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FAST TRACK COMMUNICATION

Almost periodic one-dimensional systems

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Abstract
The Schrödinger equation with potential $V(x) = 2\lambda_1 \cos x + 2\lambda_2 \cos \alpha x$ is considered. Its solution reduces to the problem of finding the eigenvectors of a matrix. The eigenvalues of this matrix show a band structure which is very sensitive to the value of the parameter α. The solutions of the Schrödinger equation are presented, and their physical meaning is discussed. The potential $V(x)$ has a complex multiwell structure, and quantum tunneling occurs. The accuracy of all approximations is carefully studied.

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There exists a lot of work on periodic systems in various contexts: partial differential equations, solid state physics, dynamical systems, etc. The solutions of the corresponding equations are based on the Floquet–Bloch theory.

An interesting generalization, which has been studied extensively more recently, is quasi-periodic systems [1–3]. These systems exhibit very interesting novel phenomena which do not appear in the periodic systems. Potential applications include quasi-crystals, electrons subject to competing incommensurate potentials, photonic crystals, etc. Both one-dimensional and higher-dimensional systems have been studied in this context, and in this article we are interested in the former case.

There are many types of one-dimensional quasi-periodic systems. A lot of work has concentrated on the study of the tight-binding Hamiltonian, which is a discrete Schrödinger equation based on the approximation that both the potential and the electron wavefunction are sharply peaked on the ionic sites. The nature of the spectrum (e.g. continuous, Cantor set, etc) and the nature of the eigenfunctions (local or non-local) for this equation with various types of the potential $V(n)$ have been studied in the literature.

Another problem in this general context is optical transmission in structures with varying refractive index. Liu, Macia and Barriuso *et al* [4–6] have studied optical beam propagation in quasi-periodic dielectric multilayers. Hollingworth *et al* [7] have studied wave propagation in media with varying refractive index in the slowly varying wave approximation. In this case, the problem reduces to the solution of the Schrödinger equation,

$$\left[-\partial_x^2 + V(x)\right]\psi(x) = \omega\psi(x), \tag{1}$$

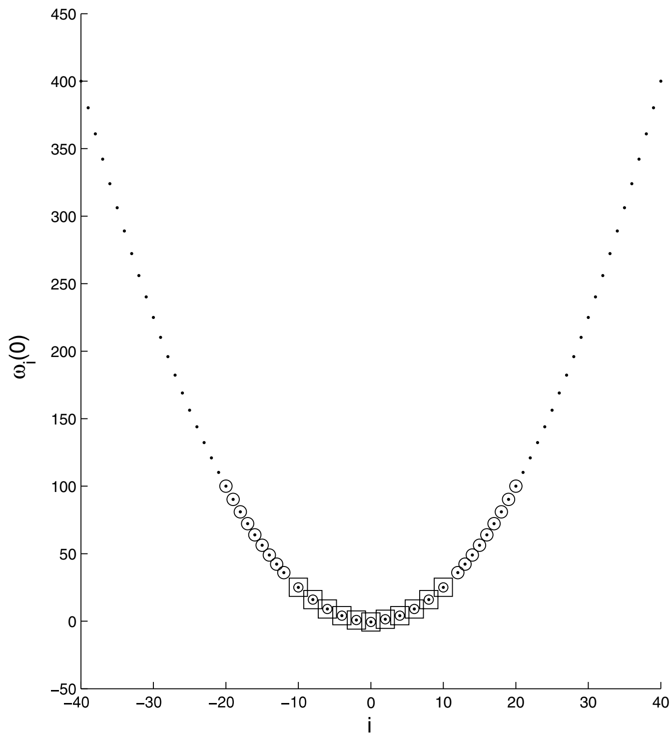

Figure 1. The eigenvalues $\omega_i(0)$ ($i = -Kq, \dots, Kq$) for the case $\lambda_1 = \lambda_2 = 0.5$, $p = 1$, $q = 2$ and for $K = 5$ (squares), $K = 10$ (circles), $K = 20$ (points). The results show that the truncation of the infinite matrices at $K = 5$ is sufficient.

with the potential

$$V(x) = 2\lambda_1 \cos x + 2\lambda_2 \cos \alpha x, \tag{2}$$

which is periodic for rational values of α and almost periodic [8] for irrational values of α. Related work has been presented in [9, 10]. The applications of these concepts to free-electron lasers have been studied in [11].

