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Dissipative Tunnelling in a Sine-Gordon Chain at High Temperatures.

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Abstract. – The dissipative tunnelling in a sine-Gordon chain driven by a weak external bias is investigated with special focus on the quantum-mechanical effects at higher temperatures where thermal activation still dominates over quantum tunnelling. Quantum-mechanical corrections to the nucleation process enhance the rate above its classical value for any intensity of the damping mechanism. However, contrary to the single-particle case, quantum effects enter the result for the nucleation rate in lowest order in \hbar , instead of \hbar^2 , and it exhibits a nonanalytic dependence on the quantum scale.

The dynamics of a sine-Gordon (SG) chain provides a conventional picture for a variety of phenomena taking place in condensed matter, *e.g.*, dislocations in crystals, charge density waves in Peierls dielectrics and tunnelling in long Josephson junctions. A problem of crucial relevance is the nucleation of soliton-antisoliton pairs driven by an external d.c.-bias field which breaks the symmetry of the SG potential. Whatever the circumstances of the nucleation process, a chain sitting in a trough of the tilted SG potential generates a soliton-antisoliton pair only after an appreciable portion of it (critical nucleus) has overcome the potential barrier which separates two adjacent troughs. The energy associated with such unstable configuration is the activation energy of the process.

The calculation of the relevant nucleation rate Γ (defined as the number of pairs created per unit of length and time) has been carried out under diverse physical conditions and approximations:

i) *Classical regime.* In ref. [1-6] the nucleation rate Γ has been determined under the assumption that the damping constant is much larger than any other characteristic frequency of the system. The temperature is taken high enough to neglect quantum-mechanical contributions, while thermal fluctuations per unit of length are always assumed to be much smaller than the activation energy. The critical nucleus grows to infinity for

vanishingly weak external biases. The interaction among nucleating pairs may not be disregarded in such a limit [3-5].

ii) *Quantum-mechanical regime.* In this case one distinguishes two threshold temperatures, T_0 and T_c . For $T < T_0$ the critical nuclei are separated and have their *temporal* dependence determined mainly by their intrinsic width, whereas for $T > T_0$ the critical nuclei coalesce and the temporal scale $\hbar\beta$ strongly affects their dynamics. The exponential factor of the nucleation rate has been determined in this temperature regime for both vanishingly small damping [6-9] and very large damping [7, 8]. For $T > T_c$, the shape of the nucleus solution ceases to possess a temporal dependence. At $T > T_c$ the thermal activation dominates the exponential factor of Γ with quantum-mechanical corrections affecting the prefactor only. A complete account of dissipation effects proved a difficult task: in ref. [9] the prefactor of Γ has been determined at zero damping, whereas the treatment of ref. [6-8] is only viable for calculating the exponential factors.

In the present letter we outline new analytical results for the *dissipative* nucleation rate in a SG chain at thermal equilibrium, restricted, for the time being, to the case of high temperatures $T > T_c$. Corrections due to the presence of both quantum-mechanical and dissipative effects are determined explicitly in the limit of very small external bias.

For the sake of convenience we adopt notations of ref. [9]. In dimensionless units, the unperturbed, undamped SG equation reads

$$\phi_{tt} - \phi_{xx} + \frac{\pi}{4} \sin \pi\phi = 0 \quad (1)$$

and admits of static localized solutions

$$\phi_{\pm} = \frac{2}{\pi} \operatorname{tg}^{-1} \exp \left[\pm \frac{\pi}{2} (x - x_0) \right], \quad (2)$$

with arbitrary centre of mass x_0 and classical energy $E_0 = 2\alpha = 4/\pi$. ϕ_{\pm} are termed soliton and antisoliton, respectively. For the quantization of the nonlinear-field theory we follow the standard scheme [10], *i.e.* in the quantum case the normal product of the SG potential $U[\phi] = 1/4 : \cos \pi\phi :$ is understood in order to regularize the ultraviolet divergence [10]. For the following, the quantity $\gamma \equiv [U''(0)]^{1/2} = \pi/2$ is the so-called plasma frequency.

