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Tunnelling at finite temperature in the LMG model

Alex H Blin, Brigitte Hiller and Li Junqing†

Centro de Física Teórica, Universidade de Coimbra, P-3000 Coimbra, Portugal

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Abstract. The Lipkin–Meshkov–Glick model is studied at finite temperature in mean field approximation. The imaginary time method is used to calculate the energy splitting due to tunnelling, by solving the equations of motion in Euclidean time and adapting the instanton approximation to finite temperatures. In this way we are also able to determine the pre-exponential factor at finite temperature.

1. Introduction

The Lipkin–Meshkov–Glick (LMG) model [1] is a good testing ground for approximation methods. Along with other schematic models it is important in present studies in many-body theory (see [4] for a review). In addition, some of its properties are reminiscent of real physical systems. As we shall see, the form of the mean field potential extracted from the LMG model is similar to the situation encountered in the NH_3 molecule. In this note we concentrate on the temperature behaviour of the LMG model. We study the form of the mean field potential and investigate the dynamical properties with the aim to determine the energy level separation of the lowest levels. To achieve this we consider motion in Euclidean time to describe barrier penetration within the imaginary time method [2]. The level separation is obtained as the energy splitting due to tunnelling in the spirit of the instanton approximation [3, 4], but this approximation is extended here to *finite* temperature. In this way we are also able to calculate the pre-exponential factor not considered in other studies, e.g. [2, 5, 6] in the context of nuclear physics or [7] in the context of the LMG model.

The extension of the instanton approximation to finite temperature is the main (and new) result of the present work, allowing us to calculate the full expression, in an approximate manner, for the energy splitting at finite temperature.

The present article is structured as follows. After this introductory section, the mean field free energy is derived in section 2 and the two possible equilibrium solutions are discussed. In section 3 we calculate the mean field Lagrangian, passing to canonical variables, and determine the equations of motion. Section 4 deals with the imaginary time method and instanton approximation, used to evaluate tunnelling processes. The results of the dynamical (tunnelling) calculations are presented and discussed in section 5, which concludes with a short summary.

† Permanent address: Institute of Modern Physics, Academia Sinica, PO Box 31, Lanzhou 730000, People's Republic of China

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2. Mean-field description of the static properties

The LMG model [1] is a two level system with N fermions. We use the quasispin operators

$$J_3 = \tfrac{1}{2}\sum_{i=1}^{N}(a_{i+}^{+}a_{i+} - a_{i-}^{+}a_{i-}) \tag{1}$$

$$J_{\pm} = \sum_{i=1}^{N} a_{i\pm}^{+}a_{i\mp} \tag{2}$$

with the indices $i+$, $i-$ indicating the creation (a^+) or annihilation (a) of a particle in the ith state of the upper or lower energy level, respectively. The LMG Hamiltonian is then expressed as

$$\hat{H} = \epsilon J_3 + V(J_+^2 + J_-^2). \tag{3}$$

Here ϵ is the (positive) parameter describing the energy level spacing and we assume V, the interaction strength, to be negative. The mean field density matrix takes the form [8–10]

$$D_0 = K_0 e^h \tag{4}$$

where

$$h = \alpha_1 J_3 + \alpha_2 J_+ + \alpha_2^* J_- \tag{5}$$

is the mean field Hamiltonian, α_1 and α_2 are real and complex numbers, respectively, and K_0 guarantees that $\mathrm{tr}\, D_0 = 1$.

Minimizing the free energy

$$F = \mathrm{tr}(D_0\hat{H}) + \frac{1}{\beta}\,\mathrm{tr}(D_0 \ln D_0) \tag{6}$$

determines the equilibrium values of the parameters α_i at a given inverse temperature $\beta = 1/kT$ (k is the Boltzmann constant). It is useful, however, to work with the diagonalized density matrix [8–10]

$$\begin{aligned} D &= K \mathrm{e}^{\gamma J_3} \\ K &= 1/\,\mathrm{tr}\, \mathrm{e}^{\gamma J_3} \end{aligned} \tag{7}$$

which is obtained from D_0 by the unitary transformation

$$D = U D_0 U^+ \tag{8}$$

where

$$U = \mathrm{e}^{\eta J_+ + \eta^* J_-}. \tag{9}$$

This means that one passes from the parameters α_i to γ and η (real and complex, respectively). The free energy thus becomes

$$F = \epsilon J \cos\left(2\sqrt{\eta\eta^*}\right) - \frac{V(N-1)}{N} J^2 \frac{\eta^2 + \eta^{*2}}{\eta\eta^*} \sin^2(2\sqrt{\eta\eta^*}) + \frac{1}{\beta}\left[\gamma J - N \ln\left(2\cosh\frac{\gamma}{2}\right)\right] \tag{10}$$

