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ABSTRACT: We calculate the energy dispersion relation for the valence band of the double sine-Gordon potential, approximating the tunneling amplitude by a sum of contributions of multi-instantons and anti-instantons trajectories. The interesting feature of this potential is that we now have to deal with two types of instantons, as there are two different potential barriers within one period of the potential. We compare our results with the standard WKB approximation.

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1. INTRODUCTION

Recently there has been great interest in the study of potentials with degenerate minima in view of their application in condensed matter physics, through the study of soliton statistical mechanics (Bishop, Krumhansl and Trullinger 1980) as well as toy models for non-perturbative phenomena in field theory (Stone 1978, Neuberger 1978, Henyey and Patrascioiu 1978). In particular there have been detailed analysis of the double-well anharmonic potential, $V(x)=\alpha(x^2-a^2)^2$ (Krumhansl and Schrieffer 1975, Gildener and Patrascioiu 1977) and the sine-Gordon periodic potential (Stone 1978, Neuberger 1978).

In this paper we consider the double sine-Gordon potential (De Leonardis and Trullinger 1979) which has the interesting feature of presenting two types of instantons, due to the different barriers within one period (figure 1). Our approach consists in using the semi-classical approximation to the path integral, in order to compute the tunneling amplitude for large Euclidean time interval. In this approximation the path integral will be dominated by a dilute gas of instantons (Coleman 1977). The new aspect of our calculation is that we have to take into account the contributions of the two different types of instantons present in this model, to the energy of the valence band. We then compare the dilute gas approximation (DGA) with the standard WKB approach in the tight-binding approximation, finding the well-known discrepancy between the two methods, by a factor of $(\frac{e}{\pi})^{1/2}=$ $=0.93$ (Gildener and Patrascioiu 1977, Neuberger 1978).

2. INSTANTONS IN THE DOUBLE SINE-GORDON POTENTIAL

The potential (figure 1) is given by

$$V(x) = \alpha(\cos\frac{x}{2} - \beta)^2 \qquad (1)$$

We will study the instanton contributions to the tunneling amplitude. Due to the tunnel effect, there will result a band structure for the energy levels of such a periodic potential.

We start with the Euclidean tunneling amplitude (Coleman 1977).

$$G(n_+,n_-,T) = \langle n_+|e^{-HT/\hbar}|n_-\rangle \qquad (2)$$

for the transition between two minima $|n_-\rangle$ and $|n_+\rangle$, separated by an integer multiple of the period (4π). Let us remark that since we are interested in obtaining the energy band of this potential, we must consider the transition between minima separated by an integer multiple of the period, so that (2) is the correct starting point.

The two types of instantons in this model connect sucessive minima separated by the small or by the large barrier. The instanton is the classical zero energy solution of the Euclidean equation of motion, which minimize the action in the large time interval limit, $T \to \infty$. We have instantons, named of type 1,

$$x_1 = 4\tan^{-1}\left[\left(\frac{1-\beta}{1+\beta}\right)^{1/2}\tanh\omega t\right] \qquad (2a)$$

which connect minima separated by the small barriers and instantons of type 2,

$$x_2 = 4\tan^{-1}\left[\left(\frac{1-\beta}{1+\beta}\right)^{1/2}\operatorname{cotanh}\omega t\right] \qquad (2b)$$

which connect minima separated by the large barriers and the respective anti-instantons obtained by making $t \to -t$. In the above equations, ω is the curvature of the potential at the minima,

$$\omega = [\alpha(1-\beta^2)/2]^{1/2} \qquad (3)$$

The Euclidean action for each type of instanton is,

$$S_1 = 8\omega - 8\omega_0\,\beta\,\cos^{-1}\beta \qquad (4a)$$

and

$$S_2 = S_1 + 8\pi\omega_0\beta \qquad (4b)$$

In the DGA, the space between the two minima n_+ and n_- is filled with non-interacting instantons and anti-instantons, separated by a large interval compared with the instanton size ω^{-1} (Coleman 77). The following condition has to be satisfied by the number of instantons and anti-instantons of the two types,

$$n - \bar{n} = m - \bar{m} = n_+ - n_- \qquad (5)$$

where $n(\bar{n})$ is the number of (anti) instantons of type 1 and $m(\bar{m})$ is the number of (anti) instantons of type 2. Summing over all such configurations, the Euclidean tunneling amplitude is written as,

$$G(n_+,n_-,T) = \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\omega T/2} \sum_{n,\bar{n}=0}^{\infty}\ \sum_{m,\bar{m}=0}^{\infty} \frac{(K_1 T\, e^{-S_1/\hbar})^{n+\bar{n}}}{n!\,\bar{n}!},$$

$$\cdot \frac{(K_2 T\, e^{-S_2/\hbar})^{m+\bar{m}}}{m!\;\bar{m}!} \quad \delta_{n-\bar{n},n_+-n_-}\;\delta_{m-\bar{m},n_+-n_-} \qquad (6)$$