In the present article, we study the solutions of equation (1) for the potential of equation (2). We show that this problem reduces to the problem of finding the eigenvectors of an infinite matrix. Numerically, we use a finite matrix, but we check very carefully that the solutions are not affected by the truncation. The fact that the results are very sensitive to the value of α makes necessary the careful study of the accuracy of the approximations. We ensure that there are no significant artefacts of the truncation in the solution. We also introduce the concept of a discretization parameter ν which defines how fine (or coarse) the discretization is. We check that finer discretizations produce almost the same results, and therefore we are confident that our results are very good approximations to the solutions of the continuous differential equation in equation (1). We then study the band structure of the eigenvalues of this system and also derive the solutions of equation (1).

For rational values $\alpha = p/q$ where p, q are coprime integers, the potential is periodic with period $2\pi q$. The Floquet–Bloch theorem states that the solution is

$$\psi_k(x) = \exp\left(\frac{\mathrm{i}kx}{q}\right)\psi_0(x), \tag{3}$$

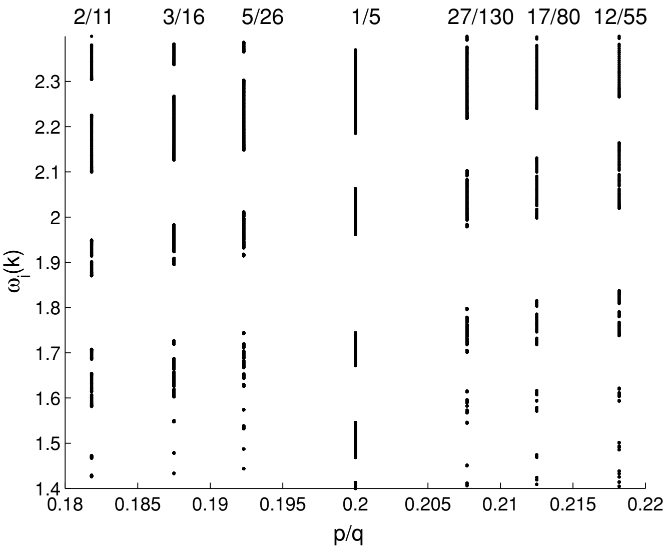

Figure 2. The eigenvalues $\omega_i(k)$ (for all k) for the case $\lambda_1 = \lambda_2 = 0.5$ and $\alpha = 2/11, 3/16, 5/26, 1/5, 27/130, 17/80, 12/55$.

