

# Electrons in a crystal lattice: A simple computer model

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A simple computer program is presented, well within the capability of sophomore students, which solves the Schrödinger equation for a "lattice" of up to 12 potential wells, and which demonstrates many features important in a discussion of semiconductor physics—energy bands, impurity states, amorphous effects, negative effective mass. The ability to present material like this to students computationally may well have a profound effect on what is taught in future physics curriculums.

The introduction of computers into undergraduate physics courses is much discussed today. Of particular interest are those schemes that teach students to use computers to solve problems in the same way as do working physicists; and one of the most successful is that developed by M.U.P.P.E.T.<sup>1</sup> Its underlying philosophy is that, with the advent of powerful personal computers with good graphics capabilities and friendly programming languages, the only things stopping students solving a wide range of problems from first principles are the time-consuming and error-prone chores of program management. What M.U.P.P.E.T. contributes are a few well-designed utilities to smooth the organization of data input, the setting up and drawing of graphs, and the making of program direction choices.

The department to which the present authors belong recently designed a course in computational physics aimed at second year students, devoted to one-dimensional quantum mechanics. By bypassing the heavy emphasis on analytical mathematics, which is so often a barrier to student understanding of this subject, students were very quickly able to construct simple models, not just of square wells and simple harmonic oscillators, but for a much more wide-ranging collection of problems, including the excitation energy of a lithium atom, alpha decay, and hydrogen molecule bonding. What is being reported here is a computer program written to extend the techniques developed in that course into research-related areas. This was to construct a computational Kronig–Penney model for a crystal lattice which would exhibit some of the features of "real" solids.

## I. BACKGROUND

Attempts to solve the Schrödinger equation for a regular array of simple potential wells date back to the earliest days of quantum mechanics. In 1928, Bloch showed that the eigenfunctions of a strictly periodic, *infinite* lattice could be written as traveling plane waves, modulated by a function with the same periodicity as the lattice.<sup>2</sup> The fact that the "wave number" associated with these waves was not necessarily real, suggested there were *ranges* of energy for which no physical states existed (*energy gaps*) and ranges for which there were a quasicontinuum of states (*energy bands*).

The same conclusion was reached independently using the *tight binding approximation*, in which the discrete energy levels of an electron in a single well are "split" by the

presence of neighboring wells into quasicontinuous bands of states with well-defined gaps between.

In 1930 Kronig and Penney published their solution for a *finite* lattice, consisting of a large number of equally spaced square wells.<sup>3</sup> A key feature of their analysis was that the solutions should be Bloch waves, an assumption only valid for a strictly infinite lattice. They therefore invoked *periodic boundary conditions*, rather than requiring that the wave function should be zero (or nearly zero) at the lattice ends, as clearly it ought. Their result gave a relation between the Bloch wave number and the energy of the state, in the form of a transcendental equation involving the parameters of the lattice. Again they predicted energy bands and gaps; and furthermore, they provided a reasonably general way to calculate the boundaries between them.

In the 1950s, with the increasing importance of semiconductors, attention was directed toward *irregular* lattices. It was found that changes to the potential at a few discrete lattice sites (equivalent to a lightly doped crystal) often resulted in energy levels which lay in the middle of the previously unoccupied energy gaps. It was suspected that these new states were strongly localized about the irregularities that generated them (as opposed to Bloch waves which extend throughout the whole crystal)—clearly important in discussions of conductivity. This was, however, not proved until the seminal paper by Anderson in 1958.<sup>4</sup> Somewhat later, when amorphous crystals became important, lattices with a small degree of randomness were extensively studied. *Inter alia*, it was found that the energy level structure was maintained, but the edges of the bands were less sharply defined than previously.<sup>5</sup>

The preceding paragraphs summarize the way the existence of energy bands is still presented in most modern textbooks on solid state physics—the basic approach has not changed since the first few years of quantum mechanics. While these ideas are straightforward *physical* concepts, the mathematical complexity necessary for any kind of quantitative analytical modeling is prohibitive, so they are usually taught by "hand waving" arguments alone.

In this paper we present the results of a simple computer program that not only demonstrates *all* of these features in a simple, straightforward, quantitative way; but also enhances understanding of the solutions.

