

## First-order phase transitions in quantum-mechanical tunneling models

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A criterion is derived for the determination of parameter domains of first-order phase transitions in quantum-mechanical tunneling models. The criterion is tested by application to various models, in particular to some that have been used recently to explore spin tunneling in macroscopic particles. In each case agreement is found with previously heuristically determined domains. [S0163-1829(99)08833-5]

### I. INTRODUCTION

It is well known that at temperatures close to zero, decay rates of metastable states are determined by quantum tunneling processes whose dynamics is described by classical configurations such as vacuum or periodic bounces, but that with increasing temperature thermal activation becomes more and more important, and beyond some critical or crossover temperature  $T_c$  becomes the decisive mechanism. It has been realized recently that this change or crossover can be regarded as a transition from quantum to classical behavior, which in turn can be looked at like a phase transition in, e.g., the thermodynamics of gases. This is a fascinating topic that has attracted considerable interest recently and application particularly in the area of macroscopic spin systems. The general idea applies also to other cases where instead of a decay rate a shift in energy is involved, such as a level splitting in quantum mechanics, which is described by vacuum or periodic instantons.

The characteristic way in which phase transitions appear in quantum-mechanical tunneling processes has been worked out in Ref. 1. In particular, a sharp first-order transition is there shown to appear in the plot of action  $S$  versus temperature  $T$ , which is very analogous to that of the free enthalpy versus pressure of a van der Waals gas, whose equation of state plotted as pressure versus volume corresponds to the plot of the period  $P(E)$  (of the periodic bounce or instanton) versus energy in the consideration of quantum-mechanical systems. It is well known<sup>2</sup> that in the case of a periodic problem in Euclidean time the derivative of the action with respect to the energy  $E$  is the negative of the oscillation time  $\tau(E)$  or period  $P(E)$  at that energy that has to be identified with  $-\hbar/T$ . If  $\tau(E)$  is a monotonically decreasing function with increasing  $E$ , one has a second-order transition; if  $\tau(E)$  has a minimum and then rises again within the domain  $0 < E < \text{barrier height}$ , one has a first-order transition, i.e., in this case there is an energy  $E_c$  within this range with  $T_c = \hbar/\tau(E_c)$  at which the first-order transition takes place. A criterion for a first-order transition can be obtained by studying the Euclidean time period in the neighborhood of the sphaleron configuration at the peak of the potential barrier, i.e., at the bottom of the well of the inverse potential, as advocated in Ref. 2. If the frequency of oscillation about the sphaleron point is  $\omega_s$  and oscillations different from  $\omega_s$  about it are possible, a first-order transition requires  $\omega^2 > \omega_s^2$  or  $\tau - \tau_s < 0$ . Thus, this is a condition one can use

as a criterion for a first-order transition. Explicit and solvable examples of both types of transitions in quantum-mechanical models have been given recently in Refs. 3–6. It was shown there that simple models, such as those of the  $(1+1)$ -dimensional scalar field theories with the familiar double-well or periodic or sine-Gordon potentials, do not lead to first-order transitions. However, as shown in Ref. 3, this changes if the mass is allowed to become field dependent, a case which occurs, for instance, in spin tunneling theories, or if an externally applied field is introduced as in Refs. 4–7, as again in the context of spin tunneling phenomena. The introduction of such extra dependences implies, of course, the introduction of appropriate parameters. Thus in Ref. 3 it was shown, for example, that in the case of a periodic potential and an effective mass with a field dependence multiplied by a parameter  $\lambda$ , the period  $P(E)$  is monotonically decreasing for  $\lambda < \frac{1}{2}$ , but for  $\lambda > \frac{1}{2}$  it has a minimum and then rises again, and so leads to a first-order transition. It is therefore of interest to find criteria for the determination of domains of such parameter values in which they lead to one type of phase transition or the other. A significant step forward in this direction on the basis of higher-dimensional arguments, was achieved in Ref. 2, where an expansion about the time-independent saddle-point configuration is considered. However, many considerations of basic interest are best illustrated by quantum-mechanical models, which serve as useful prototypes for more complicated theories, and it is natural to enquire about criteria for the occurrence of first-order transitions in these, and hence to verify the conditions obtained heuristically as in the models referred to above.<sup>3–5</sup> Thus in the following we consider a scalar theory with a field-dependent mass and suitable nonlinear potentials. Expanding the static field (quantum mechanically a coordinate) about the constant sphaleron configuration (at the top of the barrier) and proceeding to second-order perturbation theory, we obtain the deviation of the frequency from its sphaleron value (lowest-order perturbation theory) and hence the criterion for a first-order transition. We then consider various models considered earlier<sup>3–7</sup> and demonstrate the agreement of the prediction of the criterion with the results obtained there heuristically. We add that theories with effective field-dependent masses are not unusual; typical examples are, for instance, Skyrme theories.<sup>8</sup> The instability of the sphaleron configuration at the top of the barrier in various familiar models has been shown, for instance, in Ref. 9.