K_1 and K_2 are the determinants of the quantum fluctuations around the instantons 1 and 2 respectively and are given by,

$$K_{1,2} = \left(\frac{S_{1,2}}{2\pi\hbar}\right)^{1/2} \left|\frac{\det(-\partial_t^2 + \omega^2)}{\det'(-\partial_t^2 + V''(x_{1,2}))}\right|^{1/2} \qquad (7)$$

where det' is the determinant without the zero mode. The zero mode $x^0_{1,2}$ is proportional to $\frac{dx_{1,2}}{dt}$ and is normalized as follows,

$$x^0_{1,2} = (S_{1,2})^{-1/2}\,\frac{dx_{1,2}}{dt} \qquad (8)$$

It has the asymptotic behaviour

$$x^0_{1,2} \xrightarrow[|t|\to\infty]{} A_{1,2}\, e^{-\omega|t|} \qquad (9)$$

where

$$A_{1,2} = \frac{2\omega(1-\beta^2)^{1/2}}{S^{1/2}_{1,2}} \qquad (10)$$

Following Coleman (1977),

$$\left|\frac{\det(-\partial_t^2 + \omega^2)}{\det'(-\partial_t^2 + V''(x_{1,2}))}\right|^{1/2} = (2\omega)^{1/2}\; A_{1,2} \qquad (11)$$

So that,

$$K_1 = K_2 = K = \frac{2\omega^{3/2}(1-\beta^2)^{1/2}}{(\pi\hbar)^{1/2}} \qquad (12)$$

We can rewrite equation (5) as,

$$G(n_+,n_-,T) = \left(\frac{\omega}{\pi\hbar}\right)^{1/2} e^{-\omega T/2}\; I_{n_+-n_-}(2KTe^{-S_1/\hbar})\;\cdot$$

$$\cdot\; I_{n_+-n_-}(2KTe^{-S_2/\hbar}) \qquad (13)$$

(Henyey and Patrascioiu 1978), where I_n is the modified Bessel function of order n (Watson 1944).

The Bloch waves can be written as,

$$|\theta\rangle = \left(\frac{\omega}{\pi\hbar}\right)^{-1/4} \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} e^{in\theta}\;|n\rangle \qquad (14)$$

and they diagonalize equation (13), giving for the energy eigen-value $E(\theta)$, the following relation,

$$e^{-E(\theta)T/\hbar} = e^{-\omega T/2} \sum_{n_+=-\infty}^{\infty} I_{n_+}(2KTe^{-S_1/\hbar})\, I_{n_+}(2KTe^{-S_2/\hbar})\, e^{-in_+\theta} \qquad (15)$$

Using a addition theorem for Bessel functions (Watson 1944), (15) can be written as,

$$e^{-E(\theta)T/\hbar} = e^{-\omega T/2}\; I_0(z) \qquad (16)$$

where

$$z = 2KT(e^{-2S_1/\hbar} + e^{-2S_2/\hbar} + 2e^{-(S_1+S_2)/\hbar}\cos\theta)^{1/2} \qquad (17)$$

from which we obtain, in the large T limit,

$$E(\theta) = \frac{\hbar\omega}{2} - 2\hbar K(e^{-2S_1/\hbar} + e^{-2S_2/\hbar} + 2e^{-(S_1+S_2)/\hbar}\cos\theta)^{1/2} \qquad (18)$$

Using K given in (12), we arrive at the energy dispersion relation for the valence band of the double sine-Gordon model. Notice that our resulting expression for $E(\theta)$ is not a simple sum over the contributions of each of the two types of instantons, as might be naively thought before doing an explicit calculation. In the limit $\beta \to 0$ we do obtain the band structure of the sine-Gordon model (Stone 1978, Neuberger 1978), as can be easily seen from equation (18) putting $S_1 = S_2$.

