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The nature of the gaps in the electronic energy spectrum of liquid-like one-dimensional systems†

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Abstract. It is shown that the gaps which appear in the energy spectrum of a liquid-like disordered Kronig–Penney model can be explained as the energy intervals in which the phase distributions for the forward and the backward directions are almost or completely non-overlapping. Inasmuch as such a non-overlapping is intimately related to the strong localization of eigenfunctions, this explains at the same time why the wave functions near these gaps are particularly strongly localized.

1. Introduction

There have been several numerical investigations on the energy spectrum of the Kronig–Penney model with a liquid-type disorder (Makinson and Roberts 1960, Roberts 1963, Borland and Bird 1964). It has been found that when the disorder is sufficiently slight, there appear several energy gaps which are *much wider* than predicted by the phase theory (Hori 1968). The nature of these gaps has not yet been clarified, however. It has been found also that the wave functions are very strongly localized near these gaps. Some discussions have been given on the phenomenon of localization upon the basis of the variation of the phase along the system or the phase distribution thereon (Roberts and Makinson 1962, Borland 1963, Hori 1968), but no attempt seems to have been made to explain the appearance of the wide gaps upon the same basis. The purpose of the present paper is to explain the appearance of the gaps and the strong localization of the wave functions simultaneously on the basis of the behaviour of the phase on the system.

In a previous paper (Hori and Minami 1967, to be referred to as HM) we presented a phase-theoretical formalism by which the phenomenon of localization of the eigenmodes in the disordered one-dimensional systems can be conveniently discussed in terms of the phase distributions thereon. It was shown that the localization occurs as a result of the fact that in the disordered chains the phase distributions have a strong tendency to be concentrated in the L regions of the transfer matrices describing the system. It was also shown that, for each transfer matrix, the L regions for the forward and backward transfers must be mirror images of each other with respect to a point of symmetry. From these it can be concluded, as will be shown in § 3 of this paper, that if their concentration in the L regions is very strong the distributions for the forward and backward transfers tend to become almost or completely non-overlapping, provided a certain condition concerning the geometrical arrangement of the L regions is satisfied.

An energy interval throughout which the forward and backward distributions are almost or completely non-overlapping must be a quasi- or true spectral gap, since then the phase matching is very difficult to obtain or cannot occur between the solutions constructed from the opposite ends of the system. It will be shown in § 4 that the gaps in the spectrum of the liquid-like Kronig–Penney model which were found numerically just correspond to the energy intervals in which the complete or almost non-overlapping of the phase distributions occurs. Inasmuch as a strong concentration in the L regions implies a strong localization of the wave functions, this explains in a very natural way why the eigenfunctions near the gaps are particularly strongly localized.

In § 2 the theory presented in HM is reproduced somewhat in detail, in order to compensate for the too concise description in HM necessitated by severe restriction of

† This work was done during the author's stay at the Mathematics Division of the National Physical Laboratory, Teddington, Middlesex.

space. In § 3 a discussion is given which leads to the conclusion that, when the concentration in the L regions is very strong and the condition on the geometrical arrangement of the L regions is fulfilled, the phase distributions are very likely to become almost or completely non-overlapping, and consequently the quasi- or true gaps are very likely to appear. In § 4 the results of the numerical computation of the phase distributions are reported, which demonstrate that the gaps in the spectrum of the liquid-like Kronig-Penney model are none other than the intervals in which the almost or complete non-overlapping of the distributions occurs. Conclusions are given in § 5. A brief discussion on the ergodic nature of the phase distribution functions is given in the appendix.

2. Theory

Consider any one-dimensional chain which can be described by the transfer-matrix formalism.† Let the transfer matrix at a site of the chain be

$$\mathbf{Q} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \quad (2.1)$$

where the elements contain an energy parameter λ . The matrix \mathbf{Q} may be assumed to be unimodular.

