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Failure of the WKB approximation in calculations of soliton free energies

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The authors examine the accuracy of the WKB approximation used in previous work to compute soliton free energies at low temperatures; this examination is crucial in establishing the validity of a simple physical phenomenology as an alternative to the transfer-operator method of calculation. For the ϕ^4 and double sine-Gordon potentials a method developed by Goldstein (1929) is adapted which is known to give correct results in the sine-Gordon case. For all three potentials, the WKB approximation is in error by the factor $(e/\pi)^{1/2}$.

I. INTRODUCTION

The importance of nonlinear wave equations which admit "kinklike" or solitary wave (soliton) solutions has stimulated much current research in both particle and solid-state physics. The results described below were obtained in connection with soliton solutions to the equations of motion for one-dimensional (1-D) atomic chains with nonlinear on-site potentials, and are a direct outgrowth not of the dynamics of individual solitons, but of the statistical behavior of solitons in determining the thermodynamics of the system as a whole.

Since the Krumhansl and Schrieffer pioneering paper[1] [for a ϕ^4 potential, $V(\phi)=(1-\phi^2)^2$, see Fig. 1] on soliton thermodynamics, the subject has been studied extensively. Gupta and Sutherland[2] have considered the case of a general periodic potential, with special emphasis on the sine-Gordon (SG) example [$V(\phi)=2(1+\cos\phi)$, see Fig. 2(a)]; Guyer and Miller have recently made a detailed study of the sine-Gordon system in both equilibrium[3] and nonequilibrium[4] regimes. Currie, Fogel, and Palmer, in a comment[5] on the paper by Gupta and Sutherland, found the soliton component of the sine-Gordon free energy as $T\rightarrow 0$ via a WKB approximation which, it turns out, is only $(e/\pi)^{1/2} \simeq 0.93$ as large as the accepted value,[6] which is traceable to a paper[7] by Goldstein; known numerical results confirm Goldstein's formula and thereby cast doubt on the validity of WKB as used to compute soliton free energies in the cases of ϕ^4 and other potentials. In pursuing this point we have found that the ratio of WKB to Goldstein tunnel-splitting for both ϕ^4 and for double sine-Gordon [$V(\phi)=4(\cos(\frac{1}{2}\phi)-\alpha)^2$, $0<\alpha<1$, see Fig. 2(b)], is also given by $(e/\pi)^{1/2}$. [Neuberger[8] has found disagreement by the same factor of $(e/\pi)^{1/2}$ between the WKB bandwidth of the sine-Gordon quantum pendulum and the exact result.] Gildener and Patrascioiu[9-11] have used path integrals and quadratic (as opposed to standard WKB) joining formulas to obtain the ϕ^4 tunnel splitting and noticed the same $(e/\pi)^{1/2}$ discrepancy for weak tunneling, while Furry[12] has used a method more like ours and has found, for a harmonic oscillator with unsplit energy level indexed by n, that the ratio at the potential minimum of the magnitude of the standard WKB wave function to that obtained from phase integrals is $(e/\pi)^{1/2}g(n)$, where $g(0)=1$. Banerjec and Bhatnagar[13] show that the formula obtained for splitting via the methods of Gildener and Patrascioiu,[9-11] Furry,[12] and ourselves[14] agrees much better with actual numerical results than does WKB.

Our discovery of the WKB breakdown was brought about by the important role played by what amount to tunneling calculations in the statistical mechanics of classical 1-D chains. The free energy as computed *ab initio* by transfer integral techniques[1-5] is simply the lowest eigenvalue of

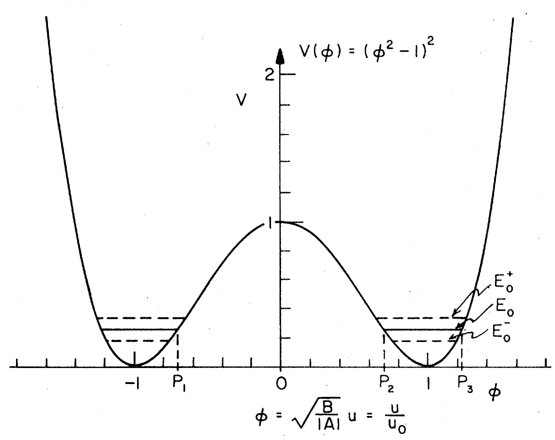

FIG. 1. Double-well dimensionless on-site potential $V(\phi)=(\phi^2-1)^2$. P_1, P_2, and P_3 are the three right-most classical turning points for the single well ground-state energy $E_0 \simeq (2m^*)^{-1/2}$ (denoted by solid line); m^*, the effective mass, goes as T^{-2}. Dotted lines denote energies E_0^+ and E_0^- of states split from this ground state; heights of all levels greatly exaggerated, since $T\rightarrow 0$.

