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2000 J. Phys. A: Math. Gen. 33 4741

(http://iopscience.iop.org/0305-4470/33/26/302)

J. Phys. A: Math. Gen. **33** (2000) 4741–4754. Printed in the UK PII: S0305-4470(00)12685-X

A quantum Peierls–Nabarro barrier

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Received 16 March 2000

Abstract. Kink dynamics in spatially discrete nonlinear Klein–Gordon systems is considered. For special choices of the substrate potential, such systems support continuous translation orbits of static kinks with no (classical) Peierls–Nabarro barrier. It is shown that these kinks experience, nevertheless, a lattice-periodic confining potential, due to purely quantum effects analogous to the Casimir effect of quantum field theory. The resulting 'quantum Peierls–Nabarro potential' may be calculated in the weak-coupling approximation by a simple and computationally cheap numerical algorithm, which is applied, for the purposes of illustration, to a certain two-parameter family of substrates.

1. Introduction

Many systems in condensed matter and biophysics may be modelled by infinite chains of coupled anharmonic oscillators. If the anharmonic substrate potential has two or more degenerate vacua, such a system may support static kink solutions interpolating between neighbouring vacua. These kinks have various interesting physical interpretations (as crystal dislocations [1], charge density waves [2] and magnetic [3] and ferroelectric [4] domain walls, for example) and their dynamics is an interesting and important subject.

Such a system of oscillators has an alternative interpretation as a spatially discrete version of an appropriate nonlinear Klein–Gordon equation. The lattice spacing h is related to the spring constant of the chain α by $\alpha = 1/h^2$, so the strong spring-coupling limit is interpreted as a continuum limit. In the continuum limit, static kinks may occupy any position in space, by translation symmetry. This is generically untrue in the discrete system: static kinks may generically occupy only two positions relative to the lattice, one of which is a saddle point of potential energy, the other a local minimum. The difference in energy between these two static solutions is the Peierls–Nabarro (PN) barrier, the barrier which a kink must surmount in order to propagate from one lattice cell to the next. It can have strong effects on the dynamics of kinks in the system (kink trapping, radiative deceleration, phonon bursts, etc [5, 6]).

One might expect the PN barrier, and hence its effects, to grow monotonically with h (of course the barrier vanishes as $h \to 0$). However, it has long been known that this is certainly not universally true [7]. In fact, recent work of Flach *et al* [8] has shown that there exist infinitely many substrate potentials with the property that for at least one non-zero lattice spacing, h_* say, the PN barrier vanishes exactly and a continuous translation orbit of static kinks is recovered. We shall say that a substrate potential with this property is 'transparent

0305-4470/00/264741+14$30.00

at lattice spacing h_*'. Such potentials may be constructed by means of the so-called inverse method, and are clearly of some theoretical interest.

The purpose of the present paper is to argue that although the kinks of such a system (at $h = h_*$) are free of the classical PN barrier, they still experience a qualitatively similar periodic confining potential due to quantum effects analogous to the Casimir effect of quantum electrodynamics. We call this the quantum Peierls–Nabarro (QPN) potential. The essential physical observation is that the total zero-point energy of the lattice phonon modes in the presence of a kink depends periodically on the kink position. It should be emphasized that the kink position itself is treated as a classical degree of freedom while the phonons are quantized. The physical regime in which this is consistent will be identified: the classical kink mass must far exceed the phonon mass, and the kink must interpolate between widely separated vacua. For the purposes of illustration, we shall compute the QPN potential numerically for a two-parameter family of substrate potentials which (in a sense) includes discrete sine–Gordon and ϕ^4 systems. As a by-product of these calculations, we will obtain numerical evidence in favour of the assumption that kinks in these models are classically stable.

2. Construction of transparent substrate potentials by the inverse method

The general discrete nonlinear Klein–Gordon system consists of a field $\phi : \mathbb{Z} \times \mathbb{R} \to \mathbb{R}$ whose evolution is determined by a second-order differential difference equation,

$$\ddot{\phi}_n = \frac{1}{h^2}(\phi_{n+1} - 2\phi_n + \phi_{n-1}) - V'(\phi_n). \tag{1}$$

Here h is the spatial lattice spacing, $\ddot{\phi}_n = \mathrm{d}^2\phi_n/\mathrm{d}t^2$ and V is the substrate potential. One interpretation of the equation of motion is as that of an infinite system of identical oscillators (each oscillating in a potential well V) with nearest neighbours coupled by identical Hooke's law springs of strength $\alpha = h^{-2}$. As the name suggests, equation (1) becomes a nonlinear Klein–Gordon equation in the continuum limit, $h \to 0$. If $V(\phi)$ has neighbouring degenerate vacua at $\phi = a_-$ and $\phi = a_+ > a_-$, say, equation (1) supports static kinks interpolating between them. To find these requires the solution of a second-order nonlinear difference equation subject to the boundary conditions $\lim_{n\to\pm\infty} \phi_n = a_\pm$, which is usual only possible numerically.