Let us denote the state vector and the state ratio at this site by $X \equiv (x, y)^T$ and $z \equiv x/y$, respectively, and the corresponding quantities at the next site by $X' \equiv (x', y')^T$ and $z' \equiv x'/y'$. Then these quantities are related by

$$X' = \mathbf{Q}X \quad (2.2)$$

and

$$z' = \frac{Az + B}{B^*z + A^*}. \quad (2.3)$$

Differentiating equation (2.3) with respect to z , we have

$$\frac{dz'}{dz} = \frac{1}{(B^*z + A^*)^2}. \quad (2.4)$$

The phase δ of a state ratio z is defined by

$$z = e^{i\delta}. \quad (2.5)$$

This is consistent with the transformation (2.3) in view of the fact that \mathbf{Q} is unimodular. Equation (2.4) then gives

$$\frac{d\delta}{d\delta'} = |Az + B|^2 = \frac{|B|^2(|x|^2 + |y|^2) + |x|^2 + 2\Re(BA^*x^*y)}{|y|^2}. \quad (2.6)$$

On the other hand, we obtain, from equation (2.2),

$$|x'|^2 + |y'|^2 = (|x|^2 + |y|^2)(2|B|^2 + 1) + 4\Re(BA^*x^*y) \quad (2.7)$$

which gives, together with (2.5), a simple relation

$$\frac{d\delta}{d\delta'} = \frac{|x'|^2 + |y'|^2}{|x|^2 + |y|^2} = \frac{\|X'\|^2}{\|X\|^2}. \quad (2.8)$$

This means that the length of the state vector, or the absolute value of the amplitude of the solution (which satisfies the boundary condition at the end of the system from which one starts the transfer), increases or decreases at the site under consideration according as $d\delta/d\delta' > 1$ or < 1 .

† For details on the formalism of the transfer matrix (phase theory), see Hori (1968).

It is an easy matter to investigate the extension of the lengthening and shortening regions of z in which the state vector is lengthened and shortened, respectively. The function $Az+B$ gives a circle-to-circle mapping on the complex plane. Since z is on the unit circle, $Az+B$ lies on the circle with the centre at B and the radius $|A|$. As $|A|^2 = |B|^2 + 1$, this circle passes through the ends C and D of the diameter of the unit circle which is orthogonal to the vector B (figure 1). The quantity $|Az+B|^2$, and hence $d\delta/d\delta'$, is smaller

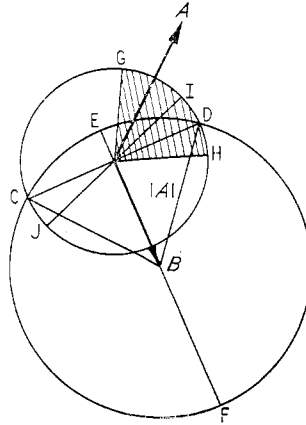


Figure 1. The construction of the L and S regions.

than unity on the arc CED of the circle $Az+B$, and larger than unity on the arc CFD . Therefore it is clear that when the state ratio z is on the arc GIH of the unit circle, which is mapped on the arc CED by the transformation $Az+B$, the length of the state vector decreases, and when z is on the arc GJH it increases. Thus the arcs GIH and GJH give the shortening and lengthening regions (in short, S and L regions), respectively. It is to be noted that the L region is always wider than the S region. The derivative $d\delta/d\delta'$ takes the maximum value $|A| + |B|$ at J and the minimum value $|A| - |B|$ at I , the product of these extremal values being equal to unity.

If \mathcal{Q} is hyperbolic, i.e. if $|\mathcal{R}A| > 1$, its two eigenvalues θ_{\pm} are real and the limit points z_{\pm} of the transformation (2.3) lie on the unit circle:

$$z_{\pm} = \frac{B}{\theta_{\pm} - A}. \tag{2.9}$$

At these points we have

$$\frac{d\delta}{d\delta'} = \theta_{\pm}^2. \tag{2.10}$$

Since $|\theta_+| < 1$ and $|\theta_-| > 1$, the source point z_+ and the sink point z_- must lie in the S and L region, respectively. When \mathcal{Q} is elliptic, z_{\pm} do not lie on the unit circle.

If the direction of the transfer is reversed (backward transfer), the transfer matrix must be replaced by

$$\mathcal{Q}^{-1} = \begin{pmatrix} A^* & -B \\ -B^* & A \end{pmatrix}. \tag{2.11}$$

Other formulae remain completely the same as above, except that A and B must be replaced by A^* and $-B$, respectively. It is easy to show that the motion of the state ratio on the unit circle now becomes a mirror image of that for the forward transfer with respect to the diameter orthogonal to B (CD in figure 1). Since it is clear that the source and sink points now interchange their role, these points must be just mirror images of each other with respect to CD , as can easily be verified. Also the positions of the S and L regions for the backward transfer must be given by the mirror images of those for the forward transfer. Now the sink z_- lies in the S region, while z_+ lies in the L region.