The dissipative SG chain is described by the equation

$$\phi_{tt} - \phi_{xx} + \frac{\pi}{4} \sin \pi\phi = -F - \eta\phi_t. \quad (3)$$

The phenomenological Ohmic friction term $-\eta\phi_t$ is equivalent in our treatment to the effective dissipation arising from coupling the chain to a heat bath of bilinearly coupled oscillators [7, 8, 11]. The d.c.-field F must be smaller than $U[0] - U[1] = 1/2$, in order for localized solutions to exist. Moreover, throughout this report, F is assumed to be sufficiently small, so that the F -dependence of the quantum-mechanical corrections is negligible. For this reason, following ref. [9], we use $F = 0$ whenever a finite value of F would lead to a mere next-to-leading order correction. The effects of the external bias on the activation energy and the prefactor of the nucleation rate have been determined explicitly for the classical limit in ref. [3] and [4].

For temperatures above the critical value T_c (which depends here on the dissipation η , see eq. (8)), the nucleation rate can be calculated in terms of the imaginary part of the relevant free energy [3, 12, 13] per unit of length, $\operatorname{Im} \mathcal{F}$, according to the formula [14],

$\Gamma = -(2T_c/T) \text{Im } \mathcal{F}$. By use of dimensionless quantities including the dimensionless time [9], the nucleation rate can be written as

$$\Gamma(\eta) = T_c(\eta) \left(\frac{2\alpha g}{\pi T} \right)^{1/2} R(T, \eta) \exp \left[-\frac{4\alpha g}{T} - \frac{b}{T} \right], \quad (4)$$

where T and g are *dimensionless quantities proportional to $(\hbar)^{-1}$* .

Before we proceed, we should comment on the regime of validity of eq. (4). By use of the $\text{Im } \mathcal{F}$ approach one implicitly neglects nonequilibrium kinetics which, in principle, is of importance in the weak-friction regime [15, 16]. In contrast to a zero-friction study [9], however, in the presence of moderate-to-strong dissipation η , eq. (4) yields the physically correct nucleation rate. In this regime, nonequilibrium kinetics does not affect the rate and, furthermore, the dissipative rate coincides with a multidimensional transition state theory (TST) in full phase space of all degrees of freedom of system plus environment [16]. Presently, there is no chance to work out a dynamical theory for the underdamped regime, $\eta \rightarrow 0$, of a nonlinear metastable field problem. Thus far, even the simple case of a single particle moving classically in a finite-dimensional metastable potential has not been entirely solved [16]. From this viewpoint our explicit results in the weak-friction regime given below, as well as the zero-friction study in ref. [9], must be interpreted as the TST-estimate to the true nucleation rate, *i.e.* in the underdamped regime the given results present a truly upper limit to the physical nucleation rate.

The contribution b/T in the exponential function of eq. (4) denotes the divergent counter-term generated by the normal product, and cancels the ultraviolet divergence inherent in the prefactor $R(T, \eta)$. The prefactor $R(T, \eta)$ is defined as

$$R(T, \eta) = \left| \frac{\det O^0}{\det' O^N} \right|^{1/2}, \quad (5)$$

where $\det' O^N$ omits the zero eigenvalues,

$$O^0 = -\frac{\partial^2}{\partial \tau^2} - i\eta \frac{\partial}{\partial \tau} - \frac{\partial^2}{\partial x^2} + \gamma^2 \quad \text{and} \quad O^N = -\frac{\partial^2}{\partial \tau^2} - i\eta \frac{\partial}{\partial \tau} - \frac{\partial^2}{\partial x^2} + U''[\phi_N].$$

$\phi_N(x)$ denotes the critical nucleus. In the limit of a weak field, $F \ll 1/2$, $\phi_N(x)$ is approximated with a linear superposition of a soliton and an antisoliton placed at the relative distance $(2\gamma)^{-1} \ln(16\gamma^2/\pi^2 F)$ [2-4, 6]. The eigenvalues $\{\lambda^{N,0}\}$ of the operators $\{O^{N,0}\}$ can be ordered as follows:

$$\lambda_m^{N,0}(n) = (2\pi T n)^2 + (2\pi T |n|) \eta + S_m^{N,0}, \quad n = 0, \pm 1, \pm 2, \dots, \quad (6)$$

