Periodic Schrödinger Operators with Large Gaps and Wannier–Stark Ladders

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We describe periodic, one dimensional Schrödinger operators, with the property that the widths of the forbidden gaps increase at large energies and the gap to band ratio is not small. Such systems can be realized by periodic arrays of geometric scatterers, *e.g.*, a necklace of rings. Small, multichannel scatterers lead (for low energies) to the same band spectrum as that of a periodic array of (singular) point interactions known as δ'. We consider the Wannier–Stark ladder of δ' and show that the corresponding Schrödinger operator has no absolutely continuous spectrum.

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In this letter we discuss spectral properties of some one dimensional, one electron Schrödinger equations. Our purpose is threefold: first, we want to point out interesting features in the band–gap structure of periodic arrays of geometric scatterers, such as the necklace shown in Fig.1; second, we show that a singular point interaction, known as δ', which leads to interesting spectral properties and has been extensively studied [1], is a useful paradigm for the finite energy behavior of appropriate geometric scatterers; and finally, we describe the spectral properties of Wannier–Stark ladders for a periodic array of δ' scatterers, which are quite unlike those of the Wannier–Stark ladders of smooth potentials (see, *e.g.*, [2, 3, 4] and references therein).

By a classical result, the spectrum of the one electron Schrödinger equation with periodic potential is in the form of bands and gaps. Recall that for smooth periodic potentials the size of the n–th gap is rapidly decreasing and the band widths increase linearly with the band index n (for more precise information see *e.g.* [5]). A common wisdom says that the Kronig–Penney model (made of a periodic array of Dirac delta functions) gives the slowest decay of gap widths. In this case the gap widths approach a constant at high energies and the gap to band ratio goes to zero like $1/n$, with n the band index. So, in general, periodic potentials are expected to have a gap to band ratios that decrease at high energies at least as fast as $1/n$.

Periodic Schrödinger operators with singular interactions may have increasing gaps and even increasing gap to band ratios. This is the case for a point interaction known as δ', which, like the usual Dirac δ, is concentrated on a lattice of points. More precisely, a δ' point scatterer of strength λ (measured in units of length), is characterized by the transfer matrix $T_{\delta'}(\lambda) \equiv \begin{pmatrix} 1 & \lambda \\ 0 & 1 \end{pmatrix}$ which relates $\begin{pmatrix} \psi \\ \psi' \end{pmatrix}$ on the two sides of the scatterer, *i.e.* the wave function has continuous first derivatives on the right and left, and a jump proportional to the first derivative. This boundary condition satisfies Kirchoff's law and leads to a self-adjoint Schrödinger operator for any real λ [1, 6].

The boundary conditions embodied in δ' appear at first to be unnatural for quantum mechanics, and some efforts have been made in order to assign δ' a quantum mechanical interpretation [6]. It turns out that unlike Dirac's δ, the δ' can not be approximated by potentials, *i.e.* functions of the coordinate with small support. In particular, it has little to do with the derivative of Dirac's δ function. Rather, the (known) approximants involve functions of both coordinate and momenta [6]. The absence of a good realization of δ' may be the reason why it has not attracted more attention. One of our aims is to rectify this situation, and to show that the unique spectral properties of δ' are, in fact, a paradigm for geometric scatterers.

Consider the band–gap structure of periodic Schrödinger operators that come from allowing complicated geometries in one dimension, *e.g.* like those of a periodic necklace of rings and its onion–like generalizations. Fig.1 illustrates one such a system, where onion–like scatterers made of four wires, or channels, are connected by wires. The gap to band ratio of such objects does not decrease at high energies, and, in particular, both bands and gaps tend to increase. As we shall show, in certain (limiting) cases, such as the periodic array of small geometric scatterers with many short channels, the band–gap structure (for low energies) approximates that of a periodic array of δ'.