an effective Schrödinger equation whose potential is just the on-site potential of the particular nonlinear system under consideration. Because each of the on-site potentials so far treated has more than one potential well, the lowest eigenvalue F (which is the configurational free energy) is given by

$$F = E_0 - t_0 , \qquad (1)$$

where for low temperatures E_0 is essentially the lowest harmonic oscillator level of an individual well and $2t_0$ is the tunnel splitting between wells, which gives two new slightly shifted eigenvalues centered about E_0. A phenomenological calculation[1,15] (in which each soliton is treated as a particle in an "ideal gas" of kinks), shows the t_0 term to be due to the solitons, and the WKB method is of course the logical first choice for the computation of t_0.

The WKB breakdown was first noted by Currie *et al.*,[15] in connection with SG tunneling; even after corrections were made to account for the periodicity of the wave functions corresponding to the tunneling eigenvalues, the WKB result was found to be only $(e/\pi)^{1/2}$ as large as the result of Ref. 6. Ordinarily such a numerical discrepancy of order unity would be insignificant; in this case, however, the determination of the correct value is essential to achieving the basic goal of the study of statistical behavior of solitons, which is to show that the thermodynamic properties of these nonlinear kinks can be obtained from a relatively simple phenomenological model, which

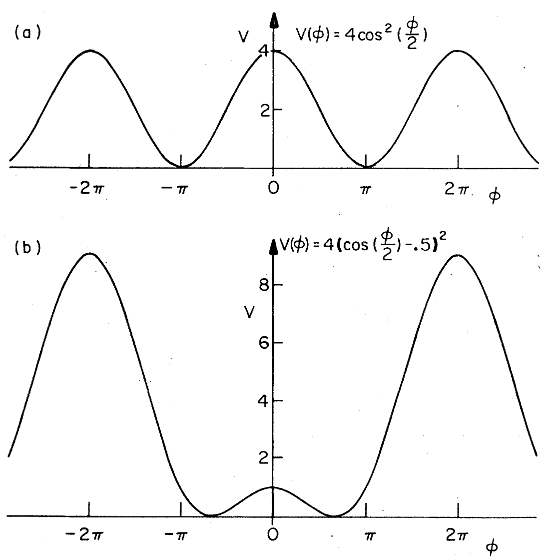

FIG. 2. Periodic soliton-bearing on-site potentials: (a) sine-Gordon, $V(\phi+2\pi)=V(\phi)=4\cos^2(\frac{1}{2}\phi)=2(1+\cos\phi)$; (b) double sine-Gordon, $V(\phi+4\pi)=V(\phi)=4[\cos(\frac{1}{2}\phi)-\alpha]^2$; here $\alpha = 0.5$.

would provide considerable insight into the physics of the system.

The starting point for the model is the fact that a kink's energy $E_k(v)$ as a function of velocity v can be straightforwardly computed via substitution of the soliton waveform into the Hamiltonian density of the atomic chain.[5] This knowledge of $E_k(v)$, along with the introduction of a chemical potential, enables one to obtain the partition function for a grand canonical ensemble of solitons thermally activated at temperature T; the calculation proceeds essentially as for a classical "relativistic" ideal gas.

The test of the model's validity is the comparison of the free energy given by it with the analytic *ab initio* value; this value depends on the results of what is mathematically a tunneling integral (even though no quantum mechanics is involved) for the particular on-site potential being considered. In computing this tunneling, however, problems arise; for it will be seen later that conditions for standard WKB to provide valid solutions to the effective Schrödinger equation are strongly violated in the wells of the potential for the low-temperature limit which we consider. We go on to show that this difficulty can be removed, and the correct numerical value for the tunnel splitting obtained, through the use, in the wells, of parabolic cylinder functions, which are especially accurate in the low-temperature domain.

