Angular Momentum Irreducible Representation and Destructive Quantum Interference for Penrose Lattice Hamiltonians

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ABSTRACT: We study the nearest-neighbor tight-binding Schrödinger equation for an electron hopping on a two-dimensional Penrose lattice in a perpendicular magnetic field. The spectrum is studied using three different approaches: (i) through closed-form expressions for small lattices, (ii) using the angular momentum decomposition of the Hamiltonian, and (iii) numerically. For any given value of the angular momentum, we observe no level crossings. According to the Wigner–von Neuman theorem, this is a clear indication that no other symmetry, hidden or not, is present. We also derive a surprising result in which destructive quantum interference occurs at a particular value of the magnetic field and localizes an *infinite* number of states with energies $\pm\sqrt{5}$. This effect does not exist in square lattices. Both the local topology and the destructive interference are responsible for this localization.

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INTRODUCTION

The excitation spectra on the one-dimensional (1D) version of quasiperiodic systems have been investigated extensively.[1] However, the electronic properties[2,3] on the 2D canonical quasiperiodic structure, the Penrose lattice, have received much less attention. Moreover, the bulk of the work[2] in this area has focused on systems without external fields. Here we would like to study the behavior of the electronic spectrum when an external magnetic field is applied. In particular, we would like to exploit the rotational symmetry of the lattice in order to explicitly obtain the block-diagonals of the Hamiltonian associated with the different values of the angular momentum. This problem is not only of interest by itself, but also directly relates to experimental measurements on 2D superconducting wire networks and arrays of Josephson junctions[4] immersed in a perpendicular magnetic field.

It has been conjectured that the energy spectrum[2] of the 2D Penrose lattice is singular. In particular, the spectrum has an isolated level at $E = 0$, whose degeneracy is proportional to the system size, and whose states are strictly localized. The existence of these localized states[2] depends on the local topology, but not on the quasiperiodicity of the lattice.

In this paper, we show, by construction, that there are also strictly localized states at $E = \pm\sqrt{5}$ at certain magnetic field values. The existence of such states also depends on the local topology, but the effect of destructive interference plays a more explicit role. The quasiperiodicity of the lattice guarantees the existence of many (proportional to the system size) identical local configurations, and therefore the degeneracy of these states.

Our model is a tight-binding Hamiltonian. Atomic orbitals, $|i\rangle$, are located on the vertices, i, of rhombuses and an electron can only hop to nearest-neighbor sites which are connected by the edges of rhombuses. All transfer integrals, t_{ij}, are set to unity. Thus, the Schrödinger equation for a wave function $|\psi\rangle = \sum_i \psi_i |i\rangle$ with an energy E is

$$\sum_j t_{ij} \exp\left(iA_{ij}\right) \psi_j = E\psi_i$$

where

$$A_{ij} = \frac{2\pi}{\Phi_0} \int_i^j \vec{A} \cdot d\vec{l}$$

and where the wave function on the left- and right-hand sides of the previous equation belong to two different sublattices. The flux quantum is denoted by Φ_0.

De Bruijn[6] first gave a global and general prescription to generate Penrose lattices. We construct our Penrose lattices by projecting a 5D cubic lattice into a 2D subspace. The centers of the cube which intersect this hypersurface are projected into it. The projected basis vectors constitute a representation of the pentagonal group. We employ open boundary conditions in which the electron is confined within the sample, i.e., ψ_i vanishes for sites outside the sample.

ANGULAR MOMENTUM IRREDUCIBLE REPRESENTATION

The magnetic field dependence of the electronic spectra for a square lattice has been studied by Hofstadter[7]. By using the Landau gauge and Bloch's theorem, the 2D tight-binding equation can be easily be reduced to a one dimensional problem known as Harper's equation. This simplification into a 1D problem *cannot* be made in the Penrose lattice case because no obvious choice of gauge will decouple one direction from the other. We need to look for a different symmetry. Penrose lattices[5] do have a vertex with perfect fivefold symmetry. Thus, we will write our Hamiltonian in a basis which is centered on that vertex. Furthermore, in order to utilize this symmetry we have used the rotationally symmetric gauge

$$\vec{A} = \tfrac{1}{2}(\vec{H} \times \vec{r})$$

Our Hilbert space will be divided into five eigensubspaces, each one of them associated with a particular value of the angular momentum. We have derived explicit expressions for the block diagonal matrices of the Hamiltonian. For instance, for a lattice with 46 sites, the zero-angular momentum, $J = 0$, block diagonal matrix is

