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INSTANTON INDUCED TUNNELING AMPLITUDE AT EXCITED STATES WITH THE LSZ METHOD

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ABSTRACT

Quantum tunneling between degenerate ground states through the central barrier of a potential is extended to excited states with the instanton method. This extension is achieved with the help of an LSZ reduction technique as in field theory and may be of importance in the study of macroscopic quantum phenomena in magnetic systems.

Quantum effects on the macroscopic scale have attracted considerable attention in recent years owing mainly to the development of technology in mesoscopic physics. Legget et al.[1] predicted that the most intriguing quantum effect which could take place on the macroscopic scale is quantum tunneling. Macroscopic magnetisation tunneling is a subject which is being investigated extensively and is of growing interest. There are two types of macroscopic quantum phenomena in magnetic systems. One appears when either a giant spin or (in bulk material) a domain wall is tunneling between degenerate states, which is the situation of macroscopic quantum coherence[1,2,3]. Quantum tunneling in this case is dominated by the instanton configuration with nonzero topological charge, and the tunneling results in the level splitting. The second phenomenon appears in macroscopic quantum tunneling dominated by the socalled bounce configuration[4] with zero topological charge which leads to the decay of metastable states[5]. In the case of the quantum depinning of a domain wall, pinned by defects, the position of the wall at the pinning centre becomes metastable in the external magnetic field, and the position tunnels out of the local minimum[6,7]. However, the usual instanton method only provides the amplitude for tunneling between ground states. It is therefore of interest to evaluate also the tunneling effect between excited states. Motivated by the study of baryon- and lepton-number violation at high energy, recently[8] a periodic (or nonvacuum) instanton configuration has been found and used to evaluate the quantum tunneling at high energy. In this note we present an approach with the LSZ reduction technique in field theory to calculate

*On leave from Department of Mathematics, Dublin City University, Dublin, Ireland the tunneling amplitude between asymptotically degenerate excited states. In the low energy limit the result is equally good as that given in the literature[8] by use of the periodic instanton. However, the procedure employed here avoids the divergence difficulty of the Feynman propagator between two turning points involved in the periodic instanton method[8], and is more adequate for the low temperature case.

The idea of a tunneling transition from one side of a potential barrier to the other has recently also been linked with the LSZ reduction mechanism of a transition from asymptotic in-states to asymptotic out-states[9,10,11]. But although this idea is very attractive and worth pursuing it has not been studied in detail. In the following we therefore go beyond a cursory employment of the method and use the LSZ reduction procedure in a modified way in order to calculate the tunneling amplitude in the one-instanton sector for the sine-Gordon potential including the contribution of quantum fluctuations up to the one-loop approximation. This example is of particular interest in the context of macroscopic tunneling phenomena in magnetic systems.

We recall first the case of a one-dimensional harmonic oscillator described by the Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 \tag{1}$$

for mass $m = 1$ and $\hbar = 1$. Here q and p are dynamical observables which become operators when subjected to the Heisenberg algebra of ordinary canonical quantisation. The solution of the Heisenberg equation of motion, $\ddot{q} + \omega^2 q = 0$, then becomes

$$q(t) = \frac{1}{\sqrt{2\omega}}[a e^{-i\omega t} + a^\dagger e^{i\omega t}] \tag{2}$$

where $a, a^\dagger$ are time-independent operators defined by the initial ($t = 0$) values of q and p, i.e.

$$q(0) = \frac{1}{\sqrt{2\omega}}[a + a^\dagger], p(0) = \frac{-i\omega}{\sqrt{2\omega}}[a - a^\dagger] \tag{3}$$

In fact, a rotation of $q(t), \frac{p(t)}{\omega}$ through angle ωt transforms these back to their initial values. The operators $a, a^\dagger$ can be obtained from $q(t), p(t) = \dot{q}(t)$. Thus

$$\begin{aligned} a^\dagger &= -\frac{i}{\sqrt{2\omega}} e^{-i\omega t}[\dot{q}(t) + i\omega q(t)] \\ &\equiv -\frac{i}{\sqrt{2\omega}} e^{-i\omega t} \frac{\overleftrightarrow{\partial}}{\partial t} q(t) \end{aligned} \tag{4}$$

and a follows with complex conjugation. One should note the extra minus sign in the definition of the symbol $\frac{\overleftrightarrow{\partial}}{\partial t}$ when acting to the left. Operators of this type are well-known in the literature[12].