The out of the ordinary band–gap structure of δ' comes together with an out of the ordinary Stark effect: recall that for a large class of Stark Hamiltonians in one dimension, including Wannier–Stark Hamiltonians, under rather week differentiability conditions on the potential, the spectrum coincides with the real axis and is (purely) absolutely continuous [4]. The Wannier–Stark ladder **is not** a ladder of eigenvalues (we refer the reader to [2], and references therein, for results on the question of existence of Wannier–Stark ladder as a ladder of resonances, and to [7] for the experimental status). In contrast, tight–binding models, which have only a finite number of bands, have Wannier–Stark ladders of (discrete) eigenvalues. Tight–binding models may be thought of as a limiting situation of the Schrödinger operator with an infinitely large gap at high energies. The question whether the Wannier–Stark ladder is a ladder of eigenvalues or not seems, therefore, to be related to the structure of gaps at high energies. This point of view has been stressed by Ao who also argued that the Kronig–Penney model is a borderline situation, which for weak electric fields has Wannier–Stark ladder of eigenvalues, but for strong electric fields does not [8]. Although we have nothing to say about this intriguing transition, our results provide some support to the overall point of view (see also [9] for related phenomena in the random setting).

Let $\lambda\delta'_x$ denote a δ' point scatterer of strength λ, located at x , and

$$H(a,\lambda,F)\,=\,-\,\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2}\,+\,\sum_{n\in Z}\lambda\delta'_{na}\,-\,eFx\,, \tag{1}$$

denote the Wannier–Stark ladder operator for δ', with a the period, and F the electric field. We choose $eF>0$. The symbol $H(a,\infty,F)$ stands for Neumann boundary conditions at each point of the lattice.

It is a general fact about the Wannier–Stark ladder Hamiltonians (which follows from the unitary translation by lattice spacing) that the spectral properties are periodic with period eFa. For example,

$$\mathrm{Spec}(H(a,\lambda,F))\,=\,\mathrm{Spec}(H(a,\lambda,F))\,+\,eFa\,. \tag{2}$$

We now state our results on Wannier–Stark ladders for δ' :

Theorem. *For $F,\lambda\neq 0$, the absolutely continuous spectrum of $H(a,\lambda,F)$ is empty.*

Remarks: 1. The proof of the Theorem is rather technical and, therefore, shall be given elsewhere [10]. Below we shall sketch the ideas and the basic intuition behind the proof.

2. The assertion of the theorem generalizes to non-identical scatterers, *i.e.*, to situations where λ is replaced by a sequence $\{\lambda_n\}$ which may be position dependent, provided $|\lambda_n|\geq\lambda>0$.

3. The essential spectrum [11] of $H(a,\infty,F)$ is given explicitly by the accumulation points of the set

$$\left\{ eFa(\gamma n^2 - k - 1/2) \mid \; n,k \in Z \,\right\}, \tag{3}$$

where $\gamma \equiv \; h^2/8meFa^3$. Thus, for $\gamma = p/q$ rational, the (Neumann) essential spectrum is contained in the set $(eFa)\,\{\ell/q - 1/2 \mid \ell \in Z\,\}$ and has gaps (in fact, it is a nowhere dense, countable set). For γ irrational it is the real axis. Our results say nothing on what is the essential spectrum (as a set) for finite λ nor if the spectrum is pure point or singular continuous.

4. The Wannier–Stark problem in one dimension and the Zeeman problem with periodic potentials in two dimensions have a dimensionless parameter which characterizes commensuration of periods. In the Zeeman problem it is the number of quantum flux units per unit cell [3]. In the Wannier–Stark problem it is γ. Aspects of this fact, in the tight binding setting, have been stressed in [12]. In the Zeeman problem it is known that the spectrum, as a set, is sensitive to number theoretic properties the of the flux per unit cell. There is, of course, no corresponding sensitivity of the spectrum for Wannier-Stark Hamiltonians with smooth periodic potentials. The sensitivity of the spectrum for the δ' Wannier–Stark Hamiltonians as function of γ, is open.

A basic intuition to the results discussed above comes from considering first the scattering properties of a single scatterer. Let us start by contrasting δ' of strength λ, with the Dirac δ interaction of strength $1/\lambda$. The Dirac delta interaction has transfer matrix $T_\delta(1/\lambda) \equiv \begin{pmatrix} 1 & 0 \\ 1/\lambda & 1 \end{pmatrix}$. For a single delta scatterer, the reflection amplitude for wave number k is [13] $r = -1/(1-2ik\lambda)$ which goes to -1 as $k\lambda \to 0$. (Here $k \equiv \sqrt{2mE/\hbar^2} \geq 0$ is the wave number associated with an energy E). Total reflection can be interpreted as a decoupling of the two sides of the scatterer which occurs here through a Dirichlet boundary condition. Decoupling is, therefore, a low energy phenomenon for Dirac's δ. On the other hand, for a single δ' the reflection amplitude is $r = ik\lambda/(ik\lambda - 2)$ which approaches $+1$ in the limit $k\lambda \to \infty$. Now the total reflection can be interpreted as decoupling the two sides of the scatterer through an approach to a Neumann boundary condition. The remarkable fact about δ' is that the decoupling is a **high** energy phenomenon! The effective decoupling at large wavenumbers is at the heart of many of the unique properties we shall discuss below.