For the potentials considered so far, the numerical prefactors of the phenomenological free energies agree with the correct prefactors calculated by the parabolic cylinder (Goldstein) formalism; herein lies the chief point of the paper, namely, that the free energy computed from a model of an ideal gas of solitons is precisely correct, which fact was hitherto obscured by the WKB method's merely approximate numerical prefactor. The results of the Goldstein method thus further strengthen the already firm foundation for the ideal gas concept.

Phenomenological treatments of three potentials (sine-Gordon,[15] ϕ^4,[15] and double quadratic[16] $[V(\phi) = \frac{1}{2}(1-|\phi|)^2]$ have now been completed; in each case, the ideal gas and *ab initio* (WKB tunneling) free energies agree to within a numerical factor of order unity. When the tunneling is calculated by the adaptation of Goldstein's method the agreement is exact, as the WKB numerical factors are multiplied by $(e/\pi)^{1/2}$ and then become small integers, which are explained[15] by phase-space modifications due to certain topological restrictions on the placement of kinks and antikinks on the chain. The Goldstein results, which agree much better than WKB with the numerics for ϕ^4 and SG, and are exact for double quadratic,[17] can be seen to put the ideal gas model on a much firmer footing than do the WKB results. In Sec. II we look more closely at the details and resolution of the disagreement between Goldstein and standard WKB approaches.

II. FORMALISM

The details and significance of WKB breakdown are best understood in the context of the formalism for a general soliton-bearing potential. The treatment is an elegant extension by Currie *et al.*[15] of the techniques used by Krumhansl and Schrieffer[1] on the ϕ^4 problem. The point of departure is the recognition that any on-site potential with two or more degenerate minima will give rise to soliton solutions for the atomic displacement. Application of this fact and appropriate boundary conditions enable one to compute the energy $E_k(v)$ carried by a soliton moving with speed v. In quantitative terms,

$$E_k(v)=E_k(0)[1-(v/v_0)^2]^{-1/2}\,, \qquad (2)$$

where v_0 is a limiting speed on the chain and $E_k(0)$ is the soliton rest energy, which appears in a Boltzmann factor in phenomenological expressions for the soliton free energy.

The tunneling contribution to the free energy arises from the potential energy (or configurational) partition function Z_ϕ, which is constructed in the standard manner from the continuumized Hamiltonian density $H(x)$ of the atomic chain[15]

$$H(x)=h\left[\frac{1}{2}A\left(\frac{\partial\phi}{\partial t}\right)^2+B_L V(\phi)+\frac{1}{2}C\left(\frac{\partial\phi}{\partial x}\right)^2\right], \qquad (3)$$

where h has units of energy/length, and where ϕ, B_L, and the entire expression in square brackets are dimensionless (ϕ is an atomic displacement, for example). Z_ϕ is then given, for N sites, by[1-3,15]

$$Z_\phi=\prod_{i=1}^{N}\int_{-\infty}^{\infty}d\tilde{\phi}_i\exp[-\beta hlf(\phi_i,\phi_{i+1})]\,, \qquad (4)$$

with l a discretization length, $\beta\equiv 1/k_BT$, $\tilde{\phi}_i$ a scaled multiple of ϕ_i, $\phi_{N+1}=\phi_1$, and

$$f(\phi_i,\phi_{i+1})=\tfrac{1}{2}(C/l^2)(\phi_{i+1}-\phi_i)^2+B_L V(\phi_{i+1})\,. \qquad (5)$$

The integration is effected by introducing an additional integration variable ϕ_1', and inserting

$$\delta(\phi_1'-\phi_1)=\sum_{n=0}^{\infty}\Psi_n^*(\phi_1')\Psi_n(\phi_1)\,, \qquad (6)$$

where the Ψ_n form a complete orthonormal set and satisfy[18] the transfer integral equation

$$\int_{-\infty}^{\infty}d\tilde{\phi}_i\,e^{-\beta hlf(\phi_i,\phi_{i+1})}\Psi_n(\phi_i)=e^{-\beta hl\epsilon_n}\Psi_n(\phi_{i+1})\,. \qquad (7)$$

This yields

$$Z_\phi=\sum_{n=0}^{\infty}e^{-\beta hL\epsilon_n}\,; \qquad (8)$$

hence the free energy per unit length is

$$F_\phi=-\frac{1}{\beta L}\ln Z_\phi\xrightarrow[L\to\infty]{}h\epsilon_0\,. \qquad (9)$$

(Here $L=Nl$ is the chain's total length.)