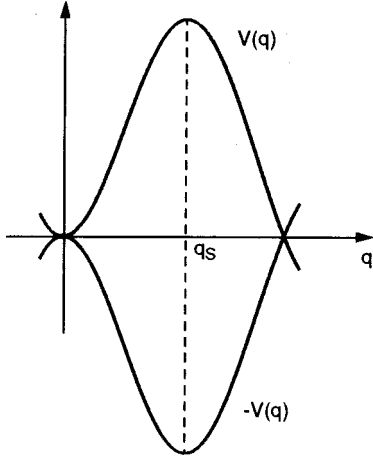


FIG. 1. The potential barrier with sphaleron coordinate  $q_s$ .

## II. CONDITION FOR A FIRST-ORDER TRANSITION

We consider a Euclidean action integral of the form

$$S = \int d\tau \left[ \frac{1}{2} M(q) \dot{q}^2 + V(q) \right] \quad (1)$$

with Euler-Lagrange equation

$$M(q) \ddot{q} + \frac{1}{2} \frac{\partial M(q)}{\partial q} \dot{q}^2 = \frac{\partial V(q)}{\partial q} \quad (2)$$

and  $q(\tau+P) = q(\tau)$ , where  $P = 1/T$  is the period and  $T$  the temperature. Since the solutions near the sphaleron solution at the top of the barrier shown in Fig. 1 have information on the order of the ‘‘phase’’ transition between quantum and thermal activity regimes, we confine ourselves to this region in solution space. We define [as for a maximum of  $V(q)$  at  $q_s$ ]

$$-\omega_s^2 \equiv \frac{V''(q_s)}{M(q_s)} \quad (3)$$

and set in Eq. (2)

$$q = q_s + \eta(\tau), \quad (4)$$

where  $q_s$  is the sphaleron position with  $V'(q_s) = 0$ . Expanding  $M[q_s + \eta(\tau)]$  and  $V[q_s + \eta(\tau)]$  and their derivatives in powers of  $\eta(\tau)$ , we obtain the fluctuation equation,

$$\begin{aligned} & [M(q_s) + M'(q_s) \eta(\tau) + \frac{1}{2} M''(q_s) \eta^2(\tau) + \dots] \ddot{\eta}(\tau) \\ & + \frac{1}{2} [M'(q_s) + M''(q_s) \eta(\tau) \\ & + \frac{1}{2} M'''(q_s) \eta^2(\tau) + \dots] \dot{\eta}^2(\tau) \\ & = V''(q_s) \eta(\tau) + \frac{1}{2} V'''(q_s) \eta^2(\tau) \\ & + \frac{1}{6} V''''(q_s) \eta^3(\tau) + \dots \end{aligned} \quad (5)$$

We are interested in small fluctuations  $\eta(\tau)$ . The first-order equation

$$M(q_s) \ddot{\eta}(\tau) - V''(q_s) \eta(\tau) = 0 \quad (6)$$

has the even solution

$$\eta(\tau) = a \cos(\omega_0 \tau), \quad \omega_0^2 = \omega_s^2. \quad (7)$$

This is the solution we choose for the following reason, which we explain for simplicity for the case  $M(q) = 1$ . The classical equation

$$\ddot{q} = \frac{\partial V}{\partial q}$$

is invariant under time translations  $\tau \rightarrow \tau + \text{const}$ . The operator of the fluctuation equation or second variational derivative of the action  $S$  at the classical configuration  $q_c$  must therefore possess a zero eigenvalue with eigenfunction  $dq_c/d\tau$ . This operator is also obtained by differentiating the classical equation and implies the fluctuation equation

