

Bound states in a nonlinear Kronig - Penney model

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1997 J. Phys. A: Math. Gen. 30 4835

(<http://iopscience.iop.org/0305-4470/30/13/031>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.108

The article was downloaded on 02/06/2010 at 05:48

Please note that [terms and conditions apply](#).

Bound states in a nonlinear Kronig–Penney model

Stavros Theodorakis and Epameinondas Leontidis

Department of Natural Sciences, University of Cyprus, PO Box 537, Nicosia 1678, Cyprus

Received 13 January 1997, in final form 17 March 1997

Abstract. We study the bound states of a Kronig–Penney potential for a nonlinear one-dimensional Schrödinger equation. This potential consists of a large, but not necessarily infinite, number of equidistant δ -function wells. We show that the ground state can be highly degenerate. Under certain conditions furthermore, even the bound state that would normally be the highest can have almost the same energy as the ground state. This holds for other simple periodic potentials as well.

1. Introduction

In this paper we shall study an unusual generalization of the one-dimensional Kronig–Penney model. We shall examine in particular the spectrum of the bound states for a Kronig–Penney potential $V(z)$, having added a nonlinear term to the Schrödinger equation. Our arguments will be valid in the case of other simple periodic potentials as well.

Such nonlinear equations with periodic potentials arise in the Ginzburg–Landau treatment of various phenomena in condensed matter physics. In layered superconductors for example, such as the high temperature ones, a periodic potential such as the Kronig–Penney potential can describe the periodically modulated superconductivity of the samples [1]. Spatially varying parameters in the nonlinear Schrödinger equation were also used to describe the periodic variation of the impurity concentration in superconductors [2], high T_c Josephson field effect transistors [3], as well as grain boundaries in superconducting bicrystals [4], while nonlinear Kronig–Penney models were used for studying twinning-plane superconductivity [5]. The nonlinear Schrödinger equation must be used in order to describe all these various phenomena, including the relevant phase transitions. The nonlinear Schrödinger equation has been studied repeatedly, but mostly with regards to its solitons [6], and usually for nonperiodic potentials. In this work the emphasis is placed on studying the bound states, rather than solitons.

We shall study the excited states for the equation

$$-\frac{\hbar^2}{2M} \frac{\partial^2 \Psi}{\partial z^2} + V(z)\Psi + \beta|\Psi|^2\Psi = 0. \quad (1.1)$$

The nonlinear term forbids the arbitrary normalization of Ψ .

The potential we have in mind is a Kronig–Penney potential, but it could be in general any simple oscillatory potential. In this work we choose

$$V(z) = V_0 \left[1 - \alpha \sum_n \delta \left(\frac{z}{d} - n - \frac{1}{2} \right) \right] \quad (1.2)$$

with α and V_0 being positive. The crucial parameter in this potential is the periodicity length d . The number of wells is large, but not necessarily infinite.

Equation (1.1) minimizes the energy functional

$$\int dz \left[V(z)|\Psi|^2 + \beta|\Psi|^4/2 + \frac{\hbar^2}{2M} \left| \frac{\partial \Psi}{\partial z} \right|^2 \right]. \quad (1.3)$$

For $M \rightarrow \infty$ we would have $|\Psi|^2 = -V(z)/\beta$, in which case $|\Psi|^2$ would follow the periodicity of $V(z)$. If the nonlinear term is omitted, the usual Kronig–Penney model is recovered. In that limit $-V_0$ is the energy, and αV_0 is the strength of each attractive δ -function.

We can write the energy functional in dimensionless form, by measuring z in units of d , the distance between successive spikes of the potential, Ψ in units of $\sqrt{V_0/\beta}$, and the energy in units of dV_0^2/β , where V_0 is the positive constant that appears in equation (1.2), and has the dimensions of $V(z)$. This constant is taken out of $V(z)$, so as to render it dimensionless. In other words, $V(z)/V_0 = u(z)$, where $u(z)$ is dimensionless. If we then define the dimensionless parameter $\nu = \hbar^2/2MV_0d^2$, the energy functional takes the dimensionless form

$$\int dz \left[u(z)|\Psi|^2 + |\Psi|^4/2 + \nu \left| \frac{\partial \Psi}{\partial z} \right|^2 \right]. \quad (1.4)$$

Note that when the quartic term is omitted, we recover the usual linear Kronig–Penney model, with energy $E = -\hbar^2/2M\nu d^2$. In this case the energy values can be found only after imposing periodic boundary conditions on $|\Psi|^2$. There are then only certain allowed values of ν , for a given value of α . The size of the wavefunction is determined by the normalization, and when we minimize the energy functional under this constraint, we find the energy eigenvalues, i.e. the minima of the energy functional.

In the nonlinear case, on the other hand, the size of Ψ is determined by the nonlinear terms, through the unconstrained minimization of the functional of equation (1.4). These nonlinear terms determine fully the behaviour of Ψ , without any need for boundary conditions. In fact, a periodic $u(z)$ will give a periodic $|\Psi|^2$. Furthermore, the parameters α and ν are now independent, and for any pair of values of α and ν we can find a solution Ψ , as long as α is sufficiently large. We shall see later what the lower bound on α is precisely. The energy of each state will be simply the value of the energy functional (1.4) at its minimum.

We see from equation (1.4) that for $\nu \rightarrow 0$, when the potential is very strong, or very weakly periodic, we obtain $|\Psi|^2 \rightarrow -u(z)$. Thus, Ψ follows the periodicity of the structure very closely, since it can change very abruptly. In this limit the sign of Ψ is arbitrary. So if the spikes of the potential are very far apart (d is long), the sign of Ψ could be positive or negative at each spike (see figure 1(a)).