At low temperatures, the integrand in (7) is negligible unless ϕ_i and ϕ_{i+1} are sufficiently close together that $\Psi_n(\phi_i)$ can be accurately approximated by a second-order Taylor expansion about $\phi_i=\phi_{i+1}$. Such an expansion leads to the effective Schrödinger equation[15]

$$-\frac{1}{2m^*}\frac{d^2}{d\phi^2}\Psi_n(\phi)+B_L V(\phi)\Psi_n(\phi)=\epsilon_n\Psi_n(\phi)\,, \qquad (10)$$

with

$$m^*=h^2C\beta^2\,. \qquad (11)$$

Equation (9) shows that only the $n=0$ term (ground state) is relevant for free energy calculations.[1,2,15] The potentials that have been treated so far [ϕ^4 and SG, see Figs. 1 and 2(a)] are symmetric about the center of the hump between adjacent minima; their eigenstates therefore have definite parity, so that, in ϕ^4, for example, Ψ_0 is the even member of the pair of states resulting from the symmetric and antisymmetric combination of the essentially simple harmonic ground states within each individual well. This is a bit more subtle in the SG case, where the analogy is more properly to a 1-D band structure problem, although the fact that m^* is large keeps the situation fairly simple since we are then in the realm of "tight binding." The even and odd tunneling eigenvalues in this case represent the bottom and top, respectively, of the lowest-energy band, and the splitting between them is exponentially small. Specifically, if the Hamiltonian density for a chain of atoms with on-site SG potential is given by

$$H(x)=h\tau^2\left[\frac{1}{2}\left(\frac{\partial\phi}{\partial t}\right)^2+\frac{1}{2}c_0^2\left(\frac{\partial\phi}{\partial x}\right)^2+\omega_0^2(1+\cos\phi)\right] \qquad (12)$$

(c_0 is the limiting velocity and τ a characteristic time), the soliton rest energy $E_k(0)$ is given by

$$E_k(0)=8h\tau^2\omega_0c_0\,, \qquad (13)$$

and the effective Schrödinger equation (10) becomes, in the notation of Goldstein,[7]

$$\frac{d^2y}{dx^2} - k^2(\cos^2 x)y + (2n+1)ky = 0\,. \tag{14}$$

Here $x = \frac{1}{2}\phi$, $y = y(x) \equiv \Psi_n(\phi)$, and $k = \frac{1}{2}\beta E_k(0)$, so that $\epsilon_n = (4\omega_0^2\tau^2/k)\ (n+\frac{1}{2})$; we are in the limit $T \to 0$ $(k \to \infty)$, so that n is an almost integral quantity given by $n = m + (a_n/k)$, where m is an integer corresponding to the mth essentially harmonic oscillator state of a single well and where a_n/k (equivalent to $A/2k$ in Ref. 19) is the exponentially small tunnel splitting within the mth band for the state indexed by n.

If the differences in ϵ_n and a_n between the top and bottom of the lowest band are given, respectively, by $\Delta\epsilon(0)$ and $\Delta a(0)$, a relation following (14) gives

$$\Delta\epsilon(0) = [4(\omega_0\tau)^2/k^2]\Delta a(0)\,, \tag{15}$$

from which the soliton free energy $\frac{1}{2}h\Delta\epsilon(0)$ (Ref. 1 and 15) follows immediately upon determination of $\Delta a(0)$. Explicitly, the bandwidth is [Eq. (23) in Sec. 3 of Ref. 7]

$$\Delta\epsilon(0) \simeq 2^5(2/\pi)^{1/2}(\omega_0\tau)^2[\beta E_k(0)]^{-1/2}e^{-\beta E_k(0)}\,, \tag{16a}$$

which is $(\pi/e)^{1/2}$ times as large as the standard WKB result

$$[\Delta\epsilon(0)]_{\rm WKB} \simeq (2^5/\pi)(2e)^{1/2}(\omega_0\tau)^2 \times [\beta E_k(0)]^{-1/2}e^{-\beta E_k(0)}\,. \tag{16b}$$