with the definition

$$J = \mathrm{Tr}(DJ_3) = \frac{N}{2}\tanh\frac{\gamma}{2}. \tag{11}$$

The equilibrium values of the new parameters are then

$$\eta = 0 \qquad \gamma = -\beta\epsilon \tag{12}$$

which we call *phase 1*, or

$$\cos 2\mathrm{i}\eta = -\frac{\epsilon\beta}{\gamma} \qquad \gamma = -2\beta V(N-1)\tanh\frac{\gamma}{2} \tag{13}$$

with $2\mathrm{i}\eta$ real, which is *phase 2*. It only exists for $V \leqslant 0$ and under the following simultaneous conditions:

$$-V(N-1)\beta \geqslant 1 \qquad -2V(N-1)/\epsilon \geqslant 1. \tag{14}$$

A third solution with $\cos 2\mathrm{i}\eta = 0$ and $\gamma = 0$ is uninteresting since it would correspond to infinite entropy.

The parameter γ diverges to $-\infty$ at vanishing temperature in both phases. This is seen in (13) by taking the limit $\beta \to \infty$; see appendix A.

3. Dynamical properties

3.1. The mean field Lagrangian

To obtain the equations of motion we proceed to determine the Lagrangian. We assume the system to be in a heat bath, which fixes γ. Then the Lagrangian is

$$L = \mathrm{Tr}\left(D_0 \mathrm{i}\hbar\frac{\partial}{\partial t}\right) - F = \mathrm{i}\hbar J\frac{\dot{\eta}^*\eta - \eta^*\dot{\eta}}{\eta\eta^*}\sin^2\sqrt{\eta\eta^*} - F. \tag{15}$$

With the substitution

$$\sqrt{-2J}\frac{\eta}{\sqrt{\eta\eta^*}}\sin\sqrt{\eta\eta^*} = \frac{p - \mathrm{i}q}{\sqrt{2}} \tag{16}$$

(p, q real) the Lagrangian takes the canonical form

$$L = \frac{\hbar}{2}(\dot{q}p - q\dot{p}) - F \tag{17}$$

with the free energy expressed as

$$F = H + \frac{1}{\beta}\left(\gamma J - N\ln\left(2\cosh\frac{\gamma}{2}\right)\right) \tag{18}$$

and the energy as

$$H = -\epsilon J + \frac{\Lambda}{4}[(p^2 - p_0^2)^2 - (q^2 - q_0^2)^2] \tag{19}$$

where

$$\begin{aligned} \Lambda &= 2V(N-1)/N \\ p_0^2 &= \frac{-\epsilon N}{2V(N-1)} - 2J \\ q_0^2 &= \frac{+\epsilon N}{2V(N-1)} - 2J. \end{aligned} \tag{20}$$

Note that contrary to η and η^*, the new variables q and p are canonically conjugate.

It is interesting also to evaluate the zero temperature limit of F. In this case, γ becomes $-\infty$ in both phases and the free energy reduces to

$$F = H\left(\tanh\frac{\gamma}{2} \to -1\right). \tag{21}$$

We show in figure 1 the behaviour of the free energy with $p = 0$ as a function of the coordinate q, at various temperatures (in dimensionless energy units with the Boltzmann