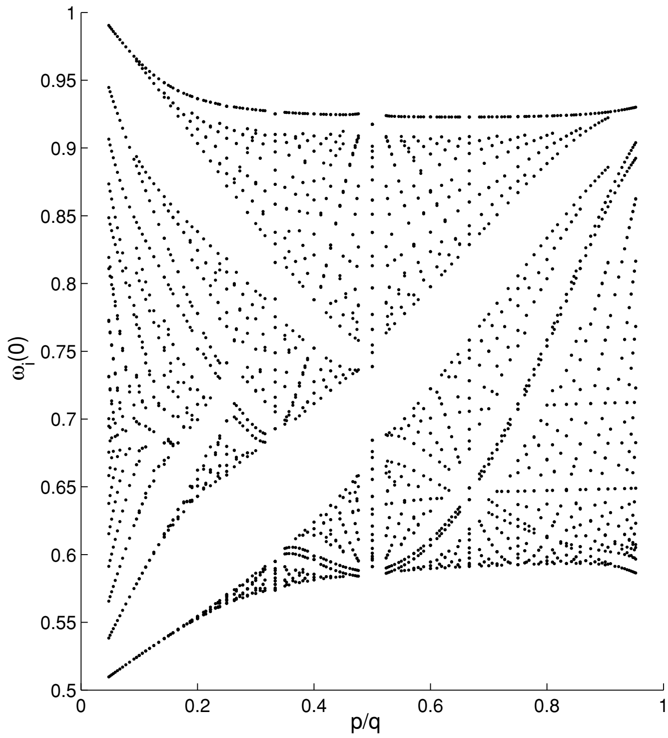

Figure 3. The eigenvalues $\omega_i(0)$ for the case $\lambda_1 = 0.5$, $\lambda_2 = 0.05$, and for all values of p/q where $1 \leqslant p \leqslant 20$ and $p < q \leqslant 21$.

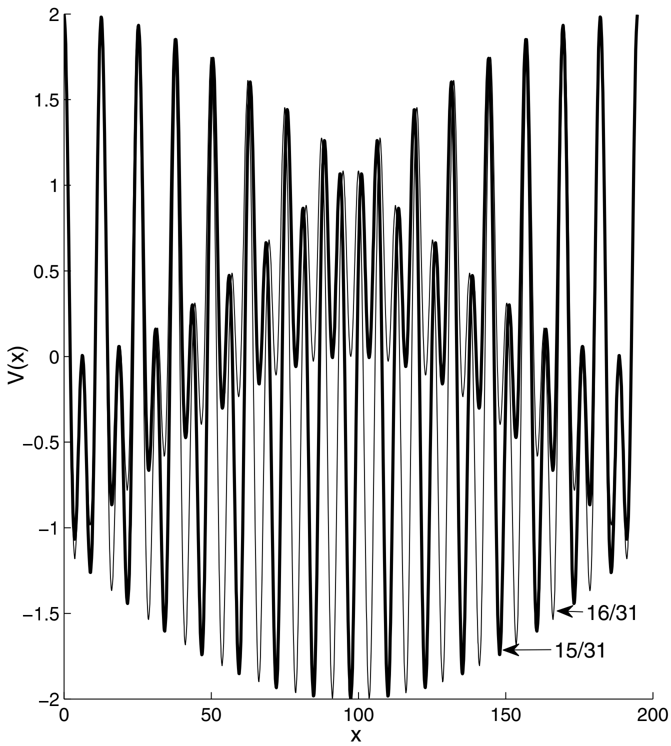

Figure 4. The potential $V(x)$ for $\lambda_1 = \lambda_2 = 0.5$ and $p/q = 15/31$ (thick line) and $p/q = 16/31$ (thin line).

where $\psi_0(x)$ is a periodic function with period $2\pi q$. The variable k takes values from 0 to 1. A Fourier series expansion of $\psi_k(x)$ gives

$$\psi_k(x) = \exp\left(\frac{\mathrm{i}kx}{q}\right) \sum_{n=-\infty}^{\infty} a_n(k) \exp\left(\frac{\mathrm{i}nx}{q}\right). \tag{4}$$

We insert equations (4) into equation (1) and get the matrix equation

$$A_{nm} a_m(k) = \omega(k) a_n(k), \tag{5}$$

where n, m take values from $-\infty$ to ∞, and

$$A_{nm} = \left(\frac{n+k}{q}\right)^2 \delta(n,m) + \lambda_1 \delta(n-q,m) + \lambda_1 \delta(n+q,m) + \lambda_2 \delta(n-p,m) + \lambda_2 \delta(n+p,m), \tag{6}$$

where $\delta(n,m)$ is Kronecker's delta. It is seen that the solution of the differential equation (1) reduces to the problem of finding the eigenvectors of the matrix A.