{In the *Handbook of Mathematical Functions*, the effective Schrödinger equation is cast in the form[20]

$$\frac{d^2y}{dx^2} + [A_0 - 2q\cos(2x)]\,y = 0\,, \tag{17}$$

so that q corresponds to $\frac{1}{4}k^2$ in Goldstein's and $\frac{1}{16}[\beta E_k(0)]^2$ in our notation; the expression[6] in this reference for the bandwidth corresponds to our $2\Delta a(0)$, and therefore gives the same value for $\Delta\epsilon(0)$ as does Goldstein.}

The WKB tunneling value can thus be corrected by a very minor adjustment, which yields exact agreement between the SG *ab initio* and phenomenological calculations. Consideration of the main features of Goldstein's method suggests that it should be generalizable, and shows why it is more accurate then WKB in the limit $T \to 0$ (so that $m^* \to \infty$ in the effective Schrödinger equation).

The most prominent feature of the Goldstein method (GM) is the use of parabolic cylinder functions to approximate the wave function in the wells (allowed region). This derives from the fact that, as $m^* \to \infty$ and the individual well's ground state thereby becomes more and more deeply bound, any of a wide class of potentials becomes more and more quadratic in an appropriate dimensionless variable centered on the well minimum.[21] Parabolic cylinder functions of proper index are exact solutions over a region where the potential is purely quadratic, so that the GM approximation gets better as m^* gets larger. The WKB value, on the other hand, is increasingly suspect as $m^* \to \infty$; this is because WKB can be relied on only when the rate of change of de Broglie wavelength with distance is much less than 2π, which condition is increasingly violated as the bound state becomes deeper. These points are especially emphasized by Furry,[12] and by Morse and Feshbach[21] when they deal with application of the WKB approximation to the "case of closely spaced classical turning points."

We have extended the GM to the calculation of tunnel splitting for the ϕ^4 and double-sine-Gordon potentials. This extension is actually a triple hybrid combining the logical systematization of Morse and Feshbach with the mathematical simplicity of Goldstein, while retaining the standard WKB functions where they are accurate. The formalism[14] used most closely resembles, but was developed independently of, that of Furry[12]; it also goes beyond Ref. 12 by treating periodic potentials. For the purposes of this paper, however, our method is best explained by example, which we now give in the form of an outline of the ϕ^4 calculation.

III. GENERALIZATION OF THE GOLDSTEIN METHOD

It turns out that the GM can be extended quite readily to ϕ^4, and that once again the WKB expression is $(e/\pi)^{1/2}$ times that of the GM; specifically, with the ϕ^4 Hamiltonian density given by

$$H(x) = h\left\{\frac{2m}{Bu_0^2}\left[\left(\frac{\partial\phi}{\partial t}\right)^2 + c_0^2\left(\frac{\partial\phi}{\partial x}\right)^2\right] + (\phi^2-1)^2\right\}, \tag{18}$$

the soliton free energy per unit length is given by the GM as

$$F_{\rm tunn} = -ht_0 \equiv F_{\rm GM} = -4\left(\frac{2}{3\pi}\right)^{1/2}\left(\frac{|A|^2}{Bl}\right) \times\left(\frac{k_BT}{E_k(0)}\right)^{1/2}\exp\left(\frac{-E_k(0)}{k_BT}\right)\,, \tag{19}$$

while the WKB free-energy density is $F_{\rm WKB} = (e/\pi)^{1/2}F_{\rm GM}$. [Our notation in Eqs. (18) and (19) follows Krumhansl and Schrieffer,[1] so that the potential (see Fig. 1) is $A^2/(4B) + \frac{1}{2}Au^2 + \frac{1}{4}Bu^4$ $(A<0)$, $u = \pm(|A|/B)^{1/2} = \pm u_0$ are the locations of the degenerate minima $(\phi \equiv u/u_0)$, c_0 is the limiting velocity, l is the discretization length, and $h = Bu_0^4/4l$ is the scale of energy density. The kink rest energy is $E_k(0) = (2\sqrt{2}/3)(|A|^3mc_0^2)^{1/2}/(Bl)$.]

