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Interaction between kinks in coupled chains of adatoms

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Abstract. A Frenkel–Kontorova type of model is proposed to describe the dynamics of excess atoms (kinks) or vacancies (anti-kinks) in two parallel chains of atoms adsorbed on a crystal surface. Various dynamic processes with kinks belonging to different adatomic chains are considered within the framework of perturbation theory for non-linear waves, the local coupling between chains being a small parameter. In particular, the interaction energy of the kinks is calculated, and the collision of kinks in the presence of dissipation and a DC driving force is considered. It is demonstrated that two slow kinks can form a bound state due to dissipative energy losses, and the threshold value of the external force for this process is obtained. Different ways of exciting the internal oscillations of the bound state are discussed. Some radiative effects accompanying collision of two kinks belonging to different chains are investigated as well.

1. Introduction

Investigation of non-linear phenomena in two-dimensional structures of atoms adsorbed on a crystal surface (adatoms) is very important from theoretical as well as practical viewpoints (see e.g. [1–5]). In some cases an adsorbed layer of atoms can be considered as a quasi-one-dimensional system. The first example is adsorption on a stepped semiconductor surface [2, 3]. The substrate atoms located on the step have unsaturated chemical bonds and, therefore, the adatoms are predominantly adsorbed close to the step where their coupling with the substrate atoms is stronger. The second example is adsorption on a 'furrowed' crystal surface (e.g. on the (112) face of a BCC metal) when the potential relief along the 'furrow' is much lower than that in the perpendicular direction [1]. In this case the atoms adsorbed in the 'furrow' can be approximately considered as a quasi-independent one-dimensional atomic chain.

To investigate the non-linear dynamics of adatoms in a one-dimensional system, the Frenkel–Kontorova model has been successfully used (see e.g. [4, 5]). The model describes a linear atomic chain in a periodic external potential (for systems of adatoms, such a periodic potential plays the role of the substrate potential relief). It is known that the long-wave excitations of the Frenkel–Kontorova model are described by the sine–Gordon (SG) equation [6]. The SG equation is used to explain a large number of physical phenomena such as motion of dislocations in crystals [7, 8], dynamics of planar domain

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walls in magnetic systems (e.g. [9]), non-linear properties of long Josephson junctions [10], the charge-density waves in quasi-one-dimensional conductors [11] and so on.

For the SG system as well as for any non-linear system for which the potential energy density has two or more equivalent vacuum states, there are solutions (the so-called kinks) that 'connect' the nearest equivalent energetic states. For adsystems described by the SG equation, the vacuum state corresponds to the commensurate structure, when all adatoms lie in the minima of the substrate potential relief. The kink (anti-kink) solution describes the dynamics of the excess atom (vacancy) in this commensurate atomic structure (e.g. [4]). The motion of the kink corresponds to the motion of the excess atom along the chain; therefore, analysis of the motion of a kink plays an important role in the investigation of surface diffusion and drift of adatoms (see [12]).

In exactly integrable systems such as the SG, one of the kinks moves freely and their collisions are elastic [6]. For real physical systems, the exact integrability of the corresponding equations is usually destroyed by additional perturbation terms describing, for example, dissipative processes, the forces between atomic chains and external forces. But in many cases the additional terms may be analysed as small perturbations of the corresponding integrable model and perturbation theory can be applied.

In the present paper we consider two parallel adatomic chains with a small local interaction between them. (The opposite case of strongly coupled adatomic chains was considered by Lyuksyutov and Pokrovskii [13].) The proposed model for such a system is described in § 2. In § 3 we investigate the motion of a kink in one chain of this atomic system. The interaction between two kinks belonging to different chains is considered in § 4. We calculate the interaction energy and analyse the stability of the bound state of two kinks belonging to different chains. The forced motion of the kink and the interaction of kinks in the presence of dissipative losses and an external driving force are considered in § 5. The threshold value of the external force that permits the formation of a bound state of two kinks is obtained for attraction as well as repulsion between the interacting kinks. Some ways of exciting the bound-state internal oscillations are presented in § 6. In § 7 we calculate the radiative energy losses accompanying the collision of two free kinks and show that the radiative losses are usually negligible in comparison with the dissipative ones. The possibility of experimental observation of the described non-linear effects, in particular a bound state of the kinks belonging to different chains of adatoms, is discussed in § 8.

2. The model: linear excitations

Let us suppose that, for the atoms of the adsorbed chain, substrate atoms form the periodic potential $w_S(u)$, where u is the displacement of an adatom from the minima of the relief. We consider the commensurate structure of adatoms when each minimum of the substrate potential relief $w_S(u)$ is occupied by one atom. The periodic function $w_S(u)$ (a is the period of the potential in the direction of the anisotropy of the substrate) can be expanded into a Fourier series in cosines. If we limit ourselves to the first terms of this series, then the potential dependence on the displacement takes the form

$$w_S(u) = \tfrac{1}{2}\varepsilon_D[1 - \cos(2\pi u/a)] \tag{1}$$

where the height of the substrate relief ε_D is equal to the activation energy for the surface diffusion of an isolated adatom. Thus, the behaviour of one adatomic chain can be

adequately described in the continuum limit by the well known Frenkel–Kontorova model [14], which corresponds to the Hamiltonian of the SG system:

$$\mathcal{H}_{SG} = \int \frac{dx}{a}\left\{\frac{1}{2}m\left(\frac{\partial u}{\partial t}\right)^2 + \frac{1}{2}w_{\parallel}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{1}{2}\varepsilon_D\left[1-\cos\left(\frac{2\pi u}{a}\right)\right]\right\} \tag{2}$$

where m is the mass of the adatom and $w_{\parallel}$ is a coefficient characterising the linear interaction of adatoms in the chain.

For two parallel chains, it is necessary to take into account the energy of interaction between them, which is caused by the anisotropic interaction of adsorbed atoms [15, 16]. When the displacements of adatoms are not small, it is difficult to obtain the exact expression for the interaction between adatoms of different chains. In the present work we assume the following expression for the interaction energy:

$$\mathcal{H}_{int}\{u_1, u_2\} = w_{\perp}^{(1)}\int \frac{dx}{a}\left[\cos\left(\frac{2\pi}{a}(u_1-u_2)\right)-1\right] + w_{\perp}^{(2)}\int \frac{dx}{a}\frac{\partial u_1}{\partial x}\frac{\partial u_2}{\partial x} \tag{3}$$

where u_1 and u_2 are the displacements of adatoms in the first and second chains. The model expression (3) takes into account three important circumstances:

(i) the correct behaviour of the energy density $\mathcal{H}_{int}$ for small relative displacements in different chains ($\mathcal{H}_{int} \sim (u_1-u_2)^2$; the first term in (3));

(ii) the constancy of the interaction energy for the displacement of all adatoms of one chain by a value that is a multiple of the lattice constant a (i.e. $u_1(x) \rightarrow u_1(x) + na$);

(iii) the existence of an interaction between equivalent excitations of two chains, when $u_1 = u_2$ (the second term in (3)).