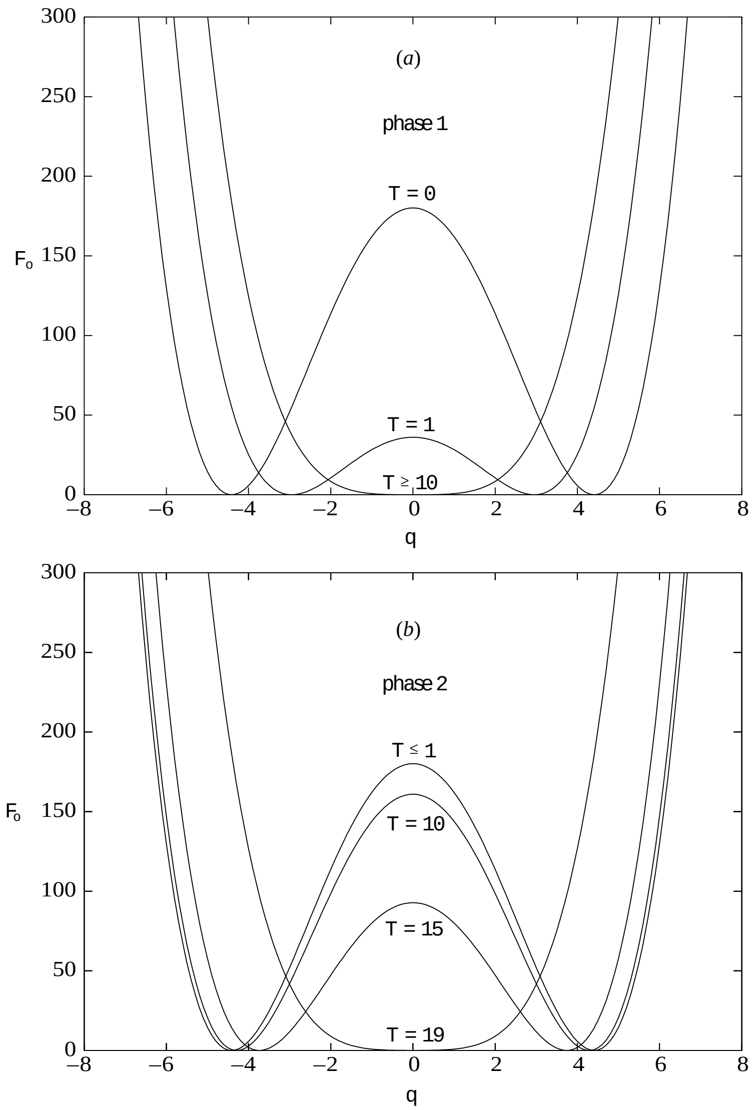
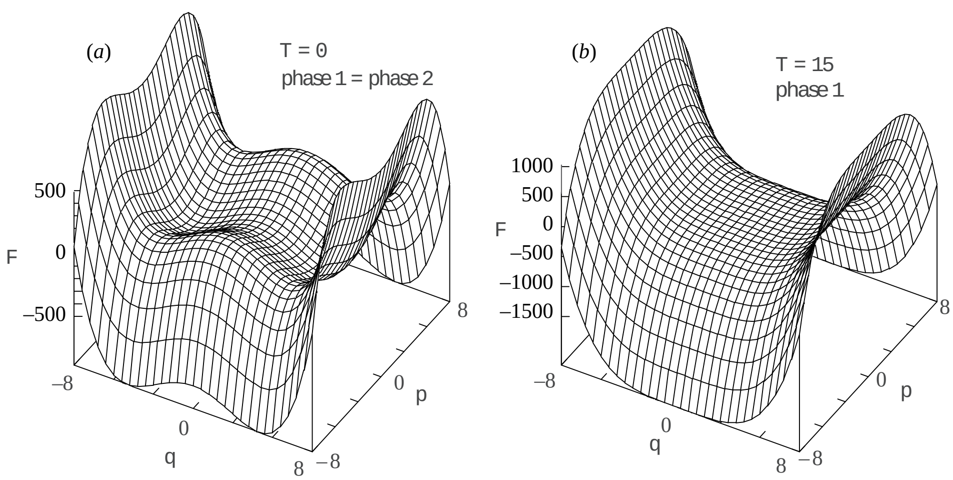


Figure 1. The shifted free energy F_0, at $p = 0$, as a function of q at different values of the temperatute T, in phases 1 (a) and 2 (b). The parameters of the model are $N = 20$, $V = -1$ and $\epsilon = 1$.

constant $k = 1$) and in both phases. The model parameters are $\epsilon = 1$, $V = -1$ and $N = 20$. Since the motion is independent of the definition of the zero point of the potential energy, the free energy displayed in figure 1 is shifted such that the minima of $F(p = 0, q)$ are zero. This shifted free energy is denoted F_0, and for $p = 0$ it takes the role of a potential energy. The potential energy as a function of q is symmetric and exhibits two pockets separated by a barrier. This situation is reminiscent of the NH_3 maser. The quantum mechanical ground state in each pocket is split due to tunnelling through the barrier and the transitions between the two neighbouring energy levels correspond to the ammonia microwave frequency. In phase 1, figure 1(*a*), the height of the barrier diminishes rapidly with increasing temperature in the range up to $T = 1$. For higher temperatures the barrier continues to decrease more slowly; the change in F_0 is not visible at the scale of figure 1(*a*), once the temperature reaches $T \simeq 10$. The barrier height in phase 2 behaves similarly, except that now the curves in the temperature range $T = 0 \ldots, 1$ are indistinguishable, and the decrease becomes more and more pronounced with increasing temperatures. At $T = 19$ the barrier vanishes in both phases, which become identical here (see the discussion in appendix A).

The dependence of the free energy on the pair of conjugate variables p and q is depicted in figure 2. At $T = 0$, figure 2(*a*), both phases coincide and the barrier has its maximum height. At $T = 15$ the barrier has virtually vanished in phase 1 (figure 2(*b*)) but not yet in phase 2 (figure 2(*c*)). Note that p is the momentum conjugate to q and not an independent variable.