## II. COMPUTATIONAL APPROACH

This program calculates the bound state wave functions and energy eigenvalues for an electron in a lattice consist-

among other things

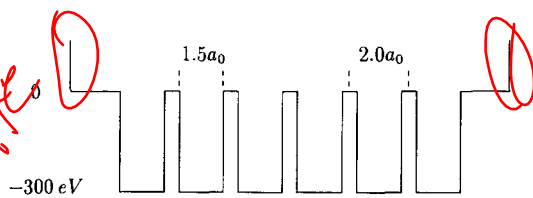


Fig. 1. The potential function for a lattice of identical square wells.

ing of a number of square potential wells arranged in one dimension. The time-independent Schrödinger equation for this problem can be expressed in dimensionless form as follows:

$$\frac{d^2}{dx^2} \psi(x) = [U(x) + E_B] \psi(x). \quad (1)$$

For convenience,  $x$  is measured in units of the Bohr radius ( $a_0$ ) and the energy  $E$  (always negative in this context) is replaced in this equation by the binding energy  $E_B$ , a dimensionless, positive number defined in terms of the real energy (in electron-volts) by

$$E_B \equiv - \left( \frac{2ma_0^2}{\hbar^2} \times 1 \text{ eV} \right) \frac{E}{\text{eV}} = -0.07357 \frac{E}{\text{eV}}. \quad (2)$$

The quantity  $U$  is related by the same factor to the potential, which has this shape shown in Fig. 1.

The program itself is simple, and is quoted in its most basic form (i.e., with no input and output features) in the Appendix.<sup>6</sup> It might easily be set as an exercise for students, provided the instructor is aware of the difficulties which can arise. The following guidelines were used in the construction of our particular version of this program.

1. Values for the width, separation, and depth of each well were fixed at  $1.50a_0$ ,  $0.50a_0$ , and 300 eV, respectively. These values have no particular significance in themselves; they are simply convenient for demonstrating the qualitative features of the lattice behavior. They represent a "realistic" interatomic spacing, and give two clear energy levels for a single well (or two bands for a series of wells).

2. The potential at the ends of the lattice was taken to be essentially infinite, making the boundary conditions to be imposed:

$$\psi(x) = 0 \text{ at } x = 0 \text{ and at } x = 2.00n, \quad (3)$$

when  $n$  is the number of "atoms" in the lattice.

However, if it were appropriate to model some real solid, the end potential could easily be set at some large but finite value, reflecting the work function of the material, with only trivial change to the calculation. The boundary condition then becomes

$$\frac{\psi'(x)}{\psi(x)} = \pm \sqrt{|U(\text{outside})| - E_B} \quad \text{at } x = 0 \text{ and at } x = 2.00n. \quad (4)$$

3. One of the most important concerns in any computer program designed to help students solve physical problems, is that the mathematical techniques used should be as simple and as straightforward as possible. Many powerful and elegant ways of solving a one-dimensional stationary Schrödinger equation exist, but there is little point in using methods that (i) only work for specific potential shapes

(e.g., piece-wise constant wells), or (ii) involve mathematical ideas likely to be beyond students in their second or third years (e.g., matrix inversion).

In the present instance we used a direct integration of the equivalent difference equation, as described in many elementary textbooks.<sup>7</sup> This involves starting with the initial condition,  $\psi(0) = 0$ , choosing a value for  $E_B$ , and integrating step-by-step to the point  $x = 2.00n$ . If the value of  $E_B$  is one of the eigenvalues, then  $\psi$  will vanish at this point. If it does not, then the "correct" value of  $E_B$  must be found by some search procedure.

Other methods of integration can give the eigenvalue spectrum directly; but again we believe it is more important that students understand what is happening. Therefore a simple binary search procedure was used (it is one of the standard M.U.P.P.E.T. tools) and the eigenvalues were found by "hunt and shoot."

4. Great accuracy is not important for its own sake. All that is really needed is an approximate value for where the bands lie and the distribution of levels within them. However, the shape of the wave functions is important. It is found, particularly for large lattices, that some pairs of levels lie very close together and, unless the integration algorithm is sufficiently accurate, "mixing" of these pairs occurs, leading to wave functions that do not have the expected symmetries. The "half-step" integration procedure referred to above (essentially equivalent to second-order Runge-Kutta) is just good enough. Even so, since many personal computers to which students have access are quite slow, it was important to keep the numbers of integration steps as small as possible. It was found that 190 steps is adequate, even for a lattice of 12 wells. But it must always be remembered that numerical results quoted below will be slightly different if any other number of integration steps or more accurate integrators are used.

5. It was also found convenient to design the program so that the number of wells in the lattice might be changed, up to a maximum of 12 (beyond which the simple integration procedure used starts to give trouble, and needs more integration steps). This enables the user, not only to observe the behavior described in this previous section, but also to investigate how this behavior "evolves" as the number of lattice elements changes.

6. Any program, such as is being described here, may be used either to allow students to explore the energy levels for themselves, and possibly to do homework exercises, or for the instructor to demonstrate to a class how the system behaves. If the latter, then it is necessary to run the program and locate all the eigenvalues beforehand.

### III. RESULTS

A lattice of ten equally spaced wells with the parameters specified in (1) and the integration procedure in (4) was chosen (although the same qualitative features may be observed with other numbers of elements).

#### A. The existence of bands

There are 25 energy levels, at these values of the binding energy (measured in electron-volts):

266.770927	266.389557	265.782635	264.994037	264.086212
263.139478	262.248352	261.513611	261.027893	260.857910
172.808222	171.112421	168.417664	164.910172	160.838928
156.519394	152.344757	148.788208	146.362183	145.496120
34.603909	30.128384	23.170090	14.273605	3.985062.