We truncate the infinite A-matrix to a $(2Kq+1) \times (2Kq+1)$ matrix with indices from $-Kq$ to Kq. In this case,

$$\psi_k(x) = \exp\left(\frac{\mathrm{i}kx}{q}\right) \sum_{n=-Kq}^{Kq} a_n(k) \exp\left(\frac{\mathrm{i}nx}{q}\right). \tag{7}$$

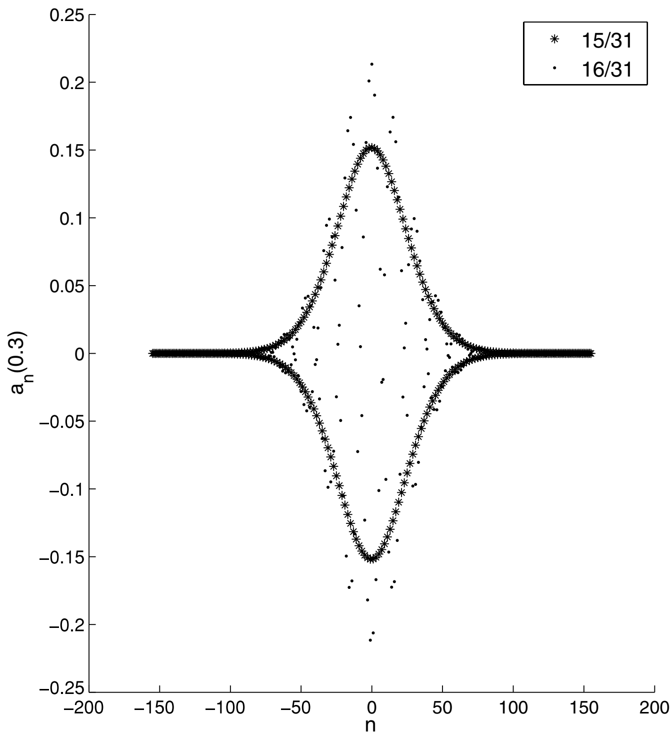

Figure 5. The components $a_n(0.3)$ of the eigenvectors for $p/q = 15/31$ and the lowest eigenvalue $\omega_0(0.3) = -1.27$ (stars), and also for $p/q = 16/31$ and the lowest eigenvalue $\omega_0(0.3) = -1.25$ (points). In both cases $\lambda_1 = \lambda_2 = 0.5$.

We label the eigenvalues of the truncated A-matrix in ascending order as follows:

$$\omega_0(k) \leqslant \omega_{-1}(k) \leqslant \omega_1(k) \leqslant \omega_{-2}(k) \leqslant \omega_2(k) \leqslant \cdots \leqslant \omega_{-Kq}(k) \leqslant \omega_{Kq}(k). \tag{8}$$

In figure 1, we plot the eigenvalues $\omega_i(0)$ $(i = -Kq, \ldots, Kq)$ for the case $\lambda_1 = \lambda_2 = 0.5$, $p = 1, q = 2$ and for $K = 5, 10, 20$. The results show that the truncation at $K = 5$ is sufficient. Consequently, all our results below are with $(10q + 1) \times (10q + 1)$ matrices.

We have said earlier that $\alpha = p/q$ where p, q are coprime integers. If we take $\alpha = \nu p/(\nu q)$ where ν is a positive integer, we have a finer discretization of the same continuous differential equation. For this reason we call ν the discretization parameter. In this case, we get the $(2K\nu q + 1) \times (2K\nu q + 1)$ matrix,

$$\mathcal{A}_{nm} = \left(\frac{n+k}{\nu q}\right)^2 \delta(n, m) + \lambda_1 \delta(n - \nu q, m) + \lambda_1 \delta(n + \nu q, m) + \lambda_2 \delta(n - \nu p, m) + \lambda_2 \delta(n + \nu p, m). \tag{9}$$

