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THERMAL NUCLEATION OF KINK-ANTIKINK PAIRS IN THE PRESENCE OF IMPURITIES: THE CASE OF A REMOISSENET-PEYRARD SUBSTRATE POTENTIAL

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Abstract

Thermal nucleation of kink-antikink pairs in a nonlinear Klein-Gordon (NKG) model with a Remoissenet-Peyrard (RP) substrate potential in the presence of impurities and coupled to an applied field is analyzed in the limits of moderate temperature and strong damping. Using the Kolmogorov method, the average velocity of particles of the lattice is calculated and its dependence on the intensity of impurities is discussed in connection with the deformability parameter or the shape of the RP substrate potential. Numerical values are carried out by making use of parameters of the hydrogen atom adsorbed in the tungsten and ruthenium substrates. We show that, for large values of the applied field, the presence of impurities in the system makes the nucleation process of kink-antikink pairs more favorable in the high-temperature regime while they contribute to make it less favorable in the low-temperature regime.

I. Introduction

Nucleation is generally defined as a phenomenon where a new phase appears locally in space. It is one of the most drastic phenomena in the various fields of physics, chemistry, biology, and also in engineering [1]. More precisely, the nucleation in condensed matter physics is most interesting in the sense that it can be controlled by parameters such as pressure, temperature, electric and magnetic fields and so on. One usually distinguishes homogeneous and heterogeneous nucleation. In the first case, embryos of a stable phase emerge from a matrix of a metastable parent phase due to spontaneous thermodynamic fluctuations. Droplets larger than a critical size will grow while smaller ones decay back to the metastable phase [2-4]. In the second case, random forces catalyze the transition by making growth energetically favorable [1].

The study of the nucleation connected to the formation of solitary structures in spatially one-dimensional (1D) and multistable systems is well developed theoretically [4-20], experimentally and numerically [21-25]. These studies offer the fundamental understanding of nucleation in homogeneous medium. More specifically, theoretical analysis of nucleation was introduced four decades ago by Seeger and Schiller [10] to describe the kinetic process of dislocation and few years later by Langer [4] to investigate the problem of reversing the direction of magnetization in a ferromagnetic system. The same ideas, but where the approach is closely related to the concepts already developed in the dislocation literature, were also developed by Büttiker and Landauer [16] to present a detailed calculation of the nucleation rate of thermal kink-antikink pairs in the over-damped sine-Gordon (SG) chain and by Yemélé and Kofané [5] to present the calculation of the nucleation rate of kink-antikink pairs in a driven and over-damped deformable chain. This theory was later improved by Marchesoni et al. [20] when analyzing the thermal nucleation of kink-antikink pairs in an elastic string.

The above studies deal with nucleation in homogeneous systems. However, most of the realistic physical systems possess impurities which may influence the nucleation process and disturb the newly formed kink-antikink pairs. Inhomogeneity may mean spatial modulation, quasiperiodicity, or disorder of several kinds. For example, local inhomogeneities (micro shunts and micro resistors) may be installed into the long Josephson junction during fabrication (see Ref. [26]). Neutron scattering experiments by Boucher et al. [27] on quasi-1D magnetic compounds (magnetic chains) which have revealed that the crossover from ballistic to diffusive behavior of soliton is driven by the impurity concentration, evidences the fact that these materials contain

impurities. In compounds whose electrical properties are due to the existence of charge density waves (CDW), that is, interacting electron-gas, impurities may also be present and represent the sites or atoms where electrical properties are different from those of the host atom; for example, Br disorder in $K_2Pt(CN)_4Br_{0.3}nH_2O$(KCP). In adatomic systems, impurities are also present due to the geometrical imperfections of the adsorbed surfaces which in general are at the origin of the spatial deformation of the nucleus, to name only a few.

The nucleation in condensed matter physics may be considered in the framework of the Frenkel-Kontorova (FK) model [28], which describes the behavior of an harmonic chain of atoms in the periodic substrate potential, known as the nonlinear Klein –Gordon (NKG) model with SG potential. This model can be generalized by considering another form of potential and by taking into account inhomogeneities in order to go beyond the mathematical problem and to obtain results that may be useful for real materials that undergo structural changes such as shape distortion, variations of crystalline structures or conformational changes in some regions of their physical parameters. By the way, the study of the effect of local inhomogeneity or single impurity on the nucleation in the case of CDW shows that the CDW can be pinned by an impurity if the external applied field is less than a threshold field [29]. Similarly, it has been demonstrated that the current carried by CDW may rise as a result of the increase in the rate of generation of solitons on fluctuations in random field of defects [30]. In quasi-1D magnetic compounds, it has also been shown that, stochastic motion of SG solitons in a random potential can be used to model their statistical properties. This random potential is generated by the presence of impurities and explains the observed crossover from the ballistic to the diffusive behavior of spin correlations [31]. Although these results are quite interesting, they are limited to the rigid substrate potential. Thus at this stage of research one may wonder what is the influence of the shape of the substrate potential on the nucleation process in these inhomogeneous systems. The answer to this question is the main objective of the present work. In this paper we focus our attention on the Remoissenet-Peyrard (RP) substrate potential whose shape can be varied continuously as a function of a deformability parameter and which has the sG shape as a particular case [32-33]. In addition, it can be successfully used to model the substrate potential along the surface of adsorbed layers in adatomic systems (see, e.g, Ref.[34] and references therein).

The organization of the paper is as follows: In Sec. 2, we present the generalized NKG model under consideration in the presence of impurities. In Sec. 3, we reformulate the basic results on the nucleation rate of kink-antikink pairs in the homogeneous system [5] by taking into account the non-Gaussian correction in the spirit of Marchesoni et al. [20]. In Sec. 4, we focus our attention on the influence of impurities on the nucleation rate of kink-antikink pairs. The mean time for a

transition of an arbitrary point on the chain to a neighboring valley of the Peierls distribution is calculated by means of the Kolmogorov method in order to obtain the mean velocity or average velocity of particles from one site to an adjacent one, due to the passing of kinks triggered by stochastic forces. In Sec. 5, experimental values of the lattice parameters for H/W and H/Ru adsystems are used as a numerical application to quantify the correction factor of the mean velocity of particles, due to the presence of impurities in the system. Finally, Sec. 6 is devoted to concluding remarks.

2. Model description

We consider a generalized NKG model describing the dynamics of a chain of particles in a periodic nonsinusoidal substrate potential in the presence of external forces and impurities. The dynamical behavior of the system is governed by the nonlinear Langevin equation (NLE)

$$Mu_{tt} - ku_{xx} + V_0 \frac{dV_{RP}(u,r)}{du} = -\gamma u_t + F + \zeta(x,t) - \frac{dV_{imp}(u)}{du}, \tag{1}$$

where u is the longitudinal dimensionless displacement of the particles from their equilibrium position along the x axis. The subscripts x and t denote the derivative with respect to space and time, respectively. V_0 is the amplitude of the substrate potential. The constant force F is related to the applied field f through the relation $F = f/2\pi$. To model the "on-site" potential $V_{RP}(u,r)$, we shall use the nonsinusoidal substrate potential introduced by Remoissenet and Peyrard [32,33]

$$V_{RP}(u,r) = (1-r)^2 \frac{1-\cos u}{1+r^2+2r\cos u}, \tag{2}$$

where r is the shape parameter, $|r| < 1$. As this parameter varies, the amplitude of the potential remains constant with degenerate minima $2\pi n$ and maxima $(2n+1)\pi$ while its shape changes. When $r > 0$, it has flat bottoms separated by thin barriers while for $r < 0$, it has the shape of sharp wells separated by flat wide barriers (see Fig. 1). At $r = 0$, the RP potential reduces to the well-known SG potential. This parameter depends on the physical characteristics of each system. For example, in quasi-1D compounds whose electrical properties are due to the existence of CDW, the substrate potential which corresponds to the interaction of CDW with the host atom may be calculated up to higher order of the perturbation theory. Up to the first order of this perturbation theory, we obtain the SG potential which is a good approximation only in the weak-and strong coupling cases. Thus, at higher order, in addition to the first harmonic which describes the sG potential, one also obtains the second, third and higher harmonics [35]. The compact form of this interaction between CDW and host atoms may then be approximated by the RP-type function where

the parameter describing the shape of the substrate potential depends on the amplitude of the CDW gap, the Fermi velocity and the quasi-particle energy. Similarly, for the adatomic systems, the parameter r of the substrate potential is related to the frequency ω_0 of oscillation of an isolated adatom at the bottom of the adsorption site, the adatom mass m_a and the period a_s of the substrate potential [36]; more precisely, $r = (1-\kappa)/(1+\kappa)$, with $\kappa = \omega_0(a_s/2\pi)(2m_a/V_0)^{1/2}$. Note that the above parameters for the adatomic systems are related to the characteristic parameters of the system described by the NLE (1).

The coupling of the scalar field $u(x,t)$ to the heat bath at absolute temperature T is described by a viscous term $-\gamma u_t$ and a zero-mean Gaussian noise source $\zeta(x,t)$. At Boltzmann equilibrium, the damping constant $\gamma = M\gamma_0$, where γ_0 corresponds to the rate of the energy exchange with the substrate, and the noise intensity are related through the fluctuation-dissipation relationship

$$<\zeta(x,t)\zeta(x',t')>= 2k_B T\gamma\delta(x-x')\delta(t-t'). \quad (3)$$

Finally, the last term of the NLE (1), $V_{imp}(u)$, is the potential energy density of impurities and its analytical expression depends on the nature of these impurities since various types of impurities may exist such as the local variations of masses of particles, of elastic constants and of substrate potential barriers, respectively. It has been shown that in the presence of impurities, the nonlinear waves may be trapped, reflected or transmitted with more or less distortion of their structure according to the intensity of the impurities [37,38]. We assume here that impurities are randomly distributed in the system and then cause the deformation of any spatially localized structure as a main effect. A simple realization of the proposed model is obtained by considering the following analytical expression

$$V_{imp}(u) = V_f(x)\frac{\partial u}{\partial x}, \quad (4)$$

where $V_f(x)$ is a random function of the spatial coordinate. Thus, the quantity $dV_{imp}(u)/du$ in the NLE (1) is then equal to $dV_f(x)/dx$. In addition, we restrict our analysis to the case where impurities are weak and where their mean separation is less than the characteristic length of the system (or the size of kink solitons), $\xi_0 = \left(k/V_0\right)^{1/2}$, which enables us to describe the statistical properties of this random field by

$$<V_f(x)V_f(x')>_V = \chi\delta(x-x'), \quad (5)$$

with zero-mean ($< V_f(x) >_V = 0$), where χ describes the intensity of impurities and $< ... >_V$ denotes the average over the different realizations of the random potential $V_f(x)$. Note also that the expression (4) can be successfully used to describe forward scattering of CDW in the quasi-1D compounds whose electrical properties are due to the existence of CDW [30]. In the next sections, we shall have occasion to use the Hamiltonian derived from the NLE (1) which is given by

$$H = \int \frac{dx}{a} \left\{ \frac{M}{2} u_t^2 + \frac{k}{2} u_x^2 + V_0 V_{RP}(u,r) - Fu + V_{imp}(u) \right\}, \tag{6}$$

where a is the lattice constant. In this expression, since u is the dimensionless displacement of particles, the parameters M, k and V_0 have the dimension of (mass)x(length), (energy)x(length), and (energy)(length)$^{-1}$, respectively.