$$\begin{pmatrix}
0 & \sqrt{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sqrt{5} & 0 & 0 & 0 & \beta & 0 & \alpha + \bar{\alpha} & 0 & \bar{\beta} & 0 \\
0 & 0 & 0 & 0 & \gamma & \delta & 0 & 0 & \bar{\gamma} & \bar{\delta} \\
0 & 0 & 0 & 0 & 0 & \epsilon & 0 & 0 & 0 & \bar{\epsilon} \\
0 & \bar{\beta} & \bar{\gamma} & 0 & 0 & 0 & 0 & \gamma & 0 & 0 \\
0 & 0 & \bar{\delta} & \bar{\epsilon} & 0 & 0 & 0 & \delta & 0 & 0 \\
0 & \alpha + \bar{\alpha} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & \bar{\gamma} & \bar{\delta} & 1 & 0 & \gamma & \delta \\
0 & \beta & \gamma & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 \\
0 & 0 & \delta & \epsilon & 0 & 0 & 0 & \bar{\delta} & 0 & 0
\end{pmatrix}$$

where

$$\alpha = e^{iHS_l}$$

$$\beta = e^{iHS_s}$$

$$\gamma = \alpha\beta$$

$$\delta = \alpha\alpha\beta$$

$$\epsilon = \alpha\alpha\beta\beta$$

and where S_l (S_s) refers to the area of a large (small) tile and H refers to the applied magnetic field. The expressions for the block diagonal submatrices of the Hamiltonian associated with the $J = 1, 2, 3, 4$ values of the angular momentum quantum numbers are

$$\begin{pmatrix}
0 & 0 & 0 & \beta & 0 & \alpha + \bar{\alpha}\bar{\theta} & 0 & \bar{\beta}\bar{\theta} & 0 \\
0 & 0 & 0 & \gamma & \delta & 0 & 0 & \bar{\gamma}\bar{\theta} & \bar{\delta}\bar{\theta} \\
0 & 0 & 0 & 0 & \epsilon & 0 & 0 & 0 & \bar{\epsilon}\bar{\theta} \\
\bar{\beta} & \bar{\gamma} & 0 & 0 & 0 & 0 & \gamma & 0 & 0 \\
0 & \bar{\delta} & \bar{\epsilon} & 0 & 0 & 0 & \delta & 0 & 0 \\
\alpha\theta + \bar{\alpha} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & \bar{\gamma} & \bar{\delta} & 1 & 0 & \gamma & \delta \\
\beta\theta & \gamma\theta & 0 & 0 & 0 & 0 & \bar{\gamma} & 0 & 0 \\
0 & \delta\theta & \epsilon\theta & 0 & 0 & 0 & \bar{\delta} & 0 & 0
\end{pmatrix}$$

where

$$\theta = e^{i\frac{2\pi}{5}J}$$

Figure 1 shows the energy levels versus magnetic flux, $E_n(\phi)$, for a Penrose lattice with 46 vertices. It was obtained by numerically diagonalizing the Schrödinger equation for a very large number of values for the magnetic field.

Notice in figure 1 the presence of groups of five energy levels moving in a more or less coherent way, either monotononically increasing or decreasing. In order to disentangle this spaghetti of energy levels we need to focus on a single value of the angular momentum (our only good quantum number).

If we numerically diagonalize the block diagonal matrix corresponding to, say, the $J = 0$ quantum number for the angular momentum, then we obtain the spectrum shown in Figure 2. Notice that the energy levels sometimes get very close to each other and that occasionally it seems that they actually either touch or cross. A close look at a magnified version of the spectra shows that the energy levels neither cross nor touch. Furthermore, we know that energy levels corresponding to the same quantum number repel each other. Thus, the Wigner–von Neumann theorem[8] tells us that this lack of level crossing is a clear indication that no other symmetry, hidden or not, is present.

