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BRST–INVARIANT APPROACH TO QUANTUM MECHANICAL TUNNELING

JIAN-GE ZHOU, F. ZIMMERSCHIED, J.-Q.LIANG*and H.J.W. MÜLLER-KIRSTEN
Department of Physics, University of Kaiserslautern, P.O.Box 3049
67653 Kaiserslautern, Germany
E-mail: zimmers@.physik.uni-kl.de

ABSTRACT

A new approach with BRST invariance is suggested to cure the degeneracy problem of ill defined path integrals in the path–integral calculation of quantum mechanical tunneling effects in which the problem arises due to the occurrence of zero modes. The Faddeev–Popov procedure is avoided and the integral over the zero mode is transformed in a systematic way into a well defined integral over instanton positions. No special procedure has to be adopted as in the Faddeev–Popov method in calculating the Jacobian of the transformation. The quantum mechanical tunneling for the Sine–Gordon potential is used as a test of the method and the width of the lowest energy band is obtained in exact agreement with that of WKB calculations.

1. Introduction

Quantum tunneling has attracted considerable interest because of its wide application in areas ranging from condensed matter to high energy physics. The instanton method is a powerful tool for the calculation of tunneling effects. Recent interests in tunneling effects were initiated by the work of Ringwald[1], who argued that although the cross section of the standard electroweak theory is proportional to an exponentially small WKB suppression factor, it is nevertheless rapidly growing with energy due to multiple production of Higgs and vector bosons. However, it has been observed that instantons interpolate between neighbouring vacua and satisfy vacuum boundary conditions and therefore may not be adequate for a description of tunneling at high energy[2]. Motivated by the instanton–induced baryon–number violating processes the instanton method of quantum tunneling has recently been extended to tunneling at finite, nonzero energy by means of nonvacuum or periodic instantons[3] which have become the subject of extensive investigation under the name of sphalerons[4,5].

It is well known that due to the translational invariance of the action, functional integrals in nonlinear field theory are not well defined when expanded about the classical solutions of the field equations. The translational symmetry results in zero eigenmodes of the second variation operator of the action which are a reflection of

*On leave from Institute of Theoretical Physics, Shanxi University, Taiyuan, Shanxi 030006, P. R. China, and Institute of Physics, Academia Sinica, Beijing 100080, P. R. China

the arbitrariness of locations in space of solitons or instantons (in Euclidean time). Obviously physical quantities are independent of such center–of–mass–like locations. A consequence of the existence of these normalizable "zero modes" which belong to the spectrum of linearised fluctuations in the soliton's background is a divergence one encounters when quantizing the theory in the background of these solitons or instantons. In essence the change of variables in field theory converts the zero modes into corresponding collective coordinates. However, calculation of the Jacobian of the transformation of variables in the path integral formalism usually involves a Faddeev–Popov procedure[8,9].

Here we report an alternative method to carry out the transformation of variables and the evaluation of the related Jacobian in a systematic way with BRST invariance, and we apply it to quantum tunneling processes. The crucial point of the method is the exploitation of a shift invariance of the fluctuation action. As a test case the quantum tunneling effect in $1+0$ dimensions is calculated for the Sine–Gordon (SG) potential. In the usual collective coordinate method [10,11,12] time–dependent collective coordinates are associated with the D (spatial) dimensional (static) solitons indicating the motion of the kink or center of mass and one has to deal with phase–space functional integrals in $1+D$ dimensions. Unlike this procedure our BRST invariant treatment does not evoke the time–dependence in one higher dimension and works on configuration–space path–integrals. Tunneling in the case of the Sine–Gordon potential is itself an interesting subject in view of similar features of the $O(3)$ nonlinear sigma model in the discussion towards understanding instanton induced baryon–number violating processes [13,14].