Consider now the onion–like scatterers with N channels, *i.e.* replace the $N=4$ channels of Fig.1 by a general N. For simplicity sake, suppose that all the wires are ideal identical conductors of length L, and that the boundary conditions at the two vertices are that the wave function has a unique limit at the vertices, and that $\sum \psi'\Big|_{\text{Vertex}} = 0$ (all legs are considered outgoing from the vertex). The transfer matrix across the scatterer is

$$T_{N,L}(k) \;=\; \begin{pmatrix} \cos(kL) & \sin(kL)/Nk \\ -Nk\sin(kL) & \cos(kL) \end{pmatrix} \tag{4}$$

(in the special case $N = 1$ it corresponds to an ideal wire of length L). The reflection amplitude from one such scatterer is

$$r(kL; N) \;=\; \frac{-N^2 + 1}{N^2 + 2iN\cot(kL) + 1}\,. \tag{5}$$

The reflection is periodic in k, something one expects for a geometric structure; there is no limit at high energies.

Note first that in the $k \to 0$ limit, $T_{N,\ell}(k) \to T_{\delta'}(L/N)$, expressing the fact that in the long–wavelength limit a geometric scatterer looks point–like. This, however, does not yet say that geometric scatterers are like δ', because, from our perspective, the crucial point of δ' is the high energy decoupling. In fact, as Eq. (5) shows, the reflection has no limit as $k \to \infty$. However, the reflection from certain geometric scatterers can mimic the reflection from a δ' in the following sense: consider the limit of a small scatterer with many channels: $L \to 0, \quad NL = \beta$,

$$r(kL; N) \;\to\; -(1 + 2i/\beta k)^{-1}\,. \tag{6}$$

When $k \to \infty$ (but still $kL \ll 1$) the reflection amplitude goes to -1, which gives the requisite decoupling at high energies (albeit through Dirichlet). One should therefore expect that such geometric scatterers will share with δ' some of its remarkable features. We shall now discuss evidence for this.

By stringing geometric scatterers or point scatterers with wires, or with a second type of geometric scatterers, to a periodic necklace as *e.g.* in Fig.1, we get a one dimensional system with spectrum made of bands and gaps. Let $T_{\rm Period}(k)$ be the transfer matrix for one period, for wave number k. The discriminant is $\Delta(k) \equiv {\rm Tr}\,(T_{\rm Period})$. By Floquet theory, the bands are given by the condition $-2 \le \Delta(k) \le 2$. It is a straightforward exercise to show that for the Kronig–Penney δ' model [1]

$$\Delta_{KP\delta'}(k) = 2\cos(ka) - \lambda k \sin(ka)\,. \tag{7}$$

For a necklace made of a pair of interlacing geometric scatterers

$$\begin{aligned}\Delta_{\rm Necklace}(k) \;=&\; \left(1 + \frac{N_1}{2N_2} + \frac{N_2}{2N_1}\right)\cos\left(k(L_1 + L_2)\right)\\ &+ \left(1 - \frac{N_1}{2N_2} - \frac{N_2}{2N_1}\right)\cos\left(k(L_1 - L_2)\right)\end{aligned} \tag{8}$$

(for the necklace of Fig.1, $N_1 = 1$ and $N_2 = 4$). It is known [1], and can easily be shown to follow from Eq. (7), that the band–gap structure of the Kronig–Penney δ' model has gaps that increase linearly with the band index n while the bands at large energies approach a constant width which is $4\hbar^2/ma\lambda$. This narrowness of the bands (compared with the large gaps) can be understood as a consequence of the fact that at high energies, the unit cells get decoupled since δ' approximates Neumann boundary conditions.