Let us now switch on slowly the parameter ν , bringing the teeth of the potential comb closer together. Then the wavefunction between neighbouring spikes could have two forms. If the wavefunction on two successive spikes A and B is positive, say, then the wavefunction in the intervening region will be reduced, and it will go through a positive minimum value, although always remaining positive (figure 1(b)). If, however, the wavefunction changes sign in going from spike B to spike C, then it must pass through a point halfway between the spikes where it is exactly zero (see figure 1(b)). Since the wavefunction $\Psi(z)$ minimizes the functional of equation (1.4), the energy equals $-\int dz |\Psi|^4/2$, as can be deduced by combining the dimensionless forms of equations (1.1) and (1.3). Consequently the wavefunction has less energy if it does not go through zero, always maintaining the

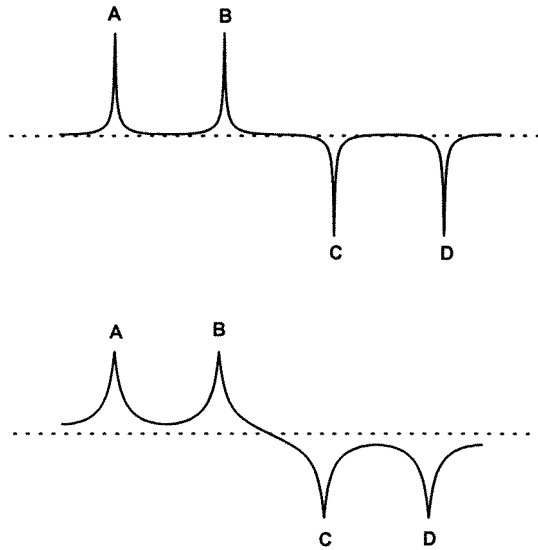


Figure 1. (a) A typical wavefunction when the potential wells are very far apart ($\nu \approx 0$). (b) A typical wavefunction when the potential wells are closer together ($\nu \ll 1$).

same sign. Indeed, in that case the minimum of $|\Psi|^4/2$ is not zero, and hence the area under $|\Psi|^4/2$ is greater.

It seems therefore more favourable for the wavefunction to have the same sign on all spikes of the potential. We say that the ground state is a *uniformly positive* state then. If the spikes of the potential are too far from each other however, the minimum value of the wavefunction between them would be practically zero, and in that case the *uniformly positive* state (where Ψ has the same sign at all spikes) becomes degenerate in energy with states that may have Ψ take on negative values at some spikes, and positive values at others.

We can, for example, have a state that is infinitesimally higher in energy compared with the uniformly positive ground state, and hence practically equally preferable, even for spikes not too far apart. This state, with $\Psi(0) = 0$, $\Psi(z) > 0$ when $z > 0$, and $\Psi(z) < 0$ when $z < 0$, connects regions of different signs of the wavefunction (see figure 2). Then in the intermediate region Ψ has to go through zero, and we obtain a region that reminds us of a domain wall. For a potential with *infinitely* many spikes, the energetically costly root of Ψ occurs only once, and hence the energy of this state is equal to the energy of the uniformly positive ground state.

Therefore there can be bound states of equation (1.1) that are degenerate to the ground state, not being positive everywhere. It is the purpose of this paper to study such bound states, first through a general variational model (section 2), and then through an exact study of the Kronig–Penney potential (section 3), as well as through a numerical study of a periodic potential with Gaussian wells (section 4). We summarize our conclusions in section 5.

2. Variational study

In this section we shall examine the possibility of having Ψ change sign in going from one spike of the potential to the next, as well as the possibility of having Ψ with the same sign

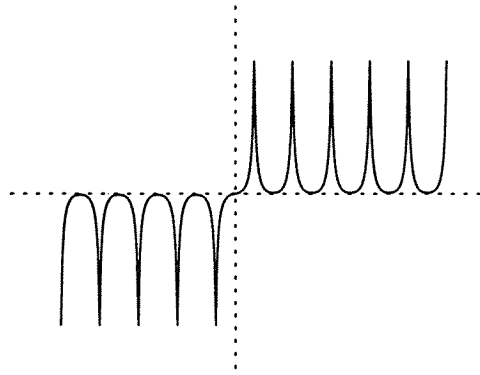


Figure 2. First excited state with the root at $z = 0$, for δ -function wells.

on neighbouring spikes. In the first case Ψ is odd with respect to the midpoint between the two spikes, while in the second case it is even. An arbitrary state of the system will then be a combination of even and odd pieces. In other words, Ψ will be even between certain neighbouring spikes of the potential, and odd between others. Thus, Ψ will maintain its sign between some spikes, and it will change sign between others. For example, in figure 1(b) Ψ is odd in one interval, and even in the other two, while in figure 2 it is even everywhere, except for the interval at the centre.

We have assumed that the spikes of the potential are at $z = n + \frac{1}{2}$, where n is any integer. Let us examine then the two neighbouring quantum wells at the ends of the interval $[n - \frac{1}{2}, n + \frac{1}{2}]$. We adopt the following odd and even trial wavefunctions, with respect to the midpoint ($z = n$), defined on the interval $[n - \frac{1}{2}, n + \frac{1}{2}]$:

$$\Psi_{on}(z) = \pm\psi \frac{\sinh[\gamma(z-n)]}{\sinh(\gamma/2)} \quad (2.1)$$

$$\Psi_{en}(z) = \pm\psi \left[\frac{\cosh[\gamma(z-n)]}{\cosh(\gamma/2)} - \operatorname{sech}^2(\gamma/2) \right] \coth^2(\gamma/2) \quad (2.2)$$

where ψ and γ are variational parameters. We note that $\Psi_{on}(n) = 0$, $\Psi_{on}(n + \frac{1}{2}) = -\Psi_{on}(n - \frac{1}{2}) = \pm\psi$, and $\Psi'_{on}(n + \frac{1}{2}) = \Psi'_{on}(n - \frac{1}{2}) = \pm\psi\gamma \coth(\gamma/2)$. Similarly $\Psi_{en}(n) = \pm\psi[\cosh(\gamma/2) - 1]/\sinh^2(\gamma/2)$, $\Psi_{en}(n + \frac{1}{2}) = \Psi_{en}(n - \frac{1}{2}) = \pm\psi$, and $\Psi'_{en}(n + \frac{1}{2}) = -\Psi'_{en}(n - \frac{1}{2}) = \pm\psi\gamma \coth(\gamma/2)$.

These wavefunctions are such that they can be joined together in any order to form a continuous wavefunction everywhere, consisting of even and odd pieces. We could have, for example, $\Psi = \Psi_{on}$ in $[n - \frac{1}{2}, n + \frac{1}{2}]$, $\Psi = \Psi_{e,n+1}$ in $[n + \frac{1}{2}, n + \frac{3}{2}]$, $\Psi = -\Psi_{o,n+2}$ in $[n + \frac{3}{2}, n + \frac{5}{2}]$, etc. Furthermore, regardless of the order in which the even and odd pieces are connected, the slope of the wavefunction is symmetric around the spikes of the potential.