$$\left( \frac{d^2}{d\tau^2} - V''(q_c) \right) \psi_i = \omega_i^2 \psi_i.$$

If  $q_c$  is the constant  $q_s$ , and if this is a saddle point, we must have (at and around  $q_s$ )  $\omega_1^2 = 0$ ,  $\psi_1$  odd (the first excited state), and  $\omega_0^2 < 0$ , and  $\psi_0$  even (the ground state). Thus in this case,  $\psi_0$  is proportional to  $\cos(\omega_0 \tau)$ . This explains our ansatz (7), which is the component of a general fluctuation in the direction of the negative eigenmode of the fluctuation equation. The fluctuation equation for the case  $M(q) \neq \text{const}$  has been discussed in Ref. 10.

For the solution in the next order of perturbation theory we set

$$\eta(\tau) = a \cos(\omega \tau) + a^2 \eta_1(\tau), \quad \omega^2 = \omega_0^2 + a \Delta_1 \omega^2. \quad (8)$$

We insert this again into Eq. (5) and retain only terms up to and including those of  $O(a^2)$ . Also we reexpress powers of  $\cos(\omega \tau)$  in terms of  $\cos(n\omega \tau)$ , where  $n$  is an integer and use Eq. (6). Then

$$\begin{aligned} & a^2 \left[ M(q_s) \frac{d^2}{d\tau^2} - V''(q_s) \right] \eta_1(\tau) \\ & = a^2 \Delta_1 \omega^2 M(q_s) \cos(\omega_0 \tau) \\ & + a^2 \left[ \frac{\omega^2 M'(q_s) + V'''(q_s)}{4} \right. \\ & \left. + \left( \frac{3\omega^3 M'(q_s)}{4} + \frac{V''''(q_s)}{4} \right) \cos(2\omega_0 \tau) \right]. \end{aligned} \quad (9)$$

We now expand the fluctuation  $\eta_1(\tau)$  in terms of lowest-order functions, i.e., we set

$$\eta_1(\tau) = \sum_{n=0,1,2,\dots} c_n \cos(n\omega_0 \tau)$$

and use the orthonormality of the latter, i.e.,

$$\int_{-P/2}^{P/2} \cos(m\omega_0 \tau) \cos(n\omega_0 \tau) d\tau = \frac{P}{2} \delta_{mn}, \quad P = \frac{2\pi}{\omega_0}.$$

The remaining steps are standard in perturbation theory. Thus, multiplying Eq. (9) by  $\cos(\omega_0 \tau)$  and integrating one obtains immediately that

$$\Delta_1 \omega^2 = 0$$

and the fluctuation  $\eta_1(\tau)$  is obtained to be

$$\eta_1(\tau) = g_1 + g_2 \cos(2\omega_0\tau), \tag{10}$$

with

$$g_1(\omega) = -\frac{\omega^2 M'(q_s) + V'''(q_s)}{4V''(q_s)},$$

$$g_2(\omega) = -\frac{3M'(q_s)\omega^2 + V'''(q_s)}{4[4M(q_s)\omega_0^2 + V''(q_s)]}, \tag{11}$$

where in these first-order expressions  $\omega^2 = \omega_0^2$ . Thus, in order to obtain a nonvanishing deviation from the sphaleron value, we have to proceed to the next order of perturbation theory. Hence we set

$$\eta(\tau) = a \cos(\omega\tau) + a^2 \eta_1(\tau) + a^3 \eta_2(\tau),$$

$$\omega^2 = \omega_0^2 + a\Delta_1\omega^2 + a^2\Delta_2\omega^2, \tag{12}$$

and insert this into Eq. (5) and expand up to and including terms of  $O(a^3)$ . The procedure is the same as before but the calculations are now much more involved, so that we can only cite a main intermediate result. The equation corresponding to Eq. (9) above and multiplied by  $\cos(\omega_0\tau)$  and integrated over yields the equation

$$-aM(q_s)a^2\Delta_2\omega^2\frac{P}{2}$$

$$= a^3 \left[ V'''(q_s) \left( \frac{g_1}{2} + \frac{g_2}{4} \right) P + \frac{1}{6} V''''(q_s) \frac{3}{8} P \right.$$

$$+ 4M'(q_s)\omega^2 g_{2\frac{P}{4}} + M'(q_s)\omega^2 \left( \frac{g_1}{2} + \frac{g_2}{4} \right) P$$

$$\left. + \frac{1}{2} M''(q_s)\omega^2 \frac{3}{8} P - 2M'(q_s)\omega^2 g_{2\frac{P}{4}} - \frac{1}{2} M''(q_s)\omega^2 \frac{P}{8} \right]. \tag{13}$$

