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 $\delta'$. We consider the Wannier-Stark ladder of $\delta'$ 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 $\delta'$, 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 $\delta'$ scatterers, which are quite unlike those of the Wannier-Stark ladders of smooth potentials (see, e.g., [2-4] 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 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 $\delta'$, which, like the usual Dirac $\delta$, is concentrated on a lattice of points. More precisely, a $\delta'$ point scatterer of strength $\lambda$ (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 $\psi$ 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 Kirchhoff's law and leads to a self-adjoint Schrödinger operator for any real $\lambda$ [1,6].

The boundary conditions embodied in $\delta'$ appear at first to be unnatural for quantum mechanics, and some efforts have been made in order to assign $\delta'$ a quantum mechanical interpretation [6]. It turns out that unlike Dirac's $\delta$, the $\delta'$ cannot 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 $\delta$ function. Rather, the (known) approximants involve functions of both coordinate and momenta [6]. The absence of a good realization of $\delta'$ 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 $\delta'$ 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 onionlike generalizations. Figure 1 illustrates one such system, where onionlike 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 $\delta'$.

The out of the ordinary band-gap structure of $\delta'$ comes together with an out of the ordinary Stark effect: recall that for a large class of Stark Hamiltonians in one di-

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FIG. 1. A necklace made of geometric scatterers in the form of "onions," each made of four wires joined at two vertices. The onions are strung together by connecting wires.
mension, including Wannier-Stark Hamiltonians, under
rather weak 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 the Wannier-Stark ladder as a ladder of resonances,
and to [7] for the experimental status). In contrast,
tight-binding models, which have a finite number of
bands, have Wannier-Stark ladders of (discrete) eigen-
values. Tight-binding models may be thought of as a
limiting situation of the Schrödinger operator with an
infinite 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
the 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 \( \lambda \delta'_a \) denote a \( \delta' \) point scatterer of strength \( \lambda \),
located at \( x \), and

\[
H(a, \lambda, F) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \sum_{n \in \mathbb{Z}} \lambda \delta'_a - eFx
\]

denote the Wannier-Stark ladder operator for \( \delta' \), 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,

\[
\text{Spec}(H(a, \lambda, F)) = \text{Spec}(H(a, \lambda, F)) + eFa.
\]

We now state our results on Wannier-Stark ladders for
\( \delta' \):

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 tech-
nical 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
nonidentical scatterers, i.e., to situations where \( \lambda \) is
replaced by a sequence \( \{ \lambda_n \} \) which may position depen-
dent, provided \( \{|\lambda_n| \geq \lambda > 0 \} \). (3) The essential spectrum
[11] of \( H(a, \infty, F) \) is given explicitly by the accumula-
tion points of the set

\[
\{eFa(\gamma n^2 - k - 1/2) \mid n, k \in \mathbb{Z}\},
\]

where \( \gamma \equiv \hbar^2/8meFa^2 \). Thus, for \( \gamma = p/q \) rational,
the (Neumann) essential spectrum is contained in the
set \( \{eFa(\gamma n^2 - k - 1/2) \mid n, k \in \mathbb{Z}\} \) and has gaps (in fact, it
is a nowhere dense, countable set). For \( \gamma \) irrational it
is the real axis. Our results say nothing about what is
the essential spectrum (as a set) for finite \( \lambda \) nor if the
spectrum is pure point or singular continuous. (4) The
Wannier-Stark problem in one dimension and the Zeen-
man problem with periodic potentials in two dimensions
have a dimensionless parameter which characterizes com-
mensuration 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 \( \gamma \). 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 of the
flux per unit cell. There is, of course, no corresponding
sensitivity of the spectrum for Wannier-Stark Hamiltoni-
as with smooth periodic potentials. The sensitivity of
the spectrum for the \( \delta' \) Wannier-Stark Hamiltonians as
a function of \( \gamma \), 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 \( \delta' \) of strength \( \lambda \),
with the Dirac \( \delta \) interaction of strength \( 1/\lambda \). The Dirac
delta interaction has transfer matrix

\[
T_D(1/\lambda) = \begin{pmatrix} 1 & 0 \\ 1/\lambda & 1 \end{pmatrix}
\]