The state with the lowest energy would consist of a chain of even pieces, because, unlike the odd pieces which have a root at the midpoint, the even pieces are equal to zero nowhere. Thus the odd pieces have a higher $-\int dz |\Psi|^4/2$, which is the exact energy if Ψ is an exact solution of the equations that minimize the energy functional.

The next lowest energy would correspond to the state with only one odd piece. This is the state in figure 2. It is presumed here that the change from the chain of negative pieces to the chain of positive pieces occurs within just one spacing. The circumstances under

which this will happen will be explored later.

The state mentioned above is followed by the state with two odd pieces, and so on, up to the highest state, which has only odd pieces. In fact, if F_e and F_o is the energy in $[n - \frac{1}{2}, n + \frac{1}{2}]$ for the even and odd trial wavefunctions respectively, then the energy of a state with m even pieces and n odd pieces is $mF_e + nF_o$. Thus, the total energy per interval is $(mF_e + nF_o)/(m+n)$. In particular, the energy per interval is F_e for the uniform chain of even pieces, i.e. the ground state, and $(mF_e + F_o)/(m+1)$ for the state with only one odd piece, i.e. the state of figure 2. For an *infinite* number of spikes ($m \rightarrow \infty$), the two states are *degenerate*, as expected. Of course, the same holds for a state with infinitely many even pieces, but only two odd pieces. If the number of odd pieces becomes substantial, then the energy of the state will definitely be higher than that of the ground state.

For a large but finite number of spikes we still expect all these various states to be degenerate, as long as the minimum value of the even pieces is practically zero, because in that case $|\Psi|^4$ is essentially the same for both even and odd pieces. We shall verify this by explicit calculation, using our variational wavefunctions.

We note that $\Psi_{en}(n) \rightarrow 0$ when $\gamma \rightarrow \infty$. Therefore the degeneracy mentioned above requires that γ is very large. Therefore, we shall neglect terms such as $\text{sech}(\gamma/2)$. In this limit,

$$F_e \approx v\gamma|\psi|^2 + \frac{|\psi|^4}{4\gamma} + \int_{n-\frac{1}{2}}^{n+\frac{1}{2}} dz u(z)|\psi|^2 \frac{\cosh^2[\gamma(z-n)]}{\cosh^2(\gamma/2)} + O(e^{-\gamma}) \quad (2.3)$$

$$F_o \approx v\gamma|\psi|^2 + \frac{|\psi|^4}{4\gamma} + \int_{n-\frac{1}{2}}^{n+\frac{1}{2}} dz u(z)|\psi|^2 \frac{\sinh^2[\gamma(z-n)]}{\sinh^2(\gamma/2)} + O(e^{-\gamma}). \quad (2.4)$$

Hence, since $\cosh^2(\gamma/2) \approx \sinh^2(\gamma/2) \approx e^\gamma/4$,

$$F_o - F_e \approx - \int_{n-\frac{1}{2}}^{n+\frac{1}{2}} dz 4e^{-\gamma} u(z)|\psi|^2. \quad (2.5)$$

And since γ is large, and terms of order $O(e^{-\gamma})$ have been dropped in this calculation, equation (2.5) implies that $F_o \approx F_e$. In other words, if $\Psi_{en}(n) \approx 0$, then all the possible states are practically degenerate, even for a finite large number of spikes, because they consist of odd and even pieces only, pieces which were shown to have the same energy. Note that our results are very general so far. The only restriction is that the γ that minimizes equation (2.3) is large. Our conclusions are valid for *any* $u(z)$ that can lead to a large γ .

We illustrate the above general conclusions by restricting ourselves now to the Kronig–Penney model:

$$u(z) = 1 - \sum_n \alpha \delta(z - n - \frac{1}{2}). \quad (2.6)$$

This choice of $u(z)$, where α is a positive constant, implies that there is a periodic chain of deep quantum wells along the z -axis.

For this choice of $u(z)$ then, and in the limit of large γ , we obtain

$$F_o \approx F_e \approx |\psi|^2 \left[v\gamma + \frac{1}{\gamma} - \alpha \right] + \frac{|\psi|^4}{4\gamma}. \quad (2.7)$$

Minimization with respect to $|\psi|^2$ gives

$$|\psi|^2 = 2\gamma \left[\alpha - v\gamma - \frac{1}{\gamma} \right] \quad (2.8)$$

and

$$F_o \approx F_e \approx -\gamma \left[\alpha - \nu\gamma - \frac{1}{\gamma} \right]^2. \quad (2.9)$$

Minimization with respect to γ yields

$$\gamma = \frac{\alpha + \sqrt{\alpha^2 + 12\nu}}{6\nu} \quad (2.10)$$

or equivalently $3\nu\gamma - \alpha = 1/\gamma$, in which case $|\psi|^2 = 4\nu\gamma^2 - 4$. Since $\gamma \gg 1$, we shall have

$$\gamma \approx \alpha/3\nu \gg 1. \quad (2.11)$$

Since $|\psi|^2 \geq 0$, we must also have $\gamma \geq 1/\sqrt{\nu}$, which implies

$$\alpha^2 \geq 4\nu. \quad (2.12)$$

Therefore, whenever ν and α satisfy the restrictions of equations (2.11) and (2.12), we expect all the possible states to be essentially degenerate. In particular, the *highest* excited state, the one consisting of odd pieces only, is *degenerate* with the *ground* state, which is a chain of even pieces. Note furthermore that the wavefunction is only nonzero if $\nu \leq \alpha^2/4$. When in fact $\nu = \alpha^2/4$, we have a transition to a zero wavefunction, even though γ , which then takes the value $1/\sqrt{\nu}$, may be quite large.

As a numerical illustration, we choose the case $\nu = 0.01$, $\alpha = 1$. Then the ground state and the highest excited state (only even or only odd pieces respectively) have an energy of -13.5207 in this variational model, with $\gamma = 34.305$ and $\psi = 6.56$. The exact energy can be found using the methods of section 3, and it is -14.933 for both the ground state and the highest state, while $\psi = 6.93$. So both calculations indicate that all the states are degenerate, for this particular choice of ν and α .

The example where $u(z)$ is given by equation (2.6) will also be examined in section 3, since it can be solved exactly. We can generalize for *any* simple oscillatory $u(z)$, as long as γ is very large.