In this section we will construct, for a given lattice spacing $h_* > 0$, a substrate potential $V_{h_*}(\phi)$ which supports a continuous translation orbit of static kinks, and so by construction is transparent at lattice spacing h_*. To do this we shall use a variant of the inverse method of Flach *et al* [8, 9] (which was originally devised to construct substrate potentials which support exact *propagating*, rather than static, kink solutions). The idea is to *choose* a static kink profile, that is an analytic, monotonic surjection $f : \mathbb{R} \to (a_-, a_+)$, satisfying exponential decay criteria as $z \to \pm\infty$,

$$f(z) = a_\pm + \mathrm{O}(\mathrm{e}^{-\mu|z|}) \qquad \mu > 0 \tag{2}$$

and the symmetry requirement,

$$f(z) + f(-z) \equiv a_+ + a_- \tag{3}$$

then *impose* that the translated kink $\phi_n^b = f(nh - b)$ be a static solution of the system (with $h = h_*$) for all $b \in \mathbb{R}$. From equation (1), this condition holds provided one chooses V_{h_*}

such that

$$V'_{h_*}(f(z)) = \frac{1}{h_*^2}[f(z+h_*) - 2f(z) + f(z-h_*)] \tag{4}$$

for all $z \in \mathbb{R}$. This uniquely determines $V'_{h_*} : (a_-, a_+) \to \mathbb{R}$ by monotonicity of f, and hence $V_{h_*} : (a_-, a_+) \to \mathbb{R}$ up to an arbitrary constant. To complete the definition of this transparent substrate, one should extend its definition appropriately to all $\mathbb{R}$. How one does this is somewhat arbitrary, but will have no bearing on our results, so we shall merely demand that V_{h_*}, V'_{h_*}, V''_{h_*} be continuous at $a_\pm$. Equations (2) and (4) then imply

$$V'_{h_*}(a_\pm) = 0 \tag{5}$$

$$V''_{h_*}(a_\pm) = \frac{2}{h_*^2}(\cosh \mu h_* - 1) > 0. \tag{6}$$

Hence $\phi = a_\pm$ are both stable equilibria. To see that these are degenerate vacua, note that from (4),

$$\begin{aligned} h_*^2[V_{h_*}(a_+) - V_{h_*}(a_-)] &= \int_{-\infty}^{\infty} [f(z+h_*) - 2f(z) + f(z-h_*)]f'(z)\,\mathrm{d}z \\ &= \int_{-\infty}^{\infty} [f(z+h_*) + f(-(z+h_*))]f'(z)\,\mathrm{d}z - (a_+^2 - a_-^2) \\ &= (a_+ + a_-)[f(z)]_{-\infty}^{\infty} - (a_+^2 - a_-^2) \\ &= 0 \end{aligned} \tag{7}$$

using the symmetry constraint on f, (3).

So given a kink profile f, the inverse method generates a one-parameter family of double-well substrate potentials $\{V_{h_*} : h_* > 0\}$ each of which is transparent at spacing $h = h_*$. Moreover, one has as explicit formula for the continuous translation orbit of static kink solutions, namely $\phi_n^b = f(nh_* - b)$, $b \in \mathbb{R}$. On physical grounds, one expects the static kinks to be stable to small perturbations, although strictly speaking this is not assured. One would need to check that the Hessian of the potential energy functional,

$$E_P = \sum_{n\in\mathbb{Z}} \left[\frac{1}{2h_*^2}(\phi_{n+1} - \phi_n)^2 + V_{h_*}(\phi_n) \right] \tag{8}$$

about ϕ^b has a strictly positive spectrum (except for the zero-mode associated with translation). The quantum calculation described in section 3 may be reinterpreted as the calculation of this spectrum. The results of section 5 then constitute numerical confirmation of kink stability for the family of transparent substrates considered therein.

3. The quantum Peierls–Nabarro potential

In this section we shall quantize the system using a weak-coupling approximation, essentially following the method outlined in [10], adapted to the infinite lattice. The method has previously been applied in the spatially discrete context to a certain non-standard lattice sine–Gordon model [11].

One may regard E_P as a potential energy function on the infinite-dimensional space Q of sequences $\phi : \mathbb{Z} \to \mathbb{R}$. The vacua $\phi = a_\pm$ lie at the bottom of identical potential wells,

cut off from each other, and all configurations with kink boundary behaviour, by an infinite energy barrier. Assuming that V is transparent at the lattice spacing under consideration (e.g. $V = V_{h_*}$ and $h = h_*$, as in section 2), the continuous kink translation orbit is an equipotential curve in Q: the classical energy of a static kink is independent of its position. If the kinks are stable, this is a level valley bottom winding through Q.

Quantum mechanically, a particle cannot sit at the bottom of a potential well, or on the low-dimensional floor of a valley: it always possesses a zero-point energy dependent on the shape of the well bottom. In this section we will semiclassically quantize motion both in the vacuum and kink sectors of the system. A physical regime will be identified in which the kink is very heavy, so that the kink position b may be treated as a classical degree of freedom, while the comparatively light phonon modes orthogonal to the translation mode are quantized perturbatively, by Taylor expansion of E_P. Computation of the kink ground state energy then amounts to summing the zero-point energies of an infinite system of harmonic oscillators, resulting in a divergent series. The quantity of physical significance is not this energy, but rather the difference between the kink and vacuum ground state energies, which is expected to be finite. Since translation is not a symmetry of the discrete system, there is no reason to expect this energy to be independent of b, that is, one expects the quantum kink energy to vary periodically with kink position, which is the origin of the quantum PN potential.

It is convenient to introduce a dimensionless coupling constant λ into the model so that the (classical) Hamiltonian of the system is

$$H = \sum_{n\in\mathbb{Z}} \left[\frac{1}{2}\pi_n^2 + \frac{1}{2h^2}(\phi_{n+1} - \phi_n)^2 + \frac{1}{\lambda^2} V(\lambda\phi) \right] \tag{9}$$

where $\pi_n = \dot{\phi}_n$ is the momentum conjugate to ϕ_n. Assuming that V is transparent at spacing h, this system supports a continuous translation orbit of static kinks

$$\phi_n^{b,\lambda} = \frac{1}{\lambda} f(nh - b) \qquad b \in \mathbb{R} \tag{10}$$

interpolating between a_-/λ and a_+/λ. The classical energy of these kinks is independent of b and clearly scales with λ as

$$E_P[\phi^{b,\lambda}] = \frac{1}{\lambda^2} E_P[\phi^{0,1}]. \tag{11}$$

The physical regime of interest is that of small λ where the kinks interpolate between widely separated vacua, by (10), and are very heavy, by (11). In this regime, one may approximate motion about any stable static solution $\widetilde{\phi} = \varphi/\lambda$ by using a truncated Taylor series approximation for $E_P[\widetilde{\phi} + \delta\phi]$:

$$E_P[\widetilde{\phi} + \delta\phi] = \frac{1}{\lambda^2} E_P[\varphi] + \frac{1}{2h^2} \sum_{n,m} W_{nm}\delta\phi_n\delta\phi_m + \mathrm{O}(\lambda) \tag{12}$$

where

$$W_{nm} = \delta_{nm}[2 + h^2 V''(\varphi)] - \delta_{n,m+1} - \delta_{n,m-1}. \tag{13}$$