In these, only the first three figures are *physically* significant, because of the limitations of the integration algorithm used. Nevertheless, the full nine figures are *computational*-ly significant, in the sense that, without that degree of accuracy, the computed solutions may not converge to zero at large values of  $x$ .

These energy levels are clearly arranged in “bands” in the usual meaning of the term. See Fig. 2. (Note: the top-most band appears “incomplete” because several of its states lie above the line  $E = 0$ .)

It is instructive for students to repeat the same exercise for differing values of  $n$ . They should gain the insight—not explicitly proved, but strongly suggested—that, however large  $n$  is, that number of levels will arrange themselves within more or less the same energy range. Hence, by extrapolation, a “real” lattice with  $10^5$ – $10^8$  atoms (in one dimension) will exhibit a band structure which is qualitatively the same.

Note that the Kronig–Penney analysis of this problem (described in standard textbooks<sup>8</sup>) predicts that energies within any band must satisfy a transcendental equation (quoted here for comparison purposes only). It relates the effective Bloch wave number  $k$  to the parameters of the lattice—the atomic spacing  $a$ , the well width  $w$ , and the well depth  $V_0$ :

$$\cos(ka) = \cos(\lambda w) \cosh[\mu(a-w)] + \frac{\mu^2 - \lambda^2}{2\lambda\mu} \sin(\lambda w) \sinh[\mu(a-w)], \quad (5)$$

where

$$\lambda^2 \equiv 2m(|V_0| - |E|)/\hbar^2 \text{ and } \mu^2 \equiv 2m|E|/\hbar^2.$$

This equation has solutions only when the right-hand side is between  $\pm 1$ , and is usually solved numerically, as in Fig. 3. For the quoted well parameters the band boundaries should be 261.2–267.5 and 145.7–175.5 eV. Agreement between the two approaches is within 0.2%—well inside the limits of accuracy of the numerical integrator used.

## B. The Bloch-like character of the eigenfunctions

Solutions to the time-independent Schrödinger equation corresponding to bound states in one dimension can always be chosen to be real. Hence, the eigenfunctions in this prob-

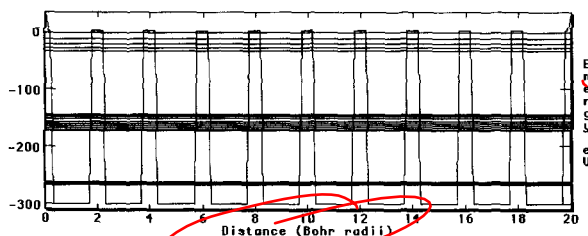


Fig. 2. The energy levels of a ten atom lattice.

lem cannot have the character of Bloch traveling waves, assumed by the Kronig–Penney approximation, which are necessarily complex. Figure 4 shows the shape of the lowest three eigenfunctions in each of the three bands.

Clearly the solutions are what might be called “Bloch standing waves,” i.e., the product of (i) a function with the periodicity of the lattice, and the number of modes appropriate to the band it is in; and (ii) a free electron standing wave—having the shape of the modes of vibration of a violin string.

It is a simple exercise, which can easily be left to students, to demonstrate that all these eigenfunctions are orthogonal to one another.

## C. Probability distributions within bands

Each eigenfunction is “nonlocalized” in the sense that it exists throughout the whole lattice. An interesting exercise is to square each of the wave functions belonging to one of the bands, forming the corresponding probability distribution; and then to sum these probabilities over the band. Figure 5 shows the result of this calculation.

It suggests that the likelihood that the electron should be found in the vicinity of any one atom (averaged over the band) is uniform across the lattice. This, in turn, implies that the bands are not just arbitrary collections of energy levels, but physical entities in their own right. It suggests a quasicompleteness property, and an exercise that can be left to the student is to show that linear combinations of eigenfunctions within a band can be found which “localize” the electron about any desired lattice site.

## D. Discrete impurities in the lattice

Conceptually, the next important step is to make the lattice *irregular*—most easily done by making one of the wells different from the others (simulating a “doped” crystal). In the program being described, this was done by leaving the central position and the depth of all wells unchanged but reducing the width of one of them by 25% to  $1.125a_0$ . (See Fig. 6.)

The energy eigenvalues were then found to be:

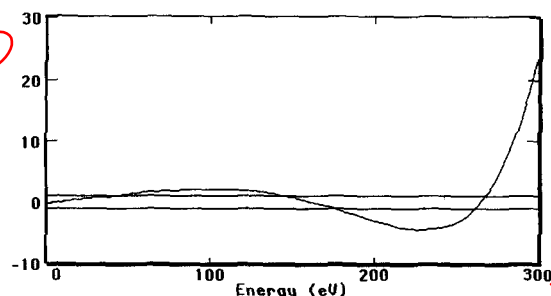


Fig. 3. The Kronig–Penney solution for a ten atom lattice. The plotted function is the right-hand side of Eq. (5), which is equal to  $\pm 1$  (the horizontal lines) at the edges of the bands.