3. Exact solutions

In this section we shall solve the model of equations (1.4) and (2.6) exactly, verifying thus the variational results of the previous section. We shall be interested in *those* values of the parameters ν and α that yield excited states *almost degenerate* with the ground state.

We should note that a large ν would imply that the kinetic energy is dominant, making thus the wavefunction too stiff. In other words, the ground-state wavefunction would come as closely as possible to a constant, a choice that minimizes the kinetic energy. In that case the minimum value of the ground-state wavefunction would be far from zero.

On the other hand, if ν were exactly zero, then the wavefunction would follow the variations of $u(z)$ exactly. Hence, we need a small value of ν if we are going to have an excited state that is close in energy to the ground state, since the wavefunction of such a state varies dramatically between the spikes. Furthermore, if ν is zero the wavefunction will have arbitrary signs at the wells, in which case the various excited states will all be degenerate with the ground state. For small ν , this degeneracy will not be altered too drastically.

We shall be interested therefore in the exact solutions of this model, for small ν . The energy functional is minimized when

$$\nu \frac{\partial^2 \Psi}{\partial z^2} = \left[1 - \sum_n \alpha \delta(z - n - \frac{1}{2}) \right] \Psi + |\Psi|^2 \Psi. \quad (3.1)$$

The solution $\Psi(z)$ will have periodic features similar to those of $u(z)$. Integrating equation (3.1) gives the boundary condition for $\Psi(z)$

$$-\alpha \Psi \left(n + \frac{1}{2} \right) = \nu \left[\frac{\partial \Psi}{\partial z} \left(n + \frac{1}{2} \right)_+ - \frac{\partial \Psi}{\partial z} \left(n + \frac{1}{2} \right)_- \right]. \quad (3.2)$$

Thus $\Psi(z)$ has a kink at each spike of the potential, due to the δ -functions.

Direct integration of equation (3.1) after multiplying it by $\partial \Psi / \partial z$ gives the solution in each interval. The ground state has no node, hence Ψ will have a minimum at the middle of each interval, while it will be symmetric around each spike. Thus, the *exact* ground state is found to be

$$\Psi(z) = \frac{q}{cn \left[\sqrt{(1+q^2)/\nu} (z-n), (2+q^2)/(2+2q^2) \right]} \quad (3.3)$$

for $n - \frac{1}{2} \leq z \leq n + \frac{1}{2}$, extended periodically everywhere else. Here cn is a Jacobi elliptic function, and $q = \Psi(n)$ is the minimum value of $\Psi(z)$. The above expression is valid for *any* value of ν , large or small, and we can easily verify that it satisfies equation (3.1).

The boundary conditions of equation (3.2) require then that

$$\alpha = 2\nu \sqrt{\frac{1+q^2}{\nu}} \frac{sn \left[\sqrt{\frac{1+q^2}{4\nu}}, \frac{2+q^2}{2+2q^2} \right] dn \left[\sqrt{\frac{1+q^2}{4\nu}}, \frac{2+q^2}{2+2q^2} \right]}{cn \left[\sqrt{\frac{1+q^2}{4\nu}}, \frac{2+q^2}{2+2q^2} \right]} \quad (3.4)$$

where the dn and sn are also Jacobi elliptic functions. This equation determines q as a function of α and ν . Note that there is always a ground state, since we can always find an appropriate q for a given choice of ν and α .

In the limit of a wavefunction localized around the spikes of the potential we expect q to be small. Then equation (3.3) reduces to

$$\Psi(z) \approx q \cosh[(z-n)/\sqrt{\nu}]. \quad (3.5)$$

This is precisely the solution of the linear Kronig–Penney model, as expected, since for very small q the nonlinear terms become unimportant. If $q = 0$, equation (3.4) yields

$$\alpha = 2\sqrt{\nu} \tanh(1/2\sqrt{\nu}). \quad (3.6)$$

So a nonzero ground state will exist only if $\alpha \geq 2\sqrt{\nu} \tanh(1/2\sqrt{\nu})$. Note that for small ν this becomes the restriction of equation (2.12), as it should. Furthermore, if α is close to its lower limit, then the change of sign of Ψ for a first excited state will have to spread over a few more spikes of the potential, and it will not be restricted to just the region between two successive spikes. In this paper we shall not be concerned with this possibility, and we shall restrict our attention to values of α far from the lower bound of equation (3.6). Then the change of sign for the excited states occurs within just one spacing.

Now the Jacobi elliptic function $cn(x, m)$ is a periodic function, with roots at the odd multiples of the elliptic function $K(m)$, where $K(m) = \int_0^{\pi/2} d\theta / \sqrt{1 - m \sin^2 \theta}$. Indeed, $cn(0, m) = 1$, $cn(K(m), m) = 0$, $cn(2K(m), m) = -1$, $cn(3K(m), m) = 0$, $cn(4K(m), m) = 1$.

The ground state, as mentioned in the previous section, must consist of even pieces everywhere, of the form given by equation (3.3). It must therefore be positive everywhere, since it is continuous. So the Ψ of equation (3.3) must not be allowed to become negative. This means that the quantity $\sqrt{(1+q^2)/\nu}|z-n|$ must be smaller than $K((2+q^2)/(2+2q^2))$ within the interval $[n - \frac{1}{2}, n + \frac{1}{2}]$. Hence

$$\frac{1}{2}\sqrt{(1+q^2)/\nu} \leq K\left(\frac{2+q^2}{2+2q^2}\right). \quad (3.7)$$

This inequality holds for any values of α and ν . If ν is small, then the right-hand side of this inequality has to be large. This happens when the argument of $K(m)$ is close to 1, in which case $K(m) \approx \ln\sqrt{16/(1-m)}$. In this particular case, the argument is 1 if q is very small. Thus, if ν is small, q must be small.

Furthermore, when inequality (3.7) becomes an equality, the denominator in equation (3.3) tends to zero at $z = n + \frac{1}{2}$, and therefore the value of $\Psi(z)$ at the spikes becomes infinite. In other words, the value of Ψ at the spikes can be much larger than the value of Ψ at the midpoints.

