Periodic Instantons and Quantum-Classical Transitions in Spin Systems

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Some models, allowing explicit calculation of periodic instantons and evaluation of their action, are studied with regard to transitions from classical to quantum behavior as the temperature is lowered and tunneling sets in. It is shown that (beyond a critical value of a coupling) the spin system considered acquires a first order transition as a result of the field dependence of its effective mass, whereas models with constant mass exhibit only second order transitions.   [S0031-9007(98)06480-1]

Recently considerable progress was made in understanding macroscopic spin systems with degenerate perturbation theory vacua. This progress was achieved largely independently of developments in field theory where very similar methods were motivated by the realization that topologically nontrivial field configurations play an important role in our understanding of fundamental particle phenomena. Thus instanton methods well known in theoretical particle physics for more than two decades appeared in spin tunneling investigations about ten years later [1]. In either direction it again took several years for topologically unstable classical field configurations, which represent saddle points in path integrals, to be accepted as a convenient means to understand decay processes, although in essence the configuration now known as a bounce was already familiar to Langer [2] several decades ago. However, there are very few theories which permit an explicit calculation and investigation of such classical field configurations. The best known example to provide an instanton is quantum mechanics of the double-well and sine-Gordon potentials. This instanton is the vacuum instanton analogous to a classical particle traveling in imaginary time with zero energy; it is this instanton which is responsible for the splitting of the degenerate perturbation theory vacua into the two lowest quantum states. Tunneling at higher perturbation theory states is mediated by periodic instantons whose classical analogs are instantons traveling with nonzero energy. Peculiarly the study of these and their stability in double-well and sine-Gordon theories [3,4] began only about ten years ago, and were called thermons [5] in independent spin tunneling contexts. Since then progress in the study of spin systems uncovered a host of other model theories permitting explicit evaluation of periodic instantons and their investigation.

Very recently spin systems aroused yet again new interest with the discovery [6] that they provide examples which exhibit first order phase transitions of which simple examples were not known previously. In view of the possibility of experimental verification of such a transition in decay rates of certain spin systems, and their interpretation as a crossover from classical to quantum behavior, such systems are also of fundamental interest. Very few models are known which allow an explicit and analytic investigation of phase transitions so that these few models serve as very instructive prototypes and are of interest beyond their immediate area of relevance.

The characteristic way in which phase transitions appear in tunneling processes has been worked out by Chudnovsky [5]. In fact, the sharp first order transition is there shown to appear in the plot of action versus temperature and is completely analogous to the plot of free enthalpy versus pressure of a van der Waals gas whose equation of state plotted as pressure versus volume corresponds to the plot of period (of the periodic instanton) versus energy in the consideration of spin systems.

In the following we consider some models permitting explicit calculation of periodic instantons and the corresponding evaluation of the action. We first consider the well-known double-well [7] and sine-Gordon [8] theories and demonstrate that these theories exhibit only second order transitions. We then consider a spin model with *XOY* easy-plane anisotropy without an applied magnetic field [9] and demonstrate that this is a model exhibiting a first order transition. We can clearly pinpoint the reason for the appearance of this first order transition here as compared to the previous models and attribute it to the field dependence of the effective mass of the system which causes the period of the periodic instanton to increase again after a certain critical value of a coupling with increasing energy. This is a very important point which one can expect to appear in numerous other models, also in the context of high energy physics, e.g., in models such as the Skyrme model, which also possess field dependent masses.

A uniaxial spin model with an applied magnetic field has been considered in the work of Chudnovsky and Garanin [6] who also demonstrated that the crossover from classical to quantum behavior is, in fact, controlled by the magnetic field in their model which has the effect of producing a shallow potential well which effectively permits the period of the periodic instanton to increase after a certain critical value. In a subsequent work [10] the model considered here—which is different from the

model of Chudnovsky and Garanin in the fieldless [6] case—is investigated with an additional applied magnetic field, and a similar conclusion is arrived at.