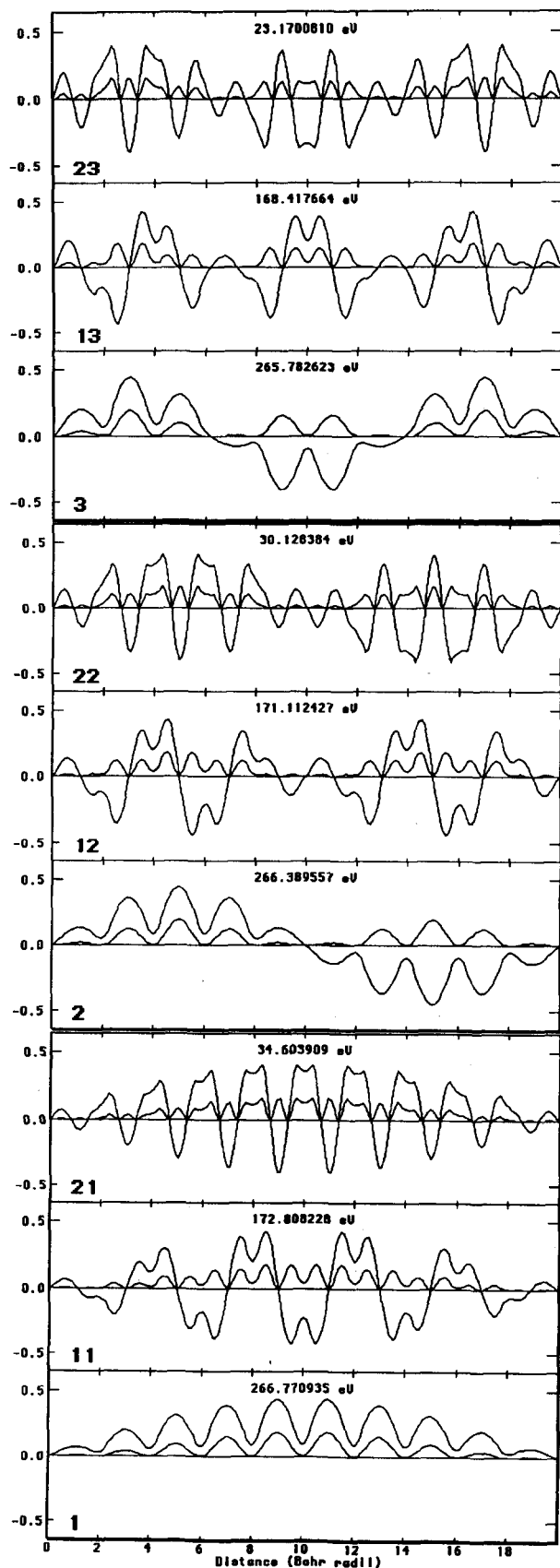


Fig. 4. The first three eigenfunctions of the three bands. Both the wave function and the probability function are plotted on each graph.

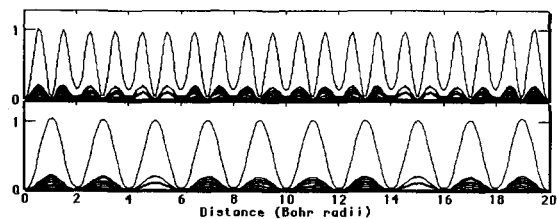


Fig. 5. The probability distributions within each band. The squares of the ten wave functions are plotted, superimposed on one another. Their sum, the free-standing curve, is also plotted on the same graph. The lower graph is for the lowest band, and the other for the second band.

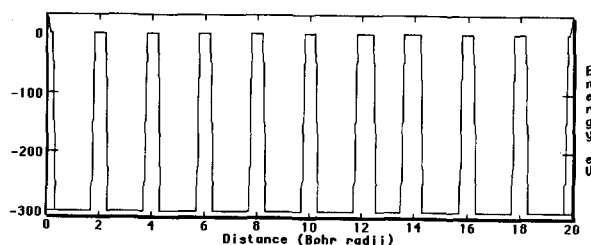


Fig. 6. A ten atom lattice "doped" with one well of different width.

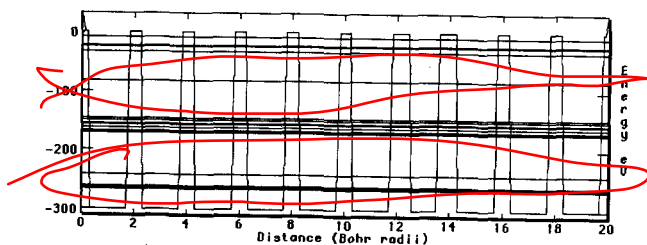


Fig. 7. Energy levels of a "doped" lattice, showing that a single level from each energy band has moved up into the gap above.