Since W is a real, symmetric matrix, there exists an orthogonal transformation R such that

$$W_{nm} = \sum_{k,l} R_{nk}^T U_{kl} R_{lm} \tag{14}$$

with U diagonal. The diagonal entries of U are the eigenvalues Λ_n of W, none of which is negative provided $\widetilde{\phi}$ is stable, as we are assuming. Introducing normal coordinates

$\xi_n = \sum_m R_{nm}\delta\phi_m$ which have conjugate momenta $\eta_n = \sum_m R_{nm}\pi_m$, the Hamiltonian for motion about $\widetilde{\phi}$ reduces to

$$H = \frac{1}{\lambda^2}E_P[\varphi] + \frac{1}{2}\sum_n \left[\eta_n^2 + \frac{\Lambda_n}{h^2}\xi_n^2\right] + \mathrm{O}(\lambda). \tag{15}$$

Neglecting the $\mathrm{O}(\lambda)$ remainder, this is the Hamiltonian for an infinite set of decoupled harmonic oscillators of natural frequencies $h^{-1}\sqrt{\Lambda_n}$.

We now quantize in standard canonical fashion in the cases where $\widetilde{\phi} = a_\pm/\lambda$ (the vacuum) and $\widetilde{\phi} = \phi^{b,\lambda}$ (the kink located at b). Let the W-matrices in these cases be denoted by W^{vac} and $W^K(b)$, respectively, with spectra $\{\Lambda_n^{vac}\}$ and $\{\Lambda_n^K(b)\}$. In each case, the quantum correction to the ground state energy is the sum of the zero-point energies of the oscillators,

$$\frac{1}{2h}\sum_n \sqrt{\Lambda_n} \tag{16}$$

in units where $\hbar \equiv 1$ (recall that h denotes the lattice spacing of the system). In the case of kinks, one should omit from this sum the eigenvalue associated with the translation mode since, the kink being very heavy, this mode is treated classically. Actually, this makes no difference since the corresponding eigenvalue vanishes, so one might as well sum over all modes, including the zero mode.

Of course, the series (16) is divergent in both the vacuum and kink sectors, and must be suitably regulated and renormalized. To this end, we truncate the lattice symmetrically about the kink centre (so $-n_0 \leqslant n \leqslant n_0$, assuming $b \in [0, h)$) and consider the spectra $\{\Lambda_n(N) : n = -1\ldots, N\}$ of the truncated W-matrices of order $N = 2n_0{+}1$. The renormalized ground state energy is then

$$\mathcal{E}(b) = \frac{E_P[\phi^{0,1}]}{\lambda^2} + \lim_{N\to\infty}\sum_{n=1}^{N}\left[\sqrt{|\Lambda_n^K(N,b)|} - \sqrt{\Lambda_n^{vac}(N)}\right] \tag{17}$$

which one expects to be finite, given the exponential spatial localization of the kink (the large-$|n|$ entries of the matrix W^K are essentially identical to those of W^{vac}). The finite size of the lattice perturbs the translation zero mode away from zero slightly, so one of the kink eigenvalues $\Lambda_n(N, b)$ may be negative for some (N, b) (although it must vanish as $N \to \infty$). This is why we have introduced an absolute value into equation (17), so that $\mathcal{E}(b)$ is the limit of a real-valued sequence. In the limit $N \to \infty$ lattice translation symmetry is recovered, so $\mathcal{E}(b)$ should be periodic with period h.

4. The $\cosh^{-\mu}$ kink family

If we now choose $V = V_h$, for some kink profile f, we see from equations (13) and (4) that the QPN potential depends on f only through f', because

