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LETTER TO THE EDITOR

A new solvable one-dimensional crystal model

L Wille, H Verschelde† and P Phariseau

Seminarie voor Theoretische Vaste Stof—en Lage Energie Kernfysica, Rijksuniversiteit—Gent, Krijgslaan 281, S9 B-9000 Gent, Belgium

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Abstract. The low-lying energy levels of electrons moving in a potential of the form $V(x)=(1-\gamma^2)/(1-2\gamma\cos x+\gamma^2)$ have been calculated. In the limits $\gamma\to 0$ and $\gamma=1$, well known results are recovered. The bandgaps are studied as a function of γ.

One-dimensional crystal models continue to play an important role in our understanding of the electronic structure and related phenomena in solids. The number of potentials for which the problem can be solved completely, however, remains very small (Lieb and Mattis 1966). In this letter we wish to investigate the one-electron Schrödinger equation with a potential function of the form

$$V(x)=(1-\gamma^2)/(1-2\gamma\cos x+\gamma^2) \qquad 0\leqslant\gamma\leqslant 1. \tag{1}$$

Our interest stems from the fact that this model reduces to the Mathieu limit for γ near zero and to the Kronig–Penney limit for $\gamma=1$. Both limits have been studied extensively and of special relevance is some recent work by Loly and Bahurmuz (1979, 1980) and by Avron and Simon (1981). We believe that the potential function (1) yields a new and meaningful way of interpolating between these two extremes.

The shape of the potential is shown in figure 1 for some typical values of the parameter γ. In the limit $\gamma\to 0$ we obtain the free electron case, but with a shift in energy zero. In the other extreme, $\gamma\to 1$, the function reduces to a periodic array of delta functions with strength 2π

$$\lim_{\gamma\to 1} V(x)=\sum_{n=-\infty}^{+\infty} 2\pi\delta(x-2n\pi). \tag{2}$$

The potential can be expanded in a Fourier series (Gradshteyn and Ryzhik 1965)

$$V(x)=1+2\sum_{n=1}^{+\infty}\gamma^n\cos nx, \tag{3}$$

a result that remains valid when $\gamma=1$ (Oberhettinger 1973). Upon the substitution $x\to 2x$, the Schrödinger equation, in atomic units, becomes

$$\psi''+4\left(E-1-\sum_{n=1}^{+\infty}\gamma^n\cos 2nx\right)\psi=0 \tag{4}$$

where E is the energy and determines the bandstructure.

† Aspirant NFWO (Belgium).

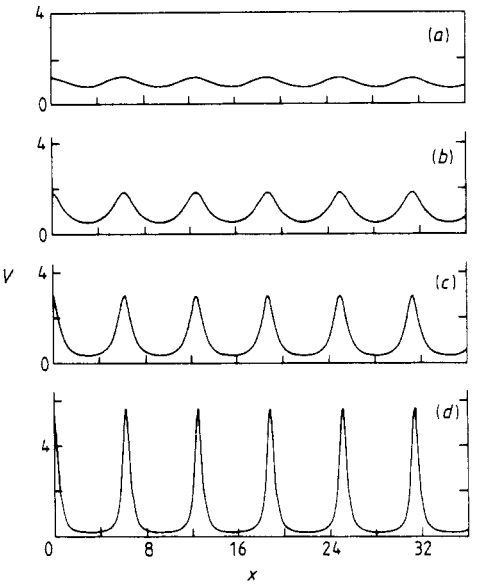

Figure 1. The potential function (equation (1)) for a few values of γ. (*a*) $\gamma=0.1$, (*b*) $\gamma=0.3$, (*c*) $\gamma=0.5$, (*d*) $\gamma=0.7$.

This differential equation is of the form

$$d^2w/dz^2+(\theta_0+2\theta_1\cos 2z+2\theta_2\cos 4z+\ldots)w=0 \tag{5}$$

i.e. it is a Hill equation (Ince 1956, Magnus and Winkler 1966). In our case the coefficients have the following values

$$\theta_0=4(E-1) \qquad \theta_n=-4\gamma^n \qquad n=1,2,\ldots. \tag{6a, b}$$

The general theory asserts that the complete solution is given by

$$w=e^{\alpha z}\sum_{n=-\infty}^{+\infty} b_n\, e^{niz} \tag{7}$$

where α is a root of

$$\sin^2(\tfrac{1}{2}\pi\alpha\,\mathrm{i})=\Delta(0)\sin^2(\tfrac{1}{2}\pi\sqrt{\theta_0}) \tag{8}$$

and $\Delta(0)$ is a Hill determinant of the form

$$\Delta(0)=\begin{vmatrix} \vdots & \vdots & \vdots & \\ \cdots & 1 & \dfrac{-\theta_1}{2^2-\theta_0} & \dfrac{-\theta_2}{2^2-\theta_0} & \cdots \\ \cdots & \dfrac{-\theta_1}{0^2-\theta_0} & 1 & \dfrac{-\theta_1}{0^2-\theta_0} & \cdots \\ \cdots & \dfrac{-\theta_2}{2^2-\theta_0} & \dfrac{-\theta_1}{2^2-\theta_0} & 1 & \cdots \\ & \vdots & \vdots & \vdots & \end{vmatrix}. \tag{9}$$

General theorems have been proven about the convergence of such infinite determinants.

