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1987 J. Phys. A: Math. Gen. 20 1695

(http://iopscience.iop.org/0305-4470/20/7/016)

J. Phys. A: Math. Gen. **20** (1987) 1695-1712. Printed in the UK

Classical statistical mechanics of kink-bearing systems with parametrised double-well and asymmetric non-linear on-site potentials

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Received 17 June 1986, in final form 27 August 1986

Abstract. The thermodynamical properties of non-linear systems capable of supporting more than one kink excitation and more than one kind of extended mode are studied in the displacive limit and at very low temperatures. Our attention is concentrated on a class of parametrised non-linear potentials $V(\Phi, r)$ whose shapes can be varied continuously as a function of a parameter r and which are doubly periodic, such as the double-well doubly periodic (DWDP) and the asymmetric doubly periodic (ASDP) cases proposed by Remoissenet and Peyrard. In the chosen limits, the Fredholm integral equation of the transfer integral operator can be converted into an 'effective' Schrödinger equation depending on a large parameter. An asymptotic method recently developed by Croitoru *et al* for the evaluation—to leading order in the large parameter—of the eigenspectrum of the Schrödinger-like equation corresponding to systems that admit a single kink solution, as well as a single type of extended mode, is extended to treat systems supporting polykink solutions and two types of extended modes.

1. Introduction

In the low-temperature regime the classical thermodynamics of kink-bearing systems has been of considerable recent interest, the important role which the kinks (solitons) play being very well established. Though the results concerning the sine-Gordon (SG) model as well as the Φ^4 and double quadratic (DQ) chain (Currie *et al* 1980) are very encouraging, they remain nevertheless limited in their applicability to real physical systems because of an important fact: in real physical systems the shape of the non-linear on-site potential may deviate considerably from that attributed to the local potentials involved in the above-mentioned models. Therefore the study of the 'elementary excitations' (phonons and kinks) of one-dimensional systems with a new periodic parametrised potential was pursued, the shape of which could be varied continuously as a function of a parameter (Remoissenet and Peyrard 1981, Peyrard and Remoissenet 1982). The main feature of this potential consists in the fact that, depending on the value of the parameter, there can exist either sharp wells separated by flat tops or flat bottoms flanked by sharp tops. However, this new system supports a single kink solution. It seemed far more interesting to investigate systems in which the non-linear periodic potential possesses either barriers of different heights or bottoms of different curvatures. An obvious consequence of such local potentials will be the appearance

0305-4470/87/071695+18$02.50

of more than one kink solution, and more than one phonon dispersion relation, this latter feature being related to the existence of potential wells of different shapes.

A prototype of a 'polykink-bearing' system is the double sine-Gordon (DSG) model, which possesses two qualitatively different potential barriers, and consequently two different kink solutions (Condat *et al* 1983, DeLeonardis and Trullinger 1983, Leung 1982, 1983, Pandit *et al* 1983a, b, Giachetti *et al* 1984). Another model responsible for disolitonic behaviour is the doubly periodic quadratic (DPQ) chain, whose properties have been investigated by DeLeonardis and Trullinger (1983). Some common features with the DSG system represent the double-well doubly periodic system (DWDP), whose dynamical properties have been analysed by Peyrard and co-workers (Remoissenet and Peyrard 1984, Peyrard and Campbell 1986). The latter authors also studied the kink-small oscillation and kink-kink scattering for an asymmetric doubly periodic (ASDP) potential. A very interesting property of the ASDP system consists in the fact that it supports not only two asymmetric 'kink solutions' but also two different extended modes (different 'media'), characterised by two different dispersion relations. With respect to this property we remark that the asymmetric kinks evolve the system from one 'medium' to the other. The main characteristic of all the above-mentioned 'polykink'-bearing systems, although they are not completely integrable, is that kink properties are very close to those of completely integrable ones (Remoissenet and Peyrard 1984, Peyrard and Campbell 1986, Bullough and Caudrey 1978, Schiefman and Kumar 1979, Maki and Kumar 1976). Thus the 'kinks' of these systems can be assimilated with quasiparticles, and it is an interesting task to study the role they play in the thermodynamics of these systems.

One of the methods which allows us to exactly determine the partition function of a kink-bearing system is the transfer integral method (TIM) (Scalapino *et al* 1972). This approach, developed for one-dimensional systems with a singly periodic on-site potential, has been extended by Condat *et al* (1983) and DeLeonardis and Trullinger (1983) to models with potentials with double periodicity (DSG, DPQ).

The purpose of this paper—in order to determine the free energy per unit length—is to extend the TIM (as well as the generalised Langer transformation (Croitoru *et al* 1984, Nayfeh-Hasan 1973)) to the DWDP and ASDP models introduced by Remoissenet and Peyrard (1984). In § 2 we present the description of the models under study and also define the associated quantities of interest. For both models, in § 3 we calculate the temperature dependence of the free energy in the low-temperature regime and in the displacive limit. Section 4 summarises the main results.

2. Model description

Let us consider a one-dimensional chain of N harmonically coupled oscillators governed by the Hamiltonian

$$H = \sum_i lA[\tfrac{1}{2}\dot{\Phi}_i^2 + \tfrac{1}{2}(c_0^2/l^2)(\Phi_{i+1} - \Phi_i)^2 + \omega_0^2 V(\Phi_i)]. \tag{1}$$

Here Φ_i is the dimensionless field variable of the ith oscillator, l the lattice constant, A a constant which sets the energy scale, and c_0 and ω_0 are a characteristic velocity and frequency, respectively. The non-linear on-site potential $V(\Phi)$ to which the

harmonic oscillators are submitted will be considered to be of two parametrised forms, namely (Remoissenet and Peyrard 1984)

$$\text{DWDP potential:} \qquad V(\Phi) = (1-r)^4 \frac{1+\cos\Phi}{(1+r^2+2r\cos(\frac{1}{2}\Phi)^2} \tag{2a}$$

$$\text{ASDP potential:} \qquad V(\Phi) = (1-r^2)^2 \frac{1-\cos\Phi}{(1+r^2+2r\cos(\frac{1}{2}\Phi)^2} \tag{2b}$$

where the parameter r is supposed to be confined to the interval $0 \leqslant r < 1$.

The potentials (2*a*, *b*) possess the following symmetry and periodicity properties:

$$\begin{aligned} &V(\Phi) = V(-\Phi) \\ &V(\Phi) = V(\Phi + p) \qquad \text{with } p = 4\pi. \end{aligned} \tag{3}$$

For $r = 0$, both potentials recover the well known sine-Gordon potential. While the DWDP potential (2*a*) is characterised by potential barriers of different heights and potential wells of the same shape (see figure 1(*a*)), the ASDP potential (2*b*) possesses potential barriers of the same height, but two adjacent minima have different curvatures (figure 1(*b*)).