Before ending this section, we would like to mention that the NLE (1) with the Hamiltonian (6) is well known as the generalized NKG model. This NKG model has been successfully used in investigations of a number of physical phenomena such as CDW, adsorbed layers of atoms, domain walls in ferromagnetic and antiferromagnetic systems, crowdions in metals, and hydrogen-bonded systems (see, e.g., the review paper in [39] and references therein for applications of the NKG model). The use of the RP potential as a substrate potential is justified by the fact that it can be invoked to describe a large amount of physical systems. As a result, an appropriate choice of the shape parameter enables us to employ a suitable form of the shape of the potential close to the system under consideration such as epitaxial or incommensurate structure [36] in crystals and other various systems.

3. Nucleation of kink-antikink pairs in the homogeneous system

The dynamics of the pure system obtained from the NLE (1) by setting its right hand side equal to zero is dominated by elementary excitations: phonons and solitons (kink and antikink). While phonons are extended modes of the system, solitons are localized modes and may be viewed as effective particles characterized by a mass and an energy. In a number of situations, kink dynamics may be described by equations of its collective coordinates, namely the kink center of mass. If one assumes periodic boundary conditions on the chain of length L, $u(x,t) = u(x+L,t)$, kinks are only present as a result of thermal activation. These thermal kinks are created in pairs involving a kink and an antikink. On the other hand, if the system is not subjected to periodic boundary conditions or in other words, if the ends of the string are free, the so-called “geometric” solitons of the same sign appear in the system. Characteristic parameters of kink solitons in the pure

system governed by the NLE (1) are well known [5]. For example, the pseudo-kink width d, the static kink (antikink) energy (E_s), and the rest mass (M_s) are given by

$$d^{(1)} = \xi_0/\alpha,\ d^{(2)} = \xi_0\alpha\,, \quad \alpha = \frac{1-|r|}{1+|r|}, \tag{7.a}$$

$$E_s^{(\ell)} = 8(kV_0)^{1/2} G^{(\ell)}(\mathrm{r}),\ M_s^{(\ell)} = (8/\zeta_0) G^{(\ell)}(r), \tag{7.b}$$

with $\ell = 1, 2$, and

$$G^{(\ell)}(r) = \alpha/\alpha_* \tanh^{-1}\alpha_*,\ G^{(2)}(r) = \alpha_* \tan^{-1}(\alpha_*/\alpha),\ \alpha_* = \sqrt{1-\alpha^2}\,, \tag{7.c}$$

where the superscripts ($\ell = 1$) and ($\ell = 2$) stand for $0 \le r < 1$ and $-1 < r \le 0$, respectively, and ξ_0 designates the characteristic length of the system. For $r = 0$, the above equations reduce to those of the usual sG kink soliton.

In the presence of the applied field, the total on-site potential energy given by

$$V(u,F) = V_0 V_{RP}(u,r) - Fu\,, \tag{8}$$

is the sum of the substrate potential energy $V_0 V_{RP}(u,r)$ and the energy due to the applied field $-Fu$. The minima (u_{sn}) and the maxima (u_{in}) of the above on-site potential energy (8) which are known as Peierls valleys and Peierls hills, respectively, are different from those of the substrate potential energy and may disappear if the applied field F is greater than the threshold value F_m [5]

$$F_m/V_0 = \frac{2\sqrt{2}\alpha^2\left[(3\alpha^2-1)+\sqrt{\Delta}\right]\sqrt{\sqrt{\Delta}-3(1-\alpha^2)}}{\left(5\alpha^2-3+\sqrt{\Delta}\right)}, \tag{9}$$

with $\Delta = 9\alpha^4 - 14\alpha^2 + 9$. This means that kink solutions of the NLE (1) can only exist if $F << F_m$. Note that these Peierls valleys and Peierls hills obey $dV(u,F)/du = 0$. More specifically, the NLE (1) describing the configuration of the nucleus in a pure system may also be viewed as the equation of motion of a classical "particle" with mass "k", time "x" in a potential $-V(u,F)$, where $V(u,F)$ is given by Eq.(8). The critical nucleus of amplitude Δu_m will be a configuration which deviated only in a localized region from the uniform state u_{sn} followed by the motion to the right until the turning-point $u_{sn} + \Delta u_m$ is reached. Then, the particle again returns asymptotically to the local maxima at u_{sn}. The corresponding stationary solution of the NLE (1) is the saddle-point configuration or the critical nucleus which departs from the stationary uniform state u_{sn} at $x = \pm\infty$. Its amplitude Δu_m strongly depends on the applied field. Furthermore, Δu_m decreases monotonically with respect to F: $\Delta u_m = 2\pi$ for $F = 0$ and $\Delta u_m = 0$ for $F = F_m$. The transition between two adjacent Peierls valleys due to thermal fluctuations called critical nucleus are the

newly formed kink-antikink pairs, whose size depends on the applied field F. This transition is possible only if the fluctuations produce, within the system, a minimum of energy $\Delta E_N >> k_B T$ necessary to create a critical nucleus $u_N(x, X)$, where X designates the position of the newly formed kink which in the continuum limit is linearly time dependent, that is, $X(t) = X_0 + \mathrm{v}t$, X_0 being the critical initial position of the kink center of mass and v the kink velocity. For $F << F_m$, the nucleus $u_N(x, X)$ can be well approximated by the linear superposition of a kink and an antikink centered at $\pm X$, respectively, that is,

$$u_N(x, X) = u_+(x + X, 0) + u_-(x - X, 0), \tag{10}$$

where the solutions $u_\pm(x,t)$ satisfies the NLE (1) without the right hand side.

In the overdamped limit $(\gamma >> V_0^{1/2})$, where the inertial term (Mu_{tt}) is neglected, the substitution of Eq.(10) into the NLE (1) in the absence of the impurity leads to the following equation for the nucleus

$$\frac{dR}{dt} = -\frac{dV_N^{(\ell)}}{dR} + \eta_R(t), \tag{11}$$

with the reduced coordinate $R = 2X$, where the potential of the critical nucleus is given by

$$V_N^{(\ell)}(R) = -\frac{2\pi F}{\gamma M_s^{(\ell)}} R - \frac{4E_s^{(\ell)} \upsilon^{(\ell)}}{\gamma M_s^{(\ell)}} e^{-|R|/d^{(\ell)}}, \tag{12}$$

with

$$\upsilon^{(1)} = \alpha_* \frac{\exp(-2\alpha_* \tanh^{-1}\alpha_*)}{\alpha^2 \tanh^{-1}\alpha_*}, \quad \upsilon^{(2)} = \alpha\alpha_* \frac{\exp[2(\alpha_*/\alpha)\tan^{-1}(\alpha_*/\alpha)]}{\tan^{-1}(\alpha_*/\alpha)}. \tag{13}$$

The noise $\eta_R(t)$, associated with Eq.(11) for the nucleus, verifies the following fluctuation-dissipation relationship

$$<\eta_R(t)\eta_R(t')> = 2\gamma^2 D_R^{(\ell)} \delta(t - t'), \quad D_R^{(\ell)} = \frac{2k_B T}{\gamma M_s^{(\ell)}}. \tag{14}$$

Following the procedure outlined in Ref.[20] useful for the calculation of the nucleation rate of kink-antikink pairs, it is necessary to determine the size of the critical nucleus $R_N^{(\ell)}$ and the negative eigenvalue $\lambda_0^{N(\ell)}$ of the non-uniform state. Thus, the nucleus size is set by the condition that $V_N^{(\ell)'}(R)\big|_{R_N} = 0$, leading to

$$R_N^{(\ell)} = d^{(\ell)} \ln\left[\frac{2E_s^{(\ell)}\upsilon^{(\ell)}}{\pi F d^{(\ell)}}\right], \tag{15}$$

and the negative eigenvalue of the non-uniform state, which is the eigenvalue of the RP scattering

potential in the presence of the applied field defined as $[d^2V(u,F)/d^2u]_{u_N}/[d^2V(u,F)/du^2]_{u_{sn}}$, is given by

$$\lambda_0^{N(\ell)} = \left.\frac{d^2V_N^{(\ell)}(R)}{dR^2}\right|_{R_N} = -\frac{2\pi F}{\gamma M_s^{(\ell)} d^{(\ell)}}. \tag{16}$$

In the limit where the shape parameter $r \to 0$, Eq.(13) reduces to 1 and then, Eq. (16) reduces to that obtained for the sG systems.

With the results above stated, in the Gaussian approximation, the improved formula of the number of kink-antikink pairs per unit time and length is then given by

$$\tilde{J}_0^{(\ell)} = \Omega^{(\ell)} K^{(\ell)}(F) \exp\left(-\beta \Delta E_N^{(\ell)}\right), \tag{17}$$

with $\beta = 1/k_B T$, and the prefactor

$$\Omega^{(\ell)} = \left(\frac{\Gamma}{2\pi}\right)^{3/2} \left(\frac{\gamma}{k}\right)^{1/2} \left(\frac{\left|\lambda_0^{N(\ell)}\right|}{\Gamma}\right)^{1/2} \prod_{n>1}^{p-1} \left(\frac{\Gamma}{\lambda_n^{N(\ell)}}\right)^{1/2} \left(\frac{\Delta E_N^{(\ell)}}{k_B T}\right)^{1/2} (Q), \tag{18}$$

where $\lambda_n^{N(\ell)}$ are the eigenvalues of the non-uniform state, $\Gamma = (V_0/\gamma)[d^2V(u,F)/du^2]_{u_{sn}}$ and Q the product of the eigenvalues of the localized eigenmodes of the critical nucleus. In addition, p is the number of localized modes and strongly depends on the shape parameter r. In fact, when $r \geq 0$, the system possesses two bound states (p=2), with $\lambda_n^{N(\ell)} = 0$ and $\lambda_0^{N(\ell)}$, given by Eq.(16). More over, internal modes appear when r decreases from 0 to –1. For example, $p = 5$ for $r = -0.5$ and $p = 21$ for $r = -0.9$.