For a single delta scatterer, the reflection amplitude for
wave number \( k \) is \[ r = -1/(1-2ik\lambda) \] which goes to
\( -1 \) as \( k\lambda \rightarrow 0 \). (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 phe-
nomenon for Dirac's \( \delta \). On the other hand, for a single
\( \delta' \) the reflection amplitude is \( r = ik\lambda/(ik\lambda - 2) \) which
approaches +1 in the limit \( k\lambda \rightarrow \infty \). Now the total
reflection can be interpreted as decoupling the two sides of
the scatterer through an approach to a Neumann bound-
ary condition. The remarkable fact about \( \delta' \) is that the
decoupling is a high energy phenomenon. The effective
decoupling at large wave numbers is at the heart of many
of the unique properties we shall discuss below.

Consider now the onionlike 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 bounda-
ry conditions at the two vertices are that the wave func-
tion has a unique limit at the vertices, and that \( \sum |\psi|^2 \rightarrow 0 \) (all legs are considered outgoing from the vertex). The
transfer matrix across the scatterer is

\[
T_{N,L}(k) = \begin{pmatrix} \cos(kL) & \sin(kL)/Nk \\ -Nk\sin(kL) & \cos(kL) \end{pmatrix}
\]

(in the special case \( N = 1 \) it corresponds to an ideal
wire of length \( L \)). The reflection amplitude from one
such scatterer is
\[ r(kL; N) = \frac{-N^2 + 1}{N^2 + 2iN \cot(kL) + 1}. \] (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, $T_{N,\ell}(k) \to T_{\ell}(L/N)$, expressing the fact that in the long-wavelength limit a geometric scatterer looks pointlike. This, however, does not yet say that geometric scatterers are like $\delta'$, because, from our perspective, the crucial point of $\delta'$ 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 $\delta'$ in the following sense: consider the limit of a small scatterer with many channels: $L \to 0$, $NL = \beta$,
\[ r(kL; N) \to - (1 + 2i/\beta k)^{-1}. \] (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 $\delta'$ 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 $T_{\text{period}}(k)$ be the transfer matrix for one period, for wave number $k$. The discriminant is $\Delta(k) \equiv \text{Tr} (T_{\text{period}})$. By Floquet theory, the bands are given by the condition $-2 \leq \Delta(k) \leq 2$. It is a straightforward exercise to show that for the Kronig-Penney $\delta'$ model [1]
\[ \Delta_{\text{KPE}}(k) = 2 \cos(ka) - \lambda k \sin(ka). \] (7)

For a necklace made of a pair of interlacing geometric scatterers
\[ \Delta_{\text{necklace}}(k) = \left[ 1 + \frac{N_1}{2N_2} + \frac{N_2}{2N_1} \right] \cos[k(L_1 + L_2)] + \left[ 1 - \frac{N_1}{2N_2} - \frac{N_2}{2N_1} \right] \cos[k(L_1 - L_2)] \] (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 $\delta'$ model has gaps that increase linearly with the band index $n$ while the bands at large energies approach a constant width which is $4\hbar^2/\pi a \lambda$. 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 $\delta'$ 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 $E = \hbar^2 k^2 / 2 m$. 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.

Figure 2 shows the discriminant and the bands for the necklace of Fig. 1 as a 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 $\delta'$ 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
\[ \Delta_{\text{necklace}}(k) = 2 \cos[k(a + L_2)] + \left( N_2 + \frac{1}{N_2} - 2 \right) \sin(kL_2) \sin(ka) \to 2 \cos(ka) - \beta k \sin(ka). \] (9)

The lower part of the spectrum coincides, therefore, with that of the Kronig-Penney $\delta'$ model with $\lambda = \beta$. This sup-
ports the point of view that the $\delta'$ 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 $\delta'$ 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 $\lambda_{n_j}$ 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 $\lambda_{n_j}$ 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 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 $\Delta(k_j) \sim O(j)$ 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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[13] Left reflection is related to right reflection by conjugation. Here we have chosen $r$ to stand for the left reflection.