Indeed $\Psi(n - \frac{1}{2})/\Psi(n) = 1/cn[\sqrt{(1+q^2)/4\nu}, (2+q^2)/(2+2q^2)]$. Hence, if $q \rightarrow 0$, $\Psi(\frac{1}{2})/\Psi(1) \approx \cosh(1/\sqrt{4\nu})$, which tends to infinity when ν tends to zero. Thus, the even pieces of Ψ become very deep if ν is small, because in that case $q \rightarrow 0$ and $\Psi(n \pm \frac{1}{2})$ is very large.

We say in that case that the wells are weakly coupled. Note that in that case the $|\Psi|^4$ of an even piece would not differ too much from the $|\Psi|^4$ of an odd piece. In other words, we expect the various possible states to be very close in energy to the ground state, as already mentioned in section 2. Indeed, the case $\nu = 0$ would correspond to a complete decoupling of the values of the wavefunctions at the spikes of the potential, and hence to a complete degeneracy of all the various states.

Let us examine more thoroughly the singularities that may arise in the behaviour of Ψ . We said that $\Psi(z)$ becomes very large at the spikes of the potential when inequality (3.7) becomes almost an equality:

$$\sqrt{(1+q^2)/4\nu} \approx K\left(\frac{2+q^2}{2+2q^2}\right). \quad (3.8)$$

But if m is very close to 1, then $K(m) \approx \ln\sqrt{16/(1-m)}$. Hence, this approximate equality reduces for small q to $1/2\sqrt{\nu} \approx \ln(\sqrt{32}/q^2)$, whence

$$q \approx \sqrt{32}e^{-1/2\sqrt{\nu}}. \quad (3.9)$$

Hence, if ν is small, and if the ground-state wavefunction has deep cups, we must have $q \approx \sqrt{32}\exp(-1/2\sqrt{\nu})$. Note that even though q is small, the value of the wavefunction at the minima of the potential is large. None the less, since $q \rightarrow 0$, the wavefunction is again given by equation (3.5), an equation that tells us that $\Psi(z)$ falls to $1/e$ of its value within a distance of $\sqrt{\nu}$ from the spikes. In that sense we can say that the 'thickness' of Ψ at each spike is $2\sqrt{\nu}$. But the peaks of Ψ would overlap when the thickness of each peak equals the distance between successive peaks. This happens when $\nu = \frac{1}{4}$. When we speak therefore of weakly coupled wells, we mean that $\nu \ll \frac{1}{4}$. And it is only such wells that can lead to an essentially degenerate spectrum of states.

Let us then summarize our results for the ground state. There is always a ground state, with $q = \Psi(n)$ being the minimum value of Ψ in the interval $[n - \frac{1}{2}, n + \frac{1}{2}]$. This is a symmetric series of even pieces, and it resembles a chain of symmetric cups (see figure 3). The absolute value of the slope of Ψ at the layers is $\alpha\Psi(n + \frac{1}{2})/2\nu$. This ground state

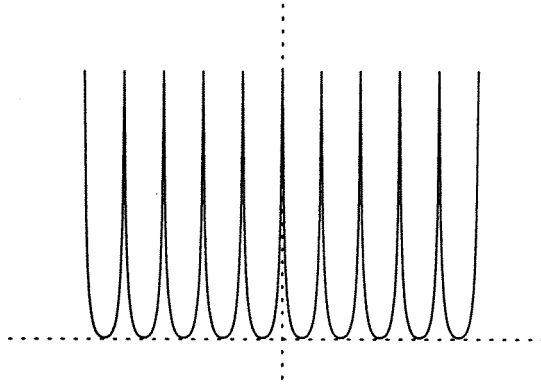


Figure 3. The ground state, for δ -function wells.

will be degenerate with any other states if their $|\Psi|^4$'s are approximately the same. This can happen only if q is almost zero, as explained in section 2, because then the minimum of the $|\Psi|^4$ of the even piece approaches the minimum of $|\Psi|^4$ of the odd piece, i.e. zero. But q can be tiny, and Ψ still have a substantially nonzero value, only close to the roots of the Jacobi elliptic function cn (see equation (3.3)), i.e. for $q \approx \sqrt{32}e^{-1/2\sqrt{\nu}}$. Furthermore, q needs to be small in order to have the degeneracy. Hence, ν must be small. Indeed, the thickness $2\sqrt{\nu}$ of each well implies that the wavefunctions around the spikes will not overlap substantially, provided $\nu \ll \frac{1}{4}$. For small ν we then obtain a ground state which resembles a chain of deep cups (see figure 3).

Let us now proceed to the first excited state (see figure 2). Here we assume again that ν is small, and hence the even pieces will resemble deep cups. There will be only one odd piece, in the interval $[-\frac{1}{2}, \frac{1}{2}]$, connecting a chain of negative even pieces with a chain of positive even pieces. The characteristics of the many even pieces will not be altered, because there is only one odd piece. In contrast, the characteristics of the odd piece will be determined from those of the even pieces, through the boundary conditions.

Direct integration of equation (3.1) after multiplying it by $\partial\Psi/\partial z$ will give the solution in the interval $[-\frac{1}{2}, \frac{1}{2}]$, as long as we use the fact that $\Psi(0) = 0$, since there is one node there. For the first excited state there is only one node, thus all the pieces outside the interval $[-\frac{1}{2}, \frac{1}{2}]$ will be even.

One can show thus that for $-\frac{1}{2} \leq z \leq \frac{1}{2}$ we obtain the *exact* solution

$$\Psi(z) = \sqrt{1-\epsilon} \frac{sn[z\sqrt{(1+\epsilon)/2\nu}, 2\epsilon/(1+\epsilon)]}{cn[z\sqrt{(1+\epsilon)/2\nu}, 2\epsilon/(1+\epsilon)]} \quad (3.10)$$

with $\Psi'(0) = \sqrt{(1-\epsilon^2)/2\nu}$ and $0 \leq \epsilon \leq 1$. We can easily verify that this expression satisfies equation (3.1). The value of $\Psi(z)$ at $z = \frac{1}{2}$, as calculated from equation (3.10), must be equal to the one that can be calculated from equation (3.3). This relation determines the parameter ϵ . If the even pieces are deep enough, i.e. if ν is small enough, then the slope of $\Psi(z)$ at $(\frac{1}{2})_-$ will turn out to be $\alpha\Psi(\frac{1}{2})/2\nu$.