For the DWDP potential the local minima are found at

$$\Phi = (2n+1)\pi \qquad n = 0, \pm 1, \pm 2, \ldots \tag{4a}$$

while the local maxima are found at

$$\Phi = 4\pi n \qquad \Phi = 2\pi + 4\pi n \qquad n = 0, \pm 1, \pm 2, \ldots . \tag{4b}$$

We note that for $\Phi = 4\pi n$ the potential (2*a*) takes the value

$$V(4\pi n) = 2\left(\frac{1-r}{1+r}\right)^4 \tag{5a}$$

and for $\Phi = 2\pi + 4\pi n$ we have

$$V(2\pi + 4\pi n) = 2. \tag{5b}$$

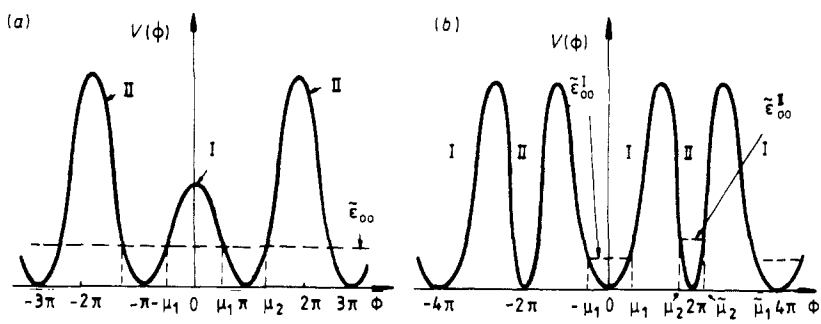

Figure 1. Representation of the potentials $V(\Phi, r)$ (*a*) for the DWDP and (*b*) for the ASDP model. The different barriers, as well as the different wells, are specified by the notations I and II. In case (*a*) $\tilde{\varepsilon}_{00}$ is the lowest isolated-well eigenvalue, and in case (*b*) $\tilde{\varepsilon}_{00}^{(I)}$ and $\tilde{\varepsilon}_{00}^{(II)}$ are the two different isolated-well eigenvalues.

While the higher barrier (5*b*) is of constant value, the smaller one (5*a*) depends on the parameter r, and for $r \to 1$ it becomes very small. At the local minima the second derivative $V''(\Phi)$ is also a function of r, namely

$$V''[(2n+1)\pi] = \frac{(1-r)^4}{(1+r^2)^2}. \tag{6}$$

For increasing values of r the potential wells become flatter and flatter.

In the case of the ASDP potential (2*b*) the local minima are situated at

$$\Phi = 2\pi n \qquad n = 0, \pm 1, \pm 2, \ldots \tag{7a}$$

and the local maxima are found at

$$\Phi = (2n+1)\pi \pm 2\cos^{-1}\left(\frac{2r}{1+r^2}\right) \qquad n = 0, \pm 1, \pm 2, \ldots . \tag{7b}$$

At the points (7*b*), the potential barrier has the constant value

$$V(\Phi) = 2. \tag{8}$$

The second derivative $V''(\Phi)$ corresponding to adjacent minima takes different values, namely

$$V''(\Phi = 4\pi n) = \left(\frac{1-r}{1+r}\right)^2 \tag{9a}$$

$$V''(\Phi = 2\pi + 4\pi n) = \left(\frac{1+r}{1-r}\right)^2. \tag{9b}$$

If the parameter r approaches unity ($r \to 1$) (9*a*) becomes very small (flat bottom) and (9*b*) becomes very large (sharp bottom).

In the following we restrict the parameters in (1) to the displacive limit ($d \equiv c_0/\omega_0 \gg l$) in which the non-linear kinks become well defined 'elementary excitations' with long lifetimes. In this regime the Hamiltonian (1) becomes

$$H = A \int \mathrm{d}x \{\tfrac{1}{2}[\Phi_t(x,t)]^2 + \tfrac{1}{2}c_0^2[\Phi_x(x,t)]^2 + \omega_0^2 V(\Phi)\} \tag{10}$$

and the associated equation of motion is

$$\Phi_{tt} - c_0^2\Phi_{xx} + \omega_0^2 V'(\Phi) = 0. \tag{11}$$

Here

$$V' = \mathrm{d}V/\mathrm{d}\Phi \qquad \Phi_{tt} = \partial^2\Phi/\partial t^2 \qquad \Phi_{xx} = \partial^2\Phi/\partial x^2.$$

For the two non-linear on-site potentials (2*a*, *b*) equation (11) supports soliton-like solutions as well as small amplitude oscillations. Their analytical expressions, together with the kink rest masses, have been derived by Remoissenet and Peyrard (1984), and are listed in table 1. From there we recognise the essential particulars of the two models under study, as follows.

(*a*) In the case of the DWDP potential (2*a*) the system supports a single type of extended mode, but two kinds of kink solutions with different rest masses. The type-I kink evolves the system from one well to the adjacent one over the type-I barrier (small barrier) while the type-II solution describes the evolution of the system over the type-II barrier (high barrier).

Table 1. Various quantities of the DWDP and ASDP systems associated with the kink (+) and antikink (−) solutions of equation (11), as well as of its small amplitude solutions. $M_K^{I,II}$ are the rest masses and $(\omega_k^2)^{I,II}$ the phonon dispersion relations, $\gamma = (1 - v^2/c_0^2)^{-1/2}$, $s = x - vt$, v being the velocity of the moving kink.

$V(\Phi, r)$	DWDP	ASDP
$\frac{\gamma s^{I}}{d}$	$\frac{1+r^2}{(1-r)^2}\ln[\tan(\frac{1}{4}\Phi+\frac{1}{4}\pi)]+\frac{r\Phi}{(1-r)^2}$	$\frac{1+r^2}{1-r^2}\ln[\tan(\frac{1}{4}\Phi)]+\frac{2r}{1-r^2}\ln[\sin(\frac{1}{2}\Phi)]$
$\frac{\gamma s^{II}}{d}$	$\frac{1+r^2}{(1-r)^2}\ln[-\operatorname{cotan}(\frac{1}{4}\Phi+\frac{1}{4}\pi)]$	$\frac{1+r^2}{1-r^2}\ln[-\operatorname{cotan}(\frac{1}{4}\Phi)]$
	$-\frac{4}{(1-r)^2}(\Phi-2\pi)$	$-\frac{2r}{1-r^2}\ln[-\sin(\frac{1}{2}\Phi)]$
M_K^{I}	$\frac{8A}{d}\frac{(1-r)^2}{r}\left(\frac{\pi}{4}-\frac{1+r^2}{1-r^2}\tan^{-1}\left(\frac{1-r}{1+r}\right)\right]$	$\frac{8A}{d}\frac{1-r^2}{2r}\ln\left(\frac{1+r}{1-r}\right)$
M_K^{II}	$\frac{8A}{d}\frac{(1-r)^2}{r}\left[-\frac{\pi}{4}+\frac{1+r^2}{1-r^2}\tan^{-1}\left(\frac{1+r}{1-r}\right)\right]$	$\frac{8A}{d}\frac{1-r^2}{2r}\ln\left(\frac{1+r}{1-r}\right)$
$(\omega_k^2)^{I}$	$\omega_0^2\frac{(1-r)^2}{1+r^2}+c_0^2k^2$	$\omega_0^2\left(\frac{1-r}{1+r}\right)^2+c_0^2k^2$
$(\omega_k^2)^{II}$		$\omega_0^2\left(\frac{1+r}{1-r}\right)^2+c_0^2k^2$

(*b*) In the case of the ASDP potential (2*b*) there exist two different kinds of extended modes, each confined to one of the two different wells. The kinks are asymmetric possessing the same rest mass, and the type-I kink evolves the system from well I to well II while the type-II kink evolves the system from well II to well I.