As stated we begin with the discussion of periodic instantons of double-well and sine-Gordon potentials and demonstrate that these lead only to smooth, i.e., second order transitions. In either case we use the notation and results of Refs. [7,8]. We write the double-well potential

$$V(\phi) = \frac{\eta^2}{2}\left[\phi^2 - \frac{m^2}{\eta^2}\right]^2. \qquad (1)$$

Solving the Euclidean time classical equation in the usual way one obtains the Jacobian elliptic function $\mathrm{sn}[b(k)\tau]$ as the periodic instanton solution with period

$$P(E) = \frac{4}{b(k)}\,\mathcal{K}(k), \qquad (2)$$

where

$$b(k) = m\sqrt{\frac{2}{1+k^2}}, \qquad k^2 = \frac{1-u}{1+u},$$

$$u = \frac{\eta}{m^2}\sqrt{2E}. \qquad (3)$$

Here k is the elliptic modulus of the Jacobian elliptic functions, $\mathcal{K}(k)$ is their quarter period, m and η are parameters of the potential, and E is the integration constant which can be interpreted as the energy of the periodic instanton. As is well known, in statistical mechanics the period is related to temperature T through the relation $P(E) = \hbar/k_B T$ where k_B is Boltzmann's constant. One can show that the equation

$$\frac{dP(E)}{dE} = 0 \qquad (4)$$

does not have a solution in the domain $0 < E < \frac{m^4}{2\eta^2} = E_0$ where E_0 is the energy of the pseudoparticle at the top of the barrier, also known as the sphaleron. The monotonically decreasing behavior of the period in this domain is shown in Fig. 1(a). The thermon defined in Ref. [5] is a configuration traveling through one complete period, whereas the periodic instanton, in keeping with its name, is defined as a configuration over half the complete period. Thus the action of the former is twice that of the latter, and hence (with $\hbar = 1 = k_B$) is as shown in Ref. [7]

$$S_T = \frac{E}{T} + \frac{8m^3}{3\eta^2}\sqrt{1+u}\,[E(k) - u\mathcal{K}(k)], \quad (5)$$

where $E(k)$ is the complete elliptic integral of the second kind [11]. The thermodynamic action, i.e., that of the sphaleron at the top of the barrier, is correspondingly given by

$$S_0 = \frac{m^4}{2\eta^2}\frac{1}{T}. \qquad (6)$$

Figure 1(b) displays the behavior of S_T, S_0 versus temperature T for $m = 1, \eta = 1$. One can clearly see the
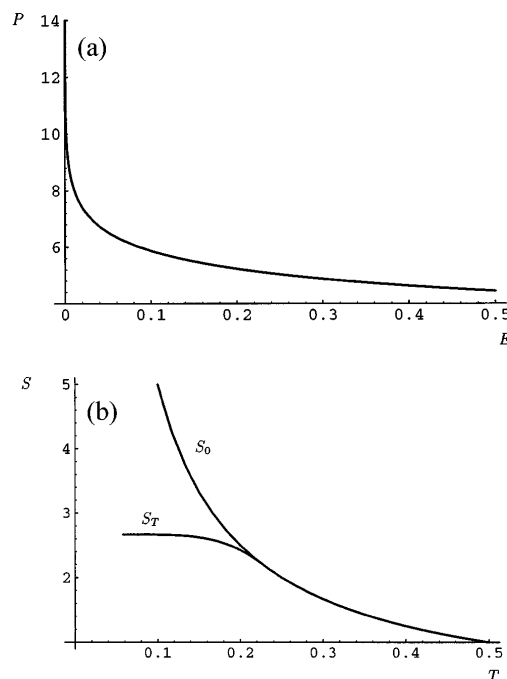

FIG. 1. (a) The period of the periodic instanton of the double-well potential as a function of energy E for $\eta = 1, m = 1$; (b) the thermodynamic and thermon actions S_0, S_T as functions of temperature T demonstrating the smooth second order transition for the same values of parameters.

typically smooth behavior of a second order transition from the thermal to the quantum regime as the temperature is lowered. Conversely, we can argue that as the temperature is increased, the number of periodic instantons and anti-instantons or thermons increases and the dilute gas approximation breaks down. The temperature corresponding to that of harmonic oscillations [5] around the sphaleron configuration is the critical temperature at which the periodic instantons and anti-instantons condense and disorder the system.