$$2 + h^2 V_h''(f(z)) = \frac{f'(z+h) + f'(z-h)}{f'(z)}. \tag{18}$$

For the purposes of illustration we will consider the one-parameter family

$$f'(z) = \frac{1}{\cosh^\mu z} \tag{19}$$

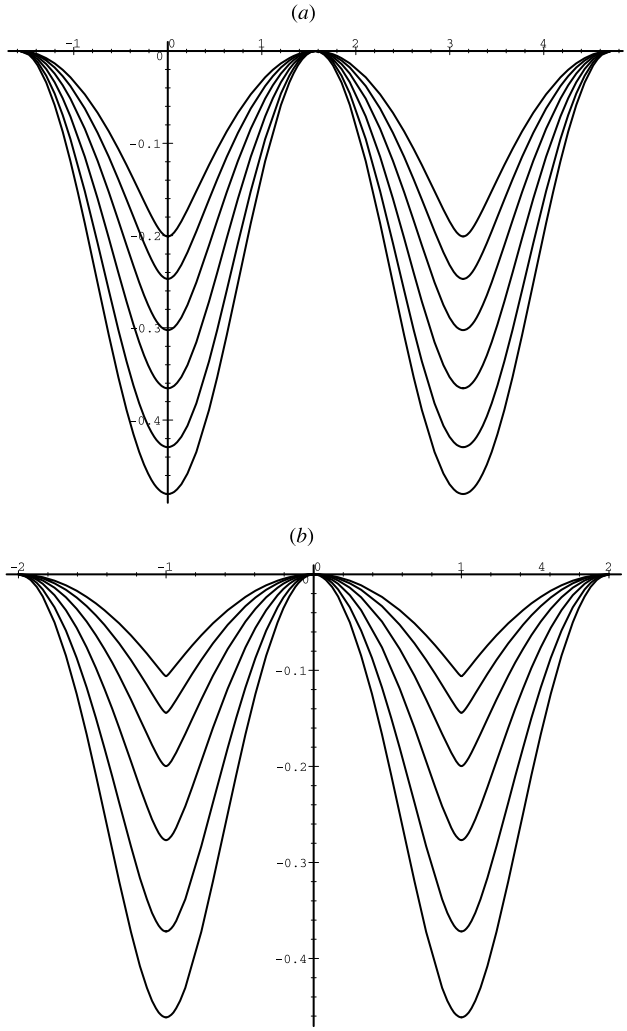

Figure 1. Transparent substrate potentials generated by (*a*) the sine–Gordon kink profile ($\mu = 1$) and (*b*) the ϕ^4 kink profile ($\mu = 2$), with lattice spacings from $h = 0.5$ (bottom curve) to $h = 3.0$ (top curve) in steps of 0.5.

with $\mu > 0$. Note that this includes the cases of the sine–Gordon ($f(z) = 2\tan^{-1}\mathrm{e}^{z}$) and ϕ^4 ($f(z) = \tanh z$) kink profiles: $\mu = 1$ and 2, respectively. The corresponding transparent substrates in these two cases are shown in figure 1.

The neighbouring vacua $a_{\pm}$ may be any real numbers separated by

$$a_+ - a_- = \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\cosh^{\mu} x}. \tag{20}$$

Since $f(z)$ has order $\mathrm{e}^{-\mu|z|}$ exponential decay, $V_h''(a_{\pm})$ is given by equation (6), and the vacuum W-matrix takes the simple form

$$W_{nm}^{vac} = 2\cosh \mu h\, \delta_{nm} - (\delta_{n,m-1} + \delta_{n,m+1}). \tag{21}$$

The spectrum of the system truncated to N lattice sites is easily computed:

$$\Lambda_n^{vac}(N) = 2(\cosh \mu h - 1) + 4 \sin^2 \left(\frac{n\pi}{2(N+1)} \right) \qquad n = 1, 2, \ldots, N. \tag{22}$$

In the limit $N \to \infty$, the spectrum densely fills the interval $[2(\cosh \mu h - 1), 2(\cosh \mu h + 1)]$.

The eigenvalue problem for the kink W-matrix,

$$W_{nm}^K(b) = \frac{f'(nh + h - b) + f'(nh - h - b)}{f'(nh - b)} \delta_{nm} - (\delta_{n,m-1} + \delta_{n,m+1}) \tag{23}$$

is intractable analytically, and will be solved numerically in section 5. One can show, however, that the quantum kink energy is (for all b) *lower* than the classical kink energy, that is, the quantum energy correction is *negative*. To see this, let $\Delta(b)$ be the real diagonal matrix

$$\Delta_{nm}(b) = h^2 \delta_{nm} [V_h''(f(nh - b)) - V_h''(a_\pm)] \tag{24}$$

so that $W^K(b) = W^{vac} + \Delta(b)$. Let $\{\Lambda_n^K(b)\}$, $\{\Lambda_n^{vac}\}$ and $\{\Gamma_n(b)\}$ be the eigenvalues of $W^K(b)$, W^{vac} and $\Delta(b)$, each spectrum arranged in non-increasing order ($\Gamma_1 \geqslant \Gamma_2 \geqslant \Gamma_3 \geqslant \cdots$). Then standard matrix perturbation theory [12] asserts that

$$\Lambda_n^K(b) \leqslant \Lambda_n^{vac} + \Gamma_1(b) \tag{25}$$

for all n, where Γ_1 is the greatest eigenvalue of $\Delta(b)$,

$$\Gamma_1(b) = \max_n h^2 [V_h''(f(nh - b)) - V_h''(a_\pm)]. \tag{26}$$

So if $V_h''(f(z)) < V_h''(a_\pm)$ for all $z \in \mathbb{R}$ then $\Gamma_n < 0$ and the perturbation of W^{vac} by $\Delta(b)$ must reduce each eigenvalue $\Lambda_n^K(b)$ relative to its vacuum counterpart, with the result (always assuming kink stability) that

$$\sum_n \left(\sqrt{|\Lambda_n^K(b)|} - \sqrt{\Lambda_n^{vac}} \right) < 0. \tag{27}$$

This condition on $V_h''(\phi)$ (a maximum second derivative at the vacua) is quite natural, and can easily be shown to hold for the whole $\cosh^{-\mu}$ family ($\mu > 0$, $h > 0$). Note that

$$h^2 [V_h''(f(z)) - V_h''(a_\pm)] = g(z) - \lim_{x \to \infty} g(x) \tag{28}$$

where

$$g(z) = \left[\frac{\cosh z}{\cosh(z + h)} \right]^\mu + \left[\frac{\cosh z}{\cosh(z - h)} \right]^\mu. \tag{29}$$

Now g is differentiable and even, and

$$g'(z) = -\mu \sinh h \cosh^{\mu-1} z \left[\frac{1}{\cosh^{\mu+1}(z + h)} - \frac{1}{\cosh^{\mu+1}(z - h)} \right] \tag{30}$$

so the only critical point of g is $z = 0$, a local minimum, whence it follows that $g(z) < \lim_{x \to \infty} g(x)$ for all z.