From this the condition of a first-order phase transition, i.e.,  $\Delta_2\omega^2 > 0$ , becomes

$$\left[ V'''(q_s) \left( g_1 + \frac{g_2}{2} \right) + \frac{1}{8} V''''(q_s) + M'(q_s)\omega^2 g_2 \right.$$

$$\left. + M'(q_s)\omega^2 \left( g_1 + \frac{g_2}{2} \right) + \frac{1}{4} M''(q_s)\omega^2 \right]_{\omega_0} < 0. \tag{14}$$

The first two terms of the expression on the left can be seen to be contained in the appropriate formula of Ref. 2 [their Eq. (31)], where  $M = \text{const}$ .

### III. APPLICATION OF THE CRITERION TO VARIOUS MODELS

In the following we focus our interest on the criterion for a first-order transition in various model theories and not on the physical contexts of these theories. We therefore do not elaborate on the latter that are discussed in the appropriate sources cited.

#### 1. Spin tunneling model with variable mass but without applied magnetic field

In Ref. 3 a large-spin tunneling model was considered in which

$$M(\phi) = \frac{1}{2K_1(1-\lambda \sin^2 \phi)}, \quad V[\phi] = K_2 s(s+1) \sin^2 \phi. \tag{15}$$

Thus, identifying  $\phi$  with our previous coordinate  $q$ , we have

$$\phi_s = \frac{\pi}{2}, \quad V[\phi_s] = K_2 s(s+1), \quad V'[\phi_s] = 0,$$

$$V''[\phi_s] = -2K_2 s(s+1), \quad V'''[\phi_s] = 0,$$

$$V''''[\phi_s] = 8K_2 s(s+1),$$

and

$$M[\phi_s] = \frac{1}{2K_1(1-\lambda)},$$

$$M'[\phi_s] = 0, \quad M''[\phi_s] = -\frac{\lambda}{K_1(1-\lambda)^2}.$$

From Eq. (3) we then obtain

$$\omega_0^2 = 4K_1 K_2 s(s+1)(1-\lambda). \tag{16}$$

It follows that  $g_1 = 0$ ,  $g_2 = 0$ , and Eq. (14) becomes

$$K_2 s(s+1) + \left( -\frac{\lambda}{K_1} \right) \frac{1}{(1-\lambda)^2} K_1 K_2 s(s+1)(1-\lambda) < 0,$$

i.e.,

$$\lambda > \frac{1}{2}. \tag{17}$$

This is precisely the condition found heuristically in Ref. 3 for the existence of a first-order transition in the model. The result implies, of course, the necessity of a significant field dependence of the effective mass to generate the first-order transition. In the next model this effect is produced by an applied magnetic field.

#### 2. Spin tunneling model with constant mass and applied magnetic field

In Ref. 6 a large-spin tunneling case was considered in which (in our present notation)

$$M = \text{const}, \quad V[\phi] = (s + \frac{1}{2})^2 D (h_x^2 \sinh^2 \phi - 2h_x \cosh \phi). \tag{18}$$