3. General considerations

It is known that for any regular lattice, that is the lattice which can be described by only one transfer matrix \mathbf{Q} , the eigenmodes cannot be localized. This means that the sample degree of localization L , or the average value of $\log(d\delta/d\delta')$, must vanish, i.e. the distribution function $f(\delta)$ of the phase must be such that

$$L = \left\{ \log \left(\frac{d\delta}{d\delta'} \right) \right\}_{\text{av}} \equiv \int f(\delta) \log \left(\frac{d\delta}{d\delta'} \right) d\delta = 0. \quad (3.1)$$

For this to be the case, the distribution must be more concentrated in the S region than in the L region, since the S region is always narrower than the L region, as was shown above, and the values of $d\delta/d\delta'$ in these regions are roughly inversely proportional to each other (see (2.10)). The state ratio must 'walk' on the unit circle by adjusting its speed in such a manner that its 'footprints' are denser in the S region than in the L region.

In the case of a disordered system, however, such a self-adjustment cannot be expected. For such a system cannot be described by only one transfer matrix \mathbf{Q} , but must necessarily be described by a set of matrices $\mathbf{Q}^{(i)}$ ($i = 1, 2, \dots, S$; $S > 1$). The state ratio z is successively transformed by a random sequence of $\mathbf{Q}^{(i)}$'s, and its motion on the unit circle becomes a random walk. Unfortunately, it is, in general, difficult to investigate analytically how the distribution $f(\delta)$ is modified by such a randomness, and we are obliged to compute it numerically. However, a qualitative argument can be given. As a simple example, let us consider an isotopically disordered diatomic chain. Let the masses of isotopes be $m^{(0)}$ and $m^{(1)}$ ($m^{(0)} < m^{(1)}$), and let us take $m^{(0)}$ as the standard mass, i.e. we define the wave-number parameter β by

$$\omega^2 = \frac{4K}{m^{(0)}} \sin^2 \beta \quad (3.2)$$

where K is the force constant. Then the transfer matrices at the light and heavy atoms become

$$\mathbf{Q}^{(0)} = \begin{pmatrix} e^{2i\beta} & 0 \\ 0 & e^{-2i\beta} \end{pmatrix} \quad (3.3)$$

and

$$\mathbf{Q}^{(1)} = \begin{pmatrix} (1 + iQ \tan \beta) e^{2i\beta} & iQ \tan \beta e^{-2i\beta} \\ -iQ \tan \beta e^{2i\beta} & (1 - iQ \tan \beta) e^{-2i\beta} \end{pmatrix} \quad (3.4)$$

respectively, where $Q \equiv m^{(0)}/m^{(1)} - 1$.

For the matrix $\mathbf{Q}^{(0)}$ we have

$$\frac{d\delta}{d\delta'} = |e^{2i\beta} z|^2 = 1 \quad (3.5)$$

so that there is neither an L nor an S region. This can be considered as a reflection of the fact that in $\mathbf{Q}^{(0)}$ the elements B and B^* vanish, so that there is no definite mirror image axis.

First, let us consider the β values at which $\mathbf{Q}^{(0)}$ and $\mathbf{Q}^{(1)}$ are both elliptic. When the chain is composed of heavy atoms only, the state ratio walks more slowly in the S region than in the L region (of the matrix $\mathbf{Q}^{(1)}$), so that its footprints are denser in the former. If the light atoms are introduced, however, it walks at these atoms always by the constant step 4β . Hence the tendency to walk slowly in the S region and rapidly in the L region must more or less be weakened, and the overall distribution of the footprints must become more or less uniform. In other words, the introduction of the randomness brings about the tendency for the phase distribution to be concentrated in the L region. As a result, the average value of $\log(d\delta/d\delta')$ becomes positive, so that the state vector is lengthened on the average.

When $\mathbf{Q}^{(1)}$ is hyperbolic, the state ratio is strongly attracted by the sink point α_- at the heavy atoms. Since α_- lies in the L region, as was noted above, the tendency for the distribution to be concentrated in the L region must be enhanced greatly, and the state vector must be lengthened still more rapidly.

