\zeta) = \int_{-\infty}^{\zeta} e^{\omega(\zeta - \zeta')} q(\zeta')\, d\zeta' \tag{III-5}$$

and

$$\phi_0(q) = N_0\left(\frac{dW}{dq}\right)^{-1/2}\exp(-W(q)/\hbar), \tag{III-6}$$

which is the BKW wave function for the barrier $\mathcal{V}(q)$ in the absence of the coupling.

The corresponding decay width is givewn by

$$\Gamma = \Gamma_0 \left(\frac{N}{N_0}\right)^2 \exp(G(\omega)) \qquad \text{(III-7)}$$

when Γ_0 is the width calculated in the absence of coupling and the function $G(\omega)$ given by

$$G(\omega) = -\frac{c^2}{2m\hbar\omega} \int_{-\infty}^{\infty} d\tau \int_{0}^{\infty} d\tau' \exp[-\omega|\tau-\tau'|]\, q(\tau)\, q(\tau')$$

It is possible to show the following inequality (1)

$$\Gamma_0 \leq \Gamma \leq \Gamma^{ad}$$

wher Γ^{ad} is the width associated with the adiabetic potetnial. This inequality can be proven for any form of the coupling hamiltonian.

III-1 Interpretation of the results in the limit $\omega \gg \omega_0$

In this limit, the function I( )(eq.III-5) can be expanded as follows

$$I(\tau) = \frac{1}{\omega}\, q(\tau) - \frac{1}{\omega^2}\, \dot{q}(\tau) + \ldots\ldots$$

also

$$\bar{x}(\tau) = \frac{-c}{m\omega^2}\, q(\tau) + \frac{c}{m\omega^2}\, \dot{q}(\tau) - \ldots\ldots$$

and

$$G(\tau) = \frac{c^2}{m\hbar}\left(\frac{1}{\omega^2}\int_{-\infty}^{\tau} q^2(\tau')d\tau' - \frac{1}{w^4}\int_{-\infty}^{\tau} \dot{q}^2(\tau')d\tau' + \ldots\right)$$

These two terms in the expansion of $G(\tau)$ represent a potential normalization and a mass renormalization, respectively, and can be incorporated in $\phi_0(q)$ (eq III-6) provided one defines an adiabatic potential and a renormalized mass in the following manner

$$V_{ad}(q) = V(q) - \frac{c^2}{2m\omega^2}\, q^2 \qquad \text{(III-8)}$$

$$M^* = M + \frac{c^2}{m\omega^4} \qquad \text{(III-9)}$$

In this limit $(\omega \ggg \omega_0)$ the wave function can then be written as

$$\psi^{eff}(q,\tau) = N\psi_0{}^{eff}(q)\, \exp\left\{\frac{-1}{2b^2}\left(x - \frac{cq(\tau)}{m\omega^2}\right)\right\} \qquad \text{(III-10)}$$

$$W^{eff}(q) = \int^{q} \sqrt{2M^*\, V_{ad}(q')}\, dq'$$

In order to understand the term involving x in eq (III-10), we make a variable tansformation

$$x = y - \frac{c}{m\omega^2}\, q$$

and write the hamiltonian in the new variable

$$H = \frac{-\hbar^2}{2M}\frac{\partial^2}{\partial q^2} + V_{ad}(q) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2} + \frac{1}{2}m\omega^2 y^2 + \frac{\hbar^2}{m}\frac{\partial^2}{\partial q \partial y}$$

Thos transformation eliminates the coupling term c q from the hamiltonian and it is replaced by a momentum dependent coupling. In the adiabatic approximation this coupling can be neglected and the wave function can be written

$$\psi = N\psi_0^{eff}(q)\ \exp(-\frac{1}{2b^2}\ y^2)$$

which agrees with eq. (III-10) showing that the mean position of the wave packet for fixed q follows the adiabatic path y = 0.

A similar result holds for the decay width, namely, the effect of the coupling between the q and x variables can be taken into account by replacing V(q) by the adiabatic potential $V_{ad}(q)$ and M by M^* appropriate for the adiabatic path in the limit for large ω.

$$\Gamma = (\frac{N}{N_0})^2\ \Gamma_0^{eff}$$

III-2 A generalization of the Bohr-Wheeler formula

This method can also be applied to study the modification in the transmission coefficient of barriers, due to the p ence of other degrees of freedom. In the case of parabolic barrier, one can obtain analytical results for any value of the ratio $\frac{\omega}{\omega_0}$ (3). The result in the high frequency limit ($\omega \gg \omega_0$) is physically very transparent

$$T = T_0\ \exp\frac{\pi|E-V_0|c^2}{2m\ M\ \omega^2\omega_0^3\ \hbar} \qquad \text{(III-11)}$$

where V_0, ω_0 and M are defined by the collective potential

$$V(q) = V_0 - \frac{1}{2}M\omega_0^2\ q^2$$

$$T_0 = \exp\left[-\frac{2\pi|E-V_0|}{\hbar\omega_0}\right]$$

In order to interpret the result, let us recall again the potential energy of our problem

$$W(q,x) = V(q) + \frac{1}{2}\ m\omega^2x^2 + cqx \qquad \text{(III-12)}$$

In the limit when $\omega \ggg \omega_0$, the x degree of freedom *will follow* the "adiabatic path", or it will adjust itself to the q motion according to the following condition

$$\frac{\partial\ W(q,\bar{x})}{\partial\bar{x}} = 0 \quad ,$$

which gives $\bar{x} = -\frac{cq}{m\omega^2}$

Inserting this average x-value in eq. (III-19), we get an effective potential given by

$$W^{eff}(q,\bar{x}) = V(q) + \frac{1}{2}\ m\omega^2\ (-\frac{cq}{m\omega^2})^2 + cq(-\frac{cq}{m\omega^2})$$

$$= V_0 - \frac{1}{2}M\ q^2\ (\omega^2 + \frac{1}{2}\ \frac{c^2}{Mm\omega^2}) = V_0 - \frac{1}{2}M\ \overline{\omega_0}^2\ q^2 \qquad \text{(III-13)}$$

We see from this equation that the effect of the coupling in this case, is to make the barrier thinner and therefore the transmission coefficient will be enhanced. This effect might help us understand the too large experimental sub-barrier fusion cross sections , which cannot be systematically reproduced by one dimensional potetnials.

If one would calculate the transmission coefficient for this new barrier, one would get the Bohr-Wheeler formula with the corresponding renormalized frequency $\bar{\omega_0}$:

$$T = e^{-\frac{2\pi |E-V_0|}{\hbar\omega_0}}$$

If, furthermore, one assumes

$$\frac{c^2}{Mm\omega^2\omega_0^2} \lll 1$$

one gets

$$T \simeq T_0 \exp\left[\frac{\pi |E-V_0| c^2}{2mM\omega^2 w_0^2 \hbar}\right]$$

a result which is identical to eq. (III-11)

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References

(1) D.M. Brink, M.C. Nemes, and D. Vautherin, Preprint IPNO (TH 82-31)

(2) J.L. Gervais and B. Sakita, Phys. Rev. D16 (1977), 3507

(3) B.V. Carlson, M.C. Nemes, A.F.R. de Toledo Piza, unpublished.