Indeed, we saw that if for small ν the value of Ψ at the spikes of the potential is very large, then $q \approx \sqrt{32}e^{-1/2\sqrt{\nu}}$. In general, the even and odd pieces correspond to the same energy if Ψ is very large at the spikes, q being quite small. But if $\Psi(\frac{1}{2})$ is very large, then equation (3.10) implies that $cn[\sqrt{(1+\epsilon)}/8\nu, 2\epsilon/(1+\epsilon)] \approx 0$, so as to make $\Psi(z)$ almost

diverge. Consequently

$$\sqrt{(1 + \epsilon)/8\nu} \approx K[2\epsilon/(1 + \epsilon)] \quad (3.11)$$

where K is the elliptic function $K(m) = \int_0^{\pi/2} d\theta/\sqrt{1 - m \sin^2 \theta}$. And since ν is small, the value of K will have to be rather large, which means that $2\epsilon/(1 + \epsilon) \rightarrow 1$, i.e. $\epsilon \rightarrow 1$. Indeed, remembering that $K(m) \approx \ln \sqrt{16/(1 - m)}$ when $m \rightarrow 1$, we can easily find that equation (3.11) is solved by the value

$$1 - \epsilon \approx 32e^{-1/\sqrt{\nu}}. \quad (3.12)$$

So this value of ϵ yields a very large $\Psi(\frac{1}{2})$, for small ν . In fact, we must have in general, for any ν ,

$$\sqrt{(1 + \epsilon)/8\nu} \leq K[2\epsilon/(1 + \epsilon)] \quad (3.13)$$

otherwise the elliptic function cn would obtain a root in $[0, \frac{1}{2}]$ and $\Psi(z)$ would have a vertical asymptote there.

We can now check the value of $\Psi(\frac{1}{2})$. The second argument of the elliptic functions sn , dn and cn is $(2 + q^2)/(2 + 2q^2)$ for the even pieces and $2\epsilon/(1 + \epsilon)$ for the odd pieces, both of which will equal $1 - 16e^{-1/\sqrt{\nu}}$ when equations (3.9) and (3.12) hold, i.e. for very large values of $\Psi(\frac{1}{2})$. Therefore for very small ν this second argument is essentially 1, in which case the sn becomes \tanh , the cn becomes sech , and the dn becomes sech . Then equation (3.10) gives $\Psi(z) \approx \sqrt{1 - \epsilon} \sinh(z\sqrt{(1 + \epsilon)/2\nu})$ in $[-\frac{1}{2}, \frac{1}{2}]$, and $\Psi(z) \approx q \cosh[(z - n)/\sqrt{\nu}]$ in $[n - \frac{1}{2}, n + \frac{1}{2}]$, where $n \neq 0$. Both expressions then give the same values for $\Psi(\frac{1}{2})$ and $|\Psi'(\frac{1}{2})|$, as expected.

The procedure for finding the first excited state then consists of finding the value of ϵ that would ensure continuity of $\Psi(z)$ at $z = \frac{1}{2}$. In that case the slope at $z = (\frac{1}{2})_-$ will turn out automatically to be the exact opposite of the slope at $z = (\frac{1}{2})_+$. Finding the ground state, on the other hand, simply requires finding a q such that $|\Psi'(n + \frac{1}{2})| = (\alpha/2\nu)\Psi(n + \frac{1}{2})$. This relation is precisely equation (3.4).

Finally, we can find the highest excited state, the one consisting of odd pieces only, by extending periodically the odd solution of equation (3.10), and finding a value of ϵ such that $|\Psi'(n + \frac{1}{2})| = (\alpha/2\nu)\Psi(n + \frac{1}{2})$. Since the minimum value q of the even piece for the solutions that interest us is $\sqrt{32}e^{-1/2\sqrt{\nu}}$, i.e. practically zero, the energy of the even piece and of the odd piece is essentially the same since they have the same $-\int dz |\Psi|^4/2$. And all the states are then degenerate.

It is interesting to note that $\alpha = 2\nu\Psi'(\frac{1}{2})/\Psi(\frac{1}{2}) \rightarrow 4\nu + \frac{1}{3}$ if $\nu \rightarrow \infty$, for the $\Psi(z)$ of equation (3.10). Hence, the highest state does not exist when $\nu \rightarrow \infty$, unless $\alpha = 4\nu + \frac{1}{3}$. Similarly, quite a few other excited states do not exist for large values of ν . The even ground state always exists, if α is above the lower bound of equation (3.6). We present numerical values of the parameters and energies of the ground state, of the first excited state and of the highest state in tables 1–3 for various choices of ν and α .

Note that for a given choice of ν , large or small, and a given value of α greater than the lower bound of equation (3.6), q is given by equation (3.4). But it is only small ν 's, and α 's quite far from their lower bound, that will lead to a ground state with deep even pieces. In that case q is given by equation (3.9), and the ground state will be practically degenerate with the first few excited states.

Table 1. Parameters of the ground state for δ -function wells, for various choices of ν and α . E_g is the energy per interval.

ν	α	$\Psi(1) = q$	$\Psi(\frac{1}{2})$	$-\Psi'(\frac{1}{2})_+$	E_g
0.002	1	7.2×10^{-5}	15.748	3 937	-81.452 6
0.01	0.25	0.012 7	1.060 8	13.260 1	-0.0271 0
0.01	1	0.031 074	6.928 21	346.41	-14.933 4
0.01	10	0.037 283	70.696 5	35 348.3	-16 646.9
0.05	1	0.346 47	2.834 02	28.340 2	-1.959 03
0.05	10	0.511 176	31.591 1	3 159.11	-3 314
0.1	1	0.497 576	1.781 92	8.909 62	-0.599 64

Table 2. Parameters of the first excited state for δ -function wells, for various choices of ν and α . E_1 is the energy in $[-\frac{1}{2}, \frac{1}{2}]$. For the other intervals, the energy is the E_g given in table 1.

ν	α	q	ϵ	$\Psi(\frac{1}{2})$	$\Psi'(\frac{1}{2})_-$	E_1
0.002	1	7.2×10^{-5}	$1.5.2 \times 10^{-9}$	15.748	3 937	-81.452 6
0.01	0.25	0.012 7	0.999 838	1.060 8	13.261 3	-0.027 094
0.01	1	0.031 074	0.999 03	6.928 2	346.41	-14.933 3
0.01	10	0.037 283	0.998 598	70.696	35 348.3	-16 646.9
0.05	1	0.346 47	0.823 56	2.834 0	28.441 7	-1.924 45
0.05	10	0.511 176	0.363 395	31.591	3 159.12	-3 313.85
0.1	1	0.497 576	0.424 940	1.781 9	9.287 66	-0.526 821

Table 3. Parameters of the highest state for δ -function wells, for various choices of ν and α . E_h is the energy per interval.