The non-Gaussian correction $K^{(\ell)}(F)$ to the nucleation rate formula of kink-antikink pairs obtained through the Gaussian approximation are given by [20]

$$K^{(\ell)}(F) = \int_{-\infty}^{\infty} \exp\left(-\frac{\left|\lambda_0^{N(\ell)}\right|}{2D_R^{(\ell)}} R^2\right) dR \Bigg/ \int_0^{\infty} \exp\left(\frac{V_N^{(\ell)}(R)}{D_R^{(\ell)}}\right) dR. \tag{19}$$

In the absence of these correction terms, that is $K^{(\ell)}(F) \to 1$, Eq. (17) reduces to that obtained by Yemélé and Kofané [5]. The presence of these factors gives rise to the better estimation of the nucleation rate of kink-antikink pairs in the system. The quantity $\Delta E_N^{(\ell)}$ interfering in Eq. (17) designates the energy of the critical nucleus whose accurate value at a given field $F \leq F_m$ is evaluated numerically through the relation

$$\Delta E_N^{(l)} = \int_{-\infty}^{\infty} dx \left[k \frac{du_N(x)}{dx}\right]^2, \tag{20}$$

where $u_N(x)$ satisfies the NLE (1) without the right hand side. However, for some particular cases, the explicit analytical expression of $\Delta E_N^{(\ell)}$ may be obtained:

For small F values ($F << F_m$), the amplitude of the critical nucleus is large and very close to 2π: $\Delta u_m^{(1)} = 2\pi - \alpha(4\pi F/V_0)^{1/2}$ and $\Delta u_m^{(2)} = 2\pi - (1/\alpha)(4\pi F/V_0)^{1/2}$. This nucleus is called large amplitude nucleus (LAN) with energy

$$\Delta E_N^{(\ell)} \approx 2E_s^{(\ell)}\left[1 - \frac{\pi d^{(\ell)} F}{E_s^{(\ell)}} - \frac{\pi d^{(\ell)} F}{E_s^{(\ell)}} \ln \frac{2E_s^{(\ell)} \upsilon^{(\ell)}}{\pi F d^{(\ell)}}\right], \tag{21}$$

where $E_s^{(\ell)}$ designates the static kink energy defined in Eq. (7).

For large F values ($F \approx F_m$), the amplitude of the critical nucleus is close to zero. This critical nucleus solution of the NLE (1) is called the small amplitude nucleus (SAN) whose analytical expression is given by

$$u_N(x) = b \sec h^2(x/2\xi), \tag{22}$$

with amplitude

$$b = 3\left(\frac{1+r^2}{1-r^2}\right)\tan u_{sn}\left[\frac{1 - 2\varepsilon\cos u_{sn} + 4\varepsilon/\cos u_{sn}}{1 - 5\varepsilon\cos u_{sn}}\right] \tag{23.a}$$

and size

$$\xi^2 = \xi_0^2\left(\frac{1+r^2}{1-r^2}\right)^2\left[\frac{(1+2\varepsilon\cos u_{sn})^3}{\cos u_{sn} + 2\varepsilon(1+\sin^2 u_{sn})}\right], \tag{23.b}$$

where $\varepsilon = r/(1+r^2)$. The energy of this SAN is also given by

$$\Delta E_N^{(\ell)} = (24/5)(kV_0)^{1/2} b (F/V_0)^{1/2}\left(\frac{1+r^2}{1-r^2}\right)\left[1/\tan u_{sn} + 4\varepsilon(1+2\varepsilon\cos u_{sn})(F/V_0)\left(\frac{1+r^2}{1-r^2}\right)^2\right] \tag{24}$$

In the presence of random fields, this critical nucleus may always exist in the system even at $T \to 0$ and resulting from the combined effects of the energy fluctuations and the applied field F. At high temperatures, thermal nucleus will play the main role. In what follows, we focus our attention on the thermally activated kink-antikink pairs. The above results constitute the starting point of the treatment of the inhomogeneous system. In order to relate the results of the nucleation rate of kink-antikink pairs to an easily accessible physical parameter we will evaluate, in the next section, the mean velocity of a particle in the chain which from a macroscopic viewpoint accounts for this microscopic phenomenon of the nucleation of kink-antikink pairs. Note that this question has been of interest in the theory of dislocation for more than four decades [6,8]. One should keep in mind that at low temperatures and in the absence of fluctuations, the particles undergo small amplitude

oscillations around their equilibrium position. In a macroscopic viewpoint, the system is at equilibrium. A remarkable displacement of particles comes from its transition from one site to an adjacent one due to the expansion of the newly formed kink-antikink pairs triggered by stochastic forces. The mean velocity of this displacement is thus determined by the number of kink-antikink pairs created per unit time and length. In other physical systems, such as compounds whose electrical properties at low temperatures are due to the existence of CDW, the above mean velocity can be interpreted as the electric current passing through the physical systems [30,40].

4. Inhomogeneous systems

4.1 Preliminaries

For real physical systems (inhomogeneous systems), the dynamics of the lattice may be described in terms of quasiparticles which, however, now interact with one another or with impurities. The interaction of nonlinear excitations with impurities plays an important role in transport properties and nucleation process of 1D systems. The kinks (antikinks) and breathers may be trapped or reflected by local inhomogeneities as in the case of a discrete lattice where the kink can be trapped in the Peierls-Nabarro energy (increment of the energy of the static kink due to the discrete character of the lattice) [41]. When the intensity χ of the random fields is weak $(\chi^{1/2} << V_0)$, the impurity has little effect on the parameters of the critical nucleus (size, shape and amplitude). However, the total energy ΔE_N^* necessary to create this nucleus is affected, that is $\Delta E_N^* = \Delta E_N + U(x)$, where $U(x)$ is the increment on the energy of a nucleus due to the random fields. From the Hamiltonian (6), we can define this increment on the energy as

$$U(x) = \int \frac{dx'}{a} V_f(x') \Phi_N(x - x'), \tag{25}$$

where $\Phi_N(x - x')$ depends on the shape of the nucleus, with $\Phi_N(x - x') = \partial u_N(x - x')/\partial x$. From the statistical properties of the random function $V_f(x)$ given by Eq.(5), it is easy to show that this increment of energy verifies the correlator

$$< U(x)U(y) >= \chi \int \frac{dx'}{a^2} \Phi_N(x - x') \Phi_N(y - x'). \tag{26}$$

Accordingly, the nucleation rate of kink-antikink pairs is given in the factored form as

$$\tilde{J} = \tilde{J}_0 \exp\left[-\beta U(x)\right], \tag{27}$$

where $\tilde{J}_0$ is, in the first order approximation in χ, the nucleation rate of kink-antikink pairs in the

homogeneous system defined by Eq.(17). Thus, we are concerned here only with the Arrhenius factor since χ is small.

As mentioned in the preceding section, we focus our attention on the mean velocity of particles $<\partial u/\partial t>$. In fact, a kink passing the point x of the chain to the right reduces the displacement field u by 2π and the antikink passing x to the right advances u by 2π. In the presence of an applied field, the kink current is $j_k = -vn_k$ and the antikink current $\bar{j}_k = v\bar{n}_k$, where v is the kink velocity and, n_k and $\bar{n}_k$ are the kink density and the antikink density, respectively. Therefore, the mean velocity of particles can then be written as $<\partial u/\partial t> = -2\pi(< j_k > - < \bar{j}_k >) = 4\pi v n_0$, where $n_0 =< n_k >=< \bar{n}_k >$ is the average kink(antikink) density in a chain. The steady state density $2n_0$ is maintained by the balance of the annihilation (recombination) and nucleation of kink-antikink pairs. From the probability that the kink encounters an antikink in the interval of time dt, one shows that the rate of recombination of n_0 kinks and n_0 antikinks per unit length and time is $2vn_0^2$ and the balance for the steady state density becomes $\tilde{J}_0 - 2vn_0^2 = 0$, where $\tilde{J}_0$ is the nucleation rate of kink-antikink pairs in the homogeneous systems. We can then write the expression of the mean velocity of particle as a function of $\tilde{J}_0$ as

$$<\partial u/\partial t> = 2\pi/<t>, \tag{28}$$

where in the homogeneous system we have $<t> = (2v\tilde{J}_0)^{-1/2}$. This result takes into account the fact that in the limit of heavy damping, the kink-antikink collision is destructive. The mean time $<t>$ may be viewed as the time for the transition of an arbitrary point on the chain to the neighboring minimum of the potential (8). In the inhomogeneous system which is under consideration, the above mean time can be generalized by means of the Kolmogorov method as

$$<t> =< \int_0^\infty dt \exp\left[-\int_0^{\tilde{x}} \tilde{J}(\tilde{z})(t - \iota(\tilde{z}))d\tilde{z} \right] >, \tag{29}$$

where $\tilde{J}(\tilde{z})$ is the nucleation rate of kink-antikink pairs whose center of mass lies at the point $\tilde{z}$ and $\iota(\tilde{z})$ is the travel time of kinks initially located at the point $\tilde{z}$ to reach the point of observation $\tilde{x}$. The exponential in the integrand (29) is the probability that the point $\tilde{x} = 0$ will be in the original minimum of the potential (8) at time t [42]. This expression of the mean time should take a simple particular form according to whether the intensities of the applied field F and of the impurities are weak or not. As we shall see below, expression (29) reduces to that obtained in the homogeneous system when the intensity of the impurity potential takes the value zero. This limiting case constitutes a proof that Eq.(29) takes into account the annihilation of kink-antikink pairs due to the strong dissipation of the system.

4.2 Mean velocity of the chain in the threshold field ($F \approx F_m$)

In the range $F \approx F_m$, the critical nucleus corresponds to a SAN defined in Eq.(22). Since the random fields are weak ($\chi^{1/2} < V_0$), impurities have little effect on the motion of kinks and their velocity v may be considered to be the same as in pure systems. Accordingly, from Eqs.(27) and (29), the mean time $< t >$ is then given by

$$< t >= \frac{\xi}{\mathrm{v}} \int_0^{\infty} dx < \exp\left[-J_0 \int_0^{x} dz \left(z e^{-\beta U(z)} \right) \right] >, \tag{30}$$

with $J_0 = \left(\xi^2 / \mathrm{v} \right) \tilde{J}_0$, where we have transformed the integration with respect to time t to integration with the dimensionless spaced variables x and z through the relation $t = \xi x / \mathrm{v}$, where $\mathrm{x}=\tilde{\mathrm{x}}/\xi$ and $\mathrm{z}=\tilde{\mathrm{z}}/\xi$. After integration, we obtain

$$< t >= \frac{\xi}{\mathrm{v}} \sqrt{\frac{2\pi}{J_0 < \exp\left[-\beta U(z) \right] >}} . \tag{31}$$

Substituting Eq.(31) into Eq.(28), yields

$$< \partial u / \partial t >= (2\pi \mathrm{v} \tilde{J}_0)^{1/2} W^{1/2}, \tag{32}$$

with

$$W =< \exp(-\beta U(z)) > . \tag{33}$$

Since in the homogeneous system the mean velocity is $< \partial u / \partial t >= (2\pi \mathrm{v} \tilde{J}_0)^{1/2}$, it follows from Eq.(32) that the factor $W^{1/2}$ designates the correction of this result when spatial inhomogeneities are taken into account. In order to evaluate *W*, we assume that the random field distribution is of Gaussian type function since the impurity assisted nucleation mechanism is local by definition [43]. This assumption is justified by the fact that the random field can take positive and negative values near zero and its intensity is weak. Thus, the probability distribution of this random field tends to 1 when $U(x)$ is zero and decreases to zero in the case of high values of $U(x)$. Accordingly, having in mind that $U(x) > -\Delta E_N$ (that is $\Delta E_N^* > 0$), the mean *W* is then defined as

$$W = \int_{-\Delta E_N}^{\infty} P(U) \exp(-\beta U) dU , \tag{34}$$

where

$$P(U) = \frac{1}{\sqrt{2\pi\tau}} \exp(-U^2 / 2\tau) \tag{35}$$

is the probability distribution with

$$\tau = < U^2 > = \frac{15}{16}\chi a^{-2} b^2 , \tag{36}$$

where b is the amplitude of the critical nucleus given by Eq.(23.a). Substituting Eq.(35) into Eq.(34) and integrating yields

$$W = \frac{1}{2}\exp\left(\beta^2\tau/2\right)\left[1-\Psi\left(\frac{\beta\tau-\Delta E_N}{\sqrt{2\tau}}\right)\right], \tag{37}$$

where Ψ is the probability integral. The correction (37) is valid for all absolute temperature satisfying the constraint $\beta\Delta E_N >> 1$. For certain regimes of temperature, the probability integral can be approximated by analytical expressions.