Now let us proceed to a short sketch of the essential relations concerning the statistical mechanics of the systems under study. The classical partition function Z for systems governed by the Hamiltonian (1) factors into kinetic and configurational parts (Currie *et al* 1980, Condat *et al* 1983, DeLeonardis and Trullinger 1983), namely

$$Z = Z_\Phi Z_\Phi \tag{12}$$

where

$$Z_\Phi = \left(\frac{2\pi Al}{\beta h^2}\right)^{N/2} \tag{13a}$$

and

$$Z_\Phi = \sum_n \exp(-\beta L A \omega_0^2 \varepsilon_n). \tag{13b}$$

Here $\beta = (k_B T)^{-1}$ (k_B being Boltzmann's constant), h is Planck's constant, N the number of atoms contained in the chain and ε_n is the nth eigenvalue of the transfer integral operator. In the thermodynamic limit ($L \to \infty$, $N \to \infty$, $L/N =$ constant) Z_Φ is dominated by the lowest eigenvalue ε_0, and the free energy per unit length ($F = -(1/\beta L)\ln Z$) becomes

$$F = -\frac{1}{2\beta l}\ln\left(\frac{2\pi Al}{\beta h^2}\right) + A\omega_0^2\varepsilon_0. \tag{14}$$

It is this quantity we shall calculate in the next section by determining the lowest eigenvalue of the transfer integral operator.

3. Asymptotic evaluation of the eigenspectrum

In the displacive limit the determination of the lowest eigenvalues of the transfer integral operator can be achieved by solving the eigenvalue problem represented by an 'effective' Schrödinger equation into which the Fredholm integral equation of the TIM can be converted (Currie *et al* 1980, Condat *et al* 1983, DeLeonardis and Trullinger 1983, Scalapino *et al* 1972), and which can be written

$$d^2\Psi_n/d\Phi^2 + \lambda^2 q(\Phi)\Psi_n(\Phi) = 0 \tag{15}$$

where

$$q(\Phi) = \tilde{\varepsilon}_n - V(\Phi) \tag{16}$$

and $\{\Psi_n(\Phi)\}$ represent the right-hand eigenfunctions of the transfer integral operator (Croitoru *et al* 1984). The parameter λ and the eigenvalue $\tilde{\varepsilon}_n$ are defined by

$$\begin{aligned} &\lambda^2 = 2m^* \qquad m^* = A^2\beta^2 c_0^2 \omega_0^2 \\ &\tilde{\varepsilon}_n = \varepsilon_n + \frac{1}{\eta}\ln\left(\frac{2\pi}{\eta_1}\right)^{1/2} \qquad \eta_1 = \eta\frac{d^2}{l^2} \qquad \eta = Al\beta\omega_0^2. \end{aligned} \tag{17}$$

Here ε_n, the nth eigenvalue of the transfer integral operator, has been introduced in (13*b*). In the following, for the sake of simplicity, the subscript n will be omitted.

With respect to equation (15), we have to make some remarks about the reasoning which determined the asymptotic method we used to solve the eigenvalue problem.

In the low temperature limit, the effective mass m^* becomes very large, thus (15) belongs to the class of second-order differential equations depending on a large parameter. This fact suggests determining its solutions in the form of an asymptotic expansion in a power series of λ. In doing so, the turning points for which $q(\Phi) = 0$ will play a special role. In the case of periodical potentials to which the parametrised potentials (2*a*, *b*) belong, the turning points appear in sequences of pairs (Croitoru *et al* 1984), each pair corresponding to a single potential well. Being faced with a problem with two turning points very close to each other, it seemed suitable to use an asymptotic method developed especially for such problems (Nayfeh-Hasan 1973). In a recent paper (Croitoru *et al* 1984) such an asymptotic procedure has been employed to obtain solutions of an equation which has the same characteristics as equation (15) but corresponds to systems which support a single kink solution, as well as a single kind of extended mode. Here this method will be extended to polykink and poly-extended mode bearing systems. Following the approach used by Croitoru *et al* (1984), equation (15) will be solved in two steps.

(1) Firstly, we look for a uniformly valid asymptotic expansion of the solution in the region between two turning points of an isolated well. The evaluation of this solution will be performed using the Langer transformation (Croitoru *et al* 1984, Nayfeh-Hasan 1973), according to which (15) will be replaced by an equivalent equation whose solutions are asymptotically equivalent to those of (15).

(2) In the second step we take into account the presence of the adjacent potential wells. As is known from previous studies (Currie *et al* 1980, Croitoru *et al* 1984), in the case of singly periodic potentials the existence of neighbouring wells leads to

the tunnel splitting of the degenerated isolated well eigenvalues into allowed narrow bands. In Croitoru *et al* (1984) this tunnelling term has been obtained by imposing on the isolated well solutions symmetry requirements which these solutions have to satisfy. In order to extend the procedure developed in Croitoru *et al* (1984) to the models under study, we have to take into account the characteristics of the potentials (2*a*, *b*) pointed out in § 2 and which can be summarised as follows.

(*a*) In the case of DWDP systems the potential (2*a*) can be imagined as a periodic repetition of a symmetric double well (see figure 2(*a*)). It is known (Currie *et al* 1980, DeLeonardis and Trullinger 1983) that the presence of two wells (see for instance the Φ^4 model) will give rise to the tunnel splitting of the degenerated isolated well eigenvalue. Afterwards, accounting also for the periodical repetition of the double well, the two double-well eigenvalues will further tunnel-split into allowed narrow bands (figure 3(*a*)). Thus the tunnelling through the type-II barrier will be responsible for the band structure, while that through the type-I barrier will be responsible for the band gap.

(*b*) A similar picture can be imagined for the ASDP case, the basic quantity, whose periodical repetition generates the potential (2*b*), being an asymmetric double well (figure 2(*b*)). Again, due to the presence of two wells, the two different degenerate

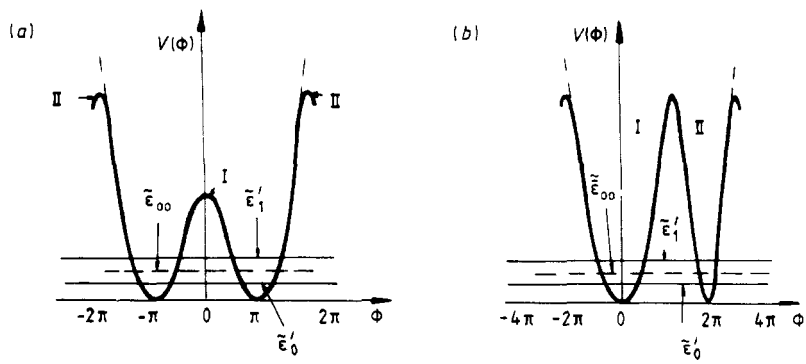

Figure 2. Schematic plot of a symmetric (*a*) and an asymmetric (*b*) 'double-well' on-site potential. The full curves represent the tunnel-split eigenvalues $\tilde{\varepsilon}'_0$, $\tilde{\varepsilon}'_1$. $\tilde{\varepsilon}_{00}$ (*b*) is the middle value of $\tilde{\varepsilon}^{\mathrm{I}}_{00}$ and $\tilde{\varepsilon}^{\mathrm{II}}_{00}$.