The states $u(x) = an$ ($n = \pm 1, \pm 2, \ldots$) correspond to the commensurate structure. Therefore, the deviation from these states is defined by the value

$$\rho(x) = -\frac{1}{a}\frac{\partial u}{\partial x}$$

which is equal to the density of the excess (with respect to the commensurate structure) adatoms. The total number of excess atoms is equal to

$$\sigma = \int_{-\infty}^{\infty}\rho(x)\,dx = -[u(+\infty) - u(-\infty)]/a.$$

The parameters $w_{\perp}^{(1,2)}$ in (2) and (3) correspond to the interaction of adatoms of different chains, and the parameter $w_{\parallel}$ characterises the interaction of adatoms along the chain. It is important to note that in our model the interaction along the chains should be repulsive (i.e. $w_{\parallel} > 0$), but the interaction between the chains may be either repulsive ($w_{\perp} > 0$) or attractive ($w_{\perp} < 0$). Let us introduce the new variables $\tilde{u} = 2\pi u/a$, $\tilde{t} = \omega_0 t$ and $\tilde{x} = x/l_0$, where $l_0 = c_0/\omega_0$, $\omega_0 = (2\pi^2\varepsilon_D/a^2m)^{1/2}$ being the frequency of oscillations of one isolated adatom, and $c_0 = (w_{\parallel}/m)^{1/2}$ being the velocity of sound in the chain. In this notation the interaction energy for two coupled adatomic chains may be represented as

$$\mathcal{H}\{u_1, u_2\} = \varepsilon_0\int dx\left[\frac{1}{2}\left(\frac{\partial u_1}{\partial t}\right)^2 + \frac{1}{2}\left(\frac{\partial u_1}{\partial x}\right)^2 + (1-\cos u_1) + (1\rightarrow 2) - \alpha[1-\cos(u_1-u_2)] + \beta\frac{\partial u_1}{\partial x}\frac{\partial u_2}{\partial x}\right] \tag{4}$$

where

$$\varepsilon_0 = \frac{\varepsilon_D c_0}{2a\omega_0} = \frac{1}{4\pi}(2\varepsilon_D w_\parallel)^{1/2} \qquad \alpha = \frac{w_\perp^{(1)}}{\varepsilon_0} \qquad \beta = \frac{w_\perp^{(2)}}{w_\parallel}.$$

From (4) one can obtain the dynamic equations

$$\frac{\partial^2 u_1}{\partial t^2} - \frac{\partial^2 u_1}{\partial x^2} + \sin u_1 = -\alpha \sin(u_1 - u_2) + \beta \frac{\partial^2 u_2}{\partial x^2} \tag{5a}$$

$$\frac{\partial^2 u_2}{\partial t^2} - \frac{\partial^2 u_2}{\partial x^2} + \sin u_2 = -\alpha \sin(u_2 - u_1) + \beta \frac{\partial^2 u_1}{\partial x^2} \tag{5b}$$

which describe the dynamics of non-linear excitations in the coupled chains of adatoms. From the linear approximation of (5) there follow two branches of the dispersion relation:

$$\omega^2 = 1 + (1 + \beta)k^2 \tag{6a}$$

$$\omega^2 = 1 + 2\alpha + (1 - \beta)k^2. \tag{6b}$$

At $\beta = 0$ equation (6*a*) is the dispersion relation for the SG system and corresponds to co-phased vibrations of adatoms, and equation (6*b*) describes anti-phased vibrations of adatoms.

We shall consider the realistic case when the signs of the parameters α and β are the same. For such a case the dispersion relations (6) intersect themselves at the point $k = k_0$, where

$$k_0^2 = \alpha/\beta = 4\pi^2(l_0/a)(w_\perp^{(1)}/w_\perp^{(2)}) \gg 1.$$

3. Motion of a kink in one of the coupled chains

In the absence of an interaction between the atomic chains (i.e. at $\alpha = \beta = 0$), the kink-type solution of the SG equation is (see e.g. [6])

$$u_K(x, t) = 4 \tan^{-1}\left[\exp\left(\sigma \frac{x - vt}{(1 - v^2)^{1/2}}\right)\right] \tag{7}$$

where v is the kink's velocity and $\sigma = \pm 1$ is its polarity (topological charge). At $\sigma = +1$ the solution (7) (so-called kink) describes an excess atom. The soliton solution (7) characterises the excitation localised on length l_0 which moves with velocity $v = V/c_0$ and has energy

$$E_K = E_0[1 - (V/c_0)^2]^{-1/2} \approx E_0 + \tfrac{1}{2}m_K V^2 \qquad E_0 = 8\varepsilon_0 \tag{8}$$

where m_K is the effective mass of the kink:

$$m_K = (2/\pi^2)ma/l_0 \ll m. \tag{9}$$

The continuum limit used may be applied when the interaction of adatoms along the chain sufficiently exceeds the height of the substrate potential relief (i.e. for $w_\parallel \gg \varepsilon_D$). In this case the kink length is large with respect to the substrate period a (i.e. $l_0 \gg a$), and the relative displacements of neighbouring atoms is small [14]:

$$\partial u/\partial x \simeq (u_{j+1} - u_j)/a \ll 1.$$

Let us consider the motion of a kink in one (e.g. the first) chain of the system of two coupled ones, when the inter-chain coupling is small, i.e. for $\alpha, \beta \ll 1$. Substituting in (5) the perturbation series

$$u_1 = u_K + u_1^{(1)} + \dots \tag{10a}$$

$$u_2 = u_2^{(1)} + \dots \tag{10b}$$

where u_K is defined by (7), and $u_{1,2}^{(1)} \sim \varepsilon$, $\varepsilon \equiv \{\alpha, \beta\}$, one can obtain to first order in α and β the equation for the wave field of the second chain:

$$\frac{\partial^2 u_2}{\partial t^2} - \frac{\partial^2 u_2}{\partial x^2} + u_2 = \alpha \sin u_K + \beta \frac{\partial^2 u_K}{\partial x^2} \tag{11}$$

where $u_2 \equiv u_2^{(1)}$. The steady-state solution of the linear equation (11) may be written as

$$u_2(z) = -2\sigma[\alpha + \beta/(1-v^2)] \operatorname{sgn} z[z \cosh z - \sinh z \lg(2 \cosh z)] \tag{12}$$

where

$$z \equiv (x - vt)/(1-v^2)^{1/2}. \tag{13}$$

The solution (12) describes the 'response' of the second chain to the non-linear excitation (kink) in the first one. In the same approximation the kink shape is also distorted. According to the perturbation theory for solitons, one can obtain (see [17])

$$u_1^{(1)} = 2\alpha \tanh z \operatorname{sech} z + O(\alpha^2, \beta^2) \tag{14}$$

and therefore the effective mass of the distorted kink is

$$\tilde{m}_K = m_K(1 + \alpha/2) + O(\alpha^2, \beta^2). \tag{15}$$

It is important to note that in the continuum limit the steady-state motion of the kink is not accompanied by emission of linear waves, i.e. the radiative losses are absent.

4. Interaction energy of kinks belonging to different chains

Let us consider another case when in the second chain of the coupled system there is a kink with velocity v_2 ($v_2 \neq v_1$). Each of the kinks creates its 'response' in the neighbouring chain, and the collision of the kinks belonging to the different chains may be considered as the interaction of the first kink with the 'response' of the second one and vice versa. This interaction we shall analyse in the framework of perturbation theory for solitons (e.g. [17–20]), i.e. under the conditions that the terms $\alpha \sin(u_1 - u_2)$, $\beta \partial^2 u_1/\partial x^2$ and $\beta \partial^2 u_2/\partial x^2$ in equation (5) are small perturbations (small coupling between the chains).