4.2.1 The low temperature regime

When the temperature satisfies the constraint $\beta\tau >> \Delta E_N$, the probability integral is then given by

$$\Psi\left(\frac{\beta\tau-\Delta E_N}{\sqrt{2\tau}}\right) = 1-(1/\pi)\exp\left\{-\left(\frac{\beta\tau-\Delta E_N}{\sqrt{2\tau}}\right)^2\right\}\sum_{i=0}^{n-1}(-1)^i\,\Gamma\left(i+\tfrac{1}{2}\right)\left(\frac{\beta\tau-\Delta E_N}{\sqrt{2\tau}}\right)^{-(2i+1)}, \tag{38}$$

where Γ designates the gamma function. Limiting this series to first order leads to the following expression for the correction factor:

$$W = \frac{\exp\left(\beta\Delta E_N\right)}{\beta\sqrt{2\pi\tau}}\exp\left(-\Delta E_N^2/2\tau\right). \tag{39}$$

In figure 2(a), we show that in this range of temperatures the correction factor $W^{1/2}$ increases when the shape of the substrate potential deviates from the sinusoidal one ($r \neq 0$). Furthermore, it appears that this factor is a decreasing function of the applied field.

4.2.2 The high temperature regime

In the high temperature regime, where the temperature satisfies the constraint $\beta\tau << \Delta E_N$ **,** Eq.(37) can be reduced, in a first order approximation, to

$$W = \exp(\beta^2\tau/2). \tag{40}$$

The analysis of this result shows that, $W^{1/2}$ is an increasing function of F if $r \leq 0$ as well as for $r > 0$, as indicated in Fig. 2(b). Note also that from the above expression, it is possible to recover the result obtained previously in the homogeneous system. In fact, in the limit $\tau \to 0$, e.g. $\chi \to 0$, the correction factor W tends to 1, in accordance with the physical expectation since, in this limit, the system is homogeneous. Finally, the correction factor strongly depends on the shape of the

substrate potential via the energy $\Delta E_N^{(\ell)}$ and/or τ at low temperatures as well as at high temperatures.

4.3 Mean velocity of the chain in subthreshold fields $(F << F_m)$

In the low applied field $(F << F_m)$, two physical situations can be obtained: the case where the applied field is greater than the intensity of impurities $(F >> \chi^{1/2})$ and the opposite situation where it is small compared to the intensity of impurities $(\chi^{1/2} >> F)$. For general the case $F << F_m$, the kink suffers the effects of thermal and stochastic fluctuations; when the temperature is lower than the specific temperature $T_0 (T << T_0 = \tau / k_B \Delta E_N^{(\ell)})$, the kink motion has an activated character whereas kink activated by impurities plays the major role for the high temperature $(T >> T_0)$.

4.3.1 Case of $\chi^{1/2} < F < F_m$

To evaluate the mean time $< t >$, here we have to take into account the distance between kink and impurities along the line. It is then convenient to rewrite Eq.(29) in the form

$$< t >= \frac{d^{(l)}}{v^{(l)}} \int_0^{\infty} dx \exp\left[-J_0 \int_0^x dz (x-z) \exp\left\{ -\int_{-\infty}^{\infty} dy \Phi_N (z-y) \psi(y) \right\} \right] > , \qquad (41)$$

where $x = \tilde{x} d^{(\ell)}$ is the dimensionless variable, $d^{(\ell)}$ the kink width defined in the preceding section, and $\psi(y) = \beta V_f(y)$ is the dimensionless random field whose properties are determined by the correlator $< \psi(y) \psi(y') >= \beta^2 \chi \delta(y - y')$ following from Eq.(5). The calculation of the mean time $< t >$ after expanding the integrand of Eq.(41) into a series, yields

$$< t >= \frac{d^{(l)}}{v^{(l)}} \left[2\pi / J_0 W \right]^{1/2} \quad , \text{with } W =< \exp\left\{ -\sum_{\alpha=1}^{m} \int_{-\infty}^{\infty} \Phi(z_\alpha - y_\alpha) \psi(y_\alpha) dy_\alpha \right\} > . \qquad (42)$$

As seen above, this quantity W describes the correction factor to the mean velocity of the chain due to the presence of impurities in the system. Its calculation depends on the temperature regime.

4.3.1.1 **The high temperature regime**

To calculate the mean W, we must remember that the statistical properties of the random field $V_f(x)$ are assumed to be delta-correlated (see Eq.5). Thus, the distribution function $P(V_f(x))$ which satisfies to this assumption is equivalent to a Gaussian probability density

$$P(V_f(x)) = \exp\left[-\frac{1}{2\chi}\int V_f^2(x)dx\right], \tag{43}$$

where χ is the intensity of the impurity. Accordingly, in the high temperature regime, the correction factor W may be written as :

$$W = \frac{\int D\psi \exp(-A)}{\int D\psi \exp(-A_0)}, \tag{44}$$

with

$$A = \frac{1}{2\beta^2\chi}\int \psi^2(y)dy + \sum_{i=1}^{m} dy_i \Phi_N(z_i - y_i)\psi(y_i), \tag{45a}$$

and

$$A_0 = \frac{1}{2\beta^2\chi}\int \psi^2(y)dy, \tag{45b}$$

where A may be viewed as the "action". We can evaluate this correction factor by minimizing the action A to obtain the extremal trajectory. The action corresponding to this particular path is equal to

$$A_c = -\frac{1}{2\beta^2\chi}\int dz\left[\sum_{i=1}^{m}\Phi_N(z - z_i)\right]^2 . \tag{46}$$

Next, we evaluated the series of these integrals. As pointed out in Ref.[30], to evaluate this series of integrals with respect to $z_1, z_2, z_3,..., z_m$, we can readily verify that the principal contribution come from the points lying close to the surfaces $z_i = z_j$, that is for $G(z_i - z_j) = G(0) \equiv G_0$ where G is related to the random field correlator as

$$< U(x)U(y) > = 4\chi d^{(\ell)} \int_{-\infty}^{\infty} \frac{dz}{a^2}\left(\frac{\partial u_N(x-z)}{\partial x}\right)\left(\frac{\partial u_N(y-z)}{\partial y}\right) \tag{47.a}$$

$$= 4\chi d^{(\ell)} G(x-y), \tag{47.b}$$

where u_N is the shape of the critical nucleus in a pure system. Using Eqs.(43)-(47), it follows that

$$W^{(\ell)} = \exp\left(\beta^2\chi G_0^{(\ell)}\right), \tag{48}$$

where the quantity $G_0^{(\ell)}$ is given by

$$G_0^{(\ell)} = 4\left[1 - \frac{\pi d^{(\ell)} F}{E^{(\ell)}} - \frac{\pi d^{(\ell)} F}{E^{(\ell)}} \ln \frac{2E^{(\ell)}\upsilon^{(\ell)}}{\pi F d^{(\ell)}}\right]. \tag{49}$$

The variation of W as a function of the applied field F is plotted in Fig. 2(c). It appears that, in this range of temperatures, the correction factor is less sensitive to the variation of the applied field in the whole range of variation of the shape parameter r.

4.3.1.2 **The low temperature regime**

In the range of low temperatures, it is necessary to take into account the fact that the random field can be cut off. For this reason, we introduce in the expression of the mean W, the Heaviside function defined as

$$\theta(x)=\frac{1}{2\pi i}\lim_{\varepsilon\to 0}\int dq\,\frac{e^{iqx}}{q-i\varepsilon}\ . \tag{50}$$

For this purpose, the correction factor (42) is then given by

$$W=\frac{\int D\psi\theta[\beta\Delta E_N+\int\Phi_N(y-Z)\psi(y)dy]\exp(-A)}{\int D\psi\theta[\beta\Delta E_N+\int\Phi_N(y-Z)\psi(y)dy]\exp(-A_0)} \tag{51}$$

Using the same procedure as before, we obtain, after some lengthy algebra

$$W=e^{\left(\beta\Delta E_N^{(l)}+\beta^2\chi G_0^{(l)}/2\right)}\left[\frac{\left(\frac{\Delta E_N^{(l)}-\beta\chi G_0^{(l)}}{\sqrt{2\chi G_0^{(l)}}}\right)+\frac{2}{3}\left(\frac{\Delta E_N^{(l)}-\beta\chi G_0^{(l)}}{\sqrt{2\chi G_0^{(l)}}}\right)^3+\frac{\pi}{4}\exp\left(\frac{\Delta E_N^{(l)}-\beta\chi G_0^{(l)}}{\sqrt{2\chi G_0^{(l)}}}\right)^2}{\frac{\Delta E_N^{(l)}}{\sqrt{2\chi G_0^{(l)}}}+\frac{2}{3}\left(\frac{\Delta E_N^{(l)}}{\sqrt{2\chi G_0^{(l)}}}\right)^3+\frac{\pi}{4}\exp\left(\frac{\Delta E_N^{(l)}}{\sqrt{2\chi G_0^{(l)}}}\right)^2}\right], \tag{52}$$

where $G_0^{(\ell)}$ is given by Eq.(49). This result is only qualitative since the perturbation approach is no longer valid. In fact, one can easily show that in the low temperature regime the main contribution to the mean velocity of particles in the chain is due to random field fluctuations which are of the order of ΔE_N. Thus, impurities can produce an appreciable change in the equilibrium shape and size of the nucleus and then the perturbation theory is no longer valid for a solution of the NLE (1).