To proceed with the calculation we first connect (18) with the notation of Eq. (3). Thus

$$C = 4mc_0^2/Bu_0^2,\quad B_L V(\phi) = (\phi^2-1)^2\,, \tag{20a}$$

so that

$$m^* = h^2 C\beta^2 = \beta^2 (u_0/l)^2 (\tfrac{1}{2}Bu_0^4)(\tfrac{1}{2}mc_0^2) . \quad (20b)$$

If we now define $\alpha \equiv 2^{5/4} m^{*1/4}$ and $z \equiv \alpha(\phi - 1)$ (z is thus centered on the minimum of the right-hand well), the effective Schrödinger equation

$$-\frac{1}{2m^*}\frac{d^2\Psi_n(\phi)}{d\phi^2} + (\phi^2 - 1)^2 \Psi_n(\phi) = \epsilon_n \Psi_n(\phi) \quad (21a)$$

becomes

$$-\frac{d^2\Psi_n(z)}{dz^2} + \frac{1}{4} z^2 \left(1 + \frac{z}{2\alpha}\right)^2 \Psi_n(z) = \left(\frac{\alpha^2 \epsilon_n}{16}\right)\Psi_n(z) , \quad (21b)$$

or, since $\alpha \to +\infty$ as $m^* \to 0$, we have roughly for the ground state (dropping subscripts)

$$\frac{d^2\Psi}{dz^2} - \frac{1}{4} z^2 \Psi + \left(a + \frac{1}{2}\right)\Psi = 0 \quad \left(a + \frac{1}{2} = \frac{\alpha^2 \epsilon_n}{16}\right) ; \quad (21c)$$

$\frac{1}{2}$ is the ground-state harmonic oscillator eigenvalue for one well, while a represents, to zeroth order in $1/\alpha$, the exponentially small shift in the eigenvalue due to tunneling. This approach thus neglects the anharmonic corrections for an individual well, and concentrates on the splitting arising from the tunneling between wells; details dealing with such subtler points and their mathematical justification will be found in Ref. 14.

Before continuing it is best to define some terms and functions which occur repeatedly in the subsequent analysis:

$$U(z) = \tfrac{1}{4} z^2 (1 + z/2\alpha)^2 \quad (22a)$$

is simply the potential in (21b):

$$b_{\rm I} \equiv -2\alpha + \sqrt{2} , \quad b_{\rm II} \equiv -\sqrt{2} , \quad b_{\rm III} \equiv +\sqrt{2} ; \quad (22b)$$

to zeroth order in $1/\alpha$ these are the three rightmost values of z for which $U(z) = \frac{1}{2}$. They correspond to classical turning points of the motion (see Fig. 1).

For $b_{\rm I} < z < b_{\rm II}$, the imaginary wave number $\kappa(z)$ will be approximated by

$$\kappa(z) \equiv [U(z) - \tfrac{1}{2}]^{1/2} ; \quad (22c)$$

finally, we also define, within the hump $b_{\rm I} < z < b_{\rm II}$, the function $K(z)$:

$$K(z) \equiv \int_{z'=z}^{b_{\rm II}} \kappa(z')\, dz' , \quad (22d)$$

so that the tunneling integral is (to order α^{-1})

$$K \equiv K(b_{\rm I}) = -\tfrac{1}{2}[1 + \ln 24 + \ln\beta E_k(0) - 2\beta E_k(0)] . \quad (22e)$$

We begin by noting that deep within the hump WKB is valid, so that the two independent solutions $\Psi^{\pm}(z)$ are well approximated by WKB functions, i.e.,

$$\Psi^{\pm}(z) = \mp \kappa^{-1/2}(z) e^{\pm K(z)} . \quad (23)$$

WKB is in particular adequate in the region $-\alpha \ll z \ll -\sqrt{2}$, where $\kappa(z) \simeq (\frac{1}{4}z^2 - \frac{1}{2})^{1/2}$; with this approximation the integral $K(z)$ takes on a simple form, and is equal to[12]

$$K(z) = \tfrac{1}{4} z^2 (1 - 2/z^2)^{1/2} - \tfrac{1}{2}\ln\{|z| + |z|[1 - (2/z^2)]^{1/2}\} + \tfrac{1}{4}\ln 2 . \quad (24a)$$

(We obtain $|z|$ since $z < 0$ in the hump.) When expanded to sufficient accuracy in $1/|z|$, $K(z)$ reduces to[12]

$$K(z) = \tfrac{1}{4} z^2 - \tfrac{1}{2}\ln|z| - \tfrac{1}{4}(1 + \ln 2) . \quad (24b)$$

Since $\kappa^{-1/2}(z) \simeq 2^{1/2}(-z)^{-1/2}$, we obtain

$$\Psi^{\pm}(z) = \mp 2^{1/2}(2)^{\mp 1/4} e^{\mp 1/4} (-z)^{-1/2 \mp 1/2} \exp(\pm\tfrac{1}{4}z^2) \quad (25)$$

for the forms of the hump functions which must be joined to the two independent solutions within the right-hand well, $b_{\rm II} < z < b_{\rm III}$. (Parity enables us to find the eigenvalues without dealing with the left-hand well.)