where $S_m^{N,0}$ denote the small-amplitude fluctuation modes about the critical nucleus, $\phi_N(x)$, and the solitonless configuration, $\phi_0(x) = 0$, respectively. The part $\{S_m^0\}$ of the spectrum is purely continuous, *i.e.* $S_m^0 \equiv S_k^0 = \gamma^2 + k^2$. On the other hand, the fluctuations about the critical nucleus $\phi_N(x)$ allow for three discrete eigenvalues λ_m^N ($n = 0$) = S_m^N , $m = 0, 1, 2$; and a continuum. There exist a negative eigenvalue (the unstable mode)

$$\lambda_0^N(0) = S_0^N = -(2\pi T_c^*)^2, \quad T_c^* = \frac{1}{\pi} \left(\frac{\gamma F}{2\alpha} \right)^{1/2}, \quad (7)$$

one zero eigenvalue $S_1^N = 0$ (the so-called Goldstone mode) and only one further discrete mode, $S_2^N > 0$, which for vanishingly small F merges into the continuous spectrum $S_2^N \rightarrow S_k^N = \gamma^2 + k^2$. The negative eigenvalue $\lambda_0^N(0)$ is linear in F , thus implying that the decay process is driven right by the external bias, *i.e.* by the mechanism which breaks the symmetry $\phi \rightarrow -\phi$ of the system. The F -dependence of the remainder of the spectra $\{\lambda^{N,0}\}$ only yields next-to-leading order corrections which we agreed to neglect on the first place. In particular, we set $S_2^N = \gamma^2$ and ignore the F -dependence of the density of states for $O^{N,0}$. Thus the dependence on the potential asymmetry $F\phi$ enters our results only through the parameter $T_c^* = T_c(\eta = 0)$. $T_c(\eta)$ is determined by the condition that there exists only one unstable mode, $\lambda_0^N(0) < 0$. From the inequality $\lambda_0^N(1) \geq 0$ we obtain for the crossover temperature $T_c(\eta)$ from $\lambda_0^N(1) = 0$ the result

$$T_c(\eta) = \frac{1}{2\pi} \left[-\frac{\eta}{2} + \sqrt{\left(\frac{\eta}{2}\right)^2 + |S_\delta^N|} \right]. \tag{8}$$

The zero eigenvalue $\lambda_1^N(0)$ is omitted in $\det' O^N$ and has been taken care of separately in the prefactor of (4).

On replacing $\det O^{N,0}$ with the product of the relevant eigenvalues (6), and working out the product over the discrete index n , explicitly, we arrive at much simpler an expression for $R(T, \eta)$, *i.e.*

$$R(T, \eta) = \frac{\prod_{m=0}^{\infty} (S_m^O)^{1/2} \prod_{n=0}^{\infty} \Gamma[1 - n_+^N(n)] \Gamma[1 - n_-^N(n)]}{\prod_{n=0, \neq 1}^{\infty} |S_n^N|^{1/2} \prod_{m=0}^{\infty} \Gamma[1 - n_+^O(m)] \Gamma[1 - n_-^O(m)]}, \tag{9}$$

where the indices in the products run over both the discrete and the continuum branches of the corresponding spectra of the operators $O^{N,0}$, and

$$n_{\pm}^{N,0}(m) = \frac{1}{2\pi T} \left[-\frac{\eta}{2} \pm \sqrt{\left(\frac{\eta}{2}\right)^2 - S_m^{N,0}} \right]. \tag{10}$$

Next, remembering that $S_1^N = 0$ and S_2^N may be approximated by γ^2 , we finally obtain after some cumbersome algebra

$$R(T, \eta) = \Gamma\left(1 + \frac{\eta}{2\pi T}\right) |S_\delta^N|^{-1/2} \Gamma[1 - n_+^N(0)] \Gamma[1 - n_-^N(0)] \cdot \exp \left[\int_0^\infty dk [\rho_O(k) - \rho_N(k)] \left(\frac{1}{2} \ln S_k - \ln \Gamma[1 - n_+(k)] - \ln \Gamma[1 - n_-(k)] \right) \right], \tag{11}$$

$\rho_{N,0}(k)$ denote here the density of states $\{S_m^{N,0}\}$, $S_k = \gamma^2 + k^2$ and $n_{\pm}(k)$ are as in (10) after replacing $S_m^{N,0}$ with S_k . Further explicit calculations have been carried out on making use of the relation [10] $\rho_O(k) - \rho_N(k) = 2/S_k$.