We now consider the (1+0)-dimensional theory defined by the Lagrangian

$$\mathcal{L} = \frac{1}{2}(\frac{d\phi}{dt})^2 - V(\phi) \tag{5}$$

with the sine-Gordon potential

$$V(\phi) = \frac{1}{g^2}(1 + \cos g\phi) \tag{6}$$

It is well-known that the classical equation of motion of this theory, for energy $E = 0$, with Euclidean time $\tau = it$, i.e.

$$\frac{1}{2}(\frac{d\phi}{d\tau})^2 - V(\phi) = 0 \tag{7}$$

possesses the instanton solution

$$\phi_c = \frac{2}{g}\sin^{-1}[\tanh(\tau - \tau_0)] \tag{8}$$

as a nontrivial (i.e. τ-dependent) and topological vacuum. Expanding $V(\phi)$ around its principal minima at $\phi = \pm\frac{\pi}{g}$ we obtain

$$V(\phi) = \frac{1}{2}[\phi - (\pm\frac{\pi}{g})]^2 + ... \tag{9}$$

Comparison with the oscillator case discussed above shows that the oscillator frequency ω around a minimum is $\omega = 1$. Crucial aspects of the LSZ procedure [13] are its asymptotic conditions which require the theory to have an interpretation in terms of observables for stationary incoming and outgoing states. We can simulate such a situation here artificially by imagining the central barrier of the potential to be extremely high and the neighbouring wells "–" and "+" on either side as extremely far apart. We therefore construct appropriate functions $\phi_\pm(\tau)$ which become oscillator-like in the limits $\tau \rightarrow \pm\infty$ respectively. These functions must be formulated in terms of the instanton ϕ_c which provides the interaction, i.e. interpolation between the asymptotic states. We define therefore the real "interaction fields"

$$\phi_\mp := \frac{\pi}{g} \pm \phi_c \tag{10}$$

which are such that

$$\lim_{\tau\rightarrow\pm\infty} \phi_\pm = 0 \tag{11}$$

and define

$$a_\pm^\dagger := \sqrt{2}e^{-\tau}\frac{\overleftrightarrow{\partial}}{\partial\tau}\phi_\pm(\tau), \tag{12}$$

$$a_\pm := -\sqrt{2}e^{\tau}\frac{\overleftrightarrow{\partial}}{\partial\tau}\phi_\pm(\tau) \tag{13}$$

These "creation" and "annihilation fields" of effective or quasi–bosons in wells "+" and "−" are related to the "interaction fields" through the formula

$$2\phi_\pm = \frac{1}{\sqrt{2}}[a_\pm e^{-\tau} + a^\dagger_\pm e^{\tau}] \tag{14}$$

Since differentiation of the defining expressions of $\phi_\pm$ in eq.(10) gives

$$\frac{\partial \phi_\pm}{\partial \tau} = \mp \frac{2}{g\cosh(\tau-\tau_0)} \stackrel{\tau\rightarrow\pm\infty}{\longrightarrow} \mp \frac{4}{g} e^{\mp\tau} \tag{15}$$

we see that

$$a^\dagger_\pm \stackrel{\tau\rightarrow-\infty}{\longrightarrow} \mp \frac{4\sqrt{2}}{g} \tag{16}$$

$$a_\pm \stackrel{\tau\rightarrow+\infty}{\longrightarrow} \pm \frac{4\sqrt{2}}{g} \tag{17}$$

and

$$\lim_{\tau\rightarrow-\infty} a_\pm(\tau) = 0, \lim_{\tau\rightarrow+\infty} a^\dagger_\pm(\tau) = 0 \tag{18}$$

i.e. comparing q of the oscillator case with $\phi_\pm$ we see that $a_{oscillator} = \frac{4}{g\sqrt{2}}$. Just as quantisation of the oscillator case is achieved by raising $a^\dagger(t), a(t), q(t), ...$ to operators $\hat{a}^\dagger(t), \hat{a}(t), \hat{q}(t), ...$, so here quantisation implies raising $a^\dagger(\tau), a(\tau), \phi(\tau), ..$ to operators $\hat{a}^\dagger(\tau), \hat{a}(\tau), \hat{\phi}(\tau), ...$ If $|0>$ is the perturbation theory vacuum state in either well of the potential (i.e. when the central barrier is infinitely high), the state $a^\dagger_-(\tau)|0>$ with $\tau\rightarrow-\infty$ represents a one-quasi-boson oscillator state in that well. We consider this as the one-quasi-boson in-state and hence write the amplitude for the one boson transition from one side ("–") of the central barrier to the other ("+")

$$A_{f,i} =< +,1|1,- >= S_{f,i}e^{-2T}$$

with the S–matrix element $S_{f,i}$ is given by

$$S_{f,i} = \lim_{\tau\rightarrow-\infty,\tau'\rightarrow+\infty} < 0|\hat{a}_+(\tau')\hat{a}^\dagger_-(\tau)|0 > \tag{19}$$