According to [17, 18], the perturbation-induced evolution of the kinks' velocities v_n ($n = 1, 2$) and coordinates ζ_n (for the unperturbed kink $\zeta_n = v_n t + \zeta_n(0)$) is described by the set of four adiabatic equations

$$\dot{v}_1 = -\tfrac{1}{4}\sigma_1(1-v_1^2)^{3/2} \int_{-\infty}^{\infty} dz_1 \, R_1(z_1, z_2) \operatorname{sech} z_1 \tag{16a}$$

$$\dot{\zeta}_1 = v_1 - \tfrac{1}{4}\sigma_1 v_1(1-v_1^2) \int_{-\infty}^{\infty} dz_1 \, R_1(z_1, z_2) z_1 \operatorname{sech} z_1 \tag{16b}$$

and two analogous equations for the second kink which follow from (16) by substituting $1 \rightleftarrows 2$. In equations (16) we introduce the notation

$$R_1 = -\alpha \sin(u_1 - u_2) + \beta \partial^2 u_2/\partial x^2$$
$$R_2 = -\alpha \sin(u_2 - u_1) + \beta \partial^2 u_1/\partial x^2. \tag{17}$$

For the slow kinks, when $v_{1,2}^2 \ll 1$, calculation of the integrals in (16) yields

$$\dot{\zeta}_1 = v_1 \qquad \dot{v}_1 = \tfrac{1}{8} I_\sigma(\zeta_1 - \zeta_2) \tag{18a}$$

and similar equations for the second kink ($1 \rightleftarrows 2$):

$$\dot{\zeta}_2 = v_2 \qquad \dot{v}_2 = -\tfrac{1}{8} I_\sigma(\zeta_1 - \zeta_2) \tag{18b}$$

where $\sigma = \sigma_1\sigma_2$ is the relative polarity of the kinks. The odd function $I_\sigma(x)$ may be represented as

$$I_\sigma(x) = -\frac{\mathrm{d}}{\mathrm{d}x} U_\sigma(x)$$

where

$$\begin{aligned} U_\sigma(x) &= -\alpha U_\sigma^{(1)}(x) + \beta U_\sigma^{(2)}(x) \\ &= (8\alpha/\sinh^3 x)[2(x - \tanh x)\cosh x - \sigma(2x - \sinh 2x + x \sinh^2 x)] \\ &\quad + 8\beta\sigma x/\sinh x \end{aligned} \tag{19}$$

and the parameter $\zeta \equiv \zeta_1 - \zeta_2$ is the relative distance between the kinks. As follows from (18) and (19), the equations for the kink parameters correspond to the 'two-particle' Hamiltonian

$$H = \tfrac{1}{16}(p_1^2 + p_2^2) + U_\sigma(\zeta_1 - \zeta_2) \tag{20}$$

where $p_1 = 8v_1$ and $p_2 = 8v_2$ are the momenta of the effective 'particles' and the last term on the RHS of equation (20) is the potential energy of their interaction. It is important that this energy is determined by the parameters of the coupling between adatoms of different chains and the relative polarity of the kinks (i.e. type of excitations).

In the case of strongly overlapping kinks, i.e. for $\zeta \ll 1$, the interaction energy $U_\sigma(\zeta)$ may be represented as

$$U_\sigma(\zeta) = A + B\zeta^2 \tag{21a}$$

$$A = 8[\tfrac{1}{3}\alpha(2 + \sigma) + \beta\sigma] \tag{21b}$$

$$B = \tfrac{1}{3}[-\tfrac{1}{3}\alpha(8 + 7\sigma) - \beta\sigma]. \tag{21c}$$

From equations (21) it follows that the first term on the RHS of (3) does not depend on the relative polarity of the kinks, but the second one is proportional to the effective parameter $\beta\sigma$. For large ζ, when the relative distance between the kinks tends to infinity, the character of their interaction is sufficiently determined by the relative polarity, i.e.

$$U_\sigma(\zeta) \simeq 16\sigma(\beta - \alpha)|\zeta| \exp(-|\zeta|) \qquad |\zeta| \gg 1. \tag{22}$$

It is easy to prove that the energy $U_\sigma^{(2)}(\zeta)$ is described for $\zeta > 0$ by a monotonic function. The dependence of $U_\sigma^{(1)}(\zeta)$ on the relative distance is more complicated, and is shown in figures 1(*a*) at $\sigma = -1$ and 1(*b*) at $\sigma = +1$. It is interesting to note that in the simpler model when $\alpha \neq 0$ the energy of kink interaction is a sufficiently non-monotonic function.

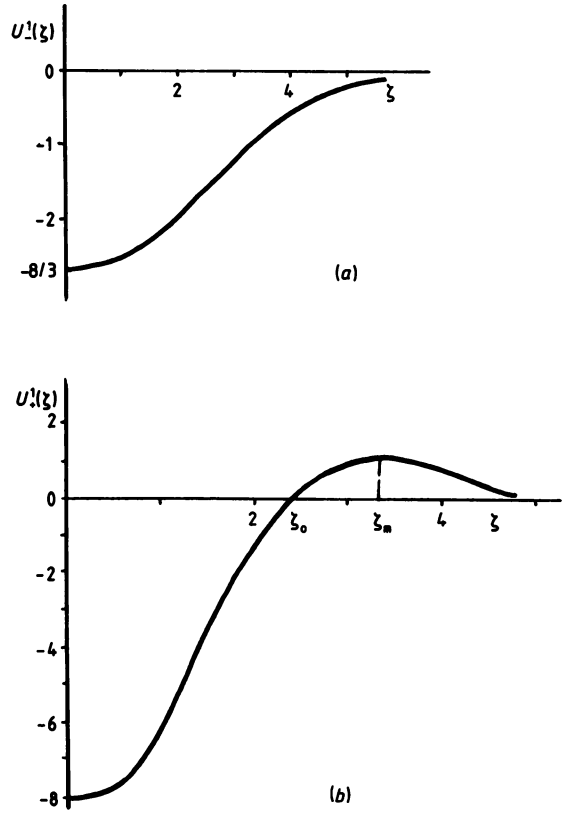

Figure 1. The dependence of energy $U_\sigma^{(1)}(\zeta)$ on relative distance between kinks belonging to different chains for $\zeta > 0$: (*a*) $\sigma = -1$; (*b*) $\sigma = +1$. $U_\sigma^{(1)}(\zeta)$ is an even function; $\zeta_0 \approx 2.39$ and $\zeta_m \approx 3.44$.

We present a more detailed analysis of kink interaction at sgn α = sgn β, i.e. for $\alpha\beta > 0$. According to (21) *kinks of equal polarities* ($\sigma = +1$) in the case of inter-chain attraction ($\alpha < 0$, $\beta < 0$) may form a stable bound state at $\zeta = 0$ with bound energy $8\varepsilon_0(\alpha + \beta)$. The bound state of the kinks belonging to different chains is similar to the well known breather of the SG equation [6], but unlike the breather this bound state may be a static one. The slightly excited bound state of the kinks is characterised by the frequency of small internal oscillations

$$\omega_b = 2\omega_0[-(\beta/3 + \alpha)]^{1/2}. \tag{23}$$

In the case of the inter-chain repulsion (i.e. $\alpha > 0, \beta > 0$), the interaction of the kinks is more complicated. For small relative distances, the kinks are repelled from one another. However, for $\alpha > \beta$ the interaction energy $U_+(\zeta)$ has a small minimum at $\zeta > \zeta_m \approx 3.44$ and the kinks may form a bound state, as for the case of inter-chain attraction. The ζ dependence of the effective energy $U_+(\zeta)$ for the interaction of kinks of equal polarities at $\alpha > 0$, $\beta > 0$ is depicted in figures 2(*a*) ($\alpha < \beta$) and 2(*b*) ($\alpha > \beta$).