4.3.2 **Case of** $F<\chi^{1/2}<F_m$

When the field F is small compared to the intensity of impurities $\chi^{1/2}$, the kink has to overcome the impurity potential. In accordance with the activation type formula, the mobility or the speed of the kink turns out to be $\approx\exp(-\beta^2\chi/2)$. Taking into account this retardation of kink by impurities in the expression of the mean time $<t>$, we obtain

$$<t>=\exp(-\beta^2\chi/2)<\int_0^\infty dx\exp\left[-J_0e^{-\beta^2\chi/2}\int_0^x dz\exp\left\{-\int\psi(y')\Phi_N(y'-z)dy'\right\}\right.$$

$$\left.\int_z^x dy\exp\left\{\int\psi(y')\Phi_s(x-y')dy'\right\}\right]\times\exp\left\{\int\psi(y')\Phi_s(y'-z)dy'\right\}>. \tag{53}$$

By expanding the exponential in series and performing the Gaussian integration over D for high temperatures, we obtain

$$< t >= \exp(-\beta^2\chi/2)\int_0^x dx e^{-\beta^2\chi B_0}\exp\left[-J_0 e^{-\beta^2\chi/2}(x^2/2)e^{\beta^2\chi\sum_{i,j=1}^{n}\left[G(z_i-z_j)-2C(z_i-z_j)+B(z_i-z_j)\right]}\right.$$

$$\left.\times e^{\beta^2\chi\sum_{i,j=1}^{n}2\left[B(z_i-x)-C(z_i-x)\right]}\right], \qquad (54)$$

where

$$B(z_i-z_j)=\int dz\Phi_s(z-z_i)\Phi_s(z-z_j), \quad C(z_i-z_j)=\int dz\Phi_N(z-z_i)\Phi_s(z-z_j). \qquad (55)$$

Integration of Eq.(54) can easily be performed if $z_i = z_j$, leading to the following expression of the mean time

$$< t >= (\pi/2)^{1/2} e^{-\beta^2\chi/2} e^{-\beta^2\chi(G_0^{(\ell)}-B_0^{(\ell)})/2} J_0^{-1/2}\ , \qquad (56)$$

and then the mean velocity of the chain

$$\left\langle \partial u/\partial t \right\rangle = (2\pi u\tilde{J}_0)^{1/2} W^{(\ell)^{1/2}} \qquad (57)$$

with the correction factor

$$W^{(l)} = \exp(\beta^2\chi/2)\exp\left[\beta^2\chi(G_0^{(\ell)}-B_0^{(\ell)})\right], \qquad (58)$$

where $B_0^{(\ell)} = \exp\left(R_N^{(\ell)}/d^{(\ell)}\right)$. Figure 2(d) shows that the correction factor W is an increasing function of the applied field F for $r \le 0$ and is less sensitive for $r > 0$.

5. Application to the diffusion of hydrogen atoms on metallic surfaces

The question of surface diffusion of atoms and molecules adsorbed on metallic surfaces is a long-standing problem which has recently attracted a renewal of interest with the introduction of new ideas from the physics of nonlinear phenomena. The experimental investigations of this problem are based on two essential classes of methods [44]: The profile evolution methods such as electron beam scanning and the equilibrium methods such as the field ion microscopy. Theoretical works are outlined by experimental studies which evidence [36,45,46] an important role of collective motion of adsorbed atoms (adatoms). According to these experimental studies, the diffusion of adatoms can be described by the nonlinear dynamics of the well known FK model which is essentially a single model allowing an accurate description of such a consistent motion of particles. In some cases, adatoms may be treated as quasi-1D systems where a chain of interacting particles is placed in a “channel”. The atomic chain is subjected to a one, two or three-dimensional

substrate potential, which is periodic in one direction and unbounded in transverse directions, so that atoms are confined transversally. However, when the concentration Θ_C of adatom is weak, i.e. closed to $1(\Theta_C \approx 1)$ one can ignore atomic displacements in transverse directions and allow atoms to move only along the direction of the chain, and the model reduces to a well-known FK model. The concentration of adatoms is characterized here by the dimensionless parameter $\Theta_C = p/q$, the so-called coverage in surface physics, where p is the number of atoms and q is the number of minima of the substrate potential. In addition, previous studies (see, e.g., Refs. [34, 36] and references therein) have proved that the system of adsorbed atoms is subjected to a nonsinusoidal substrate potential and that the RP potential (see Eq.(2)) provides an accurate description of such a substrate potential. According to these studies, the Hamiltonian model described by Eq.(6) may be successfully used to study the migration of atoms adsorbed on metallic surfaces. For the case of the H/W and H/Ru adsystems, an estimate parameter is $r \approx -0.3$ [5]. Thus, we apply the results of the above analytical study to estimate the mean velocity of a hydrogen atom on a Ru and W substrates induced by the applied field F. Note that geometrical imperfections of the adsorbed surfaces are considered here as impurities since they are at the origin of the spatial deformation of the newly created nucleus and consequently may be approximated by the impurity potential given by Eq.(4). The model parameters used in our numerical calculations are [5]: $V_0 \approx 3.62 \times 10^{-2} eV.\text{A}^{\circ -1}$, $k = 3.57 \times 10^{-1} eV\,\text{A}^{\circ}$. The lattice constant $a \approx 3\,\text{A}^{\circ}$ is taken to be the distance between the wells along a furrow on the W(112) surface since $\Theta_C \approx 1$. In addition, the shape parameter of the substrate potential is taken to be $r = -0.3$. The calculation of the correction factor from these numerical values of the characteristic parameters of the adsystem shows the following:

Firstly, for high temperatures [see Fig. 3(a)] the correction factor increases with the applied field F and tends rapidly to 1 when F becomes higher. This result is in accordance with the physical expectation since the increase of the intensity of the applied field results to the increase of the kinetic energy of the newly formed kink-antikink pairs. Consequently, impurities have little effect on the nucleation rate of kink-antikink pairs $(W \to 1)$. Note that the perturbation theory is not valid in the case of low temperatures associated to the weak applied field.

Secondly, for the value of the applied field F close to the threshold field F_m, the correction factor W increases or decreases according to whether the temperature is high [see Fig. 3(b)] or low [see Fig. 3(c)]. In fact, in the high temperature regime, the correction factor increases with the applied field. Thus, in this temperature regime, the disorder in the systems makes the nucleation of

kink-antikink pairs more favorable. However, in the low temperatures, disorder contributes to make it less favorable.

Finally, it should be noted that the correction factor, which contains all the information concerning the effect of impurities, is less than 1 [Figs. 3(a) and 3(b)] indicating the fact that the presence of impurities in the system makes the processing of nucleation of kink-antikink pairs less favorable. However, for large values of the applied field, the correction factor is greater than 1 [Fig. 3(c)] indicating the fact that the impurities catalyze the transition from the critical nucleus or saddle point configuration to the newly formed kink-antikink pairs by making the growth energetically favorable.

It is important to mention that our model is valid when the concentration of adatoms Θ_C is close to 1. When Θ_C is greater than 1, the amplitude V_0 of the substrate potential is a function of adatom concentration Θ_C and the compression forces, in the adatomic chain, overcome the forces "holding" the adatoms in a given channel and adatoms will start "creeping out" of the channel so that their motion will become more complex and can be described only in terms of a two- or three-dimensional model.

6. Conclusion

In this paper, we have investigated the influence of impurities on the nucleation of kink-antikink pairs in the nonlinear Klein-Gordon model, with the Remoissenet-Peyrard substrate potential, driven by an external constant field. We have focused our attention on the mean velocity of particles of this one-dimensional system which is a physical parameter closely related to the number of kinks and antikinks created in the system per unit time and length. Moreover, in other systems like compounds where the electrical properties are directly related to the existence of charge density waves, this mean velocity designates the electrical current carried by the CDW.

First, we have improved by taking into account the non-Gaussian correction in our calculation, the analytical expression of the nucleation rate of kink-antikink pairs in the homogeneous system previously calculated by Yemélé and Kofané [5]. This calculation is one step towards the study of the effects of impurities. Next, by means of the Kolmogorov method associated with the perturbation analysis, we have shown that the dynamics of the system may be different according to whether the intensity of the applied field is weak or not compared to the intensity of the impurity potential and the magnitude of the temperature. More precisely, we have shown that, in the range of weak values of the applied field, the quantitative effects of impurities increase with the applied field and temperature. Moreover, the presence of impurities in the system

makes the nucleation process of kink-antikink pairs less favorable. Furthermore and contrary to the preceding case, for large values of the applied field, impurities catalyze the transition from the saddle point configuration of the system to the newly formed kink-antikink pairs by making the growth of the nucleus energetically favorable.

Finally, we mention that our numerical applications are carried out by making use of the parameters of H/W and H/Ru adsystems where available data exist. However, the model may be applied to a number of various systems of condensed matter physics for which the substrate potential is used to describe its physical phenomena namely, dislocation kinetic in crystals, electrical current carried by the CDW in the compounds whose electrical properties are due to the existence of this CDW, or the electrical current in the long Josephson junctions, to name only a few. The perturbation analysis used here allows one to write down an analytical expression of the nucleation rate of kink-antikink pairs in the inhomogeneous 1D system, from which the quantitative effects of impurities on this quantity can be obtained. This calculation is one step towards a complete study of the model. The method is valid only in the case of weak impurity fields, that is, in the case where impurities have little effect on the critical nucleus parameters and on its stability. Another restriction of this study concerns the correlation length of the random field of impurities which has been taken equal to zero although the case of a spatially correlated field may be of interest for applications to much of condensed matter systems. These two limitations of our study are now under consideration.

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Figure Captions

FIG. 1: Substrate potential $V_{RP}(u,r)$ as a function of $u/2\pi$ for a few values of the deformability parameter : (1) r=-0.3, (2) r=0.0 (sG case), (3) r=0.3, and (4) r=0.9.

FIG. 2: Correction factor to the mean velocity of particles W, induced by the presence of impurities in the system, as a function of the applied field F :

(a) The case of large values of the applied field ($F \approx F_m$) and in the regime of low temperatures (T=280 K). The intensity of the impurity potential is taken to be $\chi = 1.11\times10^{-2}(eV/\mathring{A})^2$.

(b) The case of large values of the applied field ($F \approx F_m$) and in the high temperature regime (T=500 K), for $\chi = 1.11\times10^{-3}(eV/\mathring{A})^2$.

(c) The case of weak applied field satisfying the constraint $\chi^{1/2} < F << F_m$ and in high temperature regime (for example T=400 K), $\chi = 6.94\times10^{-6}(eV/\mathring{A})^2$.

(d) The case of very weak applied field ($F < \chi^{1/2}$) and in the high temperature regime. Here T=400 K and $\chi = 6.94\times10^{-8}(eV/\mathring{A})^2$.

Note that the choice of numerical values of the intensity of the impurity potential, in either case, is dictated by the condition $\beta\tau << \Delta E_N$ or $\beta\tau >> \Delta E_N$.