3. COMPARISON WITH THE WKB APPROXIMATION

Following the standard approach to tunneling processes in the WKB approximation (Merzbacher 1970), it is straightforward to generalize the method to the case of different barriers within a period. The energy dispersion relation for the band is given by,

$$\cos\theta = 2\cos^2\sigma_0 \left(e^{\tau_1} + \frac{1}{4}e^{-\tau_1}\right)\left(e^{\tau_2} + \frac{1}{4}e^{-\tau_2}\right) - \frac{1}{2}\left(e^{\tau_1-\tau_2} + e^{\tau_2-\tau_1}\right) \tag{19}$$

with $-\pi \leq \theta \leq \pi$ and

$$\sigma_0 = \frac{1}{\hbar}\int_{y_0}^{x_0}\left[2(E-V(x))\right]^{1/2} dx \tag{20a}$$

$$\tau_1 = \frac{1}{\hbar}\int_{-y_0}^{y_0}\left[2(V(x)-E)\right]^{1/2} dx \tag{20b}$$

$$\tau_2 = \frac{1}{\hbar}\int_{x_0}^{y_1}\left[2(V(x)-E)\right]^{1/2} dx \tag{20c}$$

τ_1 and τ_2 are the penetration factors for the small and large barriers respectively (y_0, x_0 and y_1 are consecutive classical turning points), σ_0 is the integral of the momentum in the classically allowed region.

Each of the integrals in equation (20) are combinations of elliptic integrals of the three kinds, furthermore, τ_2 and τ_1 are related in the same way as S_2 and S_1 before (see

equation (3b)),

$$\tau_2 = \tau_1 + \frac{8\pi\omega_0}{\hbar}\beta \tag{21}$$

Working in the tight-binding approximation (Neuberger 1978), where

$$\varepsilon = \frac{E}{\alpha} \ll 1 \tag{22}$$

and using tabulated asymptotic expansions for the elliptic integrals of the three kinds (Byrd and Friedman 1954), we find that,

$$E(\theta) = \frac{\hbar\omega}{2} - \frac{4\hbar^{1/2}\omega^{3/2}e^{1/2}(1-\beta^2)^{1/2}}{\pi}\left(e^{-2S_1/\hbar} + e^{-2S_2/\hbar} + 2e^{-(S_1+S_2)/\hbar}\cos\theta\right)^{1/2} \tag{23}$$

with S_1 and S_2 given in equation (3) and related to τ_1 and τ_2 (equation (20)) as follows,

$$\tau_1 \simeq \frac{S_1}{\hbar} - \frac{1}{2} - \ln\frac{4(1-\beta^2)}{\sqrt{\varepsilon}} \tag{24}$$

and similarly for τ_2.

Comparing equations (23) and (18) we see that the two results differ by a factor $(\frac{e}{\pi})^{1/2}$, that is,

$$\frac{\Delta E_{WKB}}{\Delta E_{inst}} = \left(\frac{e}{\pi}\right)^{1/2} = 0.93 \tag{25}$$

The same factor had been noticed before (Gildener and Patrascioiu 1977, Neuberger 1978, DeLeonardis and Trullinger 1979), for the double-well anharmonic oscillator and the sine-Gordon potential. Its origin lies in the linear interpolation formulae used in the

WKB approximation. Had we used a quadratic interpolation the agreement between the two methods would be complete (Gildener and Patrascioiu 1977, DeLeonardis and Trullinger 1979).

REFERENCES

BISHOP A.R., KRUMHANSL J.A. and TRULLINGER S.E. 1980 - Physica 1D 1-44.

COLEMAN S. 1977 - "The Uses of Instantons", International School of Physics "Ettore Majorana" (Ed. A.Zichichi).

DELEONARDIS R.M. and TRULLINGER S.E. 1979 - Phys.Rev. A20 2603-2609.

GILDENER E. and PATRASCIOIU A. 1977 - Phys.Rev. D16 423-430.

HENYEY F.S. and PATRASCIOIU A. 1978 - Phys.Rev. D18 2962-2966.

KRUMHANSL J.A. and SCHRIEFFER J.R. 1975 - Phys.Rev. B11 3535-3545.

MERZBACHER E. 1970 - "Quantum Mechanics" 2nd ed. (Wiley, N.Y.) pp.93-100.

NEUBERGER H. 1978 - Phys.Rev. D17 498-506.

STONE M. 1978 - Phys.Rev. D18 4752-4756.

WATSON G.N. 1944 - "A Treatise on the Theory of Bessel Functions" (Cambridge University Press).

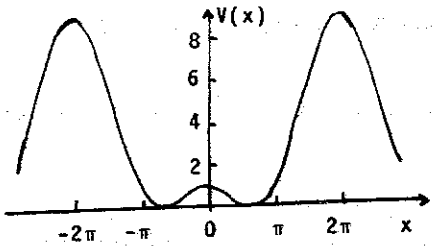

Fig.1 The double sine-Gordon potential, $V(x) = \alpha(\cos \frac{x}{2} - \beta)^2$ with period 4π, here shown for $\alpha=4$ and $\beta=0.5$.