The interaction of *kinks of opposite polarities* ($\sigma = -1$) is determined by the ratio of the parameters α and β. For $0 < \alpha < 3\beta$ the strongly overlapping kinks attract them-

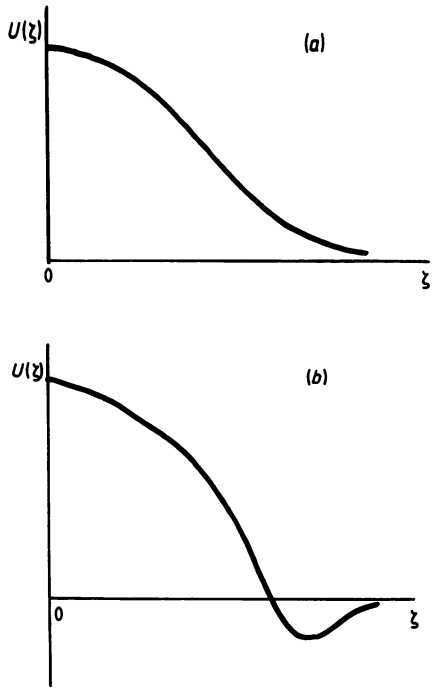

Figure 2. The effective interaction energy of kinks of the same polarities for $\alpha > 0$ and $\beta > 0$: (*a*) $\alpha < \beta$; (*b*) $\alpha > \beta$. The even function $U(\zeta)$ is shown for $\zeta > 0$ only.

selves and form a bound state with bound energy $8\varepsilon_0|-\alpha/3+\beta|$, the frequency of the excited internal oscillations being $\omega_b = 2\omega_0(\beta/3-\alpha/15)^{1/2}$. Analogously, the kink and anti-kink may form a stable bound state for $|\alpha| > 5|\beta|$ if $\alpha < 0, \beta < 0$. The ζ dependence of the interaction energy of the opposite-polarity kinks on the relative distance between them is depicted on in figures 3(*a*) ($\alpha < \beta$), 3(*b*) ($\beta < \alpha < 3\beta$), 3(*c*) ($3\beta < \alpha < 5\beta$) and 3(*d*) ($\alpha > 5\beta$) for $\alpha > 0, \beta > 0$. So, the shape of the interaction energy varies appreciably with the correlation of the parameters α and β of the inter-chain coupling.

It is interesting to note that the set of equations (5) has exact solutions for any values of the parameters α and β that correspond to bound states of kinks belonging to the different chains. Indeed, substituting

$$u_2 = \sigma u_1 \qquad \sigma = \pm 1 \tag{24}$$

one can obtain the equation for one wave field, e.g. for the function u_1: either the SG equation in the case $\sigma = +1$ (i.e. $u_1 = u_2$), or the so-called double SG equation in the case $\sigma = -1$ (i.e. $u_1 = -u_2$). One-soliton solutions of these equations are well known, but in our problem it is necessary to investigate the stability of the solutions in the framework of the general system (5). Let us consider, for example, static kinks of equal polarities ($\sigma = +1$) at $\alpha \neq 0$ and $\beta = 0$. For stability analysis one can represent the solution of equations (5) as

$$u_1 = u_K + \psi_1 \qquad u_2 = u_K + \psi_2 \qquad \psi_{1,2} \ll 1 \tag{25}$$

where u_K is the one-soliton solution (7) at $v = 0$, which describes the quiescent kink. Substituting (25) into (5), to first order in α and β ($\psi_1, \psi_2 = O(\alpha, \beta)$) one can obtain

the set of linear equations

$$\frac{\partial^2}{\partial t^2}\Psi + \hat{L}\Psi = 0 \qquad \Psi = \begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{26}$$

where

$$\hat{L} = \begin{pmatrix}L_0+\alpha & -\alpha\\ -\alpha & L_0+\alpha\end{pmatrix} \qquad L_0 = -\frac{\partial^2}{\partial x^2} + 1 - \frac{2}{\cosh^2 x}. \tag{27}$$

The operator L_0 has been investigated in the theory of the perturbed SG equation and its properties are well known (see e.g. [21]). The eigenfunction of the discrete spectrum is

$$f_b(x) = (1/\sqrt{2})\,\mathrm{sech}\,x \tag{28}$$

which corresponds to the zero eigenvalue, i.e. $L_0 f_b = 0$. The eigenfunctions of the continuous spectrum are

$$f_c(x) = \frac{1}{(2\pi)^{1/2}}\frac{e^{ikx}(k + i\tanh x)}{(1+k^2)^{1/2}} \tag{29}$$

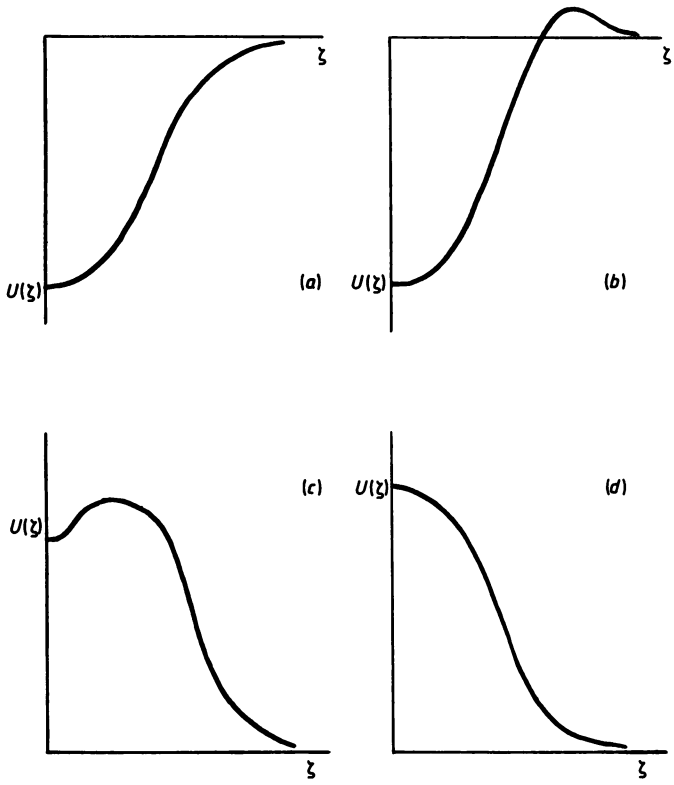

Figure 3. The effective interaction energy of kinks of opposite polarities for $\alpha > 0$ and $\beta > 0$: (*a*) $\alpha < \beta$; (*b*) $\beta < \alpha < 3\beta$; (*c*) $3\beta < \alpha < 5\beta$; (*d*) $\alpha > 5\beta$. The even function $U(\zeta)$ is shown for $\zeta > 0$ only.