The matrix A in equation (6) is a submatrix of the matrix $\mathcal{A}$ in equation (9) with $\mathcal{A}_{\nu n, \nu m} = A_{n,m}$ and with the variable k in A corresponding to νk in $\mathcal{A}$. For example, the 'q-diagonal' (with elements $(n, n + q)$ for fixed q and all n) in A consists of the elements $(\nu n, \nu n + \nu q)$ in the νq-diagonal in $\mathcal{A}$. In the terminology of image analysis, both matrices discretize the same differential operator, but the A-matrix uses $(2Kq)^2$ 'large pixels' while the $\mathcal{A}$-matrix uses $(2K\nu q)^2$ 'small pixels'. Therefore, the eigenvalue $\omega_i(k)$ of the A-matrix corresponds to the

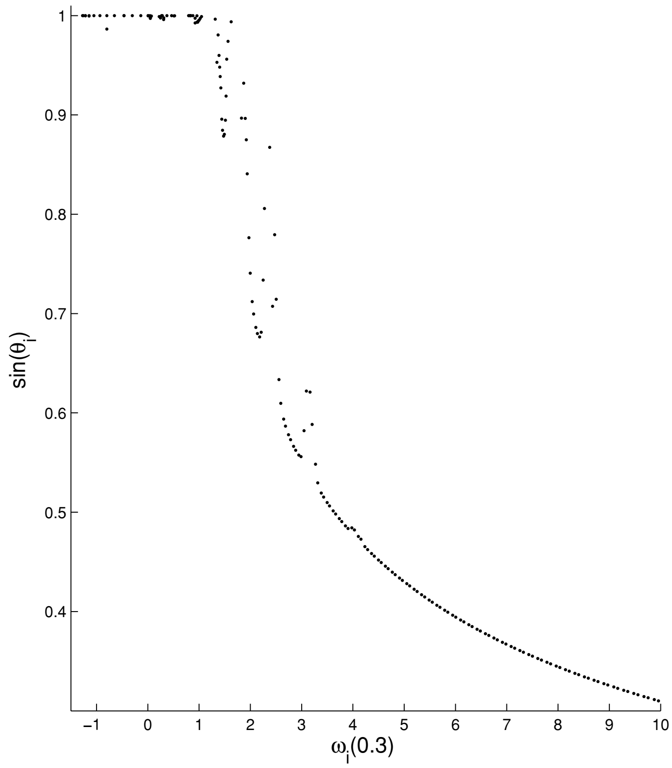

Figure 6. The $\sin(\theta_i)$ as a function of $\omega_i(0.3)$. θ_i is the angle between the eigenvectors $V[\omega_i(0.3)]$ and $V'[\omega_i(0.3)]$ for $p/q = 15/31$ and $p/q = 16/31$, and $\lambda_1 = \lambda_2 = 0.5$.

eigenvalue $\Omega_{\nu i}(\nu k)$ of the $\mathcal{A}$-matrix. We have checked that in our examples, the difference $\omega_i(k) - \Omega_{\nu i}(\nu k)$ is effectively zero. This ensures that the discretization that we have considered is fine enough for the accurate results of the continuous differential equation.

We have studied the eigenvalues $\omega_i(k)$ for various values of the parameters. The results show a band structure, i.e. there are intervals of forbidden values for $\omega_i(k)$ (which we call 'gaps'). In figure 2, we show the eigenvalues $\omega_i(k)$ for all k $(0 \leqslant k < 1)$ and for various values of p/q which are close to each other. The results show clearly that small changes in the parameter α produce major changes in the band structure. We note that in large eigenvalues $(\omega \gg \max(|V(x)|))$, there are no gaps. Physically, large eigenvalues describe particles with large energy for which the effect of the potential is almost negligible (they propagate almost as free particles).

In figure 3, we present the eigenvalues $\omega_i(0)$ for all values of p/q where $1 \leqslant p \leqslant 20$ and $p < q \leqslant 21$. We note the similarity with the 'Hofstadter butterfly' (which is produced for a very different model [2]).