2. Energy band structure for the SG potential and the transition amplitude for quantum tunneling

The $1+0$ dimensional Lagrangian we consider is

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

with the SG potential

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

where $g>0$ denotes a dimensionless coupling constant. The classical solution which extremizes the action is seen to satisfy the equation of motion which after one integration with integration constant zero is

$$\frac{1}{2}\left(\frac{d\phi_c}{d\tau}\right)^2 + V(\phi_c) = 0 \tag{3}$$

with euclidean time $\tau = it$. Mass $m=1$ and natural units $c=\hbar=1$ are used throughout. The relevant classical solution which interpolates between neighbourung vacua, say, $\phi_+ = \frac{\pi}{g}$ and $\phi_- = -\frac{\pi}{g}$, is

$$\phi_c = \frac{2}{g}\sin^{-1}[\tanh(\tau+a)] \tag{4}$$

where the integration constant a is interpreted as the position of the instanton.

In the following we consider the case of very high potential barriers with correspondingly small tunneling contributions to the eigenvalues. Thus we suppose $|0\rangle_+$, $|0\rangle_-$ are degenerate eigenstates in neighbouring wells with the same energy eigenvalue $\mathcal{E}_0$ such that $\hat{H}^0|0\rangle_\pm = \mathcal{E}_0|0\rangle_\pm$ where $\hat{H}^0$ is the Hamiltonian of the harmonic oscillator as the zeroth order approximation of the system. The degeneracy will be removed by the small tunneling effect which leads to the level splitting. The eigenstates of the Hamiltonian $\hat{H}$ then become

$$|0\rangle_o = \frac{1}{\sqrt{2}}(|0\rangle_+ - |0\rangle_-), \quad |0\rangle_e = \frac{1}{\sqrt{2}}(|0\rangle_+ + |0\rangle_-), \tag{5}$$

with eigenvalues $\mathcal{E}_0 + \Delta\mathcal{E}$ and $\mathcal{E}_0 - \Delta\mathcal{E}$ respectively. $\Delta\mathcal{E}$ denotes the shift of one oscillator level. It is obvious that

$$_+\langle 0|\hat{H} - \hat{H}^0|0\rangle_- = \Delta\mathcal{E}. \tag{6}$$

These shifts embrace the energy bands which result from the translational invariance of V. We now calculate this energy resulting from tunneling with the instanton method. The amplitude for a transition between neighbouring vacua due to instanton tunneling can be written

$$\langle\phi_f = \frac{n\pi}{g}, T|\phi_i = \frac{(n-1)\pi}{g}, -T\rangle \equiv K(\phi_f, T; \phi_i, -T) = \int_{\phi_i}^{\phi_f} \mathcal{D}\{\phi\}e^{-S} \tag{7}$$

where

$$S = \int_{-T}^{T}\left[\frac{1}{2}\left(\frac{d\phi}{d\tau}\right)^2 + V(\phi)\right]d\tau \tag{8}$$

is the Euclidean action. In the large time limit $T \to \infty$, we have

$$\begin{aligned} K &= \sum_{n,n'}\langle\phi_f|n\rangle\langle n|e^{-2\hat{H}T}|n'\rangle\langle n'|\phi_i\rangle \\ &\simeq \Psi_0(\phi_f)\Psi_0(\phi_i)e^{-2T\mathcal{E}_0}\sinh(2\Delta\mathcal{E}T). \end{aligned} \tag{9}$$

3. Translation invariance of action and zero modes

As mentioned in the introduction the degeneracy of an action which possesses a translation symmetry leads to ill defined functional integrals in perturbation expansion about the classical configuration ϕ_c since the symmetry results in zero modes of the second variation operator of the action. We consider this now in more detail. We expand $\phi(\tau)$ about the classical trajectory $\phi_c(\tau)$ and so set

$$\phi(\tau) = \phi_c(\tau) + \chi(\tau) \tag{10}$$

with the boundary conditions $\chi(T) = \chi(-T) = 0$ for the fluctuation. Substituting $\phi(\tau)$ of eq. (10) into eq. (7) and retaining only terms up to the second order in χ for the one–loop approximation we obtain

$$K = e^{-S_c}I \tag{11}$$

where the classical action is evaluated along the trajectory ϕ_c so that

$$S_c = \int_{-\infty}^{\infty} \left[\frac{1}{2} \left(\frac{d\phi_c}{d\tau} \right)^2 + V(\phi_c) \right] d\tau = \frac{8}{g^2}. \tag{12}$$