which correspond to the eigenvalues $\omega_k^2 = 1 + k^2$, where k is the wavenumber ($|k| < \infty$). Using the properties of L_0 one can obtain the eigenvalues of the operator L (27): its discrete spectrum is

$$\lambda_b^{(1)} = 0 \qquad \lambda_b^{(2)} = 2\alpha \tag{30}$$

and its continuous spectrum is

$$\begin{aligned} \lambda_c^{(1)} &= \omega_k^2 = 1 + k^2 \\ \lambda_c^{(2)} &= \omega_k^2 + 2\alpha = 1 + 2\alpha + k^2. \end{aligned} \tag{31}$$

The discrete spectrum corresponds to the displacement of the coupled kink pair as a whole ($\lambda_b^{(1)} = 0$) and to the internal oscillations of kinks in the pair ($\lambda_b^{(2)} = 2\alpha$). It is evident that, at $\alpha > 0$, the static bound state of the kinks is unstable and it decays into a pair of free kinks belonging to the different chains. For $\alpha < 0$, when $\lambda_b^{(2)} < \lambda_b^{(1)}$, the kink bound state is stable. This result corresponds to that obtained within the framework of perturbation theory (see the first part of this section) for small α. Analogously, one can investigate the stability of exact solutions of equation (5) in the more general case when $\beta \neq 0$; the corresponding results coincide with the results of the perturbation theory for solitons.

5. Dynamics of kinks in damped DC-driven coupled chains

5.1. General equations

In real physical systems the motion of an adatom is damped by the dissipative force

$$F_n = -\eta m \frac{\partial u_n}{\partial t}$$

where η is a dissipative coefficient [16]. To compensate for these dissipative losses, one can apply to an adatomic chain the external driving force $F = e^*\mathscr{E}$, where e^* is the effective charge of an adatom and $\mathscr{E}$ is the electric field along the crystal surface. Then the SG equation for adatom displacement is modified to

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + \sin u = -\gamma \frac{\partial u}{\partial t} + f \tag{32}$$

where $\gamma = \eta/\omega_0$ and $f = Fa/\pi\varepsilon_D$ are the dimensionless dissipative coefficient and driving force, respectively. The stationary solution of (32) is known to describe the steady-state motion of a kink, i.e. the drift of a kink with velocity [18, 21]

$$v_f = \tfrac{1}{4}\pi\sigma_0 f/\gamma \tag{33}$$

where σ_0 is the kink polarity. The mobility of the kink is

$$\mu_K = (v_f c_0)/F = 1/\eta m_K. \tag{34}$$

To study the dynamics of kinks in a pair of dissipative chains, one must take into account the dissipative and driving forces in equations (5). According to (32), the adiabatic equations for the kink parameters may be represented as

$$\ddot{X} = \tfrac{1}{8}\pi f(\sigma_1 + \sigma_2) - \gamma\dot{X} \tag{35a}$$

$$\ddot{\rho} = \tfrac{1}{8}\pi f(\sigma_1 - \sigma_2) - \gamma\dot{\rho} + \tfrac{1}{8}I_\sigma(2\rho) \tag{35b}$$

where the following handy notation is introduced: the coordinate of the kinks' centre of mass is

$$X = \tfrac{1}{2}(\zeta_1 + \zeta_2) \tag{36}$$

and the relative distance between the kinks is

$$\rho = \tfrac{1}{2}\zeta = \tfrac{1}{2}(\zeta_1 - \zeta_2). \tag{37}$$

According to (35), *kinks of equal polarities* interact with one another very simply. Indeed, in the case $\sigma_1 = \sigma_2 = \sigma_0$, we obtain from (35*a*) the equation

$$\ddot{X} = \tfrac{1}{4}\pi f \sigma_0 - \gamma \dot{X} \tag{38}$$

which describes for $t \gg \gamma^{-1}$ the steady-state motion of the kinks' centre of mass with velocity (cf (33))

$$\dot{X} = v_f. \tag{39}$$

The effective equation (35*b*) describes the dissipative motion of the effective particle in the potential

$$\ddot{\rho} = -\gamma\dot{\rho} + \tfrac{1}{8}I_+(2\rho) \tag{40}$$

i.e. the external force does not affect the relative motion of the kinks belonging to different chains. So, the dynamics of kinks of equal polarities under dissipative losses is determined by the shape of the effective potential. Moving in the dissipative chains, the kinks either repel one another and the relative distance between them tends to infinity, or attract one another and form bound states that correspond to the minima of the effective potential $U_+(2\rho)$. For example, at $\beta = 0$ such minima exist for $\alpha < 0$ ($\rho_{\min} = 0$) as well as for $\alpha > 0$ ($\rho_{\min} = \pm\rho_0$, where $\rho_0 \approx 1.72$) (see figure 1). In the former case the kinks strongly overlap, while in the latter they are situated at a distance $2\rho_0 \approx 3.44$. It is important to note that, in real discrete systems at a distance of order R_P, kinks should be pinned by the Peierls relief, which satisfies the condition $|U_\sigma(R_P)| \simeq \varepsilon_P$, ε_P being the Peierls energy.

5.2. *Kinks of opposite polarities: repulsion*

Let us consider the more interesting case when kinks belonging to different chains have opposite polarities (i.e. the kink–anti-kink interaction): $\sigma_1 = -\sigma_2 = \sigma_0$. In this case the external force pulls the kink and anti-kink in opposite directions, and the kinks' centre of mass is at rest, since $\dot{X} \sim \exp(-\gamma t)$. To study the kinks' dynamics, it is convenient to rewrite (35*b*) as a set of two equations

$$\begin{aligned} \dot{\rho} &= v \\ \dot{v} &= \gamma(v_f - v) + \tfrac{1}{8}I_-(2\rho) \end{aligned} \tag{41}$$

and to analyse it on the phase plane of the parameters ρ and $\dot{\rho}$. The set of equations (41) has singular points $(0, \rho_n)$, where ρ_n are the roots of the equation

$$\gamma v_f + \tfrac{1}{8}I_-(2\rho) = 0 \tag{42}$$

which exist for any signs of α and β, if

$$|f| \leqslant f_{\max} \equiv \frac{1}{2\pi}|I_-(2\rho_0)| \tag{43}$$

ρ_0 being determined by the equation

$$d^2U_-(2\rho)/d\rho^2 = 0.$$

In the cases $\alpha < \beta < 0$ and $\alpha > 5\beta > 0$ the set of equations (41) has two singular points $(0, \rho_2)$ and $(0, \rho_1)$; the former is the focus while the latter is the saddle. The phase curves are depicted in figure 4(*a*). The larger root $|\rho_2|$ (focus) corresponds to the stable bound state of two kinks, the distance between the kinks being

$$\rho_* = \max\{|\rho_1|, |\rho_2|\}$$

where $\rho_{1,2}$ are real roots of (42). At $\gamma = 0$ the frequency of the slightly excited internal oscillations of the bound state of the kinks is

$$\omega_b = \frac{\omega_0}{2}\left\{\left[\frac{d}{d\rho} I(2\rho)\right]_{\rho=\rho_*}\right\}^{1/2}. \tag{44}$$

It is obvious that the existence of a breather-like bound state of kinks in the case of their repulsion is stipulated by the compensation of the kinks' repulsion force and the external driving force.