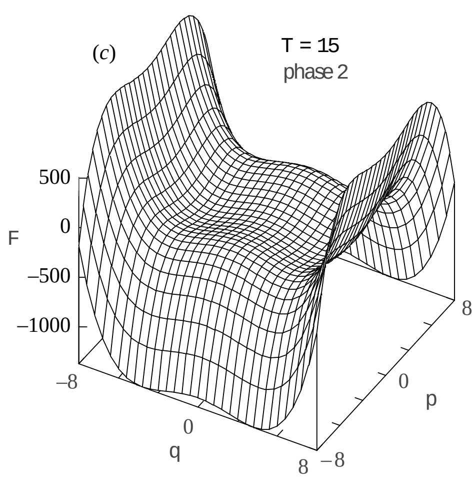


Figure 2. The free energy F in the space of variables p and q, at vanishing temperature (*a*), where the two phases are identical, and at $T = 15$ in phase 1 (*b*) and phase 2 (*c*). Note that p and q are not different degrees of freedom but canonically conjugate variables. The set of parameters is as in figure 1.

3.2. The equations of motion

The equations of motion

$$\hbar\dot{q} = \frac{\partial F}{\partial p} \qquad \hbar\dot{p} = -\frac{\partial F}{\partial q} \tag{22}$$

can be decoupled into separate equations for q and p:

$$\dot{q} = \frac{\Lambda}{\hbar}[-((q^2 - q_0^2)^2 + g_{\rm in})^{\frac{3}{2}} + p_0^2((q^2 - q_0^2)^2 + g_{\rm in})]^{\frac{1}{2}} \tag{23}$$

$$\dot{p} = \frac{\Lambda}{\hbar}[-((p^2 - p_0^2)^2 - g_{\rm in})^{\frac{3}{2}} + q_0^2((p^2 - p_0^2)^2 - g_{\rm in})]^{\frac{1}{2}} \tag{24}$$

where

$$(p^2 - p_0^2)^2 - (q^2 - q_0^2)^2 = (p_{\rm in}^2 - p_0^2)^2 - (q_{\rm in}^2 - q_0^2)^2 \equiv g_{\rm in} \tag{25}$$

is a constant of motion, fixed by the initial values of p and q, $p_{\rm in}$ and $q_{\rm in}$. This is the case since we assume γ to be kept fixed. The correct sign of the roots in evaluating the half-integer powers is determined by the initial conditions.

4. Tunnelling

To describe barrier penetration at finite temperature we have recourse to the imaginary time method [2]. The (real time) action

$$S = \int_{t_1}^{t_2} {\rm d}t\, L \tag{26}$$

is continued to imaginary time by writing the Euclidean action

$$\sigma = \int_{-\frac{\beta}{2}}^{+\frac{\beta}{2}} {\rm d}\tau\, L = \frac{{\rm i}\hbar}{2}\int_{-\frac{\beta}{2}}^{+\frac{\beta}{2}} {\rm d}\tau \left(\frac{{\rm d}q}{{\rm d}\tau}p - q\frac{{\rm d}p}{{\rm d}\tau}\right) - F\mathcal{T} \tag{27}$$

where the motion in Euclidean time $\tau = {\rm i}t \in \Re$ is constrained by the boundary condition

$$q\left(\tau = -\frac{\beta}{2}\right) = q\left(\tau = +\frac{\beta}{2}\right) \tag{28}$$

at a given temperature $T = 1/\beta$ and where $\mathcal{T}$ is the Euclidean time period of one full cycle of motion. We have made use of the fact here that the free energy is a constant of motion. Due to the replacement $t \to \tau/{\rm i}$, the equations of motion correspond to motion in imaginary time in an inverted potential.

The equations of motion in Euclidean time take the form

$$\frac{{\rm d}q}{{\rm d}\tau} = -\frac{\Lambda}{\hbar}[((q^2 - q_0^2)^2 + g_{\rm in})^{\frac{3}{2}} - p_0^2((q^2 - q_0^2)^2 + g_{\rm in})]^{\frac{1}{2}} \tag{29}$$

$$\frac{{\rm d}p}{{\rm d}\tau} = -\frac{\Lambda}{\hbar}[((p^2 - p_0^2)^2 - g_{\rm in})^{\frac{3}{2}} - q_0^2((p^2 - p_0^2)^2 - g_{\rm in})]^{\frac{1}{2}}. \tag{30}$$

The expressions for p and q necessary to evaluate σ are obtained directly from (25),

$${\rm i}q = [((p^2 - p_0^2)^2 - g_{\rm in})^{\frac{1}{2}} - q_0^2]^{\frac{1}{2}} \tag{31}$$

$${\rm i}p = [((q^2 - q_0^2)^2 + g_{\rm in})^{\frac{1}{2}} - p_0^2]^{\frac{1}{2}}. \tag{32}$$