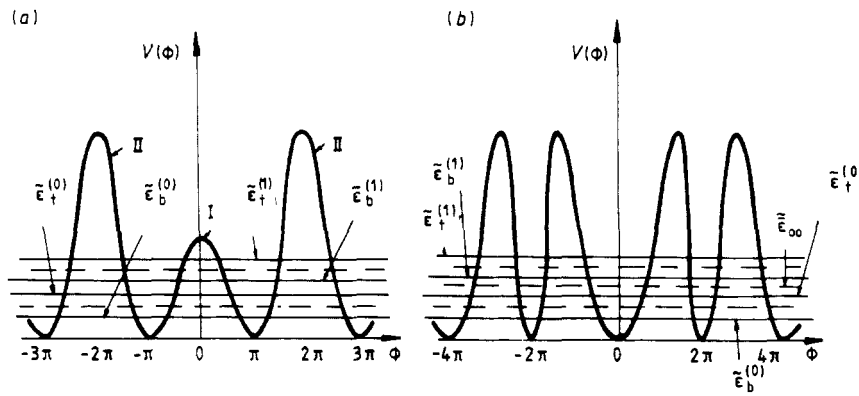

Figure 3. A schematic plot of the two lowest bands generated by the tunnel splitting of the degenerate lowest isolated-well eigenvalue.

isolated well eigenvalues will tunnel-split into two new eigenvalues corresponding to the asymmetric double well. As can be expected, the periodical repetition of the double well will lead to a further tunnel splitting into two allowed bands. We guess that the band and gap formation will not be quite so simple as in the DWDP case.

Our second remark concerns the symmetry properties of the solutions $\Psi(\Phi)$ of equation (15). According to (3), the function $q(\Phi)$ displays the following symmetry and periodicity properties:

$$\begin{aligned} &q(\Phi) = q(-\Phi) \\ &q(\Phi) = q(\Phi + p) \qquad p = 4\pi. \end{aligned} \tag{18}$$

Thus equation (15) belongs to the class of Hill equations and its eigenfunctions are the Bloch functions:

$$\begin{aligned} &\Psi_{n,k}(\Phi) = u_{n,k}(\Phi)\exp(ik\Phi) \\ &u_{n,k}(\Phi) = u_{n,k}(\Phi + p) \qquad p = 4\pi. \end{aligned} \tag{19}$$

Here n represents the band index and k the wavevector whose allowed values are contained in the first Brillouin zone $(-\frac{1}{4}, \frac{1}{4})$. In accordance with (19), the solutions $\Psi(\Phi)$ can be even or odd, depending on the value of the wavevector.

In order to proceed to the asymptotic evaluation of the eigenspectrum of (15), we have to define the Langer transformation on which, according to the introductory remarks made above, the forthcoming determinations will be based. Thus, following Langer's approach (Nayfeh-Hasan 1973) one introduces a transformation of the dependent and independent variables defined by

$$\begin{aligned} &\Psi(\Phi) = \chi^{-1/4} v \\ &\rho = \rho(z) = \int_{\mu_1}^{\Phi} d\tau \sqrt{q(\tau)} \\ &\chi = q(\Phi)/(\rho')^2 \qquad \rho' = d\rho/dz \qquad \chi^{-1/4} = (dz/d\Phi)^{-1/2} \end{aligned} \tag{20}$$

where the new independent variable z is still any undefined function of Φ. In (20) μ_1 represents one of the turning points of an isolated well (figure 1(a)). With (20), equation (15) transforms into

$$dv/dz^2 + \lambda^2(\rho')^2 v = \delta v \tag{21}$$

where

$$\delta = -\chi^{-3/4} d^2(\chi^{-1/4})/d\Phi^2. \tag{22}$$

If one can choose $\rho(z)$ such that $\delta = O(1)$, then the related equation

$$d^2v/dz^2 + \lambda^2(\rho')^2 v = 0 \tag{23}$$

has solutions which are asymptotically equivalent to the solutions of (15) for large λ. This condition is fulfilled provided that χ is a regular function in the interval of interest†. A convenient choice for $(\rho')^2$—adequate only for potentials which can be approximated with that of a harmonic oscillator—is the following (Croitoru *et al* 1984, Nayfeh-Hasan 1973):

$$(\rho')^2 = 4a^2(1 - z^2). \tag{24}$$

† For more details the reader is referred to Nayfeh-Hasan (1973) and Croitoru *et al* (1984).

According to (24), $(\rho')^2$ has two simple zeros, and we take $z=-1$ to correspond to $\Phi=\mu_1$, and choose a so that $z=1$ corresponds to $\Phi=\mu_2$, μ_2 being the second turning point of the isolated well. Then in accordance with (20) we have

$$\rho(z)=2a\int_{-1}^{z}\mathrm{d}\tau(1-\tau^2)^{1/2}=\int_{\mu_1}^{\Phi}\mathrm{d}t\sqrt{q(t)} \tag{25}$$

and consequently

$$a=\frac{1}{\pi}\int_{\mu_1}^{\mu_2}\mathrm{d}\Phi\sqrt{q(\Phi)}. \tag{26}$$

With (24) the related equation (23) becomes

$$\mathrm{d}^2v/\mathrm{d}z^2+4a^2\lambda^2(1-z^2)v=0 \tag{27}$$

and its solutions are the parabolic cylinder functions v_1 and v_2 (Abramowitz and Stegun 1965, Whittaker and Watson 1950) or any linear combination of them. For the systems under study, it seemed convenient to choose the following linear combination:

$$v(x)=v_1(x)+Cv_2(x) \tag{28}$$

where

$$x=2\sqrt{a\lambda}\,z$$

and v_1 and v_2 are defined as follows:

$$v_1(x)=\exp(-\tfrac{1}{4}x^2)M(-\nu;\tfrac{1}{2};\tfrac{1}{2}x^2) \tag{29a}$$

$$v_2(x)=x\exp(-\tfrac{1}{4}x^2)M(-\nu+\tfrac{1}{2};\tfrac{3}{2};\tfrac{1}{2}x^2). \tag{29b}$$

Here $M(b;c;\xi)$ represents the Kummer function and ν is related to a by

$$a\lambda=\tfrac{1}{2}+2\nu. \tag{30}$$

With the comments and relations given up to now we are in a position to calculate the eigenspectrum of (15).