ν	α	ϵ	$\Psi(\frac{1}{2})$	$\Psi'(\frac{1}{2})_-$	E_h
0.002	1	$1.5.2 \times 10^{-9}$	15.748	3 937	-81.452 6
0.01	0.25	0.999 838	1.060 5	13.256 5	-0.027 07
0.01	1	0.999 03	6.928 2	346.41	-14.933 2
0.01	10	0.998 598	70.696	35 348.3	-16 646.9
0.05	1	0.824 42	2.821 3	28.213	-1.895 82
0.05	10	0.363 395	31.591	3 159.11	-3 313.84
0.1	1	0.516 054	1.652 7	8.263 45	-0.401 57
1	4.34	0.730 536	0.251 8	0.546 42	-0.000 38

4. A potential with Gaussian wells

We shall examine numerically the bound states that correspond to the choice

$$u(z) = 1 - g \sum_n \exp[-b(z - n - \frac{1}{2})^2] \quad (4.1)$$

shown in figure 4. We choose the parameters so that $e^{b/4} > g > 1$. Then $u(z)$ is negative at its minima and positive at the midpoints between the minima. Therefore, if ν were exactly zero, then there would be a nonzero wavefunction at the minima of $u(z)$, but there would be a region around the midpoints where Ψ would be exactly zero. When ν is slightly positive, the stiffness of the wavefunction makes Ψ leak into the ‘forbidden’ regions (tunnelling). If, however, $b < 4 \ln g$, then there is no tunnelling. We need a large enough b in order to obtain tunnelling.

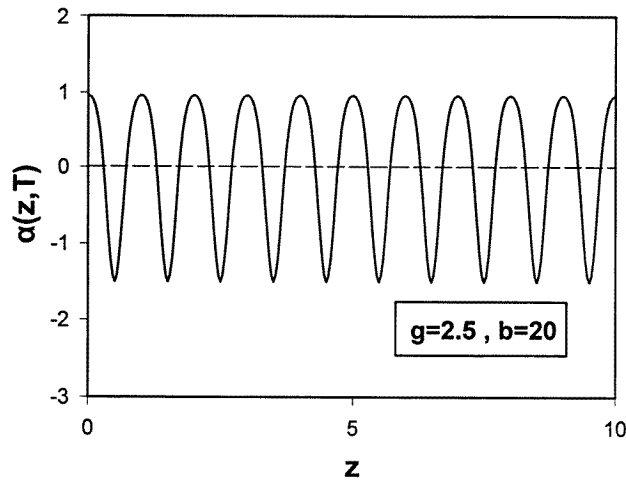


Figure 4. The potential $u(z)$ for Gaussian wells ($g = 2.5$, $b = 20$).

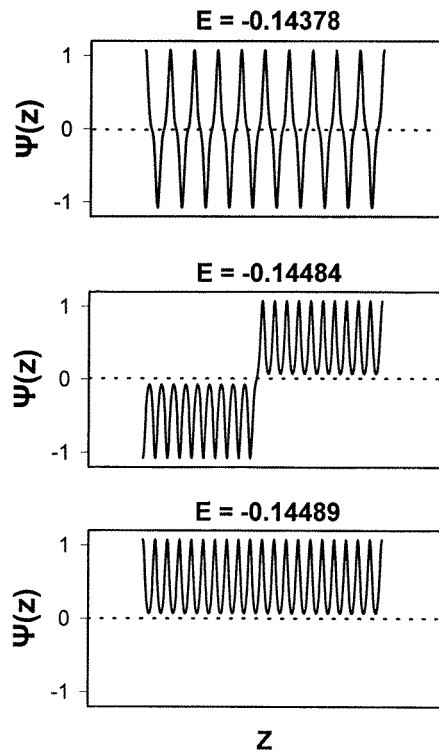


Figure 5. The ground state, the first excited state, and the highest state, for 20 Gaussian wells with $\nu = 0.01$, $g = 2.5$, $b = 20$, with the corresponding energies per interval.

If, on the other hand, b is extremely large, while g remains finite, the width of each well is reduced, its strength remaining unaltered. We expect therefore that for a given g we cannot increase b indefinitely, because we shall not be able to find a solution. The numerical calculations do indeed verify this.

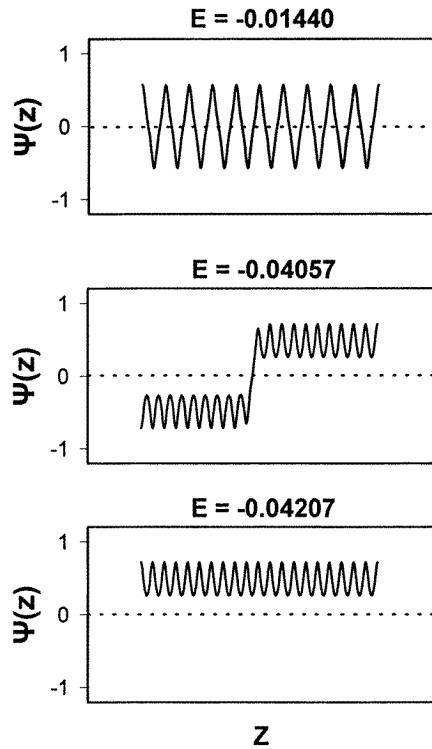


Figure 6. The ground state, the first excited state, and the highest state, for 20 Gaussian wells with $\nu = 0.05$, $g = 2.5$, $b = 20$, with the corresponding energies per interval.

Thus, if b is large enough, but not too large, and if g is large enough to allow a nonzero solution, we shall have a competition between the kinetic energy and the rest of the energy. The latter forces Ψ to follow the variations of $u(z)$. The kinetic energy, on the other hand, wants Ψ to be constant in space. Solutions such as the one in figure 2 will be relevant for small ν , since large values of ν tend to push Ψ towards a constant. Indeed, numerical calculations verify that for large ν (e.g. $\nu = 0.3$), the kinetic energy is strong enough to force Ψ_{\max} to be close to Ψ_{\min} , and $\Psi_{\min} \gg 0$. The ground state is then a chain of shallow little cups away from zero.