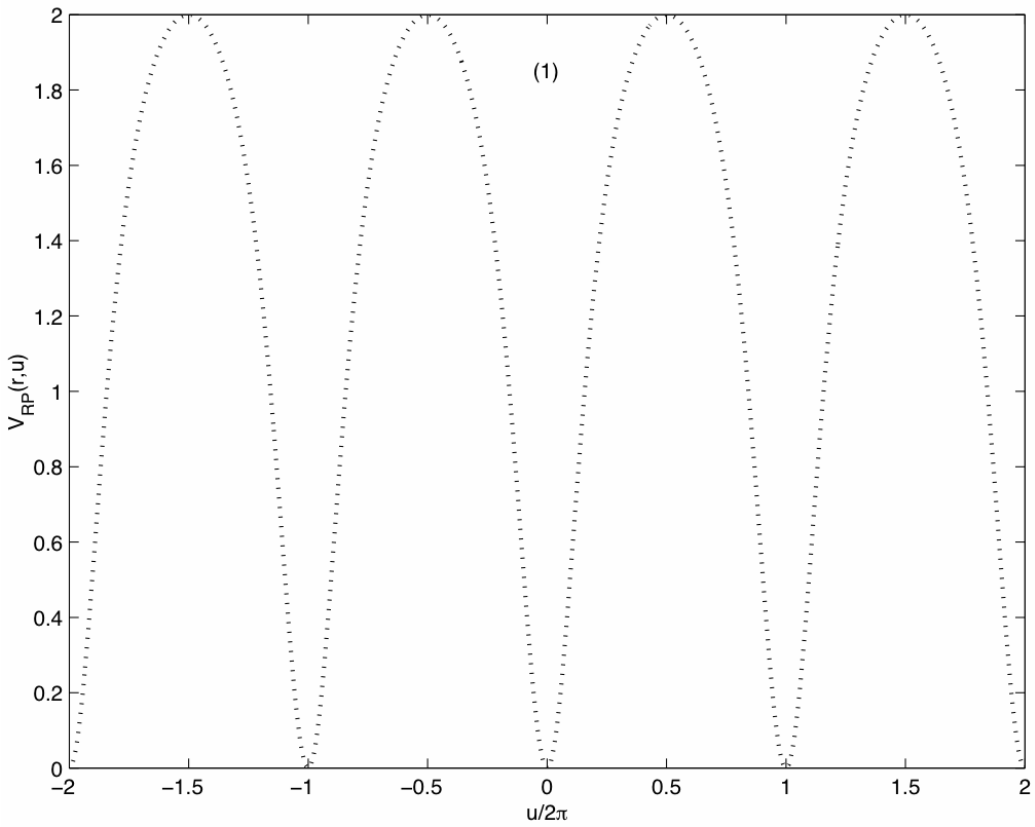
FIG. 3: Correction factor to the mean velocity of particles W, induced by the presence of impurities in the system of H/W, as a function of the applied field F and for three values of temperature:

(a) The case of weak applied field in the high temperature regime, $\chi = 6.94\times10^{-8}(eV/\mathring{A})^2$.

(b) The case of large applied field in the high temperature regime for $\chi = 1.11\times10^{-2}(eV/\mathring{A})^2$.

(c) The case of large applied field in the low temperature regime with $\chi = 1.11\times10^{-2}(eV/\mathring{A})^2$.

Note that the choice of the intensity of the impurity potential in the low and high temperature regime is dictated by the constraints verified by the quantity $\beta\tau$ in these temperature regimes. $\beta\tau >> \Delta E_N$ for the low temperature regime or $\beta\tau << \Delta E_N$ for the high temperature regime.


(1)
$V_{RP}(r,u)$
u/2π
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2

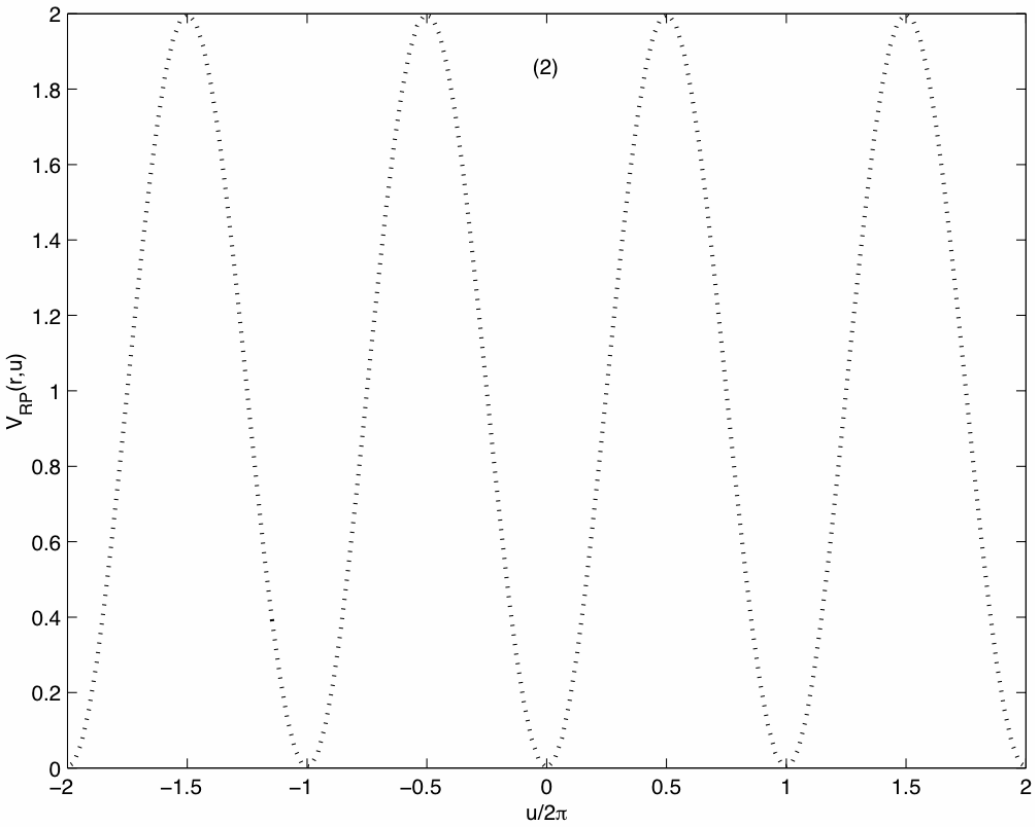
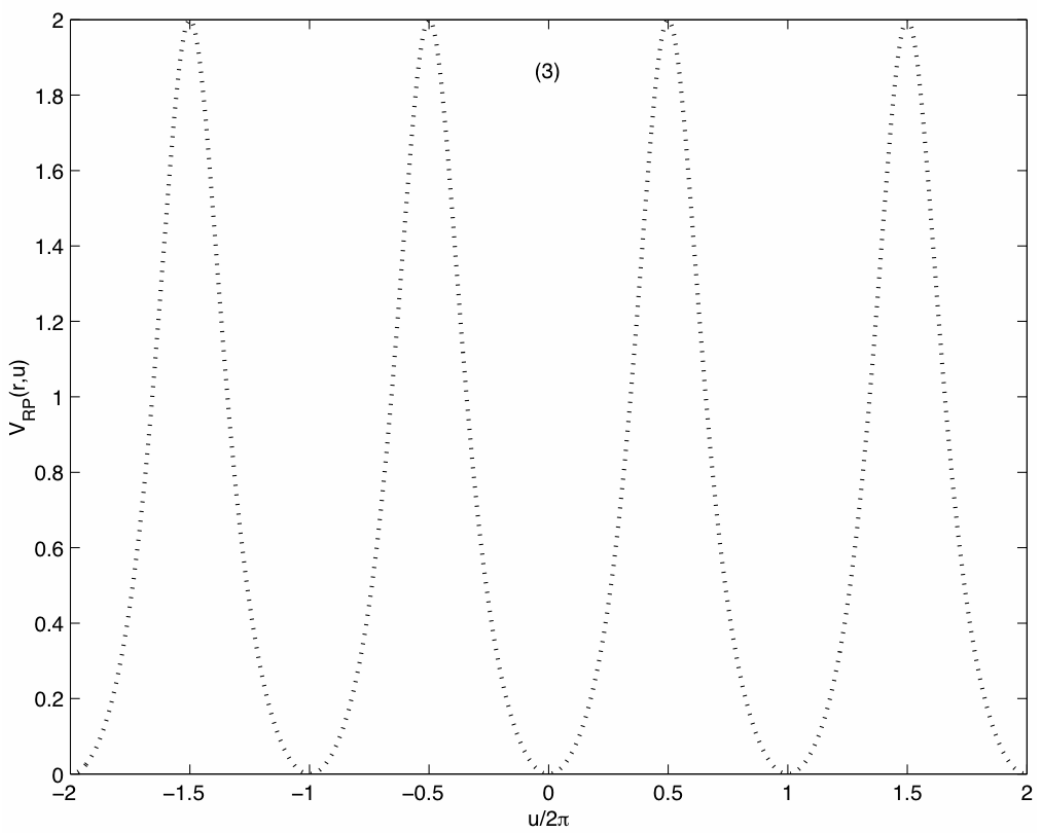

(2)
$V_{RP}(r,u)$
u/2π
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
−2
−1.5
−1
−0.5
0
0.5
1
1.5
2