Firstly, we concentrate our attention on an isolated well. Then the solution of (27) has to be an even one, i.e. $v(x)=v(-x)$. Consequently, $C=0$ and the isolated well solution will be given by $v_1(x)$. Moreover, the requirement that (29a) decays exponentially for $|x|\to\infty$ will be satisfied if and only if ν is an integer. Hence (30) becomes

$$a\lambda=\tfrac{1}{2}+2n \qquad n=0,1,2,\ldots \tag{31}$$

and represents the relation which determines to leading order in λ the eigenvalues of the isolated well. By using (31) together with (26) we obtain

DWDP potential:

$$\tilde{\varepsilon}_n\simeq(\tfrac{1}{2}+2n)\frac{1}{\sqrt{m^*}}\frac{(1-r)^2}{1+r^2} \tag{32a}$$

ASDP potential:

well I $$\tilde{\varepsilon}_n^{\mathrm{I}}\simeq(\tfrac{1}{2}+2n)\frac{m_1}{\sqrt{m^*}} \tag{32b}$$

well II $$\tilde{\varepsilon}_n^{\mathrm{II}}\simeq(\tfrac{1}{2}+2n)\frac{m_2}{\sqrt{m^*}} \tag{32c}$$

where

$$m_1 = (1-r)/(1+r) \qquad m_2 = (1+r)/(1-r). \tag{33}$$

Because $m_2 > m_1$ we also have $\tilde{\varepsilon}_n^{II} > \tilde{\varepsilon}_n^{I}$.

In the low temperature limit we are interested only in the lowest eigenvalue ($n = 0$) of the isolated well. Knowing its expression (32) we can proceed to the determination of its tunnel splitting into continuous bands due to the presence of the periodic sequence of the other potential wells. Then the lower and upper extremities of the two lowest allowed bands will result from (30), where ν now represents a very small quantity related to the small shifts from the isolated well eigenvalue. Following Croitoru *et al* (1984), it will be determined from the boundary conditions (DWDP system) or from matching requirements (ASDP system) satisfied by the isolated well eigenfunction

$$\Psi(\Phi) = \chi^{-1/4}(v_1 + Cv_2) \tag{34}$$

and its first derivative. The form (34) assumed for the eigenfunction $\Psi(\Phi)$ reflects the fact that in the DWDP case (if we take into account the neighbouring wells) the isolated well solution no longer has the same behaviour (as in the SG case (Croitoru *et al* 1984)) at the right and left boundaries (high and small barrier) of the well (see figure 1(*a*)). Moreover, in the ASDP case, to each 'medium' there corresponds a different isolated well solution of the form (34), and each type of well has as an adjacent well (on its right as well as on its left side) the other type of well (see figure 1(*b*)). Due to some basic differences the two models under consideration will be treated separately.

3.1. *DWDP system*

In the case of a symmetric double well (or a singly periodic potential such as the sine-Gordon one) the lower and upper tunnel-split eigenvalues (the bottom and top of the lowest band) result from the simple requirement that at the midpoint between two adjacent wells the eigenfunction has to be an even function of Φ if it corresponds to the fundamental level (to the bottom of the lowest band), and an odd one if it corresponds to the first excited state (or the top of the lowest band). Now, for the model under consideration we are faced up with two different barriers. Consequently the isolated well eigenfunction $\Psi(\Phi)$ (34) has to satisfy, at the midpoint between a well and its neighbouring ones, on the left (top of type-I barrier) as well as on the right side (top of type-II barrier), the following requirements:

$$\left.\frac{d\Psi}{d\Phi}\right|_{\Phi=0} = 0 \qquad \left.\frac{d\Psi}{d\Phi}\right|_{\Phi=2\pi} = 0 \qquad \text{bottom of the first band} \tag{35a}$$

$$\left.\frac{d\Psi}{d\Phi}\right|_{\Phi=0} = 0 \qquad \Psi(\Phi = 2\pi) = 0 \qquad \text{top of the first band} \tag{35b}$$

$$\Psi(\Phi = 0) = 0 \qquad \left.\frac{d\Psi}{d\Phi}\right|_{\Phi=2\pi} = 0 \qquad \text{bottom of the second band} \tag{36a}$$

$$\Psi(\Phi = 0) = 0 \qquad \Psi(\Phi = 2\pi) = 0 \qquad \text{top of the second band} \tag{36a}$$

which reflect the fact that four possibilities exist: the eigenfunction $\Psi(\Phi)$ is an even or odd function of Φ ((35*a*), (36*b*)) with respect to both barriers, or it is an even function of Φ with respect to one barrier and an odd function with respect to the other

barrier ((35*b*), (36*a*)). Obviously, in writing the conditions (35) and (36) we have accounted for (19). While the variable Φ takes finite values at the boundary points, the variable x (or z) becomes very large, namely for $\Phi \sim 0$, $x \to -\infty$ and for $\Phi \sim 2\pi$, $x \to \infty$. Therefore in these regions, the asymptotic expansions of the Kummer functions will be involved in (34) (Abramowitz and Stegun 1965). For $|x| \to \infty$ they may be approximated by

$$M(-\nu; \tfrac{1}{2}; \tfrac{1}{2}x^2) \sim 1 - 2\sqrt{\pi}\,\nu(1/|x|)\exp(\tfrac{1}{2}x^2) \tag{37a}$$

$$M(-\nu+\tfrac{1}{2}; \tfrac{3}{2}; \tfrac{1}{2}x^2) \sim \tfrac{1}{2}\sqrt{\pi}\left(\frac{2\mathrm{i}}{|x|} + \frac{2}{\sqrt{\pi}}\frac{1}{x^2}\exp(\tfrac{1}{2}x^2)\right). \tag{37b}$$

Furthermore, in order to evaulate relations (35) and (36) explicitly we need a knowledge of the relation which exists between x (or z) and Φ in the asymptotic regions. According to the definition relations (20) and (24) we have (Croitoru *et al* 1984)

$$z^2 \sim \frac{1}{a}\int_{\Phi}^{\mu_1} \mathrm{d}\tau \sqrt{|q(\tau)|} + \tfrac{1}{2} + \ln(2|z|) \qquad \text{for } z < 0 \tag{38a}$$

$$z^2 \sim \frac{1}{a}\int_{\mu_2}^{\Phi} \mathrm{d}\tau \sqrt{|q(\tau)|} + \tfrac{1}{2} + \ln(2z) \qquad \text{for } z > 0. \tag{38b}$$

In order to reveal the even and odd character of the eigenfunctions involved in (35) and (36), respectively, we introduce the following notations for the small quantity ν: ν_{ee} (in 35*a*)), ν_{eo} (in (35*b*)), ν_{oe} (in (36*a*)) and ν_{oo} (in (36*b*)). Then, by using (35) and (36) together with (37) and (38) we obtain

$$\nu_{ee} = -\nu_{oo} \qquad \nu_{eo} = -\nu_{oe} \tag{39}$$

where

$$\nu_{ee} = -\frac{1}{4\sqrt{\pi e}}[\mathcal{I}^{(I)} + \mathcal{I}^{(II)}] \tag{40a}$$

$$\nu_{eo} = -\frac{1}{4\sqrt{\pi e}}[\mathcal{I}^{(I)} - \mathcal{I}^{(II)}] \tag{40b}$$

with

$$\mathcal{I}^{(I)} = \exp\left(-2\lambda \int_0^{\mu_1} \mathrm{d}\Phi \sqrt{|q(\Phi)|}\right) \tag{41a}$$

and

$$\mathcal{I}^{(II)} = \exp\left(-2\lambda \int_{\mu_2}^{2\pi} \mathrm{d}\Phi \sqrt{|q(\Phi)|}\right) \tag{41b}$$

where

$$\mu_1 = \pi - \sin^{-1}\left(\frac{(1+r^2)}{(1-r)^2}\left(\frac{\tilde{\varepsilon}}{2}\right)^{1/2}\right) \qquad \mu_2 = \pi + \sin^{-1}\left(\frac{(1+r^2)}{(1-r)^2}\left(\frac{\tilde{\varepsilon}}{2}\right)^{1/2}\right).$$