The potential $V(x)$ has a complex multiwell structure. In each period (which is $2\pi q$) there are q wells (related to the $2\lambda_1 \cos x$ term) with different depths. The parameters λ_1, λ_2 define these depths. Physically, we expect that for the lowest energies the particle is confined in the wells with the lowest minima, and there is very little tunneling through the walls separating the wells. As the energy increases, the particle tunnels through the walls. At very high energies the particle propagates almost as a free particle.

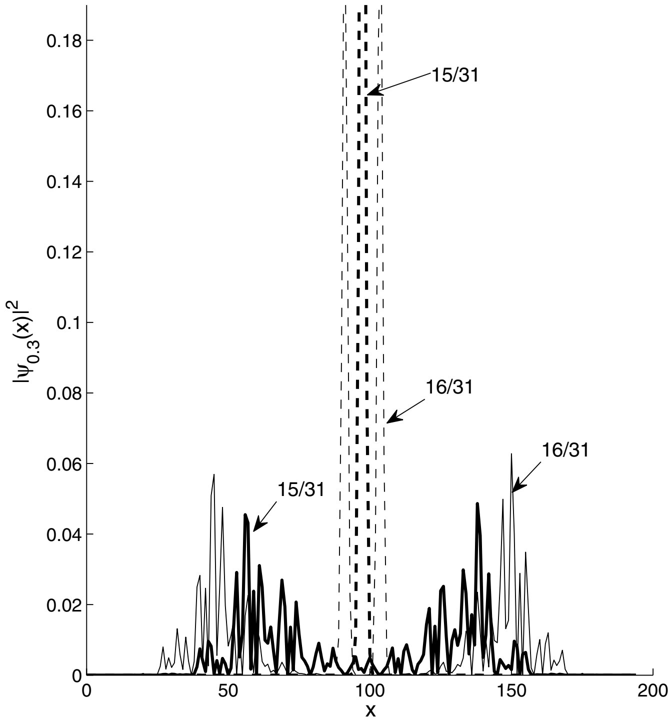

Figure 7. The $|\psi_{0.3}(x)|^2$ against x for $p/q = 15/31$ and $\omega_0(0.3) = -1.27$ (thick broken line), for $p/q = 15/31$ and $\omega_{27}(0.3) = 0.95$ (thick line), for $p/q = 16/31$ and $\omega_0(0.3) = -1.25$ (thin broken line), and for $p/q = 16/31$ and $\omega_{27}(0.3) = 0.97$ (thin line). In all cases $\lambda_1 = \lambda_2 = 0.5$. The solutions are periodic with period 62π. In the case of the thick broken line, the maximum value is $|\psi_{0.3}(\pi q)|^2 = 0.42$ (not shown in the figure).

Figure 4 shows the potentials $V(x)$ for $\lambda_1 = \lambda_2 = 0.5$ and $p/q = 15/31$ (thick line) and $p/q = 16/31$ (thin line). Let $A(k)$ and $A'(k)$ be the corresponding matrices of equation (6) for these two potentials. We call $\{\omega_i(k)\}$ and $\{\omega_i'(k)\}$ their eigenvalues, correspondingly (we label them as in equation (8)). In figure 5, we present the components $a_n(0.3)$ of the eigenvectors $\overrightarrow{a}(0.3)$ for $p/q = 15/31$ and for the lowest eigenvalue $\omega_0(0.3) = -1.27$ (stars), and also for $p/q = 16/31$ and the lowest eigenvalue $\omega_0(0.3) = -1.25$ (points). It is seen that small changes in the parameter α produce large changes in the eigenvectors corresponding to the lowest eigenvalues.