where $\lim_{\tau\rightarrow-\infty}\hat{a}_\pm(\tau)|0>= 0$. Inserting (12), (13) we have

$$S_{f,i} = \lim_{\tau\rightarrow-\infty,\tau'\rightarrow+\infty} (-\sqrt{2}e^{\tau'} \frac{\overleftrightarrow{\partial}}{\partial\tau'})(\sqrt{2}e^{-\tau} \frac{\overleftrightarrow{\partial}}{\partial\tau})G(\tau',\tau) \tag{20}$$

where G is the Green's function

$$G(\tau',\tau) =< 0|\hat{\phi}_+(\tau')\hat{\phi}_-(\tau)|0 > \tag{21}$$

The differentiations in $S_{f,i}$ imply

$$S_{f,i} = \lim_{\tau\to-\infty,\tau'\to+\infty} -2e^{-\tau}e^{\tau'}[(\frac{\partial^2 G}{\partial\tau\partial\tau'} + \frac{\partial G}{\partial\tau'}) - (\frac{\partial G}{\partial\tau} + G)] \tag{22}$$

We evaluate G by inserting complete sets of states of final and initial field configurations ϕ_f, ϕ_i. Thus

$$\begin{aligned} G(\tau',\tau) &= <0|\hat{\phi_+}(\tau')\hat{\phi_-}(\tau)|0> \\ &= \int d\phi_f d\phi_i <0|\phi_f><\phi_f|\hat{\phi_+}(\tau')\hat{\phi_-}(\tau)|\phi_i><\phi_i|0> \\ &= \int d\phi_f d\phi_i <0|\phi_f><\phi_i|0>\phi_+(\tau')\phi_-(\tau)<\phi_f|\phi_i> \end{aligned} \tag{23}$$

with

$$\hat{\phi}_-(\tau)|\phi_i>=\phi_-(\tau)|\phi_i> \tag{24}$$

Here $<0|\phi_f>, <\phi_i|0>$ are degenerate ground state wave functions in the two wells which we write

$$<0|\phi_f>\equiv\psi_0(\phi_f), \;\; <\phi_i|0>\equiv\psi_0(\phi_i) \tag{25}$$

and $<\phi_f|\phi_i>\equiv<\phi_f,\tau'|\phi_i,\tau>$ is the propagator

$$K(\phi_f,\tau';\phi_i,\tau)\equiv\int_{\phi_i}^{\phi_f}\mathcal{D}\phi e^{-S} \tag{26}$$

Considering the limits $\tau\to-\infty, \tau'\to\infty$, we can write

$$K := \lim_{\tau\to-\infty,\tau'\to\infty,\phi_i\to-\frac{2}{g},\phi_f\to\frac{2}{g}} K(\phi_f,\tau';\phi_i,\tau) \tag{27}$$

Then K representing the propagator can be removed from the integral and

$$\lim_{\tau\to-\infty,\tau'\to\infty} G(\tau',\tau) = \lim_{\tau\to-\infty,\tau'\to\infty} K\phi_+(\tau')\phi_-(-\tau)\int d\phi_f d\phi_i\psi_0(\phi_f)\psi_0(\phi_i) \tag{28}$$

$$\approx \lim_{\tau\to-\infty,\tau'\to\infty} 2\sqrt{\pi}K\phi_+(\tau')\phi_-(-\tau) \tag{29}$$

Since

$$\lim_{\tau\to-\infty}\phi_-(\tau)=0, \;\; \lim_{\tau'\to+\infty}\phi_+(\tau')=0 \tag{30}$$

we see that

$$\lim_{\tau'\to+\infty,\tau\to-\infty} G(\tau',\tau)=0 \tag{31}$$

In the combined limits $\tau\to-\infty, \tau'\to+\infty$ also $\frac{\partial G}{\partial\tau}$ and $\frac{\partial G}{\partial\tau'}\to 0$. Thus in (22) the only nonvanishing contribution in these limits results from the second derivative.

Then

$$
\begin{aligned}
\left(\frac{\partial^2 G}{\partial\tau\partial\tau'}\right)_{\substack{\tau\to-\infty\\ \tau'\to+\infty}} &= 2\sqrt{\pi}K\left(\frac{\partial\phi_+(\tau')}{\partial\tau'}\right)_{\tau'\to\infty}\left(\frac{\partial\phi_-(\tau)}{\partial\tau}\right)_{\tau\to-\infty} \\
&= -2\sqrt{\pi}K\left(\frac{\partial\phi_c(\tau')}{\partial\tau'}\right)_{\tau'\to\infty}\left(\frac{\partial\phi_c(\tau)}{\partial\tau}\right)_{\tau\to-\infty} \\
&= -2\sqrt{\pi}K\left(\frac{4}{g}\right)^2\left(e^{-\tau'}e^{\tau}\right)_{\substack{\tau'\to\infty\\ \tau\to-\infty}}
\end{aligned}
\tag{32}
$$