There are two types of solution (see also [5, 6]):

(i) $q(\tau) = 0$, called *statistical fluctuations* and

(ii) solutions with $\mathcal{T} = \beta$, called *quantum fluctuations*, i.e. tunnelling. This is the kind of solutions we study here. The boundary condition (28) fixes the initial value of q, with $p_{\rm in} = 0$, at any given temperature; i.e. $q_{\rm in}$ has to be adjusted such that the dynamical equations yield the correct period $\mathcal{T}$.

The tunnelling probability and the energy splitting are proportional to the exponential of the Euclidean action for tunnelling through the barrier. At zero temperature the energy of level splitting can be obtained in the instanton approximation [3, 4]. Generalized to finite temperature the energy splitting can be written as a pre-exponential factor multiplying the action exponential $e^{\sigma_0/2}$:

$$\Delta E = 2\sqrt{\frac{\omega m}{\pi}} B e^{\sigma_0/2}. \tag{33}$$

The generalization to finite temperature means that $|q_{\rm in}| \neq q_0$ for $T \neq 0$; $q_{\rm in}$ has to be determined to satisfy the boundary condition (28) instead. In our case there is the additional difficulty that the energy contains a p^4 dependent term. The generalization to p^4 dependence of the energy is achieved by using the equations of motion in evaluating the period $\mathcal{T}$ and the action σ (27), rather than the expressions in [3, 4] involving only the potential (valid in the absence of nonquadratic terms). We use here and in the sequel units with $\hbar = c = k = 1$. The quantity σ_0 in the above equation is

$$\sigma_0 = -2\int_{-|q_{\rm in}|}^{+|q_{\rm in}|} {\rm d}q \sqrt{\sqrt{(q^2 - q_0^2)^2 + g_{\rm in}} - p_0^2} - F_0(p_{\rm in} = 0, q_{\rm in})\mathcal{T} \tag{34}$$

with

$$F_0(p, q) = \frac{\Lambda}{4}[(p^2 - p_0^2)^2 - (q^2 - q_0^2)^2 - p_0^4] \tag{35}$$

$$B = \omega(q_0 - |q_{\rm in}|)e^{\omega\mathcal{T}/4} \tag{36}$$

$$\mathcal{T} = 2\int_{-|q_{\rm in}|}^{+|q_{\rm in}|} \frac{{\rm d}q}{{\rm d}q/{\rm d}\tau} \overset{!}{=} \beta \tag{37}$$

ω is related to the curvature of the potential near q_0,

$$\omega^2 = -2\Lambda q_0^2/m \tag{38}$$

and the mass is

$$m = -\frac{1}{p_0^2\Lambda}. \tag{39}$$

Equation (38) holds in the strict instanton approximation, i.e. for $|q_{\rm in}| = q_0$. At finite temperatures, however, we have $|q_{\rm in}| \neq q_0$ and we extract ω from the real-time oscillation period as

$$\omega = 2\pi\left[2\int_{|q_{\rm in}|}^{\sqrt{2q_0^2 - q_{\rm in}^2}} \frac{{\rm d}q}{\dot{q}}\right]^{-1} \tag{40}$$

where the integral limits are the turning points. In the limit $|q_{\rm in}| \to q_0$, this expression reduces to (38).

Note that σ_0 and F_0 differ from σ and F by shifting of the potential by a constant, such that the minima have zero potential energy (the motion is of course independent of additive constants). At zero temperature the energy of level splitting reduces to the expression given in [4]. In particular, the boundary condition (28) at $T = 0$ imposes $|q_{\rm in}| \to q_0$. At this point, however, $\mathcal{T}$ diverges and we have to evaluate explicitly the limit $|q_{\rm in}| \to q_0$ in B, which stays finite. This limit is discussed in appendix B, along with the limit $q \to q_{\rm in}$ at which the integrand in (37) diverges.

Let us mention for the sake of completeness that, according to [11], the splitting of the nth energy level is related to the level splitting of the ground state (33) by

$$\Delta E_n = \frac{(2B^2 m)^n}{n!\omega^n}\Delta E \tag{41}$$

as long as the potential well can be assumed quadratic up to the energy of this nth level.