The dependence of the discriminant of the necklace, Eq. (8), on k is, of course, trigonometric. This implies that the band–gap structure is periodic (or almost periodic) in k. In particular, both bands and gaps tend to increase, linearly with k, at large energies, as a consequence of the fact that $E = \hbar^2 k^2/2m$. Furthermore, the gap to band ratio is almost periodic as well. This behavior is qualitatively different from what one gets from periodic potentials where the dependence of the discriminant on k is not trigonometric and where, on general grounds, one has $\Delta_{\text{Period}}(k) - 2\cos(ka) \to 0$ as $k \to \infty$. The special case $L_1 = L_2$ gives rise to an amusing situation where half of the gaps (all the periodic ones) are closed.

Fig.2 shows the discriminant and the bands for the necklace of Fig.1 as function of k. The length ratio of the wire to scatterer is 5. (The discriminant is computed for the case where all four channels of the scatterer have identical lengths). As one can see, even when the number of channels is relatively small ($N_2 = 4$), and when the scatterers are not really tiny ($L_1/L_2 = 5$), a feature of δ' emerges in that the second gap is larger than the first, and the third gap is larger than the second. The pattern reverses and then repeats periodically. The figure shows one period. Taking N_2 larger and L_2 smaller leads to gap increase for many more gaps.

One can actually make the gaps grow with energy on arbitrarily large scales by taking increasingly complicated scatterers. For example, by considering the limit of Eq.(6), *i.e.*, $L_2 \to 0$ and $L_2 N_2 = \beta$, the discriminant of the necklace with $N_1 = 1$, $L_1 = a$ obeys

$$\begin{aligned}\Delta_{\text{Necklace}}(k) &= 2\cos\left(k(a+L_2)\right) + \left(N_2 + \frac{1}{N_2} - 2\right)\sin(kL_2)\sin(ka) \\ &\to 2\cos(ka) - \beta k \sin(ka)\,.\end{aligned} \tag{9}$$

The lower part of the spectrum coincides, therefore, with that of the Kronig–Penney δ' model with $\lambda = \beta$. This supports the point of view that the δ' model can be a useful paradigm for certain geometric scatterers.

Let us now make a few comments regarding the proof of the Theorem, which is an adaptation of a technique previously used by Simon and Spencer [14]. Replacing the δ' point scatterer at a lattice point n_0 by a Neumann boundary condition, *i.e.* setting $\lambda_{n_0} = \infty$, is a rank one perturbation (of the resolvent) which decouples the right of n_0 from the left. It is a general fact that the absolutely continuous spectrum is stable under finite rank perturbations. The half lattice on the left is essentially like a triangular well problem and so has discrete spectrum. This means that the absolutely continuous spectrum is determined from the half line to the right of n_0. We now repeat sending λ_{n_j} to infinity for a sequence of points n_j, $j = j_0, j_0+1, \ldots$, that march off to infinity. Although for large j the individual $\lambda\delta'_{n_j}$ are close to a Neumann boundary condition, one can actually not take any sequence of points. A judicious choice is to take a partial sequence of the points $n_j \sim const + \gamma(j+1/2)^2$, so that for large j, the Neumann decoupling takes place at points that lie deep in the forbidden gaps of the periodic problem, where the discriminant $\Delta(k_j) \sim \mathcal{O}(j)$ is large. (The effective wave number and position are related by conservation of energy: $n_j \sim \gamma(k_j a/\pi)^2$). Indeed, one can show, via the asymptotics of Airy functions, that $(H(a,\lambda,F)+iE_0)^{-1} - (H(a,\{\lambda_n\},F)+iE_0)^{-1}$, where E_0 is a finite (real) constant, $\lambda_n = \infty$ for an appropriate subsequence, and $\lambda_n = \lambda$ otherwise, is a trace class operator. By the Kuroda–Birman Theorem [15] this gives the stability of the absolutely continuous spectrum. Since $H(a,\{\lambda_n\},F)$ clearly has only pure point spectrum, the theorem follows.

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Figure captions

Fig.1. A necklace made of geometric scatterers in the form of "onions", each made of four wires joint at two vertices. The "onions" are strung together by connecting wires.

Fig.2 The discriminant for the necklace of Fig.1 as function of k. The length ratio of the connecting wires to the wires making the "onion" is 5. The two straight lines are at ± 2 and the bands are drawn thick. One period (in k) is shown and the pattern then repeats periodically.