If the direction of the transfer is reversed, the situation does not change, and it is again expected that the phase distribution tends to be concentrated in the L region (for the backward transfer) and the state vector is lengthened on the average. This can be shown to imply that the eigenfunctions must be localized, and the degree of localization is measured by \bar{L} . For this reason \bar{L} is called the degree of localization.

These observations have been confirmed in HM by numerical calculation of the phase distribution. When $\mathbf{Q}^{(0)}$ and $\mathbf{Q}^{(1)}$ were both elliptic $f(\delta)$ was more concentrated in the S region, but \bar{L} was positive. This shows that the above-mentioned tendency for $f(\delta)$ to be concentrated in the L region induced by the randomness is actually working (figure 3a of HM). When $\mathbf{Q}^{(1)}$ was hyperbolic, $f(\delta)$ was remarkably concentrated in the L region, being peaked at the sink phase δ_- of $\mathbf{Q}^{(1)}$ (figures 3b and 3c of HM), just as expected above.

In the more general case, in which the number of the transfer matrices is larger than two, the situation generally becomes much more complicated. However, if the L regions of all the $\mathbf{Q}^{(i)}$'s largely overlap one another, we may well expect the situation to be similar to the above. Let us denote the L and the S region of the i th transfer matrix by $L^{(i)}$ and $S^{(i)}$ respectively. In such a case both the intersections $\Pi L^{(i)}$ and $\Pi S^{(i)}$ are non-vanishing, and both the sums $\Sigma L^{(i)}$ and $\Sigma S^{(i)}$ have the extensions less than 2π (figure 2), and we can

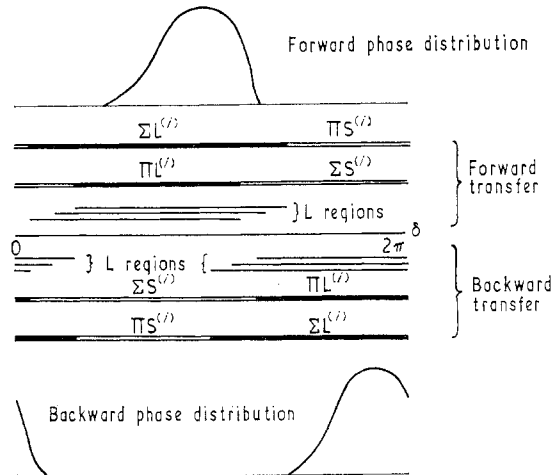


Figure 2. Concentration of the phase distributions in the neighbourhoods of $\Pi L^{(i)}$.

expect that owing to the randomness the phase distribution tends to be concentrated in $\Sigma L^{(i)}$. This tendency will be particularly remarkable when some of the matrices $\mathbf{Q}^{(i)}$ are hyperbolic, and will become stronger as the number of the hyperbolic matrices increases. In fact, if all the matrices are hyperbolic, it can be shown that the distribution must be completely concentrated in the interval spanned by the sink phases $\delta^{(i)}$ of $\mathbf{Q}^{(i)}$ (sink-phase interval), as is shown in figure 3 (Hori 1968).

Also for the backward transfer the situation must be the same, except that the geometrical arrangement of the regions $\Pi L^{(i)}$, $\Pi S^{(i)}$, $\Sigma L^{(i)}$ and $\Sigma S^{(i)}$ becomes different. (Although for each individual matrix the L regions for the forward and backward transfers are the mirror images of each other, the regions $\Pi L^{(i)}$ or $\Sigma L^{(i)}$ for the two directions of transfer are not necessarily each other's mirror images.) If all the matrices are hyperbolic, the phase distribution must be completely concentrated in the interval spanned by the source phases $\delta_-^{(i)}$ of the $\mathbf{Q}^{(i)}$ (source-phase interval), as is shown in figure 3.