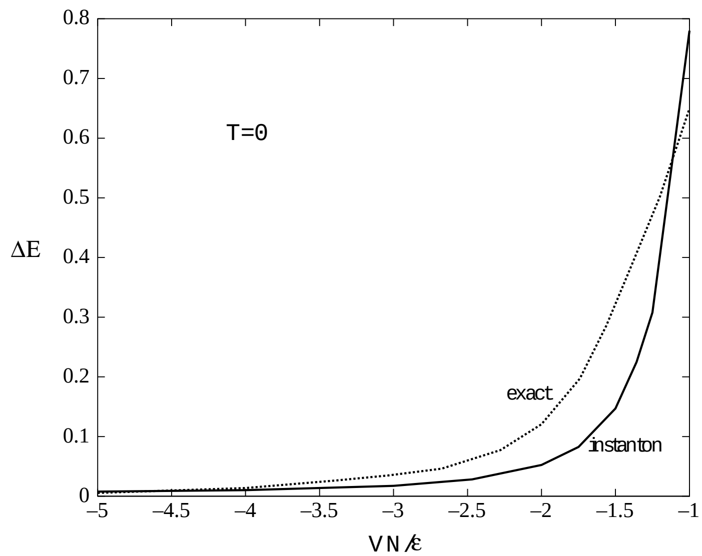


Figure 3. The energy level splitting ΔE in the instanton approximation as compared to the exact results, as a function of the potential parameter V (in units $VN\epsilon^{-1}$), for $N = 14$ at $T = 0$.

5. Results of the dynamical calculations and discussion

First let us compare the instanton approximation to the exact results [1] at zero temperature. Figure 3 shows the exact and approximate level differences of the lowest energy states in the case $N = 14$ as functions of the potential parameter V. The approximation is reasonable albeit not perfect. Note that the method breaks down for values $VN/\epsilon \simeq -1$ since the ground state energy $\omega/2$ becomes of the order of the potential barrier height so there is no longer any tunnelling.

The behaviour in terms of temperature can be understood by looking at the dependence of the potential barrier on the temperature: increasing the temperature diminishes the barrier so the energy splitting increases. This is shown in figure 4 for both phases using the same set of parameters as in figure 1. There is a limiting temperature for each phase from which it becomes impossible to fulfil the condition $\mathcal{T} = \beta$ since $\mathcal{T}$ becomes too long for any initial value of q. In any case, close to this limiting temperature the instanton approximation becomes unreliable since $|q_{\rm in}|$ cannot be chosen close to q_0, in order to have a short enough Euclidean time period; therefore the motion is not of the instanton type any longer. Note the different energy and temperature scales in both phases. At $T = 0$ both phases are

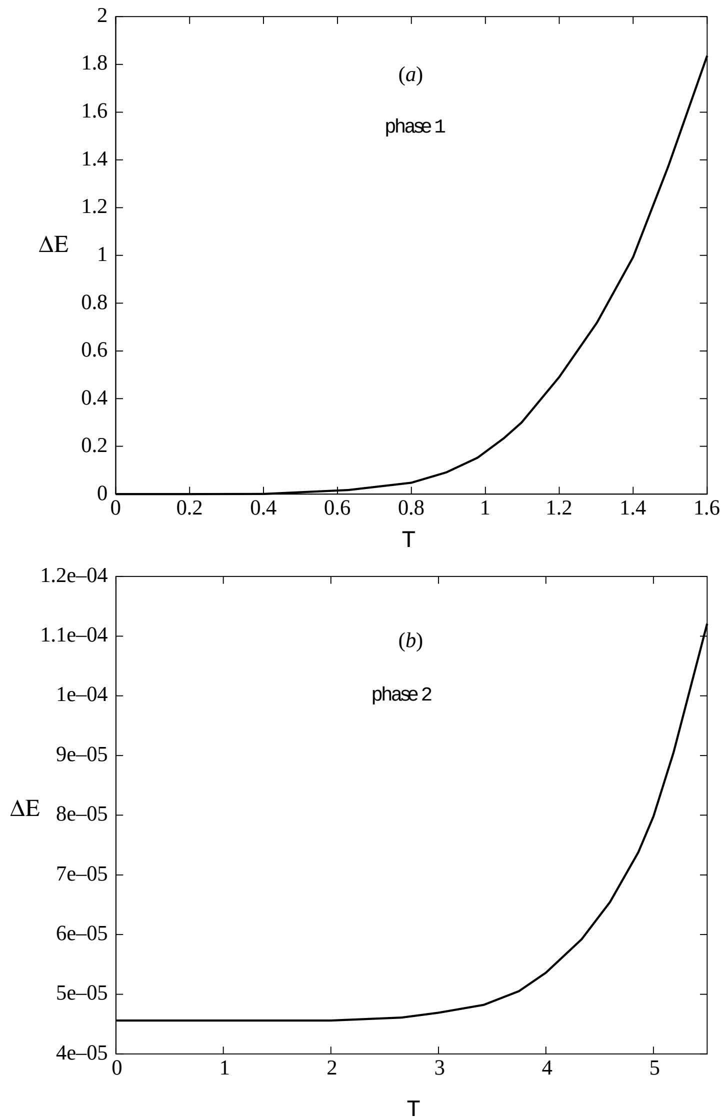


Figure 4. The energy level splitting ΔE in instanton approximation as a function of the temperature T in phase 1 (*a*) and phase 2 (*b*). The set of parameters is as in figure 1.