Moreover, the fact that the levels can get extremely close to each other for certain values of the magnetic field suggests that other approximate symmetries might exist. Since the global fivefold symmetry center is unique, the lattice has no other regions which are perfectly isomorphic to the central one (in spite of Conway's local isomorphism theorem[5]). However, very good approximants to it allow the levels to occasionally get very close. By writing the block diagonal form around the new local fivefold symmetry centers, we can express the Hamiltonian as a hierarchy of block diagonals. Only the first decomposition corresponds to an irreducible representation of the perfect fivefold symmetry and, thus, all the matrix elements outside the blocks are exactly equal to zero. The second level of the hierarchy corresponds to an almost perfect global symmetry (quasisymmetry), thus the off-diagonal elements will not be all zero, but very small numbers. This block-diagonalization procedure, can be repeated in order to obtain the other levels of the hierarchy.

For the sake of comparison, we have computed $E_n(\phi)$ for NxN finite square lattices using the same algorithm and boundary conditions employed for the Penrose lattice calculations. Figure 3 and 4 show the energy levels versus magnetic flux for the 5×5 and 8×8 cases.

For a number of small lattices, closed-form expressions for the energy spectra as a function of the magnetic fields can be obtained.

For the smallest case, five large rhombuses around a common vertex, the energy levels for the $J = 0$ angular momentum states are

$$E = \pm\sqrt{5 + 4\cos^2 A}$$

and $E = 0$. Also, we have defined $A = \frac{2\pi H S_l}{\Phi_0}$. The energy levels for the $J = 1, 2, 3, 4$ angular momentum states are

$$E = \pm 2\cos\left(A + \frac{\pi J}{5}\right).$$

A more complex example is the familiar Penrose decagon which is obtained by adding five skinny tiles to the previously considered lattice in order to complete a regular decagon. Both types of tiles are present in equal numbers. The energy levels for the $J = 0$ angular momentum states are

$$E = \pm\left\{5 + 4\left(\cos^2 A + \cos^2 B\right) \pm \left[\left(5 + 4\left(\cos^2 A + \cos^2 B\right)\right)^2 - 80\cos^2 B\right]^{\frac{1}{2}}\right\}^{\frac{1}{2}} \frac{1}{\sqrt{2}}$$

For the $J = 1, 2, 3, 4$ angular momentum states, the energy levels are

$$E = \pm 2\left\{\cos^2\left(A + \frac{\pi J}{5}\right) + \cos^2\left(B + \frac{\pi J}{5}\right)\right\}^{\frac{1}{2}}$$

and $E = 0$. We use the definitions

$$A = \frac{2\pi}{\Phi_0} H S_l \quad , \quad B = \frac{2\pi}{\Phi_0} H(S_l + S_s).$$

LOCALIZATION OF STATES DUE TO DESTRUCTIVE QUANTUM INTERFERENCE

Let us consider the Penrose decagon described above and an orbital, denoted by $|0>$, which is localized at the central site of the decagon. Let us denote the orbitals localized one (two) edge(s) away by $|1>, |2>, ..., |5>$ $(|1'>, |2'>, ..., |5'>)$. For concreteness, the site at $|1'>$ will be connected to $|1>$ and $|5>$. When the Hamiltonian, $\mathcal{H}$, is applied to a state, it provides the kinetic energy that allows it to hop one edge. We consider the effect of $\mathcal{H}^2|0>$, i.e.

$$\mathcal{H}^2 \, |0> = 5 \, |0> + \sum_{\alpha'=1}^{5} M_{\alpha'} \, |\alpha'>$$

where

$$M_{1'} = e^{i(A_{01}+A_{11'})} + e^{i(A_{05}+A_{51'})} , \quad ...$$

However, since

$$e^{i(A_{01}+A_{11'}+A_{1'5}+A_{50})} = e^{i\Phi}$$

we have

$$e^{i(A_{51'}+A_{05})} = e^{-i(A_{1'5}+A_{50})} = e^{i(A_{01}+A_{11'})} \, e^{-i\Phi}$$

where Φ is the flux enclosed by a large elementary tile. Thus, we can rewrite

$$M_{1'} = e^{i(A_{01}+A_{11'})} \left[1 + e^{-i\Phi}\right] , \quad ...$$

When $\Phi = \pi$, we have destructive interference since the factor inside the square brackets in the previous equation vanishes. Thus, $M_{\alpha'} = 0$ for all values of α' and

$$\mathcal{H}^2 \, |0> = 5 \, |0>$$

or

$$(\mathcal{H} + \sqrt{5})(\mathcal{H} - \sqrt{5})|0> = 0$$

Thus, $(\mathcal{H}-\sqrt{5})|0>$ is an eigenstate of $\mathcal{H}$ with eigenvalue $-\sqrt{5}$ and $(\mathcal{H}+\sqrt{5})|0>$ is an eigenstate of $\mathcal{H}$ with eigenvalue $+\sqrt{5}$. Thus, a particular value of the magnetic flux going through each large tile, *localizes* the state located at *every* center of a Penrose decagon.