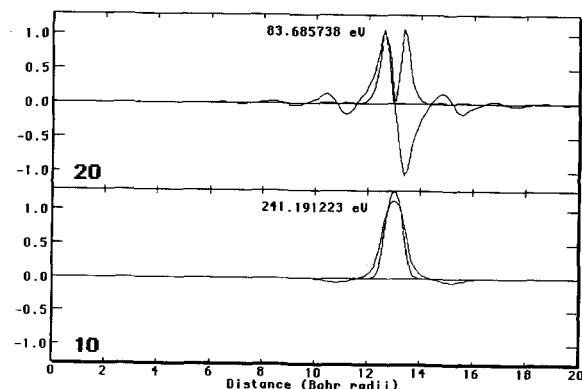


Fig. 8. The wave functions of intergap states. Both the wave functions and the probability functions are plotted on each graph.



266.591287	265.858154	265.713368	264.422563	263.366516
262.974466	261.705487	261.191101	260.957447	241.191219
172.031321	168.876227	168.176615	162.462027	157.770538
155.852938	149.785831	147.230713	146.011845	83.685734
32.699554	25.370833	22.720833	8.938789.	

It will be observed that, although individual levels have shifted slightly in energy, the bands themselves are qualitatively unchanged except that one of the levels has been shifted up into the energy gap (see Fig. 7).

These intergap states are, in a sense, decoupled from the rest of the lattice. The eigenvalues of a single well  $1.125a_0$  wide and 300 eV deep correspond to binding energies of 244 and 86 eV; hence these intergap states are basically where they would be if the rest of the lattice were not there. Clearly, the position of this state on the energy level diagram will be essentially independent of just where in the lattice the impurity is sited.

### E. Localization of wave functions in a doped lattice

Examination of the wave function shapes shows that the presence of the impurity is very disruptive to the Bloch-like structure of the wave functions. Some are spread throughout the lattice, others are "partitioned" by the crystal—restricted either to the left of the impurity site or to the right. Care is necessary when trying to interpret these shapes. The exact details of the energy levels in the band, and the shapes of the wave functions, are critically dependent on where the impurity was sited; and it would be expected that, for a two- or three-dimensional lattice, any "partitioning" would not be so extreme.

However, the shapes of the wave function corresponding to the state that has "migrated" into the gap (state numbers 10 and 20) are much the same wherever the impurity is sited, and are shown in Fig. 8.

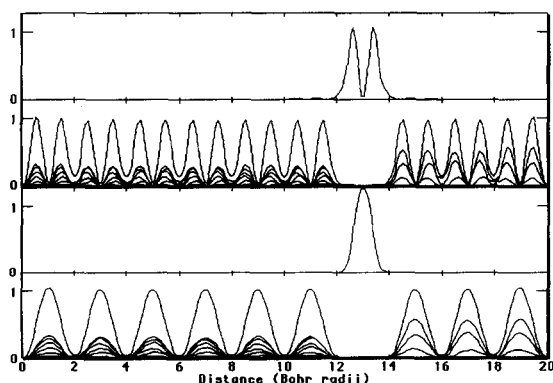


Fig. 9. Probability distributions of the "doped" bands. The squares of the lowest nine wave functions are plotted, superimposed on one another. Their sum, the free-standing curve, is also plotted on the same graph. The square of the wave function for the intergap state is plotted separately in the next graph up. The lower two graphs are for the lowest band, the upper two for the second band.

They are firmly localized around the impurity site. It is worth noting that this localization is an exceedingly sharp feature, in the following sense. If the width of the "impurity" well is set at 91.0% of that of the other wells (rather than the 75.0% used in the above calculation), the shape of the wave function is essentially the same as in Fig. 8. If however the width is made 91.5%, the wave function is virtually indistinguishable from the highest state of a regular lattice.

It is also instructive to repeat the sum-of-probabilities calculation of item (3). If the sum is done over the nine states remaining in the band, separately from the intergap state, the distribution shown in Fig. 9 results.

Clearly, although the electron is firmly localized near the impurity site when in one of the intergap states; when in one of the band states it can be thought of as spread throughout the rest of the crystal, and therefore to take part in normal conduction processes. Furthermore, the band states avoid the neighborhood of the impurity, and an electron in one of these states can be expected to "scatter" off these sites, thus contributing to resistive effects. These insights have relevance to any discussion of localization effects in semiconductors.<sup>9</sup>

### F. An amorphous lattice

This was modeled by setting up the lattice with ten equal wells (Fig. 10) separated by the following distances (in units of  $a_0$ ):

(0.25) 0.68 0.40 0.45 0.52 0.32  
0.60 0.48 0.55 0.50 (0.25).