Within the right-hand well, then [and for all z such that $|z| \ll \alpha$, so that $U(z)$ remains essentially quadratic], the solution $\Psi(z)$ will be approximated very well by a linear combination of the parabolic cylinder functions[7] (pcf's) $D_a(-z)$ and $D_{-(1+a)}(-iz)$. In the region $-\alpha \ll z \ll -\sqrt{2}$, where we will match them to the WKB's, the pcf's assume the asymptotic forms[7]

$$D_a(-z) \simeq (-z)^a \exp(-\tfrac{1}{4}z^2) \simeq \exp(-\tfrac{1}{4}z^2) \quad (26a)$$

and

$$D_{-(1+a)}(-iz) \simeq \{\exp[-\tfrac{1}{2}(1+a)\pi i]\} \times (-z)^{-(1+a)} \exp(\tfrac{1}{4}z^2) \simeq -i(-z)^{-1}\exp(\tfrac{1}{4}z^2) . \quad (26b)$$

{a[see Eq. (32)] goes as e^{-K}, where K [see Eqs. (22)] is equal to $\frac{1}{4}\alpha^2 I$; here $I = \frac{2}{3} - (2/\alpha^2)(1 + \ln 8 + \ln\alpha^2)$ which is of order unity for large α. Therefore, $|z| \ll \alpha$ implies that $\ln[(-z)^a]$ is smaller than $e^{-K}\ln\alpha$, which goes to 0 as $\alpha \to \infty$; thus in this limit, $(-z)^a \simeq 1$.} This gives the following connections from the hump into the well:

$$\Psi^-(z) \to 2q_0^{-1} D_a(-z) \quad (27a)$$

and

$$\Psi^+(z) \to -iq_0 D_{-(1+a)}(-iz) - A_0 D_a(-z) , \quad (27b)$$

where $q_0 = 2^{1/4} e^{-1/4}$ and where A_0 is an arbitrary constant much less than e^K reflecting the fact that the asymptotic form for Ψ^+, which is dominated by the exponentially large function $D_{-(1+a)}(-iz)$, may also contain an exponentially small component.

The form of the solution for $z>0$, $\sqrt{2}\ll z\ll\alpha$, is determined via the formulas[7]

$$D_a(-z)=e^{a\pi i}D_a(z)-[\sqrt{2\pi}/\Gamma(-a)]\times e^{-(1-a)\pi i/2}D_{-(1+a)}(iz) \tag{28a}$$

and

$$D_{-(1+a)}(-iz)=-e^{a\pi i}D_{-(1+a)}(iz)+[\sqrt{2\pi}/\Gamma(1+a)]e^{a\pi i/2}D_a(z)\,, \tag{28b}$$

where $\Gamma(x)$ is the gamma function. Now the tunnel splitting $a\sim\exp(-K)\ll 1$, so that $1/\Gamma(-a)\simeq -a$ and Eqs. (28) become

$$D_a(-z)\simeq D_a(z)-i\sqrt{2\pi}\,aD_{-(1+a)}(iz) \tag{29a}$$

and

$$D_{-(1+a)}(-iz)\simeq -D_{-(1+a)}(iz)+\sqrt{2\pi}\,D_a(z)\,. \tag{29b}$$

The symmetric nature of the ϕ^4 potential demands that the ground-state solution $\Psi(z)$ have zero derivative at the center of the hump ($z=-\alpha$), so that

$$\Psi(z)=\Psi^+(z)-e^K\Psi^-(z) \tag{30}$$

is an unnormalized solution to (21b); Eqs. (27) and (29) now combine to give the form of the wavefunction in the region $0<z\ll\alpha$ as

$$\begin{aligned}\Psi(z)&\simeq i(q_0+\sqrt{2\pi}A_0a+2\sqrt{2\pi}q_0^{-1}ae^K)D_{-(1+a)}(iz)\\&\quad-(2q_0^{-1}e^K+A_0+\sqrt{2\pi}iq_0)D_a(z)\\&\simeq i(q_0+2\sqrt{2\pi}q_0^{-1}ae^K)D_{-(1+a)}(iz)\\&\quad-[2q_0^{-1}e^K]D_a(z)\,.\end{aligned} \tag{31}$$