By using (30) we are now in a position to deduce compact expressions for the eigenvalues corresponding to the bottom (b) and the top (t) of the two lowest bands

$(n=0, 1)$ (see figure 3(*a*)):

$$\tilde{\varepsilon}_{\mathrm{b}}^{(0)} \simeq \tilde{\varepsilon}_{\mathrm{oo}} - \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} (\mathcal{I}^{(\mathrm{I})} + \mathcal{I}^{(\mathrm{II})}) \tag{42a}$$

$$\tilde{\varepsilon}_{\mathrm{t}}^{(0)} \simeq \tilde{\varepsilon}_{\mathrm{oo}} - \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} (\mathcal{I}^{(\mathrm{I})} - \mathcal{I}^{(\mathrm{II})}) \tag{42b}$$

$$\tilde{\varepsilon}_{\mathrm{b}}^{(1)} \simeq \tilde{\varepsilon}_{\mathrm{oo}} + \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} (\mathcal{I}^{(\mathrm{I})} - \mathcal{I}^{(\mathrm{II})}) \tag{42c}$$

$$\tilde{\varepsilon}_{\mathrm{t}}^{(1)} \simeq \tilde{\varepsilon}_{\mathrm{oo}} + \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} (\mathcal{I}^{(\mathrm{I})} + \mathcal{I}^{(\mathrm{II})}). \tag{42d}$$

Here $\tilde{\varepsilon}_{\mathrm{oo}}$ is given by (32*a*) (with $n=0$) and represents the harmonic oscillator contribution, while the second term of each of the four expressions (42) is related to the tunnelling terms. In the low temperature limit the only contribution to the partition function stems from (42*a*), and by comparison with the singly periodic systems we may write

$$\tilde{\varepsilon}_{\mathrm{b}}^{(0)} \simeq \tilde{\varepsilon}_{\mathrm{oo}} - t_0 \qquad \text{with } t_0 = t_0^{(\mathrm{I})} + t_0^{(\mathrm{II})} \tag{43}$$

where

$$t_0^{(\mathrm{I,II})} = \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{I}^{(\mathrm{I,II})} \tag{44}$$

represents the tunnelling rate through the type-I and type-II barriers, respectively. Then the free energy per unit length is

$$F = \frac{1}{\beta l} \ln\left(\frac{\beta \hbar d \omega_0}{l}\right) + A\omega_0^2 \tilde{\varepsilon}_{\mathrm{oo}} - A\omega_0^2 t_0. \tag{45}$$

The integrals involved in $\mathcal{I}^{(\mathrm{I,II})}$ can easily be evaluated by means of a procedure (Whittaker and Watson 1950) employed in Croitoru *et al.* Evaluating them, we get the following approximate expressions for the quantities $\mathcal{I}^{(\mathrm{I,II})}$:

$$\mathcal{I}^{(\mathrm{I,II})} = 2^3 \sqrt{e} \frac{1-r}{(1+r^2)^{1/2}} \exp\left(\frac{r\pi}{1+r^2}\right) (m^*)^{1/4} \exp(-\beta E_K^{(\mathrm{I,II})}). \tag{46}$$

Here $E_K^{(\mathrm{I,II})} = c_0^2 M_K^{(\mathrm{I,II})}$ represents the rest energy of the two different kink solutions. Recalling the expression (44) we see that the tunnelling through the two barriers is strictly related to the two types of kink solutions.

Each bandwidth L_{b} follows immediately from (42) and is given by

$$L_{\mathrm{b}} = \frac{1}{\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{I}^{(\mathrm{II})} \tag{47}$$

while the bandgap L_{g}, evaluated between the centres of the two bands, is given by

$$L_{\mathrm{g}} = \frac{1}{\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{I}^{(\mathrm{I})}. \tag{48}$$

As expected (recall the picture we imagined for the band formation), the bandwidth is the same for both bands and is proportional to the tunnelling through the type-II barrier, while the bandgap (representing the splitting of the isolated well eigenvalue into two eigenvalues due to the second well of the symmetric double well) is proportional to the tunnelling through the type-I barrier. These results are in complete agreement with those obtained by DeLeonardis and Trullinger (1983).

If we evaluate the gap between the top of the first band and the bottom of the second one, its width is

$$l_g = \frac{1}{\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} (\mathcal{I}^{(I)} - \mathcal{I}^{(II)}) \tag{49}$$

and for $r = 0$ it vanishes; we recover the single lowest band of the sine-Gordon system.

3.2. *ASDP system*

Now let us consider a unit cell $(0, 4\pi)$. According to figure 1(b) around $\Phi = 0$ and $\Phi = 4\pi$ we have a type-I well, while the well around $\Phi = 2\pi$ is type II. In the following we shall denote the eigenfunctions corresponding to the two different wells by $\Psi^{(I)}(\Phi)$ and $\Psi^{(II)}(\Phi)$, respectively. They will be assumed to be of the form (34). The choice of this unit cell is in accordance with the evolution of the system from well-I over the first barrier to well-II (first kink solution) and from well-II over the second barrier to well-I (second kink solution). For values of Φ which lie outside the region between the two turning points of an isolated well the variable x (or z) becomes very large. In these asymptotic regions the explicit relation between Φ and z is

well-I ($\Phi \sim 0$):

$$z^2 \sim \frac{1}{a^{(I)}} \int_{\mu_1}^{\Phi} d\tau \sqrt{|q(\tau)|} + \tfrac{1}{2} + \ln(2z) + \dots \qquad z > 0 \tag{50a}$$

well-II ($\Phi \sim 2\pi$):

$$z^2 \sim \frac{1}{a^{(II)}} \int_{\Phi}^{\mu_2} d\tau \sqrt{|q(\tau)|} + \tfrac{1}{2} + \ln(2|z|) + \dots \qquad z < 0 \tag{50b}$$

$$z^2 \sim \frac{1}{a^{(II)}} \int_{\tilde{\mu}_1}^{\Phi} d\tau \sqrt{|q(\tau)|} + \tfrac{1}{2} + \ln(2z) \qquad z > 0 \tag{50c}$$

well-I ($\Phi \sim 4\pi$):

$$z^2 \sim \frac{1}{a^{(I)}} \int_{\Phi}^{\tilde{\mu}_2} d\tau \sqrt{|q(\tau)|} + \tfrac{1}{2} + \ln(2|z|) \qquad z < 0. \tag{50d}$$