Notice that there are an infinite number of decagons of this type in a Penrose lattice. Thus, the states with energies $\pm\sqrt{5}$ have a degeneracy of finite density in the thermodynamic limit. This result crucially depends on the *local* topology and geometry of the lattice and the applied *magnetic field*. We urge the reader to check this result numerically, and also to find other states which become localized in more complex regions by the combined effect of the local geometry–topology and the external field.

The above result does not apply, for instance, to the square lattice. In order to see this, let us consider four square cells around a common vertex. It is clear that $\mathcal{H}^2\,|0>$ has additional contributions coming from four different straight paths along the horizontal and vertical axis. These (two segments each) straight paths do not cancel for any value of the magnetic flux.

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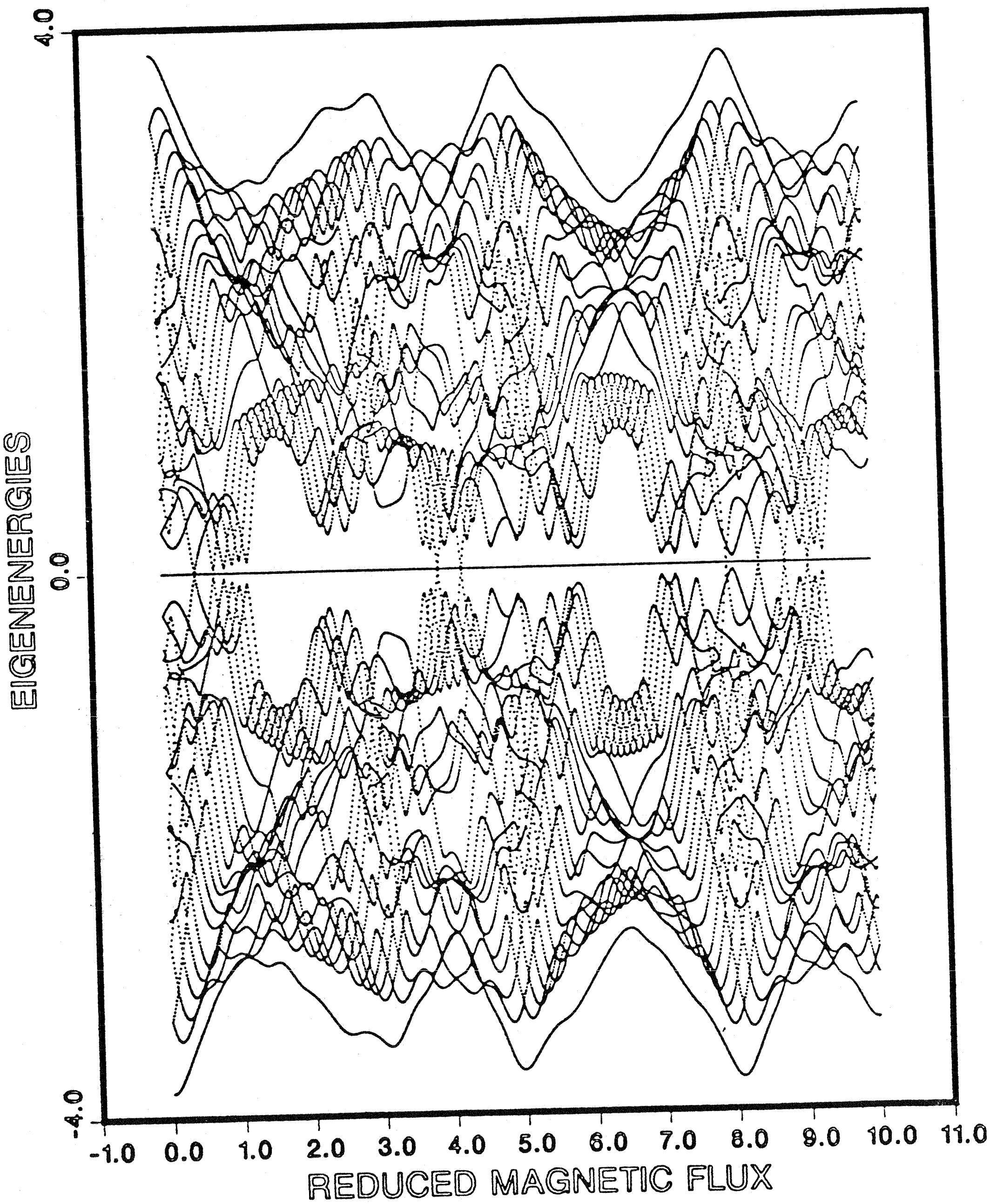
FIGURE CAPTIONS