As was seen in Eq. (26), $D_a(z)$ decreases exponentially while $D_{-(1+a)}(iz)$ increases exponentially for large z, so that the coefficient of $D_{-(1+a)}(iz)$ must vanish for $\Psi(z)$ to be well behaved as $z\to+\infty$. This requirement gives

$$a=-\tfrac{1}{2}\pi^{-1/2}e^{-1/2}e^{-K}\,; \tag{32}$$

the odd state (tunnel split from the ground state) will be shifted by an amount $a_{\text{odd}}=|a|$, so that the tunnel splitting $2t_0=a_{\text{odd}}-a$ is equal to

$$2t_0=(\pi e)^{-1/2}e^{-K}\,, \tag{33}$$

or just $(\pi/e)^{1/2}$ times the standard WKB value.[22] [θ, $\hbar^2/2m$, and $m\omega^2$ in Ref. 22 are equal, respectively, to e^{-K}, 1, and $\frac{1}{2}$ in our Eq. (21c).]

The above example hopefully gives a fairly clear idea of how our method works. In recent work on soliton statistical mechanics, we have applied to the double-sine-Gordon potential an extension of the procedure outlined above, which generalization constitutes a formalism for handling a wide class of periodic potentials. A detailed treatment of the statistical mechanics of the double-sine-Gordon system will be the subject of a later paper; here we give the results of tunneling calculations via our method and WKB. For this doubly periodic system, the Hamiltonian density $H(x)$ breaks the symmetry of that in Eq. (12) for the sine-Gordon case, and thus gives rise to the interesting feature of two different kinds of solitons. The explicit form of $H(x)$ is

$$H(x)=h\tau^2\left\{\frac{1}{2}\left(\frac{\partial\phi}{\partial t}\right)^2+\frac{1}{2}c_0^2\left(\frac{\partial\phi}{\partial x}\right)^2+2\omega_0^2\left[\cos\left(\frac{\phi}{2}\right)-\cos x_0\right]^2\right\}, \tag{34}$$

which reduces to the SG case when $x_0=\frac{1}{2}\pi$.

The effective Schrödinger equation is now

$$-\frac{1}{2m^*}\frac{d^2\Psi}{d\phi^2}+2(\omega_0\tau)^2\left[\cos\left(\frac{\phi}{2}\right)-\cos x_0\right]^2\Psi=\epsilon\Psi\,, \tag{35}$$

where $m^*=\beta^2h^2c_0^2\tau^2$, $\beta=1/k_BT$.

The double structure [see Fig. 2(b)] gives two tunneling integrals, so that each type of soliton contributes to the free energy. Through the generalized GM we obtain the following expression for the soliton free energy density F, valid for a fairly wide range of x_0 (Ref. 14):

$$F/h\equiv F_{\text{GM}}/h=-t_0=-(4/\sqrt{\pi})(\sin x_0)^{5/2}\times(k_BT/E_0)^{1/2}(e^{-\beta E_1(0)}+e^{-\beta E_2(0)})\,, \tag{36}$$

where $E_0=hc_0/\omega_0^3\tau^2$ is essentially a weighted average of $E_1(0)$ and $E_2(0)$, which are the rest energies for solitons spanning the smaller and larger hump, respectively. Once again, the WKB free energy is related to the correct expression F_{GM} by[14]

$$F_{\text{WKB}}=(e/\pi)^{1/2}F_{\text{GM}}\,. \tag{37}$$

IV. SUMMARY

Phenomenological calculations[15] for very-low-temperature soliton statistical mechanics have recently reached a stage such that they agree with the analytic functional integral results in all temperature dependence and differ only by numerical factors. In comparing the values obtained by these two approaches, it is therefore important that the numerical factor for the analytic calculation be computed correctly. For this purpose we have extended the technique of Goldstein, which gives accurate values for the sine-Gordon case, to both the ϕ^4 and double-sine-Gordon potentials;

in all three cases the ratio of the WKB to the Goldstein splitting is $(e/\pi)^{1/2}$.[23]

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[23]This result turns out to hold for a wide class of potentials (Refs. 12 and 14).