Here μ_1, μ_2 and $\tilde{\mu}_1$, $\tilde{\mu}_2$, respectively, are the turning points corresponding to the wells involved (see figure 1(b)) and their expressions in terms of $\tilde{\varepsilon}$ are

$$\mu_1 = 2\sin^{-1}(m_2\sqrt{\tfrac{1}{2}\tilde{\varepsilon}}) \qquad \mu_2 = 2\pi - 2\sin^{-1}(m_1\sqrt{\tfrac{1}{2}\tilde{\varepsilon}}) \tag{51a}$$

$$\tilde{\mu}_1 = 4\pi - 2\sin^{-1}(m_2\sqrt{\tfrac{1}{2}\tilde{\varepsilon}}) \qquad \tilde{\mu}_2 = 2\pi + 2\sin^{-1}(m_1\sqrt{\tfrac{1}{2}\tilde{\varepsilon}}). \tag{51b}$$

With respect to the two barriers, the eigenfunctions $\Psi^{(I)}(\Phi)$ and $\Psi^{(II)}(\Phi)$ can be even or odd functions of Φ. The matching relations which express the continuity of the

even and odd eigenfunctions and their first derivatives are

$$\Psi^{(\mathrm{I})}(\Phi) = \pm\Psi^{(\mathrm{II})}(\Phi) \qquad \mu_1 < \Phi < \mu_2 \tag{52a}$$

$$\mathrm{d}\Psi^{(\mathrm{I})}/\mathrm{d}\Phi = \pm\mathrm{d}\Psi^{(\mathrm{II})}/\mathrm{d}\Phi$$

$$\Psi^{(\mathrm{II})}(\Phi) = \pm\Psi^{(\mathrm{I})}(\Phi) \qquad \tilde{\mu}_1 < \Phi < \tilde{\mu}_2 \tag{52b}$$

$$\mathrm{d}\Psi^{(\mathrm{II})}/\mathrm{d}\Phi = \pm\mathrm{d}\Psi^{(\mathrm{I})}/\mathrm{d}\Phi$$

where (+) corresponds to even functions ($k = 0$) and (−) to odd ones ($k = \frac{1}{4}$). The constant C involved in the expression of the eigenfunction $\Psi(\Phi)$ (see (34)), as well as the small quantity ν contained in the asymptotic expansion of the Kummer functions (37), will be also specified by the superscript $n = \mathrm{I}, \mathrm{II}$ in accordance with the type of well to which the eigenfunction belongs. Moreover, in order to reveal the even and odd character of the eigenfunctions we introduce the notations $\nu_{\mathrm{e}}^{(\mathrm{I,II})}$ and $\nu_{\mathrm{o}}^{(\mathrm{I,II})}$. With these specifications, the explicit evaluation of the matching relations (52*a*, *b*) leads to

$$\nu_{\mathrm{e}}^{(\mathrm{I})} = -\nu_{\mathrm{o}}^{(\mathrm{I})} \qquad \nu_{\mathrm{e}}^{(\mathrm{II})} = -\nu_{\mathrm{o}}^{(\mathrm{II})} \tag{53}$$

where

$$\nu_{\mathrm{e}}^{(\mathrm{I})} = -(1/2\sqrt{\pi e})m_1\mathcal{J} \tag{54a}$$

$$\nu_{\mathrm{e}}^{(\mathrm{II})} = -(1/2\sqrt{\pi e})m_2\mathcal{J} \tag{54b}$$

with

$$\mathcal{J} = \tfrac{1}{2}(\mathcal{J}^{(\mathrm{I})} + \mathcal{J}^{(\mathrm{II})}). \tag{55}$$

Here

$$\mathcal{J}^{(\mathrm{I})} = \exp\left(-\lambda \int_{\mu_1}^{\mu_2} \mathrm{d}\Phi \sqrt{|q(\Phi)|}\right) \tag{56a}$$

$$\mathcal{J}^{(\mathrm{II})} = \exp\left(-\lambda \int_{\tilde{\mu}_1}^{\tilde{\mu}_2} \mathrm{d}\Phi \sqrt{|q(\Phi)|}\right) \tag{56b}$$

and, as expected, $\mathcal{J}^{(\mathrm{I})} = \mathcal{J}^{(\mathrm{II})}$. Finally, by using (30) together with (53)–(55) we obtain compact expressions for the extremities of the first two allowed bands into which the two isolated-well eigenvalues will tunnel-split. They are

$$\tilde{\varepsilon}_{\mathrm{b}}^{(0)} = \tilde{\tilde{\varepsilon}}_{\mathrm{oo}} - \frac{1}{2\sqrt{\pi e}}\frac{1}{\sqrt{m^*}}(m_1^2 + m_2^2)\mathcal{J} \tag{57a}$$

$$\tilde{\varepsilon}_{\mathrm{t}}^{(0)} = \tilde{\tilde{\varepsilon}}_{\mathrm{oo}} - \frac{1}{2\sqrt{\pi e}}\frac{1}{\sqrt{m^*}}(m_2^2 - m_1^2)\mathcal{J} \tag{57b}$$

and

$$\tilde{\varepsilon}_{\mathrm{b}}^{(1)} = \tilde{\tilde{\varepsilon}}_{\mathrm{oo}} + \frac{1}{2\sqrt{\pi e}}\frac{1}{\sqrt{m^*}}(m_2^2 - m_1^2)\mathcal{J} \tag{57c}$$

$$\tilde{\varepsilon}_{\mathrm{b}}^{(1)} = \tilde{\tilde{\varepsilon}}_{\mathrm{oo}} + \frac{1}{2\sqrt{\pi e}}\frac{1}{\sqrt{m^*}}(m_1^2 + m_2^2)\mathcal{J} \tag{57d}$$

where

$$\tilde{\tilde{\varepsilon}}_{\mathrm{oo}} = \frac{1}{4\sqrt{m^*}}(m_1 + m_2) \tag{58}$$

and represents a middle value of the two isolated-well eigenvalues (32*b*) and (32*c*), with respect to which the two tunnel-split lowest bands are symmetrically situated. For $r = 0$, $m_1 = m_2 = 1$, and we recover the lowest eigenvalue of the harmonic oscillator of an isolated well of the sine-Gordon system.

In the low temperature regime the only contribution to the partition function will be given by the bottom of the lowest band (57*a*) and thus the free energy per unit length can be approximated by

$$F = \frac{1}{\beta l} \ln\left(\frac{\beta \hbar c_0}{l}\right) + A\omega_0^2 \tilde{\varepsilon}_{oo} - A\omega_0^2 t_0. \tag{59}$$

The sum of the first two terms on the right-hand side of (59) is precisely equal to the free-energy density of a set of one-dimensional classical harmonic oscillators when calculated to leading order $O(l/d)$ of the displacive limit. The presence of the two 'media' appears in this limit as a new 'medium' (a weighted combination of the two 'media'), to which corresponds a harmonic oscillator whose lowest eigenvalue is given by (58). The last term $-A\omega_0^2 t_0$ can be clearly associated with the kinks, as can easily be shown.