The fluctuation integral I is seen to be

$$I = \int_{\chi(-T)=0}^{\chi(T)=0} \mathcal{D}\{\chi\} e^{-\Delta S} \tag{13}$$

with the fluctuation action

$$\Delta S = \int_{-T}^{T} \chi \hat{M} \chi d\tau \tag{14}$$

where

$$\hat{M} = -\frac{1}{2}\frac{d^2}{d\tau^2} + \frac{1}{2}\left(1 - \frac{2}{\cosh^2(\tau - a)}\right) \tag{15}$$

is the self–adjoint operator of the second variation about the classical trajectory. Expanding $\chi(\tau)$ in terms of normalized eigenfunctions of $\hat{M}$ we set

$$\chi(\tau) = \sum_m c_m \Psi_m \tag{16}$$

where

$$\hat{M}\Psi_m = E_m \Psi_m. \tag{17}$$

Changing the integration variables of (13) to $\{c_m\}$, the functional integral I can be formally evaluated to be

$$I = \left| \frac{\partial \chi(\tau)}{\partial c_m} \right| \prod_m \left[\frac{\pi}{E_m} \right]^{\frac{1}{2}} \tag{18}$$

which is seen to be divergent in view of the vanishing eigenvalue of the zero mode, $E_0 = 0$. Since the transformation (16) is linear the Jacobian $\left|\frac{\partial \chi(\tau)}{\partial c_m}\right|$ is constant and has therefore been factored out. To cure the problem one normally resorts to the so–called Faddeev–Popov procedure[7,9] in order to transform the integral over the zero mode c_0 into the continuous integration of a collective coordinate, which is the instanton position a in our case.

4. BRST invariance and "gauge fixing"

In the usual collective coordinate method, the essential ingredient is a change of variables which is such that every collective coordinate which is time–dependent is associated with a zero mode[11,12]. In our $(1+0)$ dimensional case the procedure is not appropriate. We therefore adopt an alternative method[14,15] which employs a BRST invariance in dealing with the transformation of variables. If we identify euclidean time τ with a spatial coordinate, the equivalence of the present method with that of a collective coordinate method with BRST invariance is similar to that demonstrated in a previous paper[16].

After expansion about the classical trajectory ϕ_c, the fluctuation action still retains a shift symmetry expressed by the invariance

$$\Delta S(\chi') = \Delta S(\chi) \tag{19}$$

where

$$\chi' = \chi + \frac{\partial \phi_c}{\partial a} = \chi + \frac{\partial \phi_c}{\partial \tau}. \tag{20}$$

In other words the action is invariant under a kind of "gauge transformation" of the fluctuation variable χ. This is an important observation. The key point of the BRST procedure is to enlarge the number of degrees of freedom and invent a nilpotent symmetry which mimics the structure of the gauge symmetry. Then one can achieve the effects of gauge fixing without breaking the BRST invariance of the system. To achieve this we first enlarge the configuration space by considering the parameter a as a variable. We replace the transformation (20) by the introduction of new anticommuting variables c and $\bar{c}$ and a Nakanishi–Lautrup auxiliary variable b (the latter in such a way that it implements the gauge fixing condition as its equation of motion, i. e. $b = \int \chi \frac{d\phi_c}{da} d\tau$ in analogy with the implementation of the Lorentz gauge in QED) together with conjugate momenta P_a, Π_c, $\Pi_{\bar{c}}$ such that

$$\begin{aligned} \delta\chi &= -c\frac{\partial \phi_c}{\partial a} \\ \delta a &= -c \\ \delta \bar{c} &= 2\pi b \\ \delta b &= 0 \\ \delta c &= 0. \end{aligned} \tag{21}$$

The variables a, c, $\bar{c}$, χ and their conjugate momenta are assumed to satisfy the canonical Poisson relations

$$\begin{aligned} \{a, P_a\} &= 1 \\ \{\bar{c}, \Pi_{\bar{c}}\}_+ &= 1 \\ \{c, \Pi_c\}_+ &= 1 \\ \{\chi, \pi_\chi\} &= 1. \end{aligned} \tag{22}$$