In the case of an electron moving in a potential of the form under study the parameter α must be purely imaginary, to insure the proper behaviour of the wave function, i.e.

$$\alpha = 2ik. \tag{10}$$

Of course this is just the Bloch property, and the bandstructure $E(k)$ is then determined by

$$\sin^2(k\pi) = \Delta(0)\sin^2[\pi(E-1)^{1/2}]. \tag{11}$$

One can check that this equation reduces to the correct Kronig–Penney result when $\gamma = 1$. In general however the determinant (9) cannot be calculated analytically, but it turns out that an efficient numerical procedure is possible. To this end we consider the (finite) determinant

$$\Delta_m^n = \begin{vmatrix} 1 & \dfrac{4\gamma}{(2m)^2-\theta_0} & \dfrac{4\gamma^2}{(2m)^2-\theta_0} & \cdots & \\ \dfrac{4\gamma}{(2m-2)^2-\theta_0} & 1 & \dfrac{4\gamma}{(2m-2)^2-\theta_0} & \cdots & \\ \dfrac{4\gamma^2}{(2m-4)^2-\theta_0} & \dfrac{4\gamma}{(2m-4)^2-\theta_0} & 1 & \cdots & \\ & & \cdots & 1 & \dfrac{4\gamma}{(-2n+2)^2-\theta_0} \\ & & \cdots & \dfrac{4\gamma}{(-2n)^2-\theta_0} & 1 \end{vmatrix}$$

$$m = -n+2, \ldots, n. \tag{12}$$

One then obtains the following recursion formula

$$\begin{aligned}\Delta_m^n = &\left(1 - \frac{8\gamma^2}{(2m)^2-\theta_0} + \gamma^2\frac{(2m-2)^2-\theta_0}{(2m)^2-\theta_0}\right)\Delta_{m-1}^n \\ &- \gamma^2\left(\frac{4}{(2m-2)^2-\theta_0} - 1\right)\left(\frac{4}{(2m)^2-\theta_0} - \frac{(2m-2)^2-\theta_0}{(2m)^2-\theta_0}\right)\Delta_{m-2}^n\end{aligned} \tag{13}$$

together with the initial values

$$\Delta_{-n}^n = 1 \qquad \Delta_{-n+1}^n = 1 - \frac{(4\gamma)^2}{[(-2n)^2-\theta_0][(-2n+2)^2-\theta_0]}. \tag{14a, b}$$

Taking a big enough value for n we obtain an approximation Δ_n^n for the determinant $\Delta(0)$. Thus the bandstructure can be computed very accurately.

In figure 2 we show the results of our calculations for the lowest-lying bands for a few values of γ. The case $\gamma = 0.1$ corresponds to a nearly free electron case. The low energy bands are slightly perturbed at the zone edges by the weak potential, whereas the bands that are higher up in energy are hardly affected. Upon increasing

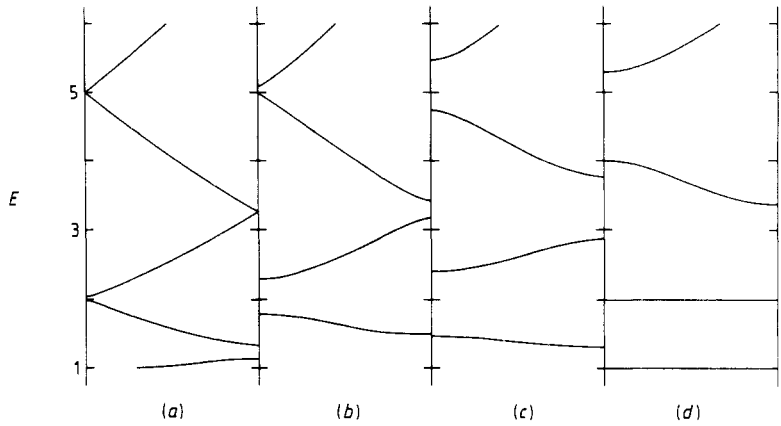

Figure 2. The bandstructure along the Γx direction. (a) $\gamma = 0.1$, (b) $\gamma = 0.4$, (c) $\gamma = 0.7$, (d) $\gamma = 1.0$.

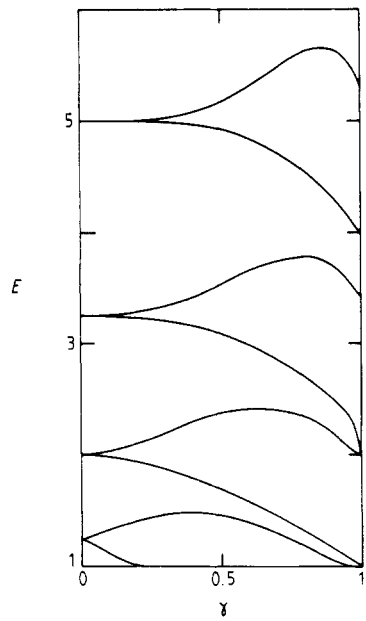

Figure 3. The gaps as a function of γ.

γ the potential becomes stronger and the bandgaps grow wider. In the limit $\gamma = 1$ the lowest bands are almost reduced to 'atomic' levels. In figure 3 we plot the edges of the gaps as a function of γ. These can be compared with the regions of stability and instability in the Mathieu problem (McLachlan 1964).

In conclusion we can say that we have determined very accurately the bandstructure for a new potential function, that promises to be relevant to other recent work. Further details will be published elsewhere.

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