A bound state of the kinks should be formed during the collision of the free kink and anti-kink when their relative velocity v is less than the threshold value. In the case of repulsion, it is rather simple to obtain the binding threshold condition: one should demand the height $4|\alpha/3 - \beta|$ of the potential barrier (see e.g. figure 3(*d*)) to be larger than the sum of the kinetic energies of the two free kinks prior to the collision: $K_1 + K_2 \simeq 8v_f^2 \approx 8(\pi f/4\gamma)^2$ (cf an analogous condition for trapping the kink by a repulsive impurity [18, 21–23]). So, the threshold inequality is

$$|f| < f_{thr} = (4\gamma/\pi)(|\alpha/3 - \beta|)^{1/2}. \tag{45}$$

Under the conditions (43) and (45) and for $\alpha > \beta > 0$ or $\alpha > 5\beta > 0$, the colliding kink and anti-kink bind themselves into a bound breather-like state and the latter is damped due to dissipative losses. These dynamic processes are presented on the phase plane (see figure 4(*a*), hatched area) by the curves ending at the focus. If at least one inequality from (43) and (45) is not valid, the kinks do not form a bound state after their collision, and their relative velocity tends to the constant value v_f.

5.3. Kinks and opposite polarities: attraction

In the cases $0 < \alpha < \beta$ or $0 > \alpha > 5\beta$, when the kinks attract themselves, the set of equations (41) also has two singular points when (43) is valid. The stable bound state of the kinks corresponds to the singular point with the smaller value $|\rho|$, so the distance between the kink and anti-kink in this case is

$$\rho_{**} = \min\{|\rho_1|, |\rho_2|\}. \tag{46}$$

Therefore, the external force moves the kinks aside, forming a bound state, and sufficiently changes their bound energy.

The calculation of the threshold value of the external driving force for the binding of the free kink and anti-kink is more difficult. To obtain the threshold condition for the attraction of kinks, it is necessary to calculate the total dissipative energy losses ΔE during the collision between the kinks; then the threshold condition may be written as

$$\Delta E \geqslant K_1 + K_2 \tag{47}$$

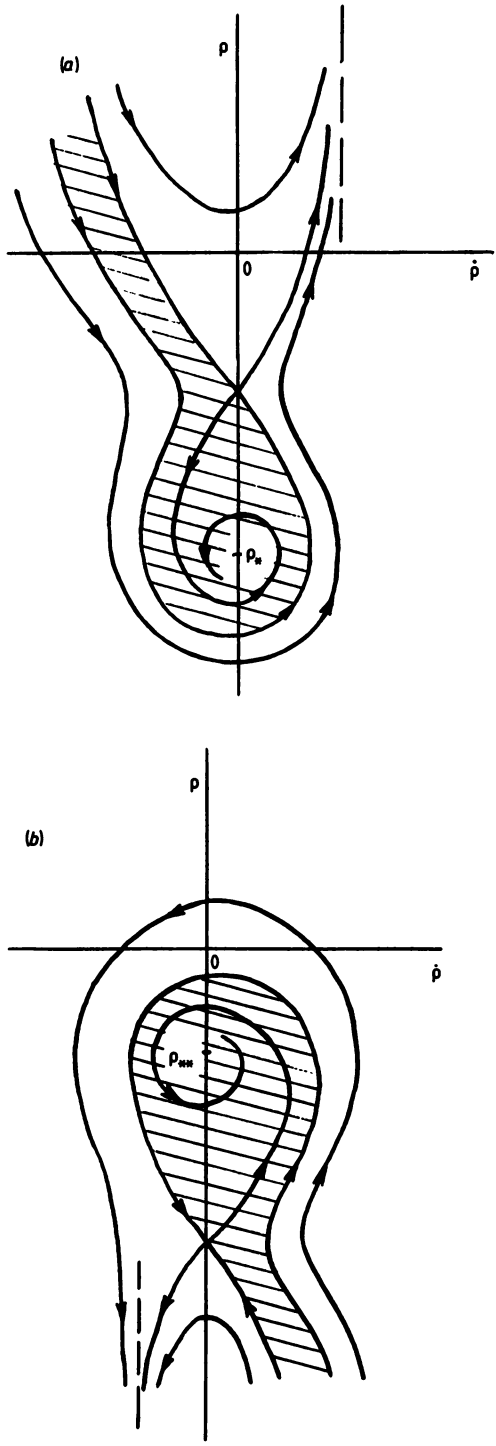

Figure 4. Phase plane for equation (41) in the case $f > 0$: (*a*) repulsion of kinks of opposite polarities (for $\alpha < \beta < 0$ or $\alpha > 5\beta > 0$); (*b*) attraction of kinks of opposite polarities (for $0 < \alpha < \beta$ or $5\beta < \alpha < 0$). The hatched areas correspond to the capture of kinks and the formation of their bound state.

where $K_{1,2}$ are, as above, the kinetic energies of the two kinks prior to the collision. The quantity ΔE can be calculated as (see [22, 23])

$$|\Delta E| = \gamma \int_{-\infty}^{\infty} \dot{X}^2(t)\,\mathrm{d}t = \gamma \int_{-\infty}^{\infty} \dot{X}(X)\,\mathrm{d}X. \tag{48}$$

To calculate (48) we have used the law of relative kink motion (41).

Therefore, the threshold value of the external force is (cf an analogous condition for trapping of the kink by an attractive inhomogeneity [22, 23])

$$f_{\mathrm{thr}} = (1/\pi)2^{1/4}\gamma^{3/2}\left(\int_{-\infty}^{\infty} \mathrm{d}x\,[|\alpha U^{(1)}(x) + \beta U^{(2)}(x)|]^{1/2}\right)^{1/2}. \tag{49}$$

So, we obtain $f_{\mathrm{thr}} \sim \gamma^{3/2}\mathrm{O}(\alpha^{1/4}, \beta^{1/4})$, i.e. in the latter case the threshold value of f is sufficiently less than in the former one (cf (45)).

6. Excitation of internal oscillations of bound kinks

The internal oscillations of the bound state of kinks belonging to different chains may be excited either by other kinks colliding with the bound ones or by the application of external alternating forces. The former way is based on the inelastic interaction of kinks in perturbed non-linear systems. Let us consider this problem without dissipative and external forces when the system of two coupled chains contains a quiescent bound state of kinks belonging to different chains. The law of relative motion for the bound kinks may be obtained from (41) as

$$4\int_{\rho_1}^{\rho_2} \frac{\mathrm{d}\rho}{[|U_\sigma(2\rho)| - E]^{1/2}} = t + \text{constant} \tag{50}$$

where $U_\sigma(2\rho)$ is determined in (19) and E is the binding energy ($0 < E < |U_{\mathrm{min}}|$). It is evident (see (50)) that the binding energy E of the kink is of the order of α and β, while the frequency of the internal oscillations is of the order of $\alpha^{1/2}$, $\beta^{1/2}$.