Here  $h_x = H_x / (2s + 1)D$ , where  $H_x$  is the magnetic field applied in the direction of coordinate  $x$ , which in our notation is also  $\phi \equiv x$ . In this case one finds

$$\phi_s = 0, \quad V[\phi_s] = -2(s + \frac{1}{2})^2 D h_x, \quad V'[\phi_s] = 0,$$

$$V''[\phi_s] = -2(s + \frac{1}{2})^2 h_x (1 - h_x), \quad V'''[\phi_s] = 0,$$

$$V''''[\phi_s] = 2(s + \frac{1}{2})^2 D h_x (4h_x - 1),$$

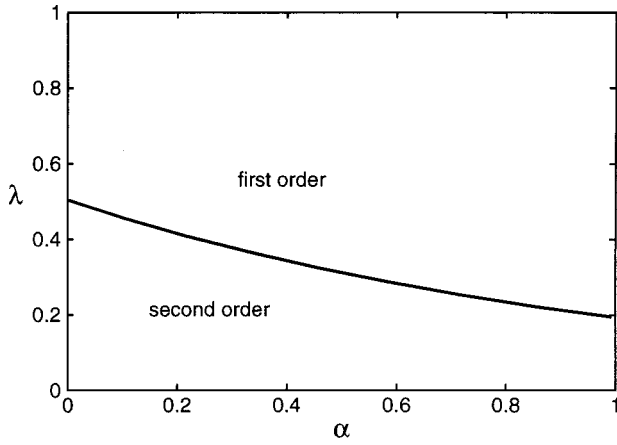


FIG. 2. The parameter domains for first- and second-order transitions through the large barrier in the spin tunneling model with field-dependent mass and field transverse to the easy axis.

and

$$M = M, M' = M'' = 0.$$

Then from Eq. (3),

$$\omega_0^2 = \frac{2}{M} (s + \frac{1}{2})^2 h_x (1 - h_x) \quad (19)$$

and  $g_1 = 0, g_2 = 0$  and the inequality (14) becomes

$$\frac{1}{8} \times 2 (s + \frac{1}{2})^2 D h_x (4 h_x - 1) < 0,$$

and hence

$$h_x < \frac{1}{4}, \quad (20)$$

as found in Ref. 6, there expressed as  $H_x < sD/2$ .

### 3. Spin tunneling model with variable mass and applied transverse magnetic field

In Ref. 4 another and more complicated spin tunneling model was investigated in which the magnetic field is applied in a direction transverse to that of the easy axis and the potential has the shape of a periodically recurring asymmetric twin barrier (i.e., a large one followed by a small one) with

$$M(\phi) = \frac{1}{2K(1 - \lambda \sin^2 \phi + \alpha \lambda \sin \phi)},$$

$$V[\phi] = K\lambda s^2 (\sin \phi - \alpha)^2. \quad (21)$$

In this case we have to distinguish between transitions in the large barrier and those in the small barrier. We therefore consider these separately.

(i) *Large barrier transitions.* In this case the sphaleron angle is (superscript  $L$  referring to the large barrier)

$$\phi_s^L = \frac{3}{2} \pi$$

and there

$$V[\phi_s^L] = K\lambda s^2 (1 + \alpha)^2, \quad V'[\phi_s^L] = 0,$$

$$V''[\phi_s^L] = -2K\lambda s^2 (1 + \alpha),$$

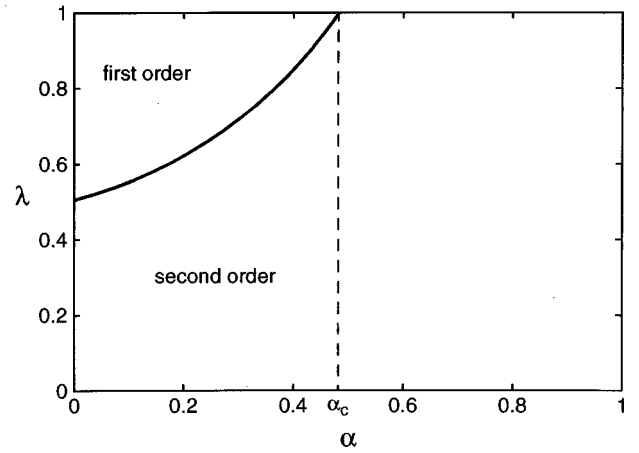


FIG. 3. The parameter domains for first- and second-order transitions through the small barrier in the spin tunneling model with field-dependent mass and field transverse to the easy axis.

$$V'''[\phi_s^L] = 0, \quad V''''[\phi_s^L] = 2K\lambda s^2 (4 + \alpha)$$

and

$$M(\phi_s^L) = \frac{1}{2K[1 - \lambda(1 + \alpha)]}, \quad M'(\phi_s^L) = 0,$$

$$M''(\phi_s^L) = -\frac{\lambda}{2K} \frac{(2 + \alpha)}{[1 - \lambda(1 + \alpha)]^2}.$$