(The mean of these number is 0.50 and the standard deviation 0.10. The outermost separations are equal to what they were in the regular lattice.)

For this potential, 25 energy levels were found:

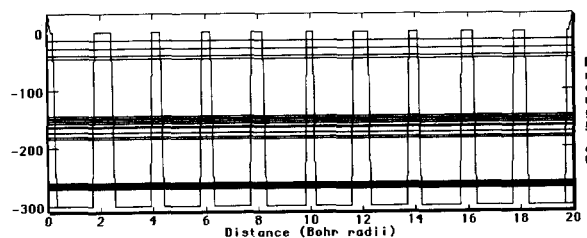


Fig. 10. The energy levels of a ten atom amorphous lattice.

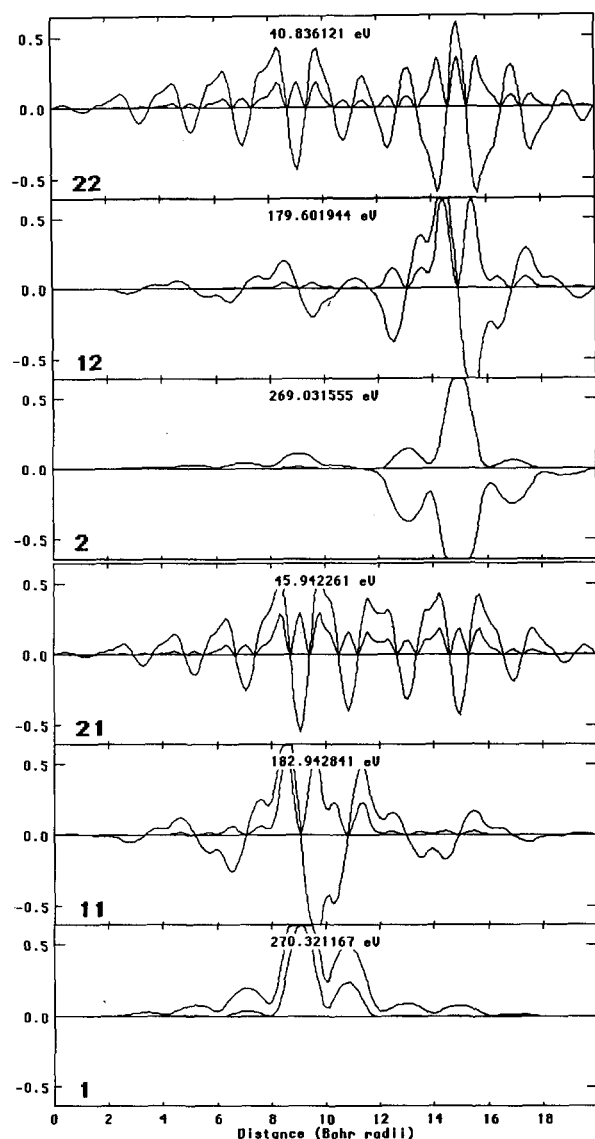


Fig. 11. The eigenfunctions of a ten atom amorphous lattice. Both the wave functions and the probability functions are plotted on each graph.

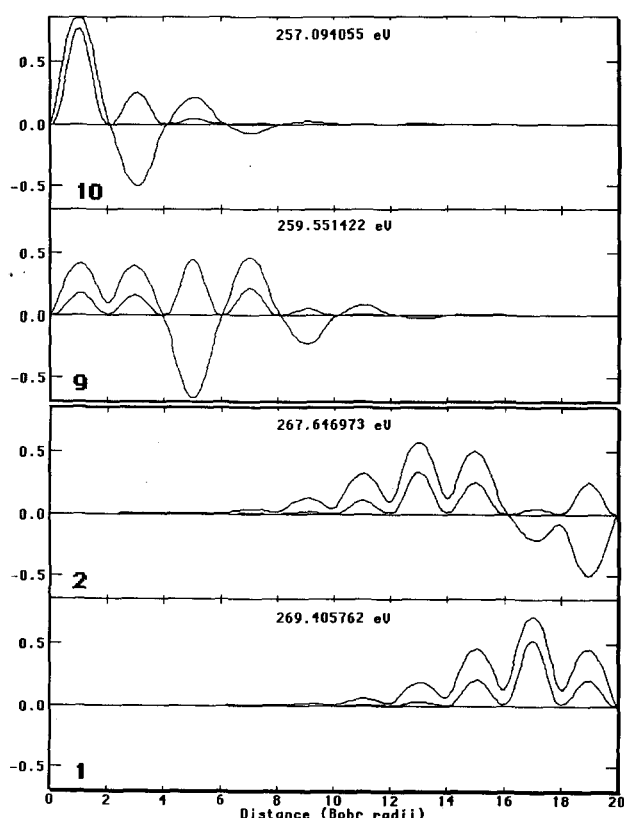


Fig. 12. The two lowest and two highest states in the lowest band for a lattice with an applied electric field. Both the wave functions and the probability functions are plotted on each graph.