Inserting the result into $S_{f,i}$ and hence into $A_{f,i}$, and taking the limits with $2T = \tau' - \tau \to \infty$ we obtain

$$
A_{f,i} = 2\sqrt{\pi}.K.\left(\frac{4}{g}\right)^2 e^{-2T} \tag{33}
$$

The factor $(\frac{4}{g})^2$ is the product of asymptotic amplitudes of the two operators as can be seen from (15). The next step is to calculate the propagator K with the instanton method. To this end we expand $\phi(\tau)$ around the instanton trajectory $\phi_c(\tau)$ such that

$$
\phi(\tau) = \phi_c + \chi(\tau) \tag{34}
$$

where $\chi(\tau)$ denotes the quantum fluctuation. The propagator is now evaluated in the one-loop approximation, and the result is found to be

$$
K = \frac{2T}{\pi}e^{-\frac{8}{g^2}}.e^{-T}.\frac{4}{g} \tag{35}
$$

The tunneling amplitude then reads

$$
A_{f,i} = \frac{2Te^{-\frac{8}{g^2}}}{\sqrt{\pi}g}4e^{-3T}\left(\frac{4\sqrt{2}}{g}\right)^2 \equiv A_{f,i}^{1\to1} \tag{36}
$$

where $2T = \tau' - \tau$. In this result the factor $2T$ can be interpreted heuristically as representing energy conservation in the sense of the relation

$$
2\pi\delta(E_f - E_i) \overset{T\to\infty}{=} \int_{-T}^{T} dt e^{i(E_f - E_i)t} \tag{37}
$$

or

$$
2\pi\delta(0) \overset{T\to\infty}{=} \int_{-T}^{T} dt = 2T \tag{38}
$$

The factor $e^{-3T} = [e^{-(n+\frac{1}{2})2T}]_{n=1}$(the one-quasi-boson case) represents in Minkowski time the free-field evolution. We can obtain the corresponding amplitude for the transition between the nth excited states on either side of the barrier in the one-instanton sector by evaluating

$$
A_{f,i}^{n\to n} = \frac{1}{n!}\prod_{i=1}^{n}\lim_{\tau_i\to-\infty,\tau_i'\to\infty}\left(-\sqrt{2}e^{\tau_i'}\frac{\overset{\leftrightarrow}{\partial}}{\partial\tau_i'}\right)\left(\sqrt{2}e^{-\tau_i}\frac{\overset{\leftrightarrow}{\partial}}{\partial\tau_i}\right)G(\tau_1', \tau_2', ..., \tau_n'; \tau_1, \tau_2, ..., \tau_n) \tag{39}
$$

and it may be surmised that with calculations analogous to those above

$$A_{f,i}^{n\to n} = 2T\frac{e^{-\frac{8}{g^2}}}{\sqrt{\pi}g}\frac{4e^{-2E_{cl}T}}{n!}(\frac{4\sqrt{2}}{g})^{2n} \tag{40}$$

where now $E_{cl} = (n+\frac{1}{2})$. Without tunneling the eigenstates in neighbouring wells are degenerate. The degeneracy is removed by the small tunneling effect which leads to the level splitting while the levels extend to bands due to the translational symmetry of the sine-Gordon potential [8]. The relation between the tunneling amplitude and the level splitting is given by [8]

$$A^{n\to n} = e^{-2E_{cl}T}\sinh(2\triangle\epsilon_n T) \tag{41}$$

where $\triangle\epsilon_n$ denotes the level splitting of the n-th energy eigenvalue. The one–instanton sector of the tunneling amplitude, eq.(37), does not show the proper hyperbolic function which, however, can be obtained by taking into account the contributions of the infinite number of instanton–antiinstanton pairs[8]. The tunneling effect is, of course, extremely small. One may expand the hyperbolic function in eq. (42) in rising powers of $2\triangle\epsilon_n$. Up to the first order we have

$$\triangle\epsilon_n \approx \frac{4e^{-\frac{8}{g^2}}}{\sqrt{\pi}gn!}(\frac{4\sqrt{2}}{g})^{2n} \tag{42}$$

which reduces to the correct value of the level splitting of the ground state when $n = 0$ [8]. To our knowledge the level splitting due to tunneling at excited states within the framework of the instanton method applied to the sine-Gordon potential has not been reported previously in the literature, and the explicit calculation of the one-loop correction in this case is also not wellknown, and of interest in the study of macroscopic quantum tunneling in magnetic systems.

The calculation of the contributions of instanton–antiinstanton pairs and the application to macroscopic tunneling in a specific system will will be considered elsewhere.

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