In this case we obtain with Eq. (3),

$$\omega_0^2 = 4K^2 \lambda s^2 (1 + \alpha) [1 - \lambda(1 + \alpha)]. \quad (22)$$

Again  $g_1 = 0, g_2 = 0$  and the condition for a first-order phase transition is found to be

$$\lambda > \frac{\alpha + 4}{(\alpha + 1)(3\alpha + 8)}. \quad (23)$$

The parameter domains for first- and second-order transitions through the large barrier are shown in Fig. 2.

(ii) *Small barrier transitions.* In the case of transitions through the small barrier we have  $\phi_s^S = \pi/2$  and

$$V[\phi_s^S] = K\lambda s^2 (1 - \alpha)^2, \quad V'[\phi_s^S] = 0,$$

$$V''[\phi_s^S] = -2K\lambda s^2 (1 - \alpha),$$

$$V'''[\phi_s^S] = 0, \quad V''''[\phi_s^S] = 2K\lambda s^2 (4 - \alpha),$$

and

$$M(\phi_s^S) = \frac{1}{2K[1 - \lambda(1 - \alpha)]}, \quad M'(\phi_s^S) = 0,$$

$$M''(\phi_s^S) = -\frac{\lambda}{2K} \frac{(2 - \alpha)}{[1 - \lambda(1 - \alpha)]^2}.$$

From Eq. (3) we find

$$\omega_0^2 = 4K^2 \lambda s^2 (1 - \alpha) [1 - \lambda(1 - \alpha)]. \quad (24)$$

Again  $g_1 = 0, g_2 = 0$  and the condition for a first-order transition through the small barrier is found to be

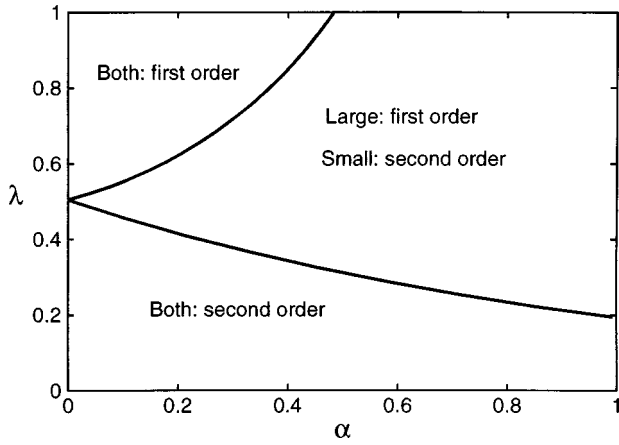


FIG. 4. The parameter domains for first- and second-order transitions in the model with field-dependent mass and transverse magnetic field.

$$\lambda > \frac{4 - \alpha}{(8 - 3\alpha)(1 - \alpha)}. \quad (25)$$

The parameter domains for first- and second-order transitions through the small barrier are shown in Fig. 3. The parameter domains for transitions through either barrier are shown in Fig. 4.

#### 4. Spin tunneling model with variable mass and applied longitudinal field

In Ref. 7 yet another model was investigated in which the applied magnetic field assumes a longitudinal, i.e., parallel, direction with respect to the easy axis. In this case it is also possible to find explicit classical configurations,<sup>11</sup> but we do not consider these here. In this model,<sup>7</sup>

$$M(\phi) = \frac{1}{2K_1 \left(1 - \lambda \sin^2 \phi - \frac{\alpha\lambda}{2} \cos \phi\right)},$$

$$V[\phi] = K_2 s^2 (\sin^2 \phi + \alpha \cos \phi + \alpha). \quad (26)$$

In this case the sphaleron value of  $\phi$  is  $\phi_s = \arccos \alpha/2$  and

$$V[\phi_s] = K_2 s^2 \left(1 + \alpha + \frac{\alpha^2}{4}\right), \quad V'[\phi_s] = 0,$$

$$V''[\phi_s] = -K_2 s^2 \left(2 - \frac{\alpha^2}{2}\right),$$

$$V'''[\phi_s] = -3K_2 s^2 \alpha \left(1 - \frac{\alpha^2}{4}\right)^{1/2},$$

$$V''''[\phi_s] = K_2 s^2 \left(8 - \frac{7}{2}\alpha^2\right),$$

and

$$M(\phi_s) = \frac{1}{2K_1(1-\lambda)}, \quad M'(\phi_s) = \frac{\lambda}{4K_1} \frac{\alpha \left(1 - \frac{\alpha^2}{4}\right)^{1/2}}{(1-\lambda)^2},$$