Now we may write

$$t_0 = t_0^{(I)} + t_0^{(II)} \tag{60}$$

where

$$t_0^{(I,II)} = \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} m_{1,2}^2 \mathcal{J}. \tag{61}$$

Here the superscript $n = I, II$ specifies the type of well from which the tunnelling process through the adjacent barrier starts. Recalling the definition relations (33) of m_1 and m_2, we observe that $t_0^{(I)} < t_0^{(II)}$. This inequality can be explained by the fact that the height of a barrier 'measured' from the lowest isolated eigenvalue $\tilde{\varepsilon}_{oo}^{(I)}$ of the type-I well is larger than that 'measured' from the isolated well eigenvalue $\tilde{\varepsilon}_{oo}^{(II)}$ corresponding to the type-II well. Taking this into account, by analogy with the DWDP results, we may expect that the bandwidth will be proportional to $t_0^{(I)}$ and the bandgap will be proportional to $t_0^{(II)}$. Indeed, from (57) we obtain

$$L_b = \frac{1}{\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} m_1^2 \mathcal{J} \tag{62}$$

and

$$L_g = \frac{1}{\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} m_2^2 \mathcal{J} \tag{63}$$

when evaluated from the centres of the two bands. If the gap is evaluated between the top of the lowest band and the bottom of the second one its width is given by

$$l_g = \frac{1}{\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} (m_2^2 - m_1^2) \mathcal{J} \tag{64}$$

and vanishes for $r = 0$; again we recover the sine-Gordon case.

The integrals involved in (55) and defined by (56*a*, *b*) can be easily calculated by using the procedure employed by Croitoru *et al.* By performing these calculations we obtain the following final (appoximate) expression for the tunnelling term t_0:

$$t_0 = (2/\pi)^{1/2} 2^2 2^{(m_1+m_2)/4} \tfrac{1}{2}(m_1^2 + m_2^2)(m^*)^{1/4} \exp(-\beta E_K) \tag{65}$$

where $E_K = c_0^2 M_K$ represents the rest energy of the two kinks. The special form (65) again shows that the tunnelling is clearly associated with the kinks. Though the tunnelling rates $t_0^{(I)}$ and $t_0^{(II)}$ are weighted by the parameters m_1^2 and m_2^2, respectively, which characterise the well from which the tunnelling process starts, they also depend weakly (note the factor $2^{(m_1+m_2)/4}$) on the well to which this process proceeds. We recall that all calculations have been based on the assumption that the potential wells can be approximated by a harmonic oscillator, i.e. we have limited our investigations to such values of the shape parameter r for which this hypothesis is fine. For very small values of r this assumption is clearly fulfilled and then $2^{(m_1+m_2)/4}$ is slightly different from $\sqrt{2}$.

4. Conclusions

In the preceeding sections we have presented the main features of two polykink-bearing systems, such as the DWDP and ASDP chain. As an interesting property of the latter system, we have pointed out the presence of two types of extended modes, each confined to one of the two different potential wells.

Extending an asymptotic procedure employed in a recent paper (Croitoru *et al* 1984) for the study of singly periodic systems such as the Φ^4 and SG chain to the investigation of the low temperature thermodynamics of polykink as well as of poly-extended mode-bearing systems, we have succeeded in calculating the temperature dependence of the free-energy density in the displacive limit. In the DWDP case the free-energy density contains two parts: a term which can be precisely attributed to the free-energy density of a set of harmonic phonons when calculated to order $O(l/d)$ of the displacive limit, and a term which can be clearly associated with the two types of kinks ((44), (46)), thus representing the free-energy density of a dilute ideal gas of two types of kinks. In the ASDP case our results again show that the free-energy density contains a part which represents the contribution of a set of harmonic oscillators and a second one strongly related to the two asymmetric kinks with the same rest energy ((61), (65)). This latter portion can be considered as the free-energy density of a dilute gas of two types of kinks: the type-I kink describes the evolution of the system from 'medium I' to 'medium II', while the type-II kink describes the system's evolution from 'medium II' to 'medium I'. We remark that, on the one hand, the phonon contribution to the free-energy density stems from a 'medium' which represents a weighted combination of the two different 'media', and on the other hand the contribution to the free-energy density of both types of kinks depends on both wells, even if the main dependence is determined by the well from which the tunnelling starts. Furthermore, the asymptotic method employed in our studies enabled us to evaluate, for the two models investigated here, the tunnel splitting of the lowest isolated-well eigenvalue (DWDP case) as well as of the two different isolated-well eigenvalues (ASDP case) into two allowed narrow bands, for whose lower and upper extremities we obtained compact expressions dependent on the shape parameter r. For $r=0$ we recovered in both cases the known sine-Gordon results. Taking in the ASDP case as reference levels for the barrier's height the two different lowest isolated-well eigenvalues, it resulted for both models that the bandwidth is due to the tunnelling through the high barrier, while the tunnelling through the small barrier determines the gap between the two bands. These latter conclusions are in complete agreement with the

picture which can be imagined to generate the two potentials $(2a, b)$, namely the periodic repetition of a symmetric and an asymmetric double well, respectively. Indeed, by starting for instance in the DWDP case, from the double well (see figure 2(a)), the degenerated lowest isolated-well eigenvalue tunnel splits into

$$\tilde{\varepsilon}_0' = \tilde{\varepsilon}_{oo} - \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{J}^{(I)} \tag{66a}$$

$$\tilde{\varepsilon}_1' = \tilde{\varepsilon}_{oo} + \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{J}^{(I)} \tag{66b}$$

the splitting being given by

$$2t' = \frac{1}{\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{J}^{(I)}. \tag{67}$$

By comparing (67) with (48), we see that $2t'$ is identical to the width of the gap between the two bands. Taking into account the periodic repetition of the double well, each eigenvalue $\tilde{\varepsilon}_0'$ and $\tilde{\varepsilon}_1'$, respectively, will tunnel-split into a narrow band. The lower and upper extremities of these bands are

$$\tilde{\varepsilon}_b^{(0)} = \tilde{\varepsilon}_0' - \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{J}^{(II)} \tag{68a}$$

$$\tilde{\varepsilon}_t^{(0)} = \tilde{\varepsilon}_0' + \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{J}^{(II)} \tag{68b}$$

and

$$\tilde{\varepsilon}_b^{(1)} = \tilde{\varepsilon}_1' - \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{J}^{(II)} \tag{68c}$$

$$\tilde{\varepsilon}_t^{(1)} = \tilde{\varepsilon}_1' + \frac{1}{2\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{J}^{(II)} \tag{68d}$$

the width of both bands being given by

$$\tilde{\varepsilon}_t^{(0)} - \tilde{\varepsilon}_b^{(0)} = \tilde{\varepsilon}_t^{(1)} - \tilde{\varepsilon}_b^{(1)} = \frac{1}{\sqrt{\pi e}} \frac{1}{\sqrt{m^*}} \frac{(1-r)^2}{1+r^2} \mathcal{J}^{(II)} = L_b \tag{69}$$

thus completely recovering the results (42), (47) and (48) and so the picture we have imagined seems completely adequate.

Much remains to be done, however, to extend the above analysis still further. For example, there may exist physical situations for which it is not always possible to assume small values for the shape parameter r for which the potential wells can be approximated by a harmonic oscillator. Thus for such situations one has to imagine a suitable change of the Langer transformation. Another challenging problem represents the extension of the phenomenological ideal-gas theory to treat the ASDP system as well, and not only polykink-bearing systems like those studied by DeLeonardis and Trullinger (1983).

Acknowledgments

We wish to thank Dr D Grecu for helpful discussions.

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