identical so the curves start off at the same value of the energy splitting ΔE. In phase 1 the rise is much more pronounced than in phase 2 and the limiting temperature is reached much earlier. This is of course due to the behaviour of the potential barrier as represented in figure 1; the decrease of the barrier height with increasing temperature is faster in phase 1 than in phase 2.

It is instructive to see the influence of the pre-exponential factor which is often neglected in this kind of calculation. Figure 5 depicts the variation of this factor, which multiplies the action exponent in expression (33), as a function of the temperature. The set of parameters is again as in figure 1, and we show the behaviour of the factor in phase 1. In figure 5

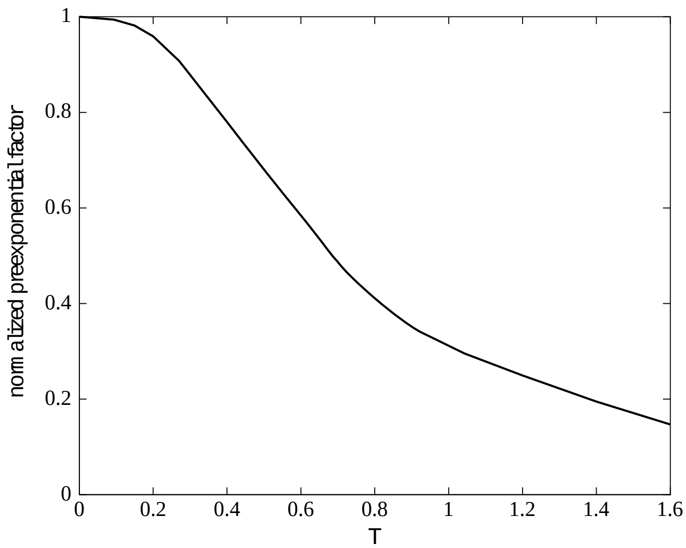


Figure 5. The pre-exponetial factor, normalized to 1 at $T = 0$, as a function of the temperature T in phase 1. The set of parameters is as in figure 1.

it is normalized to 1 at $T = 0$ so the deviation from the value 1 indicates its importance. As one can see, this factor is not constant at all but diminishes appreciably with increasing temperature.

To summarize, we have extracted a mean field Lagrangian from the LMG model at finite temperatures. Then we studied the equations of motion in Euclidean time and adapted the instanton method to finite temperature tunnelling. The instanton approximation assumes that the system spends most of the time near the initial position, and that the motion which corresponds to tunnelling is fast compared to this, hence the name instanton. This approximation is reasonable for not too large temperatures where $|q_{\rm in}|$ is close to q_0, and larger deviations from the exact behaviour at higher temperatures are expected. The advantage of the method presented here is that it makes it possible to calculate, in an approximate manner, the full expression of the energy splitting at finite temperature, and not just the exponential factor containing the action.

Appendix A

This appendix deals with the dependence of the potential on temperature.

A.1. The zero-temperature limit of the two phases

To see the behaviour of γ at $T = 0$, we observe first that $\eta = 0$ and $\gamma \to -\infty$ for $\beta \to \infty$ in phase 1. In phase 2, to have γ finite for infinite β, γ would have to vanish, see the second term of (13), which would correspond to infinite entropy. Thus γ cannot be finite and must diverge. In that case, the hyperbolic tangent goes to ± 1, depending on the sign of γ; it is the negative values of γ, however, which give the *minimum* free energy. Thus by (13)

$$\gamma \to 2\beta V(N-1) \to -\infty \qquad \text{and} \qquad \cos 2i\eta = \frac{\epsilon}{2V(N-1)}. \tag{A1}$$

A.2. The limit $q_0 \to 0$

The potential barrier disappears when the two minima at q_0 and $-q_0$ merge, so the potential becomes purely quartic. Using (20) and (11) this happens when

$$\tanh\frac{\gamma}{2} = \frac{\epsilon}{2V(N-1)}. \tag{A2}$$

Expressing γ by β, relations (12) and (13), it turns out that in *both* phases

$$\tanh -\frac{\beta\epsilon}{2} = \frac{\epsilon}{2V(N-1)} \tag{A3}$$

describes the temperature of vanishing potential barrier. Also, $\eta = 0$ in both cases, so the phases become indistinguishable at this point.