Then one finds that the BRST transformations can be generated by the following BRST charge

$$\Omega = -cP_a - c\pi\frac{\partial \phi_c}{\partial a} + \Pi_{\bar{c}} b \tag{23}$$

which is nilpotent. The following BRST invariant term may now be added to the fluctuation Lagrangian to break the shift symmetry:

$$\begin{aligned} L_B &= \int \delta\left[\bar{c}\frac{\partial \phi_c}{\partial a}\chi\right] d\tau - \pi b^2 \\ &= 2\pi b \int \frac{\partial \phi_c}{\partial a}\chi d\tau - c\bar{c}\int \left[\frac{\partial^2 \phi_c}{\partial a^2}\chi + \left(\frac{\partial \phi_c}{\partial a}\right)^2\right] d\tau - \pi b^2 \end{aligned} \tag{24}$$

Eliminating the Nakanishi–Lautrup auxiliary variable by using its equation of motion, we obtain the final expression of the fluctuation functional integral

$$\begin{aligned} I &= \int \mathcal{D}\{\chi\}\mathcal{D}\{c\}\mathcal{D}\{\bar{c}\}\mathcal{D}\{a\} \\ &\cdot \exp\left\{-\int \chi \hat{M}\chi \, d\tau - \pi\left[\int \frac{\partial\phi_c}{\partial a}\chi d\tau\right]^2 - c\bar{c}\int\left[\frac{\partial^2\phi_c}{\partial a^2}\chi + \left(\frac{\partial\phi_c}{\partial a}\right)^2\right]d\tau\right\} \end{aligned} \tag{25}$$

(In the following we neglect the term linear in the fluctuation χ since it is of higher order than the soliton mass $M = \int d\tau \left(\frac{d\phi_c}{da}\right)^2$). Expanding the fluctuation variable χ in terms of the eigenmodes of $\hat{M}$ so that

$$\chi = \sum_m c_m \Psi_m, \quad \mathcal{D}\{\chi\} = \left|\frac{\partial\chi}{\partial c_m}\right| \mathcal{D}\{c_m\} \tag{26}$$

we obtain (ignoring the higher order contribution proportional to χ in the coefficient of $c\bar{c}$)

$$I = \left|\frac{\partial\chi}{\partial c_m}\right| \int \mathcal{D}\{c_m\}\mathcal{D}\{c\}\mathcal{D}\{\bar{c}\}\mathcal{D}\{a\} \exp\left\{-\sum_{m\neq 0} c_m^2 E_m - \pi c_0^2 M - c\bar{c}M\right\} \tag{27}$$

where we used $E_0 = 0$ and the fact that Ψ_0 is a normalized eigenfunction, i. e. (from (3) and (4))

$$\Psi_0 = \frac{1}{\sqrt{M}}\frac{\partial\phi_c}{\partial\tau}, \quad \sqrt{M}\Psi_0 = \frac{d\phi_c}{da} \tag{28}$$

where $M \equiv S_c = \frac{8}{g^2}$ is the classical action or instanton mass (as it is also called). Integrating out all variables (and recalling that $\mathcal{D}\{a\} \to da$) the final result is

$$\begin{aligned} I &= 2T\left|\frac{\partial\chi}{\partial c_m}\right| \prod_{m\neq 0}\sqrt{\frac{\pi}{E_m}}\frac{1}{\sqrt{M}}M \\ &\equiv 2T I_0\sqrt{M} \end{aligned} \tag{29}$$

where

$$I_0 = \left|\frac{\partial\chi}{\partial c_m}\right| \prod_{m\neq 0}\left(\frac{\pi}{E_m}\right)^{\frac{1}{2}}. \tag{30}$$

In I the factor $\frac{1}{\sqrt{M}}$ comes from the $\mathcal{D}\{c_0\}$ integration and M from integrating out $\mathcal{D}\{c\}\mathcal{D}\{\bar{c}\}$. We see therefore that the functional integration can be done without resorting to the Faddeev–Popov method of inserting a delta function and interchanging integration and limiting procedures. The BRST procedure converts the ill defined integral over the zero mode into a Gaussian integral and leads to the integration over the instanton position, da, which gives rise to $2T$.