270.321167	269.031555	267.391052	264.907623	264.355682
263.279114	262.388885	261.725159	261.297760	260.428589
182.942841	179.601944	173.334595	164.526703	161.764755
157.142014	153.173950	149.739075	147.528595	144.111069
45.942261	40.836121	28.191851	13.758299	6.596588.

Again, the exact details of this energy level structure is dependent on the particular arrangement of wells chosen, but the following qualitative features can be observed with most such arrangements: (i) The energy bands are widened, but still preserve their band character, and (ii) the wave functions are greatly disrupted from their Bloch-like structure.

In the lower bands many of the wave functions tend to be somewhat localized around the most extreme separations. However, a comparison of the corresponding levels in the three bands suggests that, in the upper bands, these levels tend to regain at least some of the unlocalized, Bloch-like nature of the regular lattice (see Fig. 11). Since the uppermost band might well correspond to a conduction band, this is relevant to the conductivity of the whole lattice.

A further insight is to be gained by observing that the states lying towards the edge of the bands tend to be more localized than those toward the center. Experimentally, localized states are indeed observed near the edges of bands in amorphous solids, and contribute, through tunneling, to what is known as *hopping conductivity*.<sup>10</sup>

## G. An applied electric field

This was modeled by adding to the potential energy of the ten atom regular lattice, a linearly decreasing term, varying from + 10 eV at  $x = 0$  to - 10 eV at  $x = 20a_0$  (equivalent to an electric field in the negative  $x$  direction). A field of this strength may be unphysically large but it demonstrates clearly the response of the electron.

The energy eigenvalues were then found to be:

269.405762	267.646973	266.337738	265.341971	264.442291
263.463104	262.390869	261.139709	259.551422	257.094055
174.199844	171.081970	168.194122	164.778473	160.799362
156.583160	152.628418	149.697678	147.020676	142.614639
35.278491	29.998083	23.073047	14.221058	3.960253

It will be observed that these values are only slightly changed from those of the regular lattice (see Sec. A). However, the shapes of the wave functions, particularly those near the edges of the bands, are strikingly different. The two lowest and two highest states in the lowest band (numbers 1 and 2, 9 and 10) are shown in Fig. 12.

Interpretation of these shapes suggests that an electron in a state at the bottom of a band will be "pulled" in the direction in which a free electron would move in the applied field. However when in a state near the top of the band, it will be pulled in the opposite direction. Thus students can be introduced to the concept of *negative effective mass* before meeting it in the more usual dispersion-curve treatment.<sup>11</sup>

It is worth noting also that, if the sum-of-probabilities calculation (see Sec. C) is carried out, the same result as in Fig. 5 is obtained. This demonstrates that in an *insulator*, a material in which the occupied bands are full and any electron has equal probability of being in any one state, an applied electric field will produce no change to the average internal charge distribution.

There are other variations on this theme that may be explored, for example: (i) *coulombic wells (truncated in some way so that they do not become infinite) should produce upper bands that overlap*, or (ii) *two different lattices can be joined to simulate a p-n junction*.

Such exercises might easily be left to students to explore for themselves. The important feature, from a pedagogical point of view, is that, not only is the basic mathematical technique well within the capabilities of undergraduate students in their early years; but as the problems get more elaborate, *no further mathematical expertise is needed*.

It is in that sense that modern methods of computational physics can be said to relieve the barrier to student understanding that our present heavy reliance on advanced analytical mathematics represents.

## IV. CONCLUSION

Earlier we expressed the opinion that in modern textbooks and courses in introductory solid-state physics, these ideas, although of enormous importance to the study of semiconductors and electronics, cannot be taught simply and convincingly because of the mathematical intractability of any attempt to treat them quantitatively; and that this is unfortunate. We believe we have demonstrated here that a change of emphasis toward computational physics, made possible by the development of schemes such as M.U.P.P.E.T., goes a long way to alleviate this misfortune.

We further believe that a discussion of energy bands,

energy gaps, lattice irregularities, and who knows how much more, can now take the place that its importance suggests it should have, not just in courses in solid-state physics, but in courses on elementary quantum mechanics as well.

## APPENDIX: THE PROGRAM

The following is a Pascal computer program which can reproduce many of the aforementioned results. It is given in its most basic form, with no input or output features (and therefore making no explicit use of the M.U.P.P.E.T. utilities).