Excited states that will be almost degenerate in energy with the ground state will appear at small values of ν , when the minimum of the ground-state wavefunction between the wells is very small, while $\Psi_{\max} \gg 0$. Figure 5 shows the ground state, the first excited state, and the highest excited state, for $\nu = 0.01$, with the corresponding energies per interval, for a sample of 20 Gaussian wells. Figure 6 shows the same states, but for $\nu = 0.05$. We see again the characteristics mentioned earlier: full degeneracy if ν is small enough, in which case the minimum of Ψ between the wells is quite small compared with its value Ψ_{\max} at the wells. The value of Ψ_{\max} depends strongly on g .

Remember also that the energy difference between the ground state and the first excited state is strictly equal to zero for an infinite number of wells. This is due to the fact that the wavefunction of the first excited state is exactly equal or exactly opposite to the wavefunction of the ground state on almost all of the infinitely many wells. Indeed, in figures 7 and 8 we see the first excited state for a fairly large value of ν , and a series of

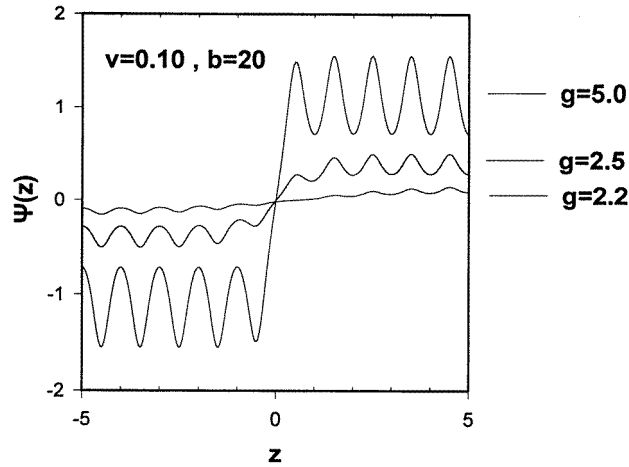


Figure 7. First excited state for Gaussian wells with $\nu = 0.1$, $b = 20$, and $g = 2.2, 2.5$ and 5 .

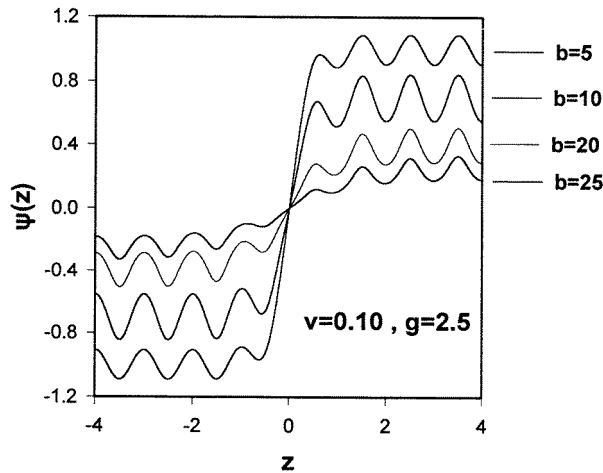


Figure 8. First excited state for Gaussian wells with $\nu = 0.1$, $g = 2.5$ and $b = 5, 10, 20$, and 25 .

values for b and g . Here the stiffness of the wavefunction is quite large, so the change of the sign cannot take place within just one interval. This change now occurs over three or four wells. For small values of ν though, when the wavefunction is quite malleable, the wavefunction changes sign within one interval.

5. Conclusions

We have studied the bound states of a nonlinear version of the Schrödinger equation for the Kronig–Penney model, a version that is relevant to quite a few phenomena in condensed matter physics.

We have seen that there is a substantial range of parameters, not just for the Kronig–Penney model but for other simple oscillatory choices of $u(z)$ as well, for which the various

states are essentially degenerate in energy. This degeneracy requires that ν is small enough, so as to allow the wavefunction to have a small, but nonnegligible, value at the midpoints between the wells. At the same time, the value of the wavefunction at the wells can be quite substantial. Then there is very little cost in having Ψ change sign in going from one well to the next. In fact, the energy differences are really small when $\Psi_{\max} \gg \Psi_{\min}$. This means that the lower excited states, which connect regions of positive Ψ with regions of negative Ψ , become as favourable as the ground state. This degeneracy is exact in the limit of infinitely many quantum wells for these lower excited states. Even the highest excited state though, which consists of odd pieces only, has an energy very close to the energy of the ground state for sufficiently small ν .

We demonstrated this basic idea in section 2 through a variational calculation valid for a generic oscillatory potential. The variational results were confirmed through the exact solution of the nonlinear Kronig–Penney model, presented in section 3, as well as through a numerical calculation for the case of another simple oscillatory potential, presented in section 4. All these calculations show the exact (for infinitely many spikes) or approximate (for finitely many spikes) degeneracy of the ground state.

References

- [1] Koyama T, Takezawa N, Naruse Y and Tachiki M 1992 *Physica* **194C** 20
Koyama T and Tachiki M 1992 *Physica* **193C** 163
Machida M and Kaburaki H 1995 *Phys. Rev. Lett.* **74** 1434
Balents L and Radzihovsky L 1996 *Phys. Rev. Lett.* **76** 3416
- [2] Ami S and Maki K 1975 *Prog. Theor. Phys.* **53** 1
- [3] Betouras J, Joynt R, Dong Z W, Venkatesan T and Hadley P 1996 *Appl. Phys. Lett.* **69** 2432
- [4] Betouras J and Joynt R 1995 *Physica* **250C** 256
- [5] Khlyustikov I and Buzdin A 1987 *Adv. Phys.* **36** 271
Abrikosov A, Buzdin A, Kulic M and Kuptsov D 1989 *Sov. Phys.—JETP* **68** 210
- [6] Hizanidis K, Frantzeskakis D and Polymilis C 1996 *J. Phys. A: Math. Gen.* **29** 7687
Frantzeskakis D 1996 *J. Phys. A: Math. Gen.* **29** 3631
Frauenkron H and Grassberger P 1995 *J. Phys. A: Math. Gen.* **28** 4987