5. Numerical results

Since the truncated kink W-matrix $W_N^K(b)$ is real, symmetric and tridiagonal, its eigenvalue problem is particularly easy to solve numerically. In this section we present data generated by implementing the QL decomposition algorithm for tridiagonal matrices with implicit eigenvalue shifts, outlined in [13].

The first thing to check is that, as expected, the spectrum of $W^K(b)$ is positive semi-definite with non-degenerate eigenvalue zero. The least and next-to-least eigenvalues of $W_N^K(b)$ for N odd, $3 \leqslant N \leqslant 90$ were computed for a large sample of parameter values in the range $1 \leqslant \mu \leqslant 3$, $0.5 \leqslant h \leqslant 10$, $0 \leqslant b/h \leqslant 0.5$. The results were similar at all points sampled: the least eigenvalue converges to zero, while the next-to-least converges to a positive number *below* the lower edge of the vacuum phonon band, that is, less than $2(\cosh \mu h - 1)$. It is instructive to look at the build up of the spectrum of $W_N^K(b)$ as N grows large, as depicted for two contrasting sets of parameter values in figure 2. This clearly shows the rapid convergence of the bottom eigenvalue to zero (convergence being faster for larger μh, since the kink structure is then more tightly spatially localized) and the next lowest eigenvalue to a positive constant below the phonon band. The eigenvector corresponding to the lowest positive eigenvalue is a spatially localized mode in which the slope of the kink oscillates about the kink centre. The rest of the eigenvalues accumulate, apparently densely, within the phonon band (delimited by horizontal broken lines in figure 2). This is precisely the right behaviour to ensure both kink stability and convergence of the quantum-corrected kink energy in the limit $N \to \infty$. The size of the truncated system needed to obtain practical convergence depends on μh, but, within the parameter range cited above, $N = 51$ seems to suffice. This is the matrix order used to obtain the remaining numerical data.

The quantity $\mathcal{E}(b)$ as defined in (17) is problematic to plot since it contains contributions of different orders in λ. For this reason it is convenient to consider $\widetilde{\mathcal{E}}(b) = \mathcal{E}(b) - \mathcal{E}(0)$, which is of order λ^0, instead. In fact, $\widetilde{\mathcal{E}}(b)$ is the quantity of most direct physical significance anyway: it gives the change in kink energy as b varies, which is precisely what is meant by the quantum Peierls–Nabarro potential.

Figure 3 shows $\widetilde{\mathcal{E}}(b)$ ($0 \leqslant b/h \leqslant 1$) for the sine–Gordon substrate potentials ($\mu = 1$), at a variety of lattice spacings. The results are qualitatively very similar to the usual classical PN potential: the kink has greatest energy when located exactly on a lattice site ($b = 0$) and least when located exactly midway between lattice sites ($b = h/2$), the energy difference (the QPN barrier) growing monotonically with h.

Figure 4 shows similar plots for the ϕ^4 substrate potentials ($\mu = 2$). Here, once again, kinks have greatest energy when $b = 0$ and least when $b = h/2$, but the QPN barrier does not grow monotonically with h, nor is the shape of $\widetilde{\mathcal{E}}(b)$ so uniform as in the $\mu = 1$ case.

Similar plots for $\mu = 3$ reveal more complicated behaviour, as shown in figure 5. For small h, $\widetilde{\mathcal{E}}(b)$ is maximum at $b = 0$ and minimum at $b = h/2$ as for $\mu = 1, 2$. However, for h above a critical value ($\sim$1.46) $b = 0$ becomes a local minimum of $\widetilde{\mathcal{E}}$ and two extra local maxima appear. The global minimum of $\widetilde{\mathcal{E}}$ remains at $b = h/2$, rather than $b = 0$, until h exceeds about 1.52, after which $\widetilde{\mathcal{E}}(h/2)$ exceeds $\widetilde{\mathcal{E}}(0)$. As h is increased further, the two local minima coalesce at $b = h/2$ (at $h \sim 1.7$), so that the QPN potential starts to resemble an inverted version of the $\mu = 1$ case: now kinks have a *minimum* energy when located exactly on a lattice site and a *maximum* energy when located exactly midway between sites. This variation of the shape of $\widetilde{\mathcal{E}}$ with h is qualitatively rather similar to the behaviour of the classical PN potential for a particular member of a one-parameter family of substrates introduced by Peyrard and Remoissnet [7].