Appendix B

This appendix shows how to treat the singularities related to the Euclidean time period $\mathcal{T}$.

B.1. The limit $|q_{in}| \to q_0$

We consider here the limiting behaviour of B (36). We split the Euclidean time period (37) into two pieces,

$$\mathcal{T} = \mathcal{T}_\Delta + \mathcal{T}_{\text{rest}} \tag{B1}$$

with

$$\frac{\mathcal{T}_\Delta}{4} = \int_{-q_0+\epsilon}^{-q_0+\epsilon+\Delta} \frac{\mathrm{d}q}{\mathrm{d}q/d\tau} \tag{B2}$$

and

$$\frac{\mathcal{T}_{\text{rest}}}{4} = \int_{-q_0+\epsilon+\Delta}^{0} \frac{\mathrm{d}q}{\mathrm{d}q/\mathrm{d}\tau} \tag{B3}$$

i.e. we perform the substitution $q_{\text{in}} = -q_0 + \epsilon$ ($q_{\text{in}} < 0$ here and $q_0 > 0$ by definition) and split $\mathcal{T}$ into its two parts at the point $q = q_{\text{in}} + \Delta$. We assume Δ to be small compared to p_0 and q_0 and $\epsilon \ll \Delta$. The expression for the derivative of q becomes

$$\mathrm{d}q/\mathrm{d}\tau = -\frac{\Lambda}{\hbar} p_0[\Delta(\Delta(2q_0^2 - 6q_0\epsilon) + 4q_0^2\epsilon)]^{\frac{1}{2}}. \tag{B4}$$

This is inserted into (B2) and the integration performed. Taking then the small ϵ limit, i.e. $q_{\text{in}} = -q_0 + \epsilon \to -q_0$, yields

$$\frac{\mathcal{T}_\Delta}{4} = \frac{1}{\omega} \ln\frac{2\Delta}{\epsilon}. \tag{B5}$$

This expression diverges obviously when $\epsilon \to 0$, which is exactly the instanton behaviour. But B (36) stays finite in this limit,

$$B = 2\omega\Delta \mathrm{e}^{\frac{\omega\mathcal{T}_{\text{rest}}}{4}} \tag{B6}$$

and therefore the energy splitting as well.

B.2. The limit $q \to q_{in}$

Independent of the initial value of $q_{\rm in}$ the integrand of $\mathcal{T}$ diverges for q close to $q_{\rm in}$. The derivative of q becomes at $q = q_{\rm in} + \Delta$ (Δ small compared to p_0 and q_0, and $q_{\rm in} < 0$ here)

$$\mathrm{d}q/\mathrm{d}\tau = -\frac{\Lambda}{\hbar} p_0[(2q_{\rm in}(q_{\rm in}^2 - q_0^2) + \Delta a)\Delta]^{\frac{1}{2}} \tag{B7}$$

with

$$a = 3q_{\rm in}^2 - q_0^2 + 6q_{\rm in}^2(q_{\rm in}^2 - q_0^2)^2/p_0^4 \tag{B8}$$

so the first part of expression for $\mathcal{T}$ becomes

$$\frac{\mathcal{T}_\Delta}{4} = \int_{q_{\rm in}}^{q_{\rm in}+\Delta} \frac{\mathrm{d}q}{\mathrm{d}q/\mathrm{d}\tau}$$

$$= \begin{cases} \dfrac{-2}{(-\frac{\Lambda}{\hbar})p_0\sqrt{-a}}\left[\tan^{-1}\sqrt{\dfrac{-\Delta a - 2q_{\rm in}(q_{\rm in}^2 - q_0^2)}{\Delta a}} - \dfrac{\pi}{2}\right] & \text{for } a < 0 \\ \dfrac{1}{(-\frac{\Lambda}{\hbar})p_0}\sqrt{\dfrac{2\Delta}{q_{\rm in}(q_{\rm in}^2 - q_0^2)}} & \text{for } a = 0 \\ \dfrac{2}{(-\frac{\Lambda}{\hbar})p_0\sqrt{a}}\ln\left[\dfrac{\sqrt{\Delta a} + \sqrt{\Delta a + 2q_{\rm in}(q_{\rm in}^2 - q_0^2)}}{\sqrt{2q_{\rm in}(q_{\rm in}^2 - q_0^2)}}\right] & \text{for } a > 0. \end{cases} \tag{B9}$$

Similar expressions are obtained in the evaluation of ω (40) in the limit $q \to |q_{\rm in}|$, changing some signs in the appropriate places, and a corresponding one in the limit $q \to \sqrt{2q_0^2 - q_{\rm in}^2}$.

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