The collision of a fast kink in the first chain with a bound kink belonging to the bound state is described by equation (50) and may result in inelastic effects analogous to those dealt with in [24, 25, 29]: kicking out the slow kink in the first chain from the bound state. If the incident kink is not too slow, we may use the expression for the collision-induced phase shift $\Delta\rho$ of the slow (bound) kink, valid in the absence of perturbations [6]:

$$\Delta\rho = \tfrac{1}{2}\lg\left(\frac{1 - (1 - v_{\mathrm{fast}}^2)^{1/2}}{1 + (1 - v_{\mathrm{fast}}^2)^{1/2}}\right) \tag{51}$$

v_{fast} being the fast kink velocity. The collision duration is of the order of v_{fast}^{-1}, which is much smaller than the bound kink oscillation period $4\pi/E^{1/2} = \mathrm{O}(\alpha^{-1/2}, \beta^{-1/2})$. Hence we may neglect the change of the bound kink's velocity during the collision. Thus, the collision does not change the slow kink's kinetic energy, while according to (50) and (51) its potential energy acquires a change

$$\Delta U = U(2\rho_0 + 2\Delta\rho) - U(2\rho_0)$$

ρ_0 being the instantaneous value of the slow kink coordinate before the collision. For example, in the case $\alpha \neq 0$, $\beta = 0$, one can obtain

$$\Delta U \approx \tfrac{4}{15}\alpha(\Delta\rho)^2.$$

So, it is evident that the bound state of the kinks decays provided $\Delta U > E$, and the kinks remain bound in the opposite case. This consideration and the final results are valid provided $v_{\text{fast}} \gg \alpha^{1/2}, \beta^{1/2}$. In the presence of dissipative and DC driving forces, the fast kink's velocity is fixed and given by (33), while the potential energy is changed as follows:

$$U_\sigma(2\rho) \rightarrow U_\sigma(2\rho) + 4\gamma v_f \rho.$$

The above consideration is valid in this case too, if (i) the dissipative forces are not very large, i.e. $\gamma_1, \gamma_2 \ll \alpha^{1/2}, \beta^{1/2}$, and (ii) when potential minima exist, i.e. for $f < f_{\text{cr}}$, where f_{cr} is determined from the condition $\gamma v_f = \frac{1}{8} I_\sigma(2\rho_{\min})$.

Another way to excite internal oscillations of bound kinks belonging to different chains is to apply an external AC force. This additional force may be taken into account in (5) by the substitution:

$$f \rightarrow f_0 + f_1 \cos(\Omega t) \tag{52}$$

Ω being the external frequency. Then the amplitude b of the forced internal oscillations of the bound kinks is

$$b = \tfrac{1}{4}\pi f_1 [(\Omega^2 - \omega_b^2)^2 + \gamma^2 \Omega^2]^{-1/2}$$

ω_b being the kink's eigenfrequency.

A system of adatoms in which a bound state of kinks belonging to different chains has been excited absorbs the energy of the microwave field, and the dependence of the average absorbed power on the external force frequency has resonant form for $\Omega \sim \omega_b$. Thus, an absorbed structure in which bound states have been created should give a response to an additional microwave pulse of frequency approximately equal to ω_b.

7. Emission of radiation from colliding kinks

In § 4 we consider the so-called adiabatic approximation to describe the collision of kinks. In the framework of this approximation, kinks collide elastically, i.e. without energy losses. Indeed, if we calculate the total changes of the kinks' velocities as

$$\Delta v_{1,2} = \int_{-\infty}^{\infty} \mathrm{d}t \, \mathrm{d}v_{1,2}/\mathrm{d}t$$

we obtain $\Delta v_1 = \Delta v_2 = 0$. However, the collision of kinks belonging to different chains stipulates the phase shifts of the kinks, caused by inter-chain interactions. For example, at $\beta = 0$ one can obtain

$$\Delta\zeta_1 = -\frac{2\alpha v_1 (1 - v_1^2)(1 - v_2^2)^{1/2}}{|v_2 - v_1|} \qquad \Delta\zeta_2 = \frac{2\alpha v_2 (1 - v_2^2)(1 - v_1^2)^{1/2}}{|v_2 - v_1|}. \tag{53}$$

On a level with the phase shifts the colliding kinks will emit radiation, i.e. dispersive linear wavepackets. We shall calculate the total energy and its spectral density emitted by colliding kinks belonging to different chains.

A general method for calculating the emitted energy radiated by colliding solitons has been put forward in [24, 29]. In this problem the emitted energy can be found explicitly for all values of the kink velocities v_1 and v_2 except for the case when their relative velocity $v = v_1 - v_2$ is very small, i.e. for $v^2 \ll v_{\text{thr}}^2$, as in this case the collision may result in dissipative (or radiative) binding of the kinks into a bound state.

In terms of the inverse scattering transform, a radiation component of the SG wave field is described by the complex amplitude $\delta(\lambda)$ (the so-called Jost coefficient [6]) where the real spectral parameter λ is related to the radiation wavenumber k and frequency ω: $k = \lambda - 1/4\lambda$, $\omega = \lambda + 1/4\lambda$. The perturbation-induced evolution for $\delta(\lambda)$ is well known (see e.g. [19, 30]). For our purpose, it can be conveniently written in the form

$$\partial B(\lambda, t)/\partial t = (\mathrm{i}/4)a(\lambda) \int_{-\infty}^{\infty} \mathrm{d}x\, P[u]\{[\Psi^{(2)*}(x, t; \lambda)]^2 - [\Psi^{(1)*}(x, t; \lambda)]^2\} \tag{54}$$

where

$$B(\lambda, t) \equiv \delta(\lambda, t) \exp[\mathrm{i}\omega(\lambda)t]$$

$P[u]$ stands for the perturbation on the RHS of the SG equation, $a(\lambda)$ is the second Jost coefficient, $|a(\lambda)|^2 \approx 1$, and $\Psi^{(1,2)}(x, t; \lambda)$ are components of the so-called Jost function. For the one-soliton solution (7) of the SG equation, these functions have been given, for example, in [30, 31]. Assuming the radiation is absent prior to the collision of kinks, i.e. $B(\lambda, t = -\infty) = 0$, we can calculate the final value $B_f(\lambda)$ of the radiation amplitude as

$$B_f(\lambda) = B(\lambda, t = +\infty) = \int_{-\infty}^{\infty} \frac{\partial B(\lambda, t)}{\partial t}\, \mathrm{d}t. \tag{55}$$

The basic physical characteristic of the emitted radiation is the spectral density $\mathscr{E}(k)$ of its total energy E_{em} (see e.g. [17, 24, 28, 29])

$$\mathscr{E}(k) = \frac{\mathrm{d}E_{\mathrm{em}}}{\mathrm{d}k} = \frac{1}{\pi}|B_f[\lambda = \tfrac{1}{2}\{k + (1 + k^2)^{1/2}\}]|^2. \tag{56}$$

The distinctive feature of the present problem is that the colliding kinks generate radiation in both chains, i.e. the radiation field is made up of the functions $\mathscr{E}_1(k)$ and $\mathscr{E}_2(k)$ for the first and second chains, respectively. Straightforward calculations based on (54)–(56) yield the following final expressions for the spectral energy densities of radiation emitted by the colliding kinks:

$$\mathscr{E}_1(k) = (\pi^3\alpha^2/v^4)(1 - v^2)^3\{2\kappa_1[k - v(1 + k^2)^{1/2}] - (1 - v^2)^{1/2}(\kappa_1^2 - 1)\}^2 \times \sinh^2[\tfrac{1}{2}\pi(\kappa_1 + \sigma_1\sigma_2\kappa_2)]/\sinh^2(\pi\kappa_1)\sinh^2(\pi\kappa_2) \tag{57}$$

and

$$\mathscr{E}_2(k) = \mathscr{E}_1(-k) \tag{58}$$

where v is the relative velocity of the kinks, and

$$\kappa_{1,2} = \frac{(1 - v^2)^{1/2}}{2v}[(1 + k^2)^{1/2} \pm vk]. \tag{59}$$

The dependence of the spectral density $\mathscr{E}_1(k)$ of energy emitted by the kinks in the first chain on the wavenumber k is shown in figures 5(a) and (b) for small relative velocity ($v^2 \ll 1$) and figures 6(a) and (b) for large relative velocity (in the latter case the kinks are 'relativistic', i.e. $1 - v^2 \ll 1$). It is important to note that the collision of the kink with the anti-kink does not generate radiation in the long-wave part of the spectrum, since $\mathscr{E}_{1,2}(k = 0) = 0$ (see figures 5(b) and 6(b)).