Fig. 1



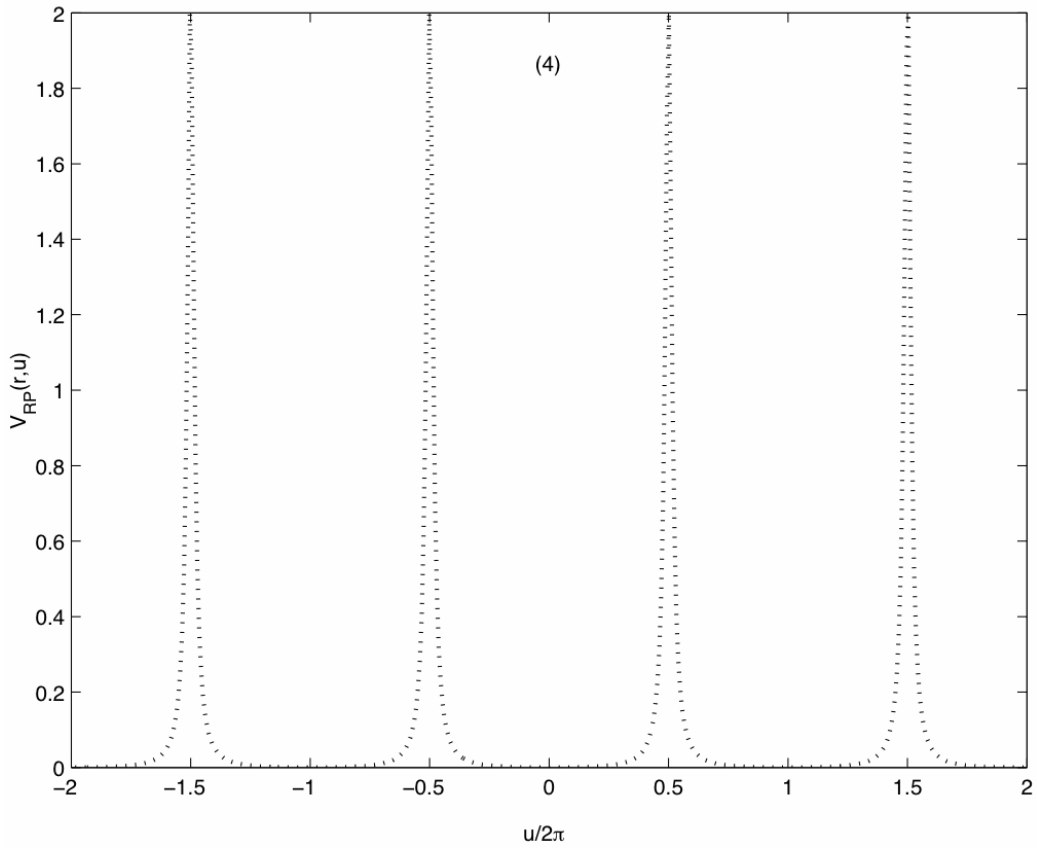


Fig. 1

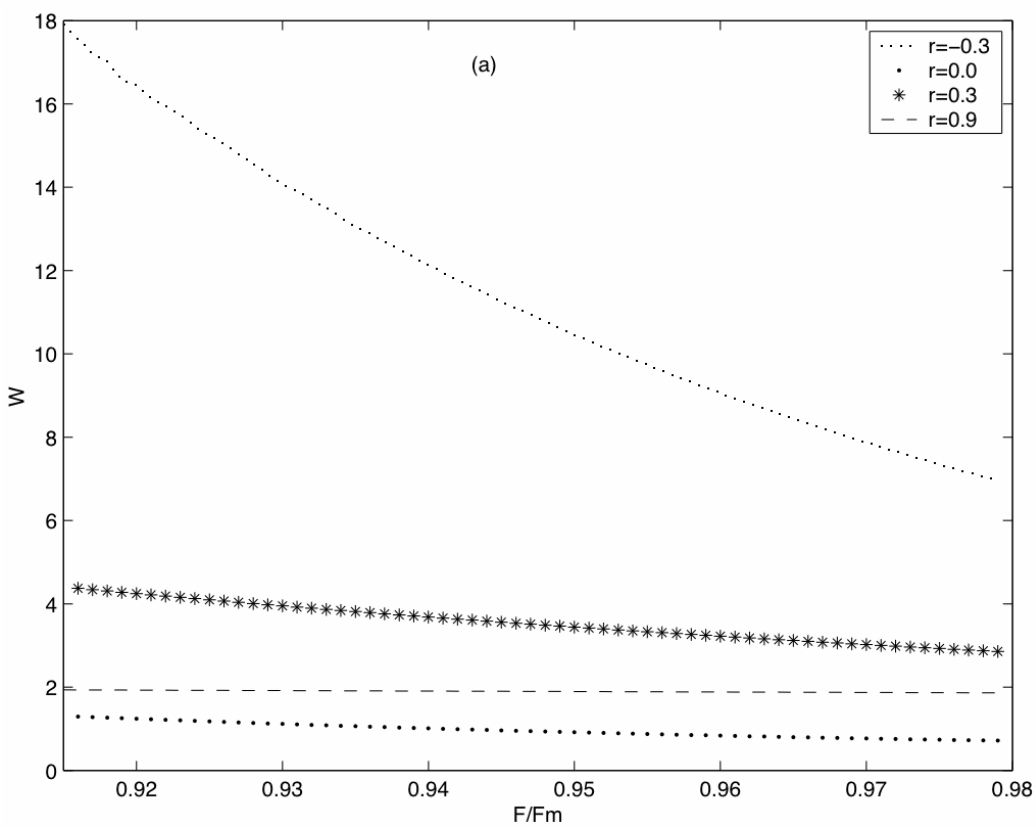

(a)
r=–0.3
r=0.0
r=0.3
r=0.9
W
F/Fm
0
2
4
6
8
10
12
14
16
18
0.92
0.93
0.94
0.95
0.96
0.97
0.98

Fig. 2(a)

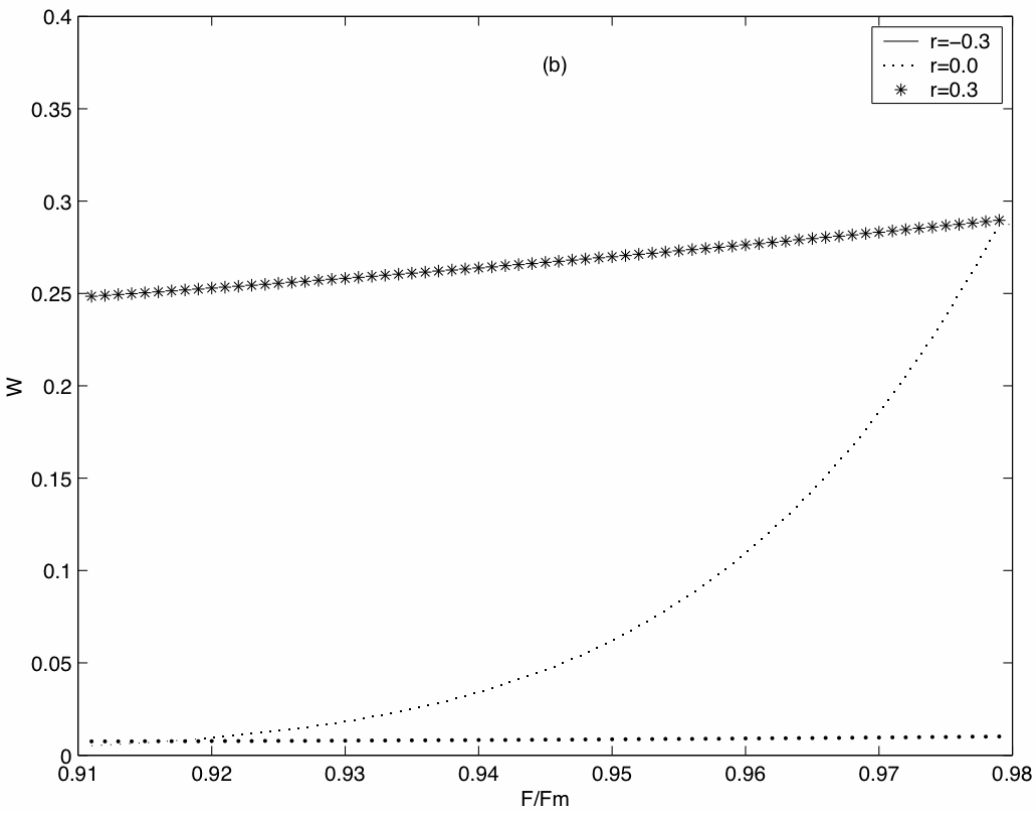

(b)
r=–0.3
r=0.0
r=0.3
W
F/Fm
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.91
0.92
0.93
0.94
0.95
0.96
0.97
0.98

Fig. 2(b)

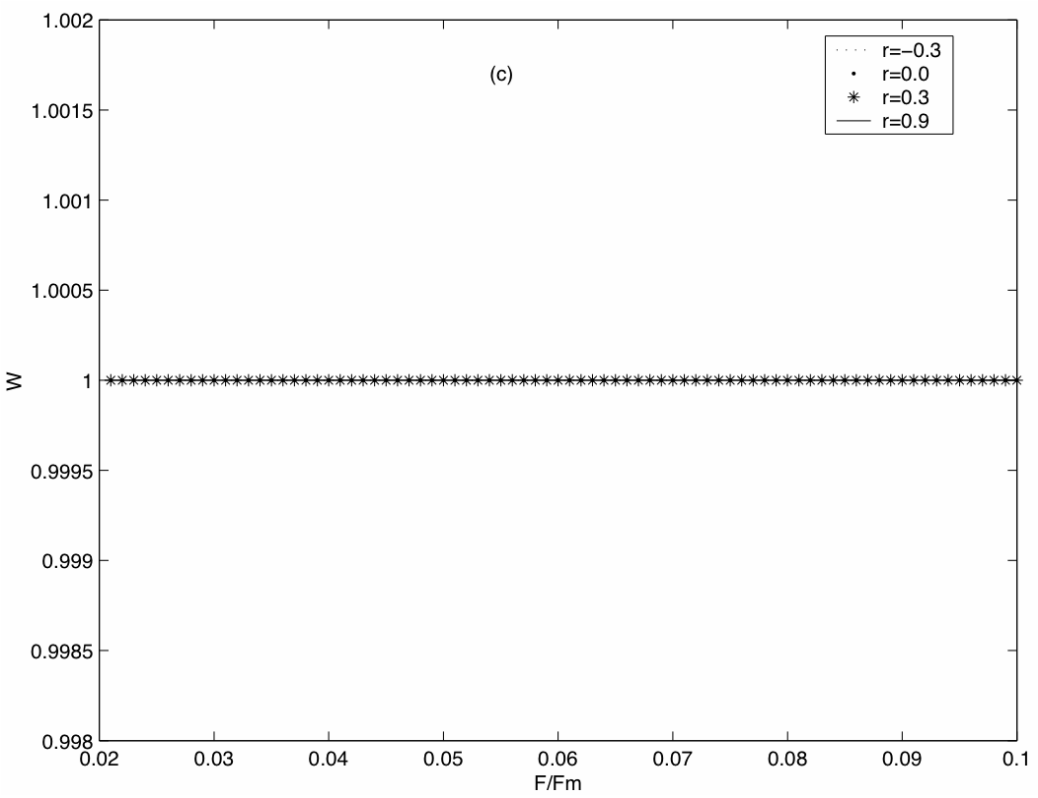

(c)
r=−0.3
r=0.0
r=0.3
r=0.9
W
F/Fm
1.002
1.0015
1.001
1.0005
1
0.9995
0.999
0.9985
0.998
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1

Fig. 2(c)