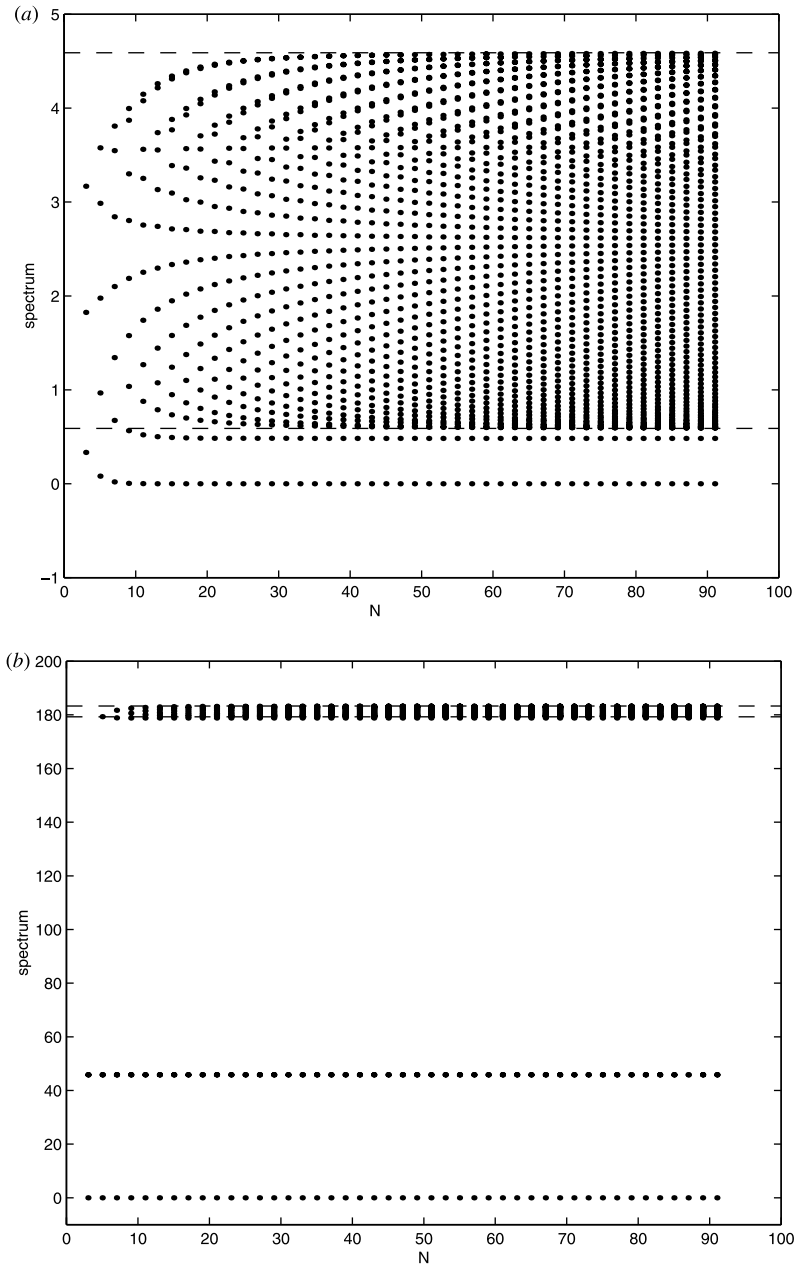

Figure 2. Build up of the spectrum of $W_N^K(b)$ as the matrix order N grows large, in the cases (*a*) $\mu = 1.5$, $h = 0.5$, $b/h = 0.2$ and (*b*) $\mu = 2.0$, $h = 2.6$, $b/h = 0$. Note how the spectrum accumulates within the vacuum phonon band, delimited by horizontal broken lines.

Periodicity and reflection symmetry of $\mathcal{E}$ imply that $b = 0$ and $h/2$ must always be critical points. There may be others (as in the case $\mu = 3.0$), but for the most part, plotting $\widetilde{\mathcal{E}}(h/2) = \mathcal{E}(h/2) - \mathcal{E}(0)$ against h gives a good account of how the QPN barrier varies with h and μ. In particular, the sign of $\widetilde{\mathcal{E}}(h/2)$ tells one whether the QPN barrier tends to trap kinks

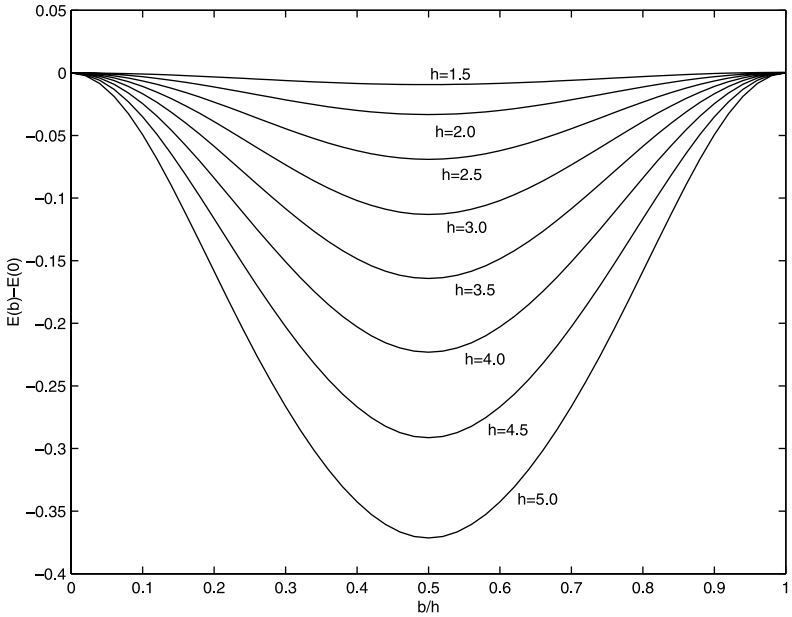

Figure 3. Position dependence of the quantum PN potential $\widetilde{\mathcal{E}}(b)$ for $\mu = 1$ and $h = 1.5$–5 in steps of 0.5.

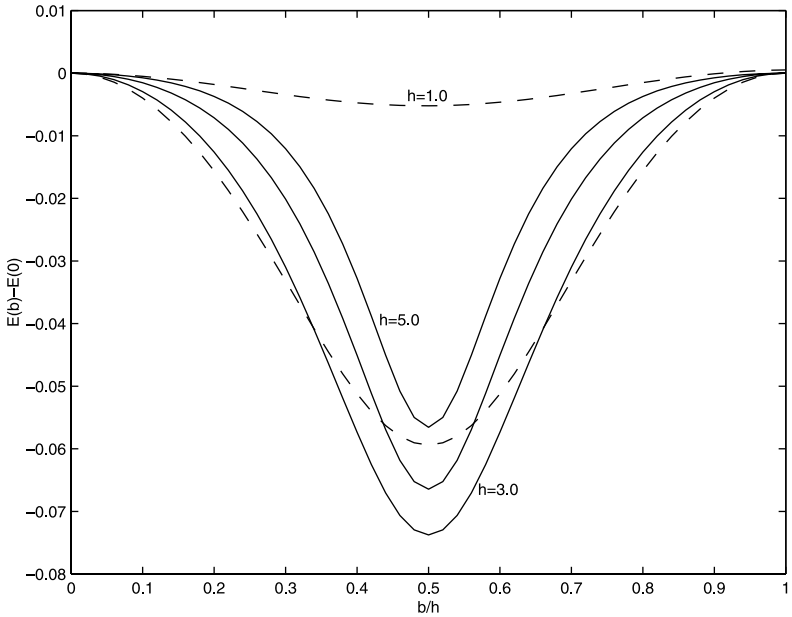

Figure 4. Position dependence of the quantum PN potential $\widetilde{\mathcal{E}}(b)$ for $\mu = 2$ and $h = 2$ to $h = 5$ in steps of 1. The unlabelled curves are $h = 2$ (broken) and $h = 4$ (full).