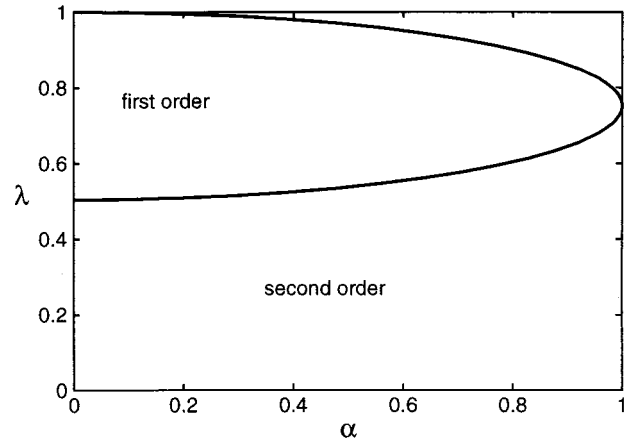


FIG. 5. The parameter domains for first- and second-order phase transitions in the model with applied longitudinal field.

$$M''(\phi_s) = \frac{\lambda}{2K_1} \frac{\left(\frac{3}{4}\alpha^2 - 2\right)(1-\lambda) + \frac{\alpha^2\lambda}{2} \left(1 - \frac{\alpha^2}{4}\right)}{(1-\lambda)^3}.$$

In this case,

$$\omega_0^2 = 2K_1 K_2 s^2 (1-\lambda) \left(2 - \frac{\alpha^2}{2}\right). \quad (27)$$

The expressions for  $g_1$  and  $g_2$  are now found to be

$$g_1 = \frac{\alpha}{8 \left(1 - \frac{\alpha^2}{4}\right)^{1/2}} \left[ \frac{\lambda}{(1-\lambda)} \left(1 - \frac{\alpha^2}{4}\right) - 3 \right],$$

$$g_2 = - \frac{\alpha}{8 \left(1 - \frac{\alpha^2}{4}\right)^{1/2}} \left[ \frac{\lambda}{1-\lambda} \left(1 - \frac{\alpha^2}{4}\right) - 1 \right]. \quad (28)$$

The condition for a first-order phase transition is now more complicated in that it reduces to the inequality

$$\frac{3}{16} \alpha^2 \xi^2 - \xi + \left(1 + \frac{\alpha^2}{2}\right) < 0, \quad (29)$$

where

$$\xi = \frac{\lambda}{1-\lambda} \left(1 - \frac{\alpha^2}{4}\right).$$

Setting

$$\xi_{\pm} = \frac{8}{3\alpha^2} \left\{ 1 \pm \left[ 1 - \frac{3}{4}\alpha^2 \left(1 + \frac{\alpha^2}{2}\right) \right]^{1/2} \right\},$$

the inequality (29) is then  $\xi_- < \xi < \xi_+$ , which reduces to

$$\frac{\xi_-}{\xi_- + \left(1 - \frac{\alpha^2}{4}\right)} < \lambda < \frac{\xi_+}{\xi_+ + \left(1 - \frac{\alpha^2}{4}\right)}. \quad (30)$$

In Fig. 5 we plot the boundary separating the parameter domain of first-order transitions from that of second-order transitions.

#### IV. CONCLUSIONS

In the above we have derived a criterion for the parameter domains of first-order phase transitions for a wide class of quantum-mechanical tunneling models. By application to specific models that received attention recently, particularly in the discussion of the tunneling of large or macroscopic spins, we demonstrated the agreement of the prediction of the criterion with previous heuristically obtained results. We envisage that considerations like those presented above and

in Ref. 2 can be useful in wider contexts, and also in field-theory models, such as those with Skyrme terms that imply an effective field-dependent mass.

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