In the case of the sine-Gordon potential written

$$V(\phi) = \frac{1}{g^2}[1 + \cos(g\phi)], \qquad (7)$$

one finds $\arcsin[k\,\mathrm{sn}(\tau)]$ as the periodic instanton (cf. Ref. [8]) with period

$$P(E) = 4\mathcal{K}(k), \qquad k = \sqrt{1 - \frac{g^2 E}{2}}, \qquad (8)$$

and again Eq. (4) can be shown not to possess a solution in the domain $0 < E < \frac{2}{g^2}$. The thermon and thermodynamic actions are obtained as

$$S_T = \frac{E}{T} + \frac{16}{g^2}[E(k) - k'^2\mathcal{K}(k)], \qquad S_0 = \frac{2}{g^2}\frac{1}{T}, \qquad (9)$$

where $k' = \sqrt{1 - k^2}$ and T is again the temperature. Again one finds a second order transition from the thermal

to the quantum regime very similar to that depicted in Fig. 1(b).

We now consider the particular spin tunneling model without applied magnetic field we investigated earlier in Ref. [9] and which allows the explicit calculation of periodic instantons as well as the evaluation of their action, and we show that this model gives rise to a first order transition. The model is described in Refs. [1,9,12–14] and a lot of further information can be found in Ref. [15]. We therefore restrict ourselves here to the essential aspects of relevance in our present consideration. With the help of the coherent-state path integral the theory defined by the original Hamiltonian, i.e., $H = K_1 S_z^2 + K_2 S_y^2$, can be shown to lead to an equivalent effective continuum theory with Hamiltonian

$$H = \frac{p^2}{2m(\phi)} + V(\phi) \qquad (10)$$

and

$$m(\phi) = \frac{1}{2K_1(1 - \lambda \sin^2 \phi)},$$
$$V(\phi) = K_2 s(s + 1) \sin^2 \phi, \qquad (11)$$

where $\lambda \equiv K_2/K_1$ is assumed to be less than 1, and the spin eigenvalue s is assumed to be large (i.e., much larger than 1). We see that the potential is again a periodic potential as in the sine-Gordon theory, but now the effective mass is field dependent. It will be seen that this field dependence is crucial in leading to a first order transition from the classical to the quantum regime. In Ref. [9] it is shown that the classical equation associated with the model possesses the following periodic instanton configuration

$$\phi = \arcsin \left[\frac{1 - k^2 \mathrm{sn}^2(\omega\tau|k)}{1 - \lambda k^2 \mathrm{sn}^2(\omega\tau|k)} \right]^{1/2}, \qquad (12)$$

where $\mathrm{sn}(\omega\tau|k)$ again denotes the Jacobian elliptic function of modulus k, and

$$k = \sqrt{\frac{n^2 - 1}{n^2 - \lambda}}, \qquad n^2 = \frac{K_2 s(s + 1)}{E},$$
$$\omega = \omega_0 \sqrt{1 - \frac{\lambda}{n^2}}, \qquad \omega_0^2 = 4K_1 K_2 s(s + 1). \qquad (13)$$

Again we consider first the energy dependence of the period $P(E)$ which is given by

$$P(E) = \frac{2}{\sqrt{K_1}} \frac{1}{\sqrt{K_2 s^2 - E\lambda}} \mathcal{K}(k),$$
$$k \equiv \sqrt{\frac{K_2 s^2 - E}{K_2 s^2 - E\lambda}}. \qquad (14)$$

We consider again Eq. (4) and inquire about a nontrivial solution corresponding to an energy E in the domain $0 < E < E_0 \equiv K_2 s^2$. Such a solution would violate the monotonically decreasing behavior of $P(E)$ observed in

the earlier examples. Using the formula

$$\frac{d\mathcal{K}(k)}{dk} = \frac{1}{k} \left(\frac{E(k)}{k'^2} - \mathcal{K}(k) \right), \qquad (15)$$

one obtains for Eq. (4)

$$\mathcal{K}(k) - \frac{K_2 s^2}{E} E(k) = 0. \qquad (16)$$

The solution of this equation can be investigated both numerically and with approximation analytically. In the numerical procedure we choose $K_1 = 1$ (thus $\lambda = K_2$), and $s = \sqrt{1000}$, and calculate the energy E_1 of the minimum of $P(E)$ for K_2 varying from 0.9 downwards. The results in Table I show that E_1 reaches the maximum energy E_0 when K_2 approaches 0.5. Thus the critical value of K_2 is $\frac{1}{2}$ implying that smaller values of K_2 correspond to unphysical values of E. We obtain the same condition analytically using the expansions of $\mathcal{K}(k)$ and $E(k)$ in rising powers of k^2 around $\pi/2$. Taking into account terms of $O(k^2)$ in these expansions, one finds two possible solutions, i.e.,

$$E = K_2 s^2 \quad \text{or} \quad E = \frac{3K_2 s^2}{1 + 4\lambda}. \qquad (17)$$

Since $E < E_0$, the nontrivial solution is obtained for

$$\frac{3K_2 s^2}{1 + 4\lambda} < K_2 s^2, \qquad \text{i.e.,} \quad \lambda > \frac{1}{2},$$

in agreement with the numerical finding.