Note that the M.U.P.P.E.T. team originally chose to work in Pascal because it is the most widely taught elementary computing language; and for students not already familiar with it, they provide tutorial handouts to teach a minimal level of competence. In our own department, we have found that students with no previous programming experience can be taught enough Pascal in a few hours to enable them to follow programs like this one:

```
PROGRAM CrystalLattice;

TYPE
  DataVector = ARRAY[1..401] OF real; {standard MUPPET type}

VAR
  NumWells      : integer;
  Depth, width, separation: real;
  HighestX, dX, E : real;
  X, V, Psi      : DataVector;

PROCEDURE SetParameters;
VAR
  i : integer;
BEGIN
  NumData := 190; {number of integration points}
  EnergyConversion := 0.074; { = (2 m a0^2 / hbar^2 * 1eV)}
  NumWells := 10; {Default value}
  Depth := 300; {electron-Volts}
  Width := 1.5; {Bohr radii}
  Separation := 0.5; {Bohr radii}
  E := 266.770927; {change for different levels}

  HighestX := NumWells*(Width+Separation);
  dX := HighestX / NumData;
  FOR i:=1 TO NumData+1 DO X[i] := (i-1)*dX;
END;

PROCEDURE MakeSingleWell(thisCenter, thisWidth, thisDepth: real);
VAR
  i : integer;
  startPt, endPt: real;
BEGIN
  startPt := thisCenter - thisWidth/2;
  endPt := thisCenter + thisWidth/2;
  FOR i:=1 TO NumData+1 DO
    BEGIN
      IF (X[i]>startPt) AND (X[i]<endPt) THEN
        V[i] := V[i] - thisDepth; {square well}
    END;
  END;
END;
```

```

PROCEDURE CalculatePotential;
VAR
  i: integer;
  center: real;
BEGIN
  FOR i:=1 TO numData+1 DO V[i] := 0;
  FOR i:=1 TO numWells DO
    BEGIN
      center := (i-0.5)*(width+separation);
      MakeSingleWell(center,width,depth);
    END;
  V[1] := 1000; { "infinite" edges }
  V[numData+1] := V[1];
END;

PROCEDURE IntegrateWaveEquation;
VAR
  i: integer;
BEGIN
  Psi[1] := 0; { Initial conditions }
  Psi[2] := dX;
  FOR i:=3 TO NumData+1 DO
    Psi[i] := 2*Psi[i-1] - Psi[i-2] +
      (E+V[i-1])*EnergyConversion*Psi[i-1]*dX*dX;
  END;
}----- MAIN PROGRAM -----{

BEGIN
  SetParameters;
  CalculatePotential;
  IntegrateWaveEquation;
END.

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<sup>1</sup>J. M. Wilson and E. F. Redish, "Using Computers in Teaching Physics," *Phys. Today* **42**(1), 34-41 (1989).

<sup>2</sup>F. Bloch, "Über die Quantenmechanik der Electronen in Kristallgittern," *Z. Phys.* **52**, 555-600 (1928).

<sup>3</sup>R. L. Kronig and W. G. Penney, "Quantum Mechanics of Electrons in Crystal Lattices," *Proc. R. Soc. London Ser. A* **130**, 499-513 (1931).

<sup>4</sup>P. W. Anderson, "Absence of Diffusion in Certain Random Lattices," *Phys. Rev.* **109**, 1492-1505 (1958).

<sup>5</sup>N. F. Mott, "Electrons in Disordered Structures," *Adv. Phys.* **16**, 49-144 (1967).

<sup>6</sup>A more extensive program, illustrating all the features described, is in preparation for the NSF funded Consortium for Upper-level Physics Software, directed by Robert Ehrlich *et al.*, George Mason University, Fairfax, VA.

<sup>7</sup>See for example: A. P. French and E. F. Taylor, *Introduction to Quantum Mechanics* (van Nostrand-Reinhold, United Kingdom, 1978), pp. 174-184.

<sup>8</sup>See for example: H. F. Hameka, *Quantum Mechanics* (Wiley, New York, 1981), pp. 134-138.

<sup>9</sup>See for example: N. F. Mott, *Conduction in Non-crystalline Materials* (Clarendon, Oxford, 1987), pp. 20-29.

<sup>10</sup>A. Miller and S. Abrahams, "Impurity Conduction at Low Concentrations," *Phys. Rev.* **120**, 745-755 (1960).

<sup>11</sup>See for example: M. A. Omar, *Elementary Solid State Physics* (Addison-Wesley, Reading, MA 1975), pp. 189-196.

## THE VALUE OF IMPRECISE DEFINITIONS

We recall in this connection Clerk Maxwell's humorous commentary on Herbert Spencer's appearance before Section A of the British Association at the memorable meeting in Belfast in 1874. Among other references Maxwell says:

"Mr. Spencer in the course of his remarks regretted that so many members of the Section were in the habit of employing the word Force in a sense too limited and definite to be of any use in a complete theory of evolution. He had himself always been careful to preserve that largeness of meaning which was too often lost sight of in elementary works. This was best done by using the word sometimes in one sense and sometimes in another and in this way he trusted that he had made the word occupy a sufficiently large field of thought."

Robert Bruce Lindsay and Henry Margenau, *The Foundations of Physics* (Wiley, New York, 1936), p. 96.