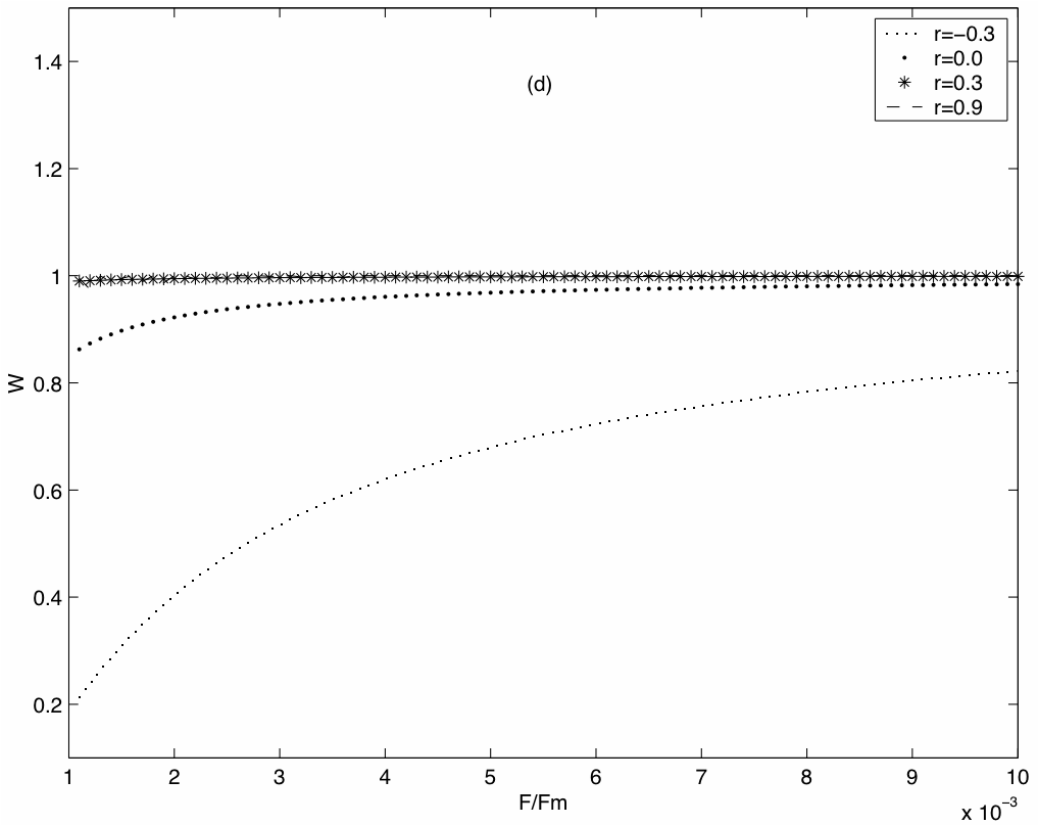

(d)
r=−0.3
r=0.0
r=0.3
r=0.9
W
F/Fm
x 10^−3
1.4
1.2
1
0.8
0.6
0.4
0.2
1
2
3
4
5
6
7
8
9
10

Fig. 2(d)

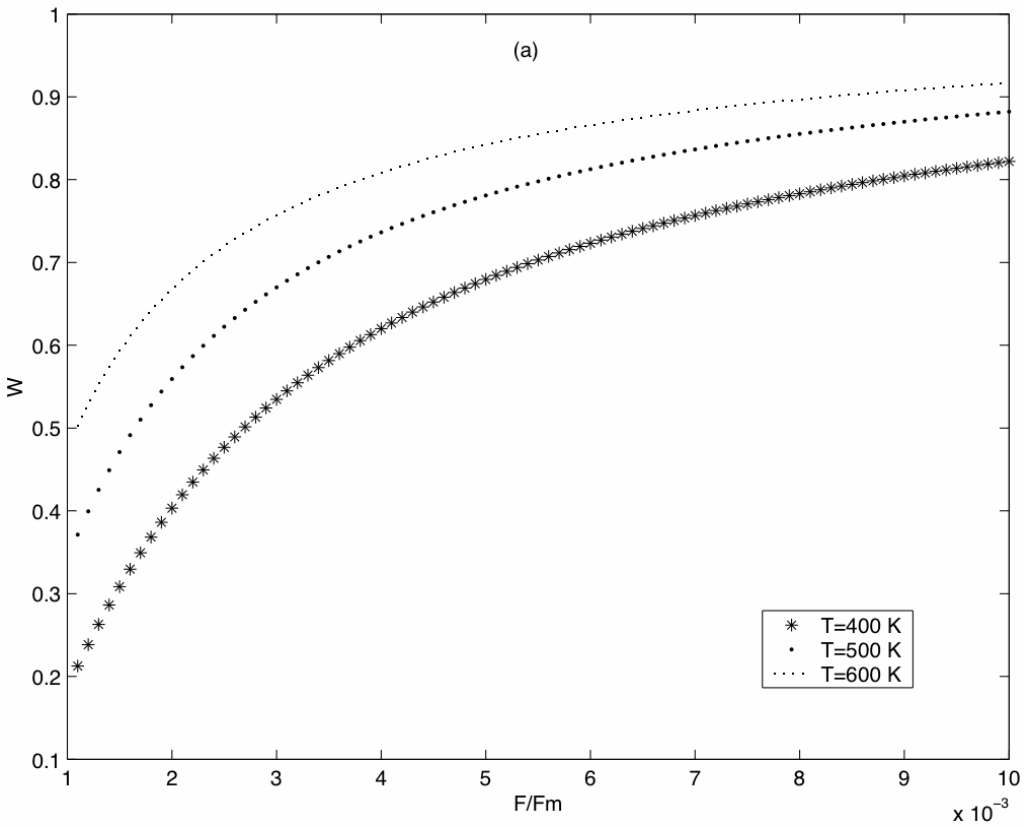


Fig. 3(a)

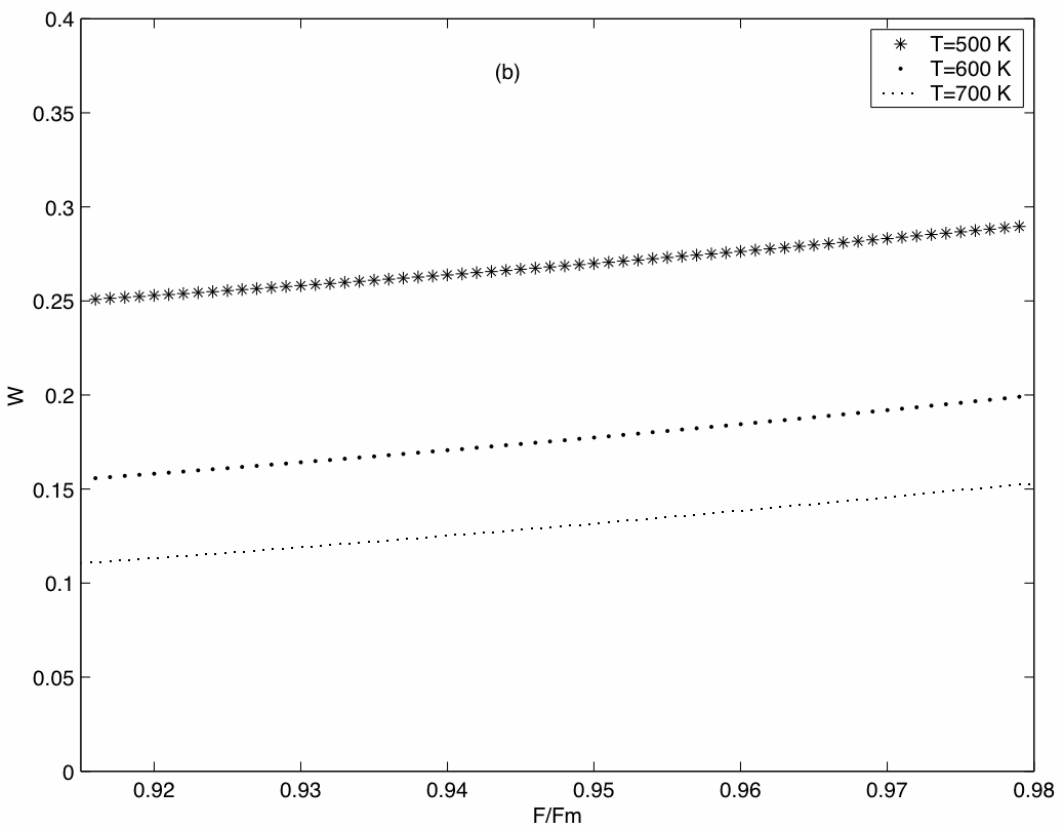


Fig. 3(b)

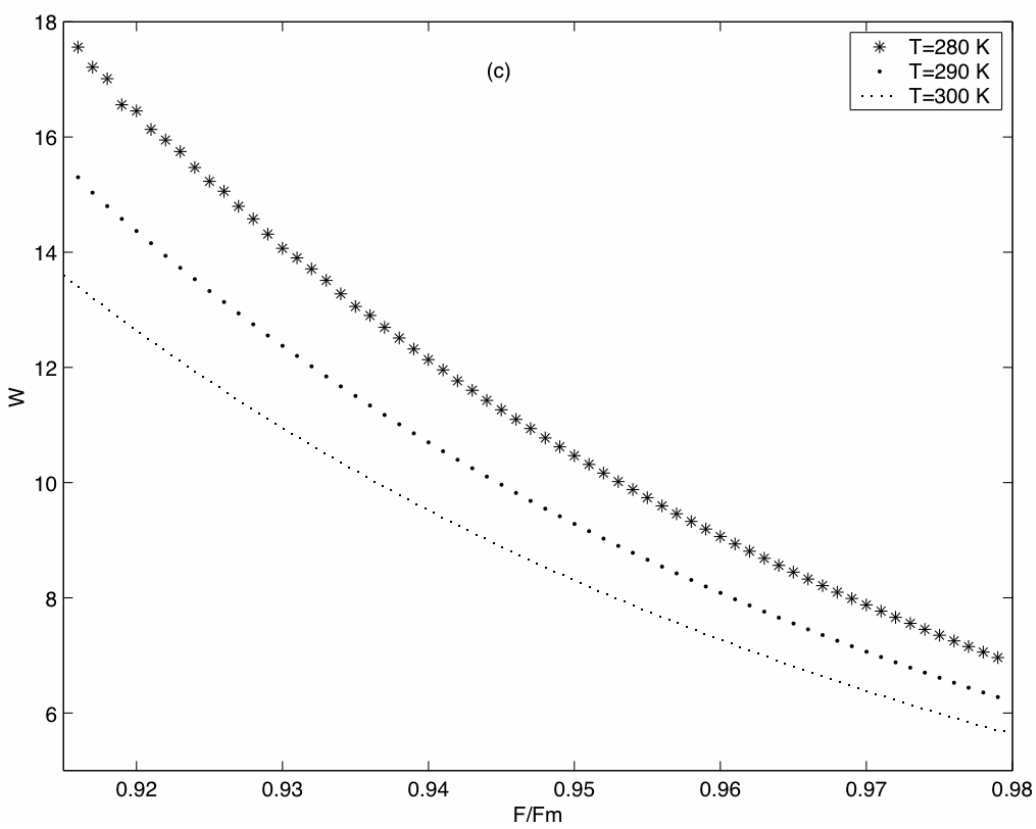

(c)
T=280 K
T=290 K
T=300 K
W
F/Fm
18
16
14
12
10
8
6
0.92
0.93
0.94
0.95
0.96
0.97
0.98

Fig. 3(c)