5. The one–instanton transition amplitude and the contributions from one instanton and an infinite number of instanton–antiinstanton pairs

The following calculations are similar to those of the level splitting for the double–well potential[7] and of the decay rate for the inverted double–well potential[9]. The shift method which is effectively defined by the transformation

$$\chi(\tau) = \xi(\tau) \int_{-T}^{T} d\tau' \frac{\dot{y}(\tau')}{\xi(\tau')} \tag{31}$$

where $\xi = \frac{d\phi_c}{d\tau}$ converts the functional integral into Gaussian form along with boundary constraints which are then implemented with a delta function trick analogout to the Faddeev–Popov method which then leads to a finite result [18]. Taking care of the boundary condition constraint, the functional integral for the field fluctuations is given by

$$I = \sqrt{\frac{1}{2\pi\xi(T)\xi(-T)\int_{-T}^{T}\frac{d\tau}{\xi^2(\tau)}}}. \tag{32}$$

Considering the large time limit one finds

$$I \stackrel{T\to\infty}{\longrightarrow} \sqrt{\frac{1}{2\pi}}. \tag{33}$$

Comparing with eq. (18) it is seen that

$$I_0 = \left|\frac{\partial\chi}{\partial c_m}\right| \prod_{m\neq 0} \sqrt{\frac{\pi}{E_m}} = \frac{1}{\pi}\sqrt{\frac{E_0}{2}}. \tag{34}$$

The eigenvalue E_0 vanishes only asymptotically when time T tends to infinity; its finite value corresponds to a finite time interval. E_0 can be evaluated with a so–called boundary perturbation method[7,9] which gives rise to a formula for the "unrenormalized" eigenvalue–zero eigenfunction $\xi = \frac{d\phi_c}{d\tau}$,

$$\xi(T)\frac{d\xi(T)}{d\tau} - \xi(-T)\frac{d\xi(-T)}{d\tau} = E_0 \int_{-T}^{T} \xi^2 d\tau. \tag{35}$$

Again we take the large time limit; the quasi zero eigenvalue due to the size effect is obtained from eq. (35) as

$$E_0 = 4e^{-2T}. \tag{36}$$

Replacing I_0 in eq. (29) by eq. (34) with the value E_0 of eq. (36), the fluctuation part of the transition amplitude of the one–instanton sector is seen to be

$$I^{(1)} = 2T\sqrt{M}\frac{\sqrt{2}}{\pi}e^{-T}. \tag{37}$$

The contribution stemming from one instanton together with an instanton–antiinstanton pair can be calculated with the help of the group property for propagators [17]. The result is

$$I^{(3)} = \frac{(2T)^3}{3!}[\sqrt{M}]^3 \left[\frac{\sqrt{2}}{\pi}\right]^3 \Delta^2 e^{-T} \tag{38}$$

where the determinant

$$\Delta = \left[\frac{\pi}{\frac{1}{2}\frac{\partial^2 S_c}{\partial \phi_f^2}}\right]^{\frac{1}{2}} \stackrel{T\to\infty}{\longrightarrow} \sqrt{2\pi} \tag{39}$$

is determined from the end point integration of the group property of the propagator and is evaluated with a formula given in the literature[3] by carefully taking the large time limit. The contribution from one instanton plus n pairs is a straightforward extension of eq. (38) and is found to be

$$I^{(2n+1)} = \frac{(2T)^{2n+1}}{(2n+1)!}(\sqrt{M})^{2n+1}\left(\frac{\sqrt{2}}{\pi}\right)^{2n+1}\Delta^{2n}e^{-T}. \tag{40}$$

The final result of the propagator is

$$\langle \phi_f, T|\phi_i, -T\rangle = \frac{1}{\sqrt{2\pi}}e^{-T}\sinh\left[2T\frac{1}{\sqrt{2\pi}}\left(\frac{2^5}{g^2}\right)^{\frac{1}{2}}e^{-\frac{8}{g^2}}\right]. \tag{41}$$

Comparing with eq. (9) we obtain the level shift, which is half of the width of the lowest energy band, i. e.

$$\Delta\mathcal{E} = J = \frac{1}{\sqrt{2\pi}}\left(\frac{2^5}{g^2}\right)^{\frac{1}{2}}e^{-\frac{8}{g^2}} \tag{42}$$

which is in exact agreement with the result in the literature[19]. The periodic potential has also been dealt with in the literature[20] but the width of the energy band has not been given explicitly there.

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