As a first check on our general result (11) we see immediately that both limiting cases for $\hbar = 0$ and for $\eta = 0$ are reproduced correctly. In the *classical regime* ($\hbar = 0$), the regularization counterterm $\frac{b}{T} \equiv \frac{1}{T} \int_0^\infty dk S_k^{1/2}$ is identically zero, $R(T, \eta) = \pi/2T_c^*$, whence

from eq. (4)

$$\Gamma_{cl}(\eta) = \frac{T_c(\eta)}{T_c^*} \left(\frac{\pi\alpha g}{2T} \right)^{1/2} \exp \left[-\frac{4\alpha g}{T} \right], \quad T \gg T_c. \quad (12)$$

In the overdamped limit, $\eta \gg \gamma$, (12) reduces to the relevant result of ref. [3], see eq. (21) therein, provided that one approximates the activation energy $2E_N(F)$ to $2E_0 = 4\alpha$, as agreed above.

In the *quantum-mechanical zero-friction case* ($\eta = 0$, $\hbar \neq 0$) our determination for Γ coincides with Ivlev and Melnikov's, see eq. (40) of ref. [9]. Taking the limit of that result for $1/T \rightarrow 0$ yields

$$\Gamma(0) = \Gamma_{cl}(0) \exp \left[\frac{1}{T} \ln T + \frac{I_1}{T} \right], \quad (13)$$

where $I_1 \approx 1.65$.

In the *underdamped case* ($\eta \ll \gamma$, $\hbar \neq 0$) dissipation effects on the quantum-mechanical corrections to $\Gamma_{cl}(\eta)$ show up at the order η/T . Indeed, on expanding the factor $R(T, \eta)$, eq. (11), in powers of η , we obtain

$$\Gamma(\eta) \approx \Gamma(0) \exp \left[-\frac{\eta}{T} I_2 \right], \quad (14)$$

where $\Gamma(0)$ is given in eq. (13) and $I_2 = \frac{1}{2} \sum_{n=1}^{\infty} (1/n \sqrt{n^2 + \gamma^2})$, which for $\gamma = \pi/2$ yields $I_2 \approx 0.54$. The validity of eq. (14) is restricted by the conditions that $\eta \ll \gamma$ and $|S_0^N|^{1/2} \ll T$.

In the *overdamped case* ($\eta \gg \gamma$, $\hbar \neq 0$), instead, the quantum corrections enhance the rate (13), *i.e.*

$$\Gamma(\eta) \approx \Gamma_{cl}(\eta) \left(\frac{\eta}{2\pi T} \right)^{(\pi/2-1)/2\gamma T}, \quad (15)$$

which with $\hbar \rightarrow 0$ exhibits a nonanalytical dependence on \hbar of the form $\hbar \ln \hbar$ ⁽¹⁾.

In conclusion, the quantum effects on the sine-Gordon nucleation rate at high temperatures $T > T_c$ produce a series of interesting features. In the single-particle case quantum corrections to the classical expressions usually enter in order of \hbar^2 [17, 18], since the underlying quantum dynamics is governed by operation equations involving the quantity $i\hbar$. The \hbar -dependence inherent in eqs. (13)-(15) thus represents a nonanalytic dependence on the quantum scale.

Moreover, quantum-mechanical corrections in the presence of dissipation always enhance the nucleation rate above its classical value. This latter finding resembles the behaviour of the quantum corrections for a single particle [15, 16]. In particular, we remark that strong dissipation does suppress the tunnelling rate by lowering T_c , $T_c(\eta \rightarrow \infty) \rightarrow 0$, but also leads to a large *quantum* prefactor, as shown in eq. (15). These new results given here are also hoped to be of relevance in future experiments on extended Josephson-junction systems for which the quantum effects at finite temperatures may not be negligible.

(¹) Recall that T denotes a dimensionless temperature scale being proportional to $(\hbar)^{-1}$ [9].

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