Figure 1: Energy levels versus magnetic flux, $E_n(\phi)$, for a Penrose lattice with 46 sites.

Figure 2: Energy levels corresponding to the block-diagonal submatrix of the Hamiltonian corresponding to states with zero angular momentum.

Figure 3: Energy levels versus magnetic flux, $E_n(\phi)$, for a 5x5 square lattice with open boundary conditions.

Figure 4: Energy levels versus magnetic flux, $E_n(\phi)$, for a 8x8 square lattice with open boundary conditions.



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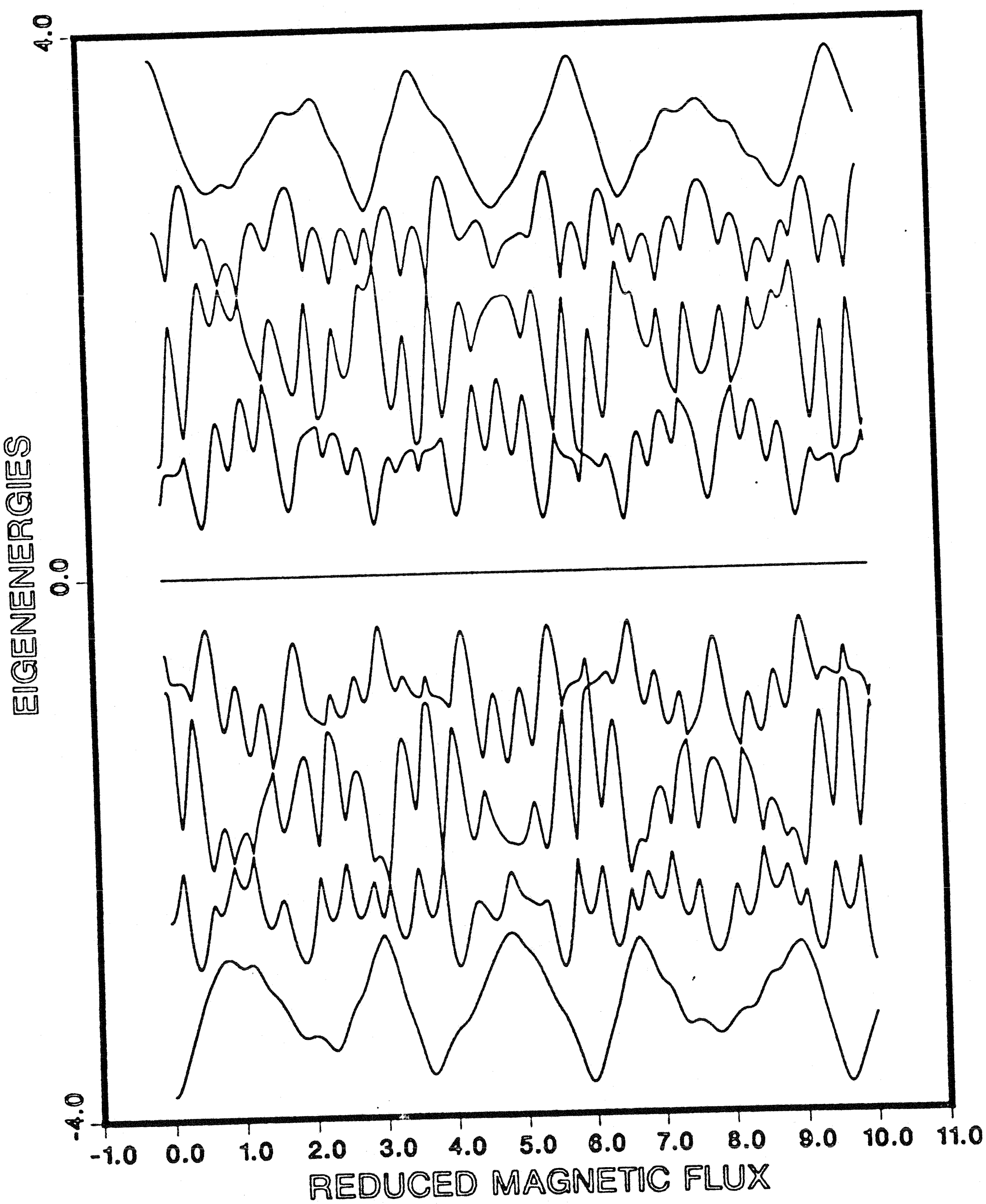
9.0
10.0
11.0