Continuing in the present case as in the earlier examples we have the thermodynamic action

$$S_0 = \frac{K_2 s^2}{T} \qquad (18)$$

and the thermon action (which is twice the action of the periodic instanton given in Ref. [9])

$$S_T = \frac{E}{T} + 2W,$$
$$W = \frac{\omega}{\lambda K_1} [\mathcal{K}(k) - (1 - k^2\lambda)\Pi(k^2\lambda, k)], \qquad (19)$$

where $\omega = 2\sqrt{K_1(K_2 s^2 - E\lambda)}$ and $\Pi(k^2\lambda, k)$ is the complete elliptic integral of the third kind. Figure 2(a) shows the monotonically decreasing behavior of the period $P(E)$ as a function of energy for $s = \sqrt{1000}$,

TABLE I. Numerical determination of critical value E_1.

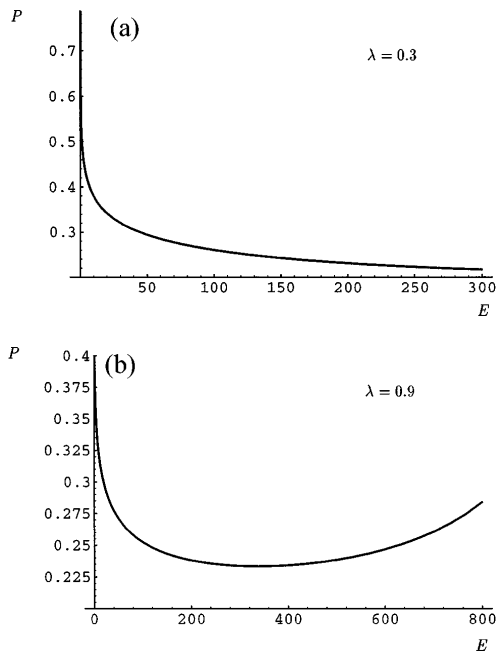| K_2	Energy E_1 at minimum of $P(E)$	$E_0 = K_2 s^2$ (Barrier height)
0.9	336.81	900
0.7	430.75	700
0.6	446.36	600
0.51	496.67	510
0.501	500	501

FIG. 2. The period of the periodic instanton in the fieldless spin model as a function of energy E for $s = \sqrt{1000}$ and $K_1 = 1$: In (a) for $\lambda = 0.3$ and in (b) for $\lambda = 0.9$.

$K_1 = 1$, and $\lambda = 0.3$, i.e., less than the critical value $\frac{1}{2}$. In Fig. 2(b) we plot the period for the corresponding case with $\lambda = 0.9$, i.e., larger than $\frac{1}{2}$. The rising behavior of the period after reaching the critical energy value of 336.81 results from the increasing importance of the field dependence of the effective mass. It is this kind of rising behavior of the period which is necessary in order to generate a first order transition. We see this in the corresponding plots of the thermodynamic and thermon actions shown in Fig. 3, again plotted for the value 0.9 of λ, in which only the two lowest branches, marked S_0 and S_T, are physical.
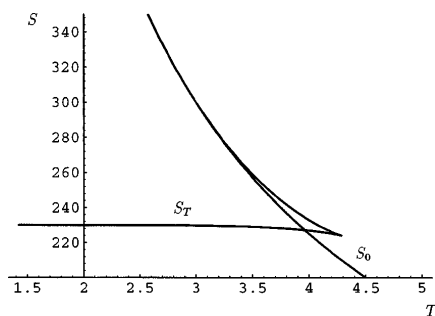

FIG. 3. The thermodynamic and thermon actions S_0, S_T of the fieldless spin model as functions of temperature T for $\lambda = 0.9$ demonstrating the first order transition.

We have therefore made a very general observation. The regulation of the transition from the classical to the quantum regime by variation of the applied magnetic field as observed by Chudnovsky and Garanin [6] can also be achieved through variation of the field dependence of the effective mass. We expect this characteristic to show up also in field theory models such as the Skyrme model and its variants.

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