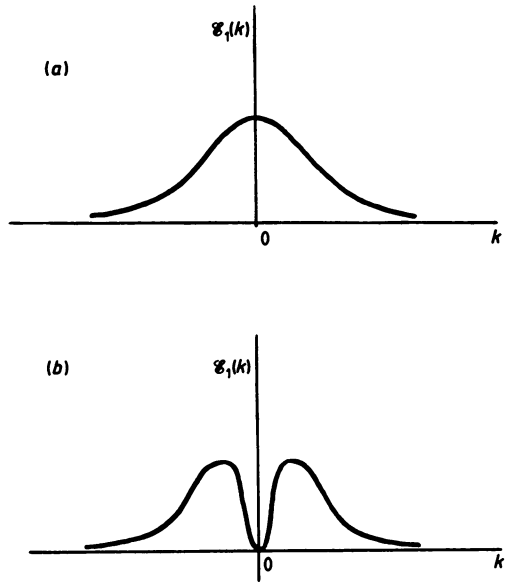

Figure 5. The spectral density of energy emitted by a slow kink in the first chain colliding with a slow kink in the other chain: (*a*) $\sigma = +1$, (*b*) $\sigma = -1$.

The corresponding emitted energies E_1 and E_2 can be obtained as

$$E_{1,2} = \int_{-\infty}^{\infty} \mathcal{E}_{1,2}(k)\,\mathrm{d}k. \tag{60}$$

The integral in (60) may be calculated in two limiting cases: when $v^2 \ll 1$ and when $1 - v^2 \ll 1$. In the former case the results for $E_{1,2}$ are exponentially small in v^{-1}:

$$E_1 = E_2 \simeq \pi^3\alpha^2 2^{-g/2} v^{-15/2} \exp(-\pi/v) \qquad \sigma_1\sigma_2 = +1 \tag{61a}$$

$$E_1 = E_2 \simeq \pi^4\alpha^2 2^{-6} v^{-13/2} \exp(-2\pi/v) \qquad \sigma_1\sigma_2 = -1. \tag{61b}$$

In the latter case, when the spectral densities are described by non-symmetric functions (see figure 6), i.e. the kinks emit radiation mostly with wavenumbers $k \approx -k_m$, where $k_m = (1 - v^2)^{-1/2}$, the results do not depend on the kinks' relative polarity:

$$E_1 = E_2 \simeq 3 \times 2^4\pi^{-4}\alpha^2(1 - v^2)^{3/2}. \tag{62}$$

Analogous results can be obtained in the more general case, when $\alpha \neq 0$, $\beta \neq 0$. In particular, for the case $\alpha = 0$, $\beta \neq 0$, the spectral density $\mathcal{E}_1(k)$ of the emitted energy has a shape similar to that depicted in figures 5(*a*) and 6(*a*), respectively, and does not depend on the relative polarity of the colliding kinks (see [32]).

Thus, for any values of the relative kink velocity the radiation losses are small, and they can be negligible in comparison with the dissipative ones if $\gamma_{1,2} \gg \alpha^2, \beta^2$.

8. Summary and conclusions

In an isolated adatomic chain, which is described by the sine–Gordon equation, kinks of equal polarities always repel one another, but a kink and anti-kink attract one another

and may form a bound state—a breather. However, in a dissipative system, even if a constant external force is present, the breather is unstable, and it either decays into a kink–anti-kink pair or damps, i.e. the kink and anti-kink bound in the breather annihilate (see e.g. [18, 30, 33]).

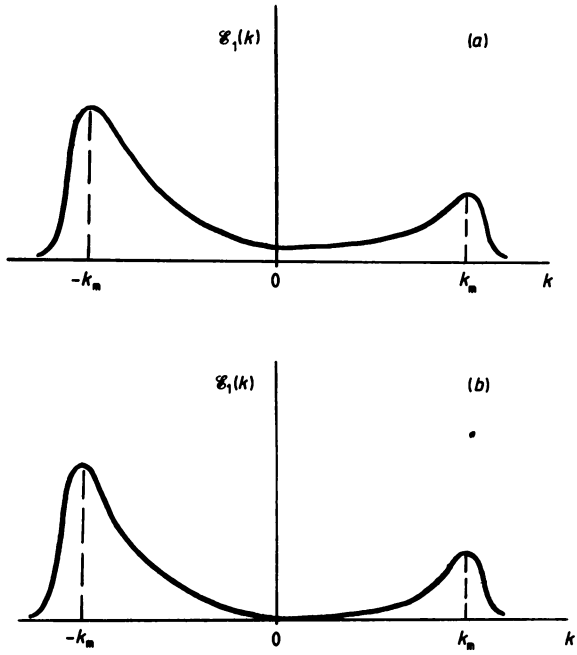

Figure 6. The spectral density of energy emitted by a fast kink in the first chain after its collision with a fast kink in the other chain: (*a*) $\sigma = +1$; (*b*) $\sigma = -1$.

In a system of two coupled adatomic chains, which is described by the set of equations (5), the interaction of kinks belonging to different chains is determined not only by the kinks' relative polarity but also by the inter-chain interaction, i.e. by the signs of the parameters α, β and σ. For example, for $0 < \alpha < \beta$ kinks of equal polarities repel one another as in an isolated chain; but for $\alpha < \beta < 0$ these kinks attract one another. It is very interesting that kinks belonging to different chains may form a breather-like bound state. Unlike a breather, such a bound state is stable even if dissipative losses are present. The slightly excited bound state of the kinks is characterised by the frequency of the internal oscillations. In the presence of a constant external force, the distance between the kinks forming the bound state increases, while the frequency of its internal oscillations decreases. Free colliding kinks belonging to different chains can be bound into a bound state if the external force is less than the threshold value. The threshold values of the external force are calculated for different ratios of parameters α, β and σ.

It is important to note that the internal oscilations of the kinks' bound state may be excited by an external AC force when the frequency of the force is of the order of the internal frequency. The response of the coupled adatomic system to the AC pumping may be observed experimentally, e.g. with the help of high-resolution spectroscopy [34].

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Addendum

The model equations (5) at $\beta = 0$ have also been applied to describe the long-wave excitations of the B form of DNA [35, 36]. The functions u_1 and u_2 are mean angles of rotation of the base pairs, which measure the deviation from the exact form of DNA. Homma and Takeno [35, 36] have considered the discrete version of this model for the special case $u_1 = -u_2$ only. In particular, they study various dynamic states of the reduced (one-component) system, most interesting from it being stochastic.

Our results at $\beta = 0$ may be applied to investigate the Homma–Takeno model and to describe its non-linear dynamics too. As was demonstrated in § 4, it is very important that in some cases exact solutions of the reduced equation (e.g. the double SG equation for $u_1 = -u_2$) may be unstable in the framework of the general set (5) at $\beta = 0$. This fact has not been taken into account by Homma and Takeno.

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