between lattice sites ($\widetilde{\mathcal{E}}(h/2) < 0$) or on lattice sites ($\widetilde{\mathcal{E}}(h/2) > 0$). Figure 6 shows plots of $\widetilde{\mathcal{E}}(h/2)$ against h for various $\mu \in [1, 3]$. Three regimes clearly emerge for large h: $1 \leqslant \mu \leqslant 2$

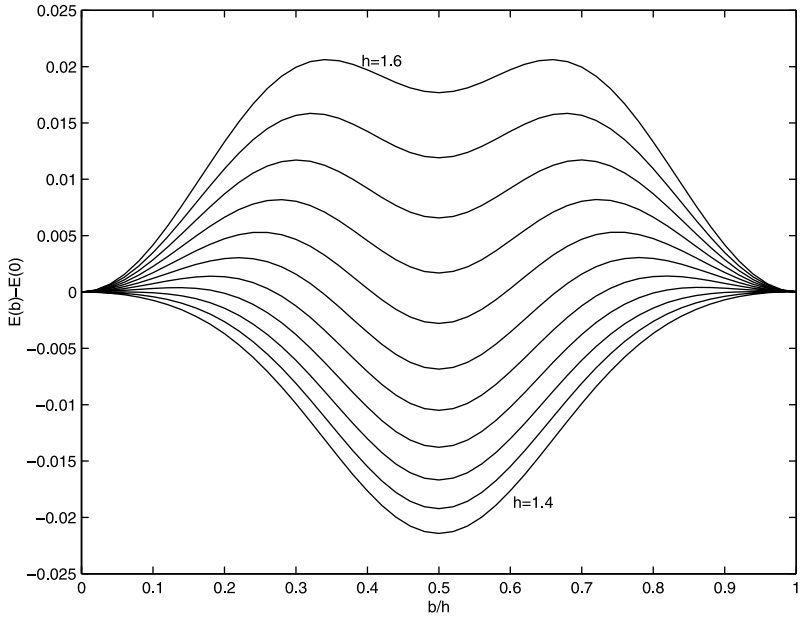

Figure 5. Position dependence of the quantum PN potential $\widetilde{\mathcal{E}}(b)$ for $\mu = 3$ and $h = 1.4$–1.6 in steps of 0.2.

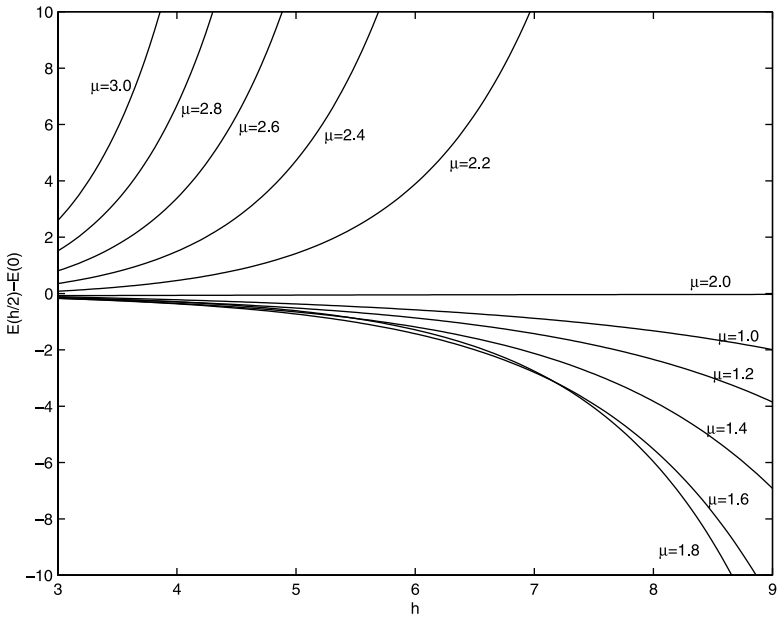

Figure 6. A rough measure of the depth of the QPN barrier: $\widetilde{\mathcal{E}}(h/2)$ as a function of h for various $\mu \in [1, 3]$.

($\widetilde{\mathcal{E}}(h/2) < 0$ growing unbounded as $h \to \infty$), $\mu = 2$ ($\widetilde{\mathcal{E}}(h/2) < 0$ remaining bounded as $h \to \infty$) and $2 \leqslant \mu \leqslant 3$ ($\widetilde{\mathcal{E}}(h/2) > 0$ growing unbounded as $h \to \infty$). This trichotomy may