We study this point in greater detail as follows. We consider the eigenvalues $\omega_i(0.3)$ and $\omega_i'(0.3)$ with same index i. They are different from each other because the corresponding matrices $A(k)$ and $A'(k)$ are different from each other. Let $V[\omega_i(0.3)]$ be the eigenvector of $A(0.3)$ corresponding to $\omega_i(0.3)$ and $V'[\omega_i'(0.3)]$ be the eigenvector of $A'(0.3)$ corresponding to $\omega_i'(0.3)$. We have calculated the angle θ_i between $V[\omega_i(0.3)]$ and $V'[\omega_i(0.3)]$ for all i. In figure 6, we present $\sin(\theta_i)$ as a function of $\omega_i(0.3)$ for the case $\lambda_1 = \lambda_2 = 0.5$. It is seen that the eigenvectors corresponding to the smaller eigenvalues are significantly different in the two cases. For large eigenvalues, the corresponding eigenvectors are almost the same ($\sin(\theta_i)$ is small). As we explained earlier, large eigenvalues ($\omega \gg \max(|V(x)|)$) describe particles with large energy for which the effect of the potential is almost negligible.

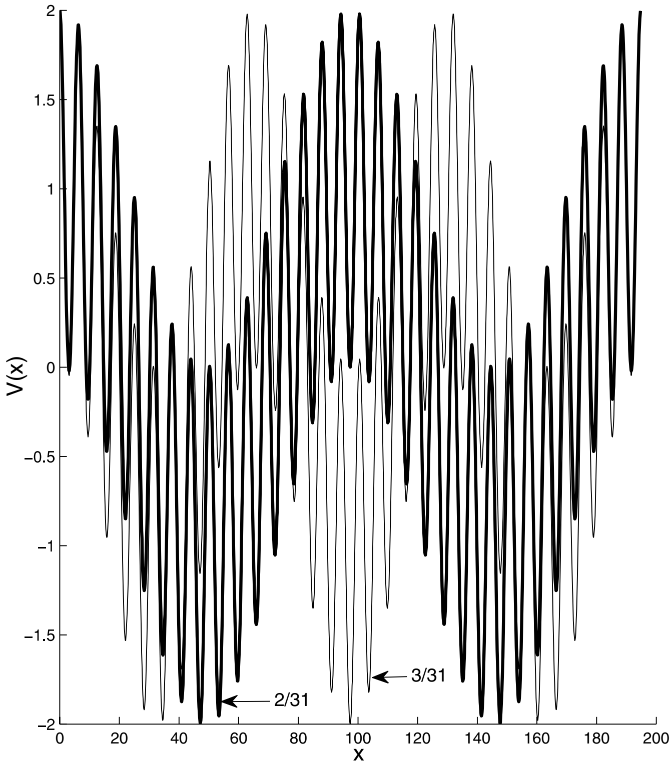

Figure 8. The potential $V(x)$ for $\lambda_1 = \lambda_2 = 0.5$ and $p/q = 2/31$ (thick line) and $p/q = 3/31$ (thin line).

Having the eigenvectors we can calculate the function $\psi_k(x)$ of equation (7). In figure 7, we present $|\psi_{0.3}(x)|^2$ for the lowest eigenvalue $\omega_0(0.3)$ and also for a higher eigenvalue $\omega_{27}(0.3)$. For $p/q = 15/31$ and for the lowest eigenvalue which is $\omega_0(0.3) = -1.27$, the potential has one global minimum (within a period), and the particle is confined in the corresponding well (thick broken line). Due to the low energy, the tunneling through the walls is negligible. For $p/q = 16/31$ and for the lowest eigenvalue which is $\omega_0(0.3) = -1.25$, there are two wells (within a period) with the lowest minimum, and the particle is confined in these two wells (thin broken line). We also show $|\psi_{0.3}(x)|^2$ for $p/q = 15/31$ and $\omega_{27}(0.3) = 0.95$ (thick line), and also for $p/q = 16/31$ and $\omega_{27}(0.3) = 0.97$ (thin line). In this case, we have significant quantum tunneling through the walls, and the particle is spread in the whole region. The results shown in this figure confirm that the solutions are very sensitive to the value of α.