REDUCED MAGNETIC FLUX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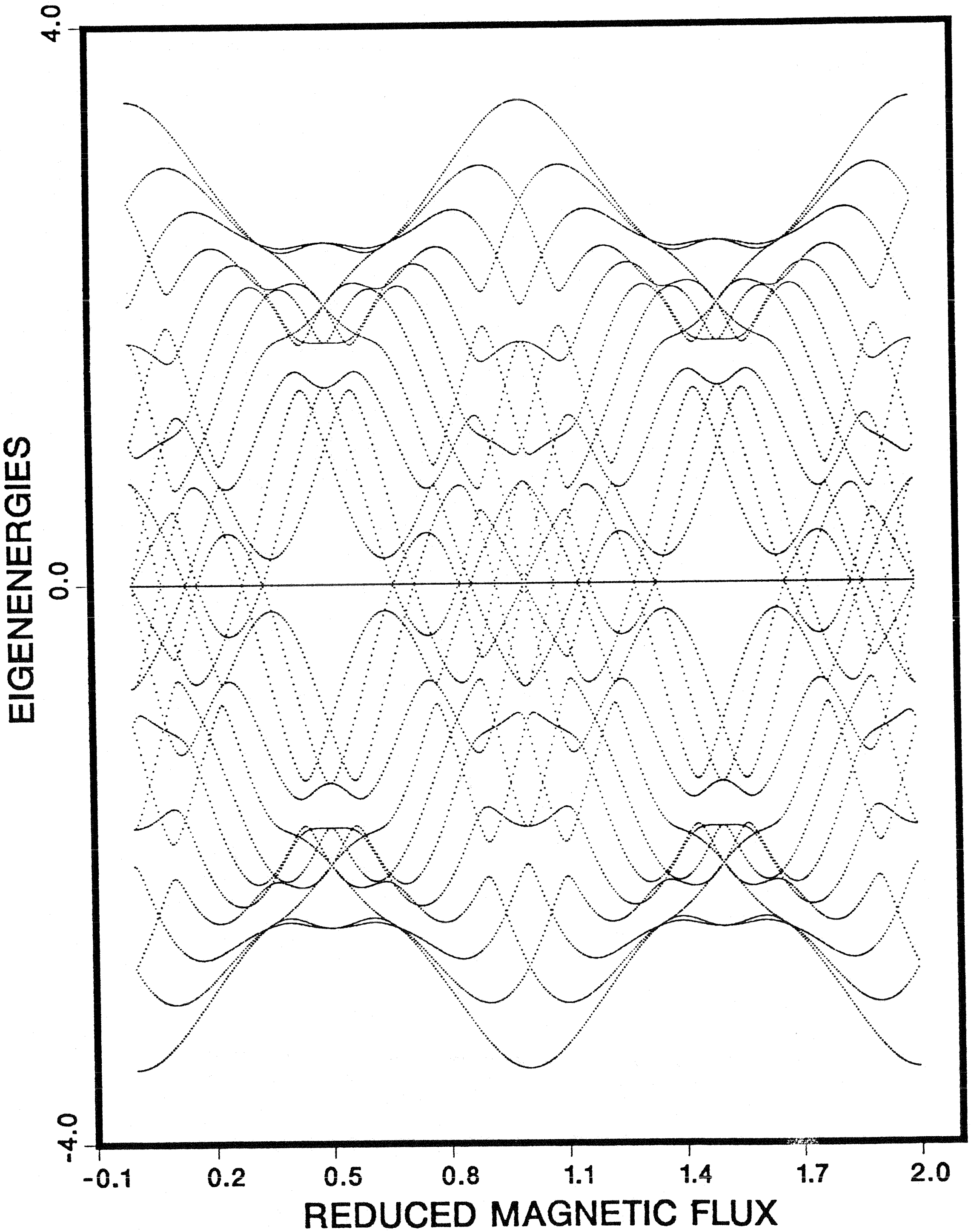
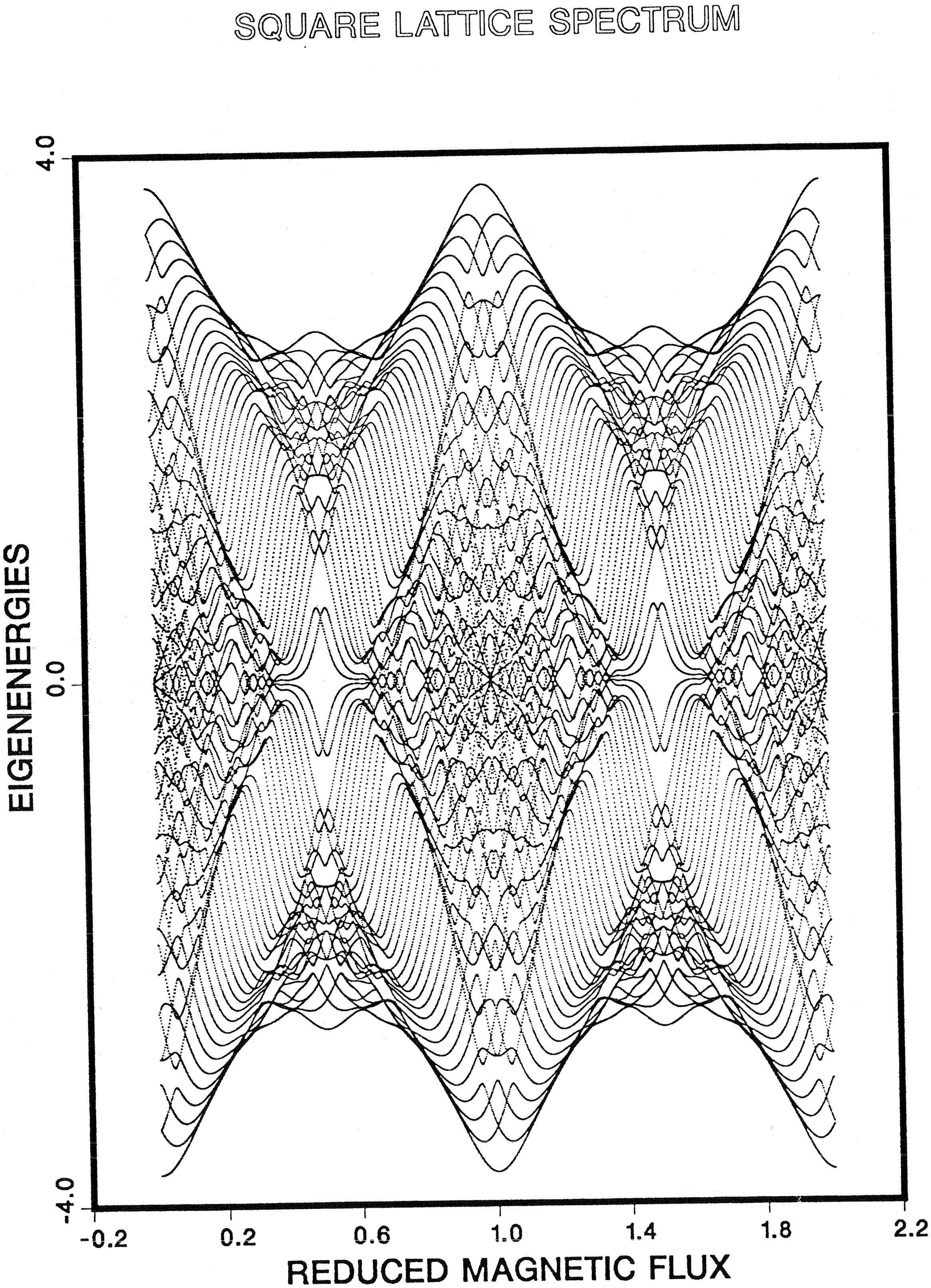
REDUCED MAGNETIC FLUX

SQUARE LATTICE SPECTRUM

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0.6
1.0
1.4
1.8
2.2
REDUCED MAGNETIC FLUX

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