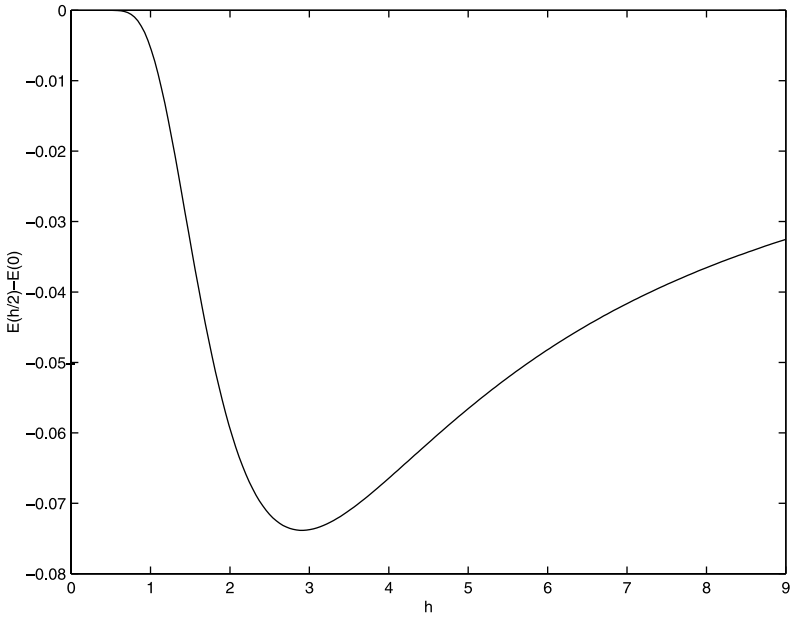

Figure 7. Dependence of the QPN barrier on the lattice spacing h in the critical case ($\mu = 2$).

be explained by consideration of the asymptotic forms of $W^K(0)$ and $W^K(h/2)$ for large h:

$$\frac{W^K(0)}{\mathrm{e}^{\mu h}} \sim \mathrm{diag}(\ldots, 1, 1, 2^{-\mu}, 0, 2^{-\mu}, 1, 1, \ldots) \tag{31}$$

$$\frac{W^K(h/2)}{\mathrm{e}^{\mu h}} \sim \mathrm{diag}(\ldots, 1, 1, 0, 0, 1, 1, \ldots). \tag{32}$$

This leads to the prediction

$$\frac{\widetilde{\mathcal{E}}(h/2)}{\mathrm{e}^{-\mu h/2}} \sim \frac{1}{2h}\left[(0-0) + (0-2^{-\mu/2}) + (1-2^{-\mu/2}) + (1-1) + (1-1) + \cdots\right] \tag{33}$$

$$\Rightarrow \widetilde{\mathcal{E}}(h/2) \sim \frac{(1-2^{1-\mu/2})}{2h}\mathrm{e}^{\mu h/2}. \tag{34}$$

Formula (34) accounts well for the asymptotic behaviour seen in figure 6. Clearly the most interesting case from this point of view is the critical value $\mu = 2$. The dependence of $\widetilde{\mathcal{E}}(h/2)$ on h for $\mu = 2$ is shown in figure 7. One sees that, rather counterintuitively, the QPN barrier actually vanishes in the extreme discrete limit, $h \to \infty$. One should remember, of course, that in varying h one also varies the shape of the transparent substrate potential V_h (which would not otherwise remain transparent). In fact, the limit $h \to \infty$ is always badly singular since the curvature of the substrate at the vacua grows unbounded, by equation (6).

6. Concluding remarks

In this paper we have considered oscillator chains with no classical PN barrier and shown that their kinks still experience a lattice-periodic confining potential due to purely quantum mechanical effects, leading to a new mechanism for kink pinning. The quantum PN potential

was computed numerically for a simple two-parameter family of substrates, revealing a rich variety of behaviour.

It remains to be seen whether the QPN potential and quantum kink pinning have any relevance to genuine physics. Given the idealized one-dimensional nature of the model, this seems unlikely (generalizing the inverse method to higher dimensions is very problematic). Another cause for doubt is that the effect exists only for certain special substrates. Just how special these 'transparent' substrates are is unknown. In order to have any physical relevance they would at least have to be structurally stable: if $V_h[f]$ is the substrate transparent at h generated by kink f, then given any sufficiently small perturbation δV there should exist a kink f_* close to f and spacing h_* close to h such that $V_h[f]+\delta V = V_{h_*}[f_*]$. Thinking of the inverse method as a mapping $K \times \mathbb{R}_+ \to P$ (where K is the space of kink profiles and P the space of potentials), the question is whether this mapping is continuous with respect to some sensible choice of topologies on K and P.

Given a non-transparent substrate V (i.e. with non-vanishing classical PN barrier) it still makes sense, in the regime of small λ, to treat the kink translation mode classically while quantizing the normal modes. Now one should quantize not about genuine static kink solutions, but rather about kinks solving a constrained energy minimization problem, necessarily determined numerically. In this situation the QPN potential is a correction to the classical PN potential. It is interesting to ask whether there exist substrates for which the two potentials exactly cancel, so that classically pinned kinks are *unpinned* by quantum effects (in contrast to the situation studied in this paper, where classically unpinned kinks are pinned by quantum effects). Unfortunately, this question lies beyond the scope of the perturbative methods used here. The classical PN potential, being a difference of kink masses, is order λ^{-2}, while the QPN potential is order λ^0, with unknown higher-order terms. Even if V could be found such that at some fixed λ the terms of order λ^0 and λ^{-2} cancel, the higher-order terms would still (presumably) produce kink pinning.

This paper also raises some rather more mathematical questions. We have presented numerical evidence to support the assumption of classical kink stability, but it should be possible to prove stability rigorously. Similarly, one should be able to prove convergence of the series defining $\mathcal{E}(b)$. In both cases one needs to understand the large-N behaviour of the spectrum of $W_N^K(b)$. Standard minimax estimates are insufficient for this purpose—a more delicate analysis is required.

Acknowledgments

This work was partially completed at the Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, where the author was a guest scientist. He wishes to thank Professor Eberhard Zeidler for the generous hospitality of the institute. The author is an EPSRC Postdoctoral Research Fellow in Mathematics.

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