We have also considered the potential $V(x)$ shown in figure 8, where $\lambda_1 = \lambda_2 = 0.5$, and $p/q = 2/31$ and $p/q = 3/31$. In figure 9, we present $|\psi_0(x)|$ for the lowest eigenvalue $\omega_0(0) = -1.35$ for $p/q = 2/31$ (thick broken line), and for $\omega_0(0) = -1.35$ and $p/q = 3/31$ (thin broken line). We also show results for $p/q = 2/31$ and $\omega_{-27}(0) = 0.88$ (thick line), and also for $p/q = 3/31$ and $\omega_{-27}(0) = 0.85$ (thin line). Again we see that for the lowest energy the tunneling is negligible, and the particle is confined in the wells with the lowest minima. For higher energies tunneling occurs, and the particle is spread in the whole region.

The study of the solutions of equation (1) is an interesting problem from both an academic and a practical point of view. From the academic point of view, it is interesting to study

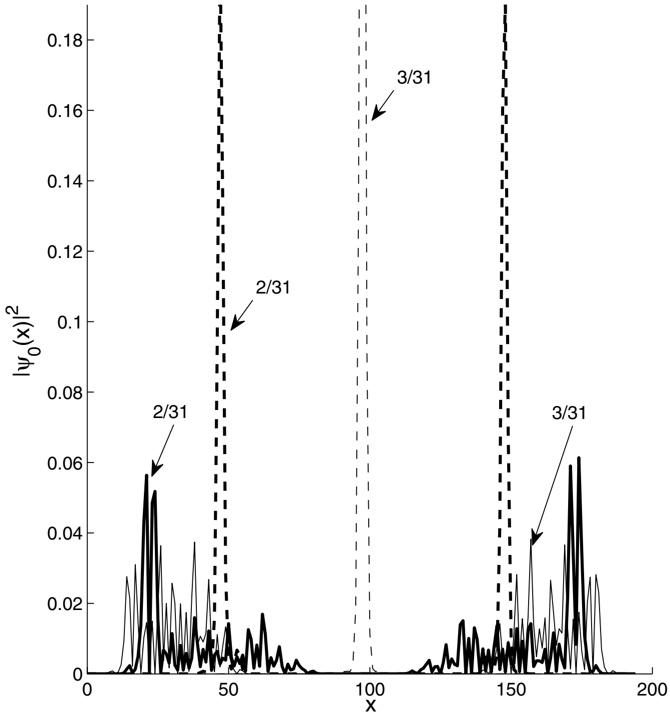

Figure 9. The $|\psi_0(x)|^2$ against x for $p/q = 2/31$ and $\omega_0(0) = -1.35$ (thick broken line), for $p/q = 2/31$ and $\omega_{-27}(0) = 0.88$ (thick line), for $p/q = 3/31$ and $\omega_0(0) = -1.35$ (thin broken line), for $p/q = 3/31$ and $\omega_{-27}(0) = 0.85$ (thin line). In all cases $\lambda_1 = \lambda_2 = 0.5$. The solutions are periodic with period 62π. In the case of the thin broken line, the maximum value is $|\psi_0(\pi q)|^2 = 0.39$ (not shown in the figure).

problems where the strict periodicity required in the Floquet–Bloch theory is relaxed. Although the potentials considered in this article are periodic (rational values of α), the study of the sensitivity of the results to small changes in the value of α is a first step towards understanding the case with almost periodic potentials (irrational values of α). The potential $V(x)$ has a multiwell structure with many wells of varying depth. For very low energies the particle is confined in the wells with the lowest minima. As the energy increases tunneling through the walls occurs.

From a more practical point of view, it has been explained in [4] that the study of equation (1) is useful in the wave propagation in media with varying refractive index in the slowly varying wave approximation. In this context, the existence of many bands in the solutions might be useful for the practically important problem of ultradense multiplexing in optical communications.

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