If all the matrices are hyperbolic and the sink- and source-phase intervals are disjoint, the forward and backward phase distributions are therefore completely non-overlapping. Since when the two distributions are non-overlapping the phase matching cannot occur between the solutions constructed from the opposite ends of the system, the energy interval

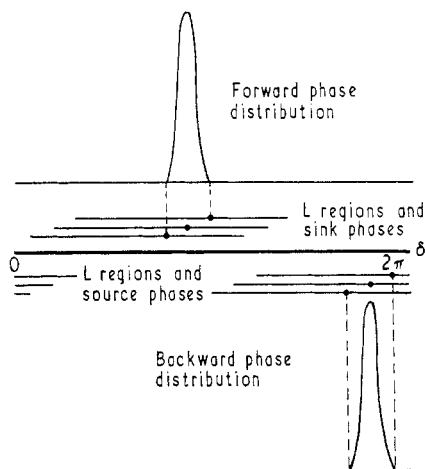


Figure 3. Concentration of the phase distributions in the case where all the transfer matrices are hyperbolic.

in which the distributions are non-overlapping must give a spectral gap. Thus, if all the $\mathbf{Q}^{(i)}$ are hyperbolic and the sink- and source-phase intervals are disjoint, the energy under consideration must lie in a spectral gap. This is just the theorem of Hori and Matsuda which plays the basic role in the phase theory (Hori and Matsuda 1964, Hori 1968). The energy gaps which have been predicted by the phase theory are no other than the energy intervals which fulfil the conditions of this theorem.

Inasmuch as there is a strong tendency for $f(\delta)$ to be concentrated in $\Sigma L^{(i)}$, in particular when the number of hyperbolic matrices is large, we obtain the following expectation. Even if not all of the $\mathbf{Q}^{(i)}$ are hyperbolic, the phase distribution is completely or almost completely concentrated in a relatively narrow interval contained in $\Sigma L^{(i)}$ (figure 2), provided the energy under consideration lies sufficiently near a gap predicted by the Hori-Matsuda theorem, or, if not, at that energy the number of the hyperbolic matrices is sufficiently large. If, in addition, the intervals in which the forward and backward phase distributions are concentrated are disjoint, or nearly disjoint, the distributions become completely or almost non-overlapping. Then the energy under consideration must lie in a gap or quasi-gap, according as the non-overlapping is complete or almost complete.

Thus it has been shown that, if the condition of disjointness of the L regions stated just above is fulfilled, we can expect that there appear true or quasi-gaps which are wider than those which have hitherto been predicted by the phase theory, or which lie at the energies where the phase theory has failed to predict any gaps. Since when $f(\delta)$ is strongly concentrated in $\Sigma L^{(i)}$ the localization must be accordingly strong, it is naturally to be expected that the wave functions near these gaps are strongly localized.

In the next section it will be shown that in the case of the liquid-like Kronig-Penney model the two distributions are in fact almost completely concentrated in certain narrow intervals, which are completely or nearly disjoint, at the energies lying in the gaps found numerically, but outside the gaps predicted phase-theoretically.

4. Numerical calculations and discussions

In order to demonstrate that the suppositions presented in the preceding section are correct, we calculated the forward and backward phase distributions at several energies for the same model considered by Borland and Bird (1964), that is, a liquid-like disordered

Kronig–Penney model described by the Schrödinger equation

$$-\frac{d^2\psi}{dx^2} - V \sum_{i=1}^{\infty} \delta(x-x_i)\psi = E\psi \quad (4.1)$$

where V is the strength of the delta potential, and the separations $l_i = x_{i+1} - x_i$ between the neighbouring potentials are distributed for all values of i according to a probability density function $P(l)$ of the form

$$P(l) = \frac{1}{b}, \quad |l - \langle l \rangle| \leq \frac{1}{2}b \quad (4.2)$$

$$P(l) = 0, \quad |l - \langle l \rangle| > \frac{1}{2}b.$$

Borland and Bird calculated the spectral density $\rho(\nu)$ of this system for several values of the parameters

$$\lambda = \frac{1}{2}V\langle l \rangle$$

$$\nu = 2\sqrt{E/V} \quad (4.3)$$

$$\sigma = b/2\sqrt{5}\langle l \rangle.$$

Some of their results are shown in figure 4. The horizontal arrows indicate the energy gaps of the regular chain with the spacing $\langle l \rangle$. The thick bar indicates the gap which has been predicted by the phase theory. It is seen that the calculated gap is slightly wider than the predicted one. The other two gaps appear at the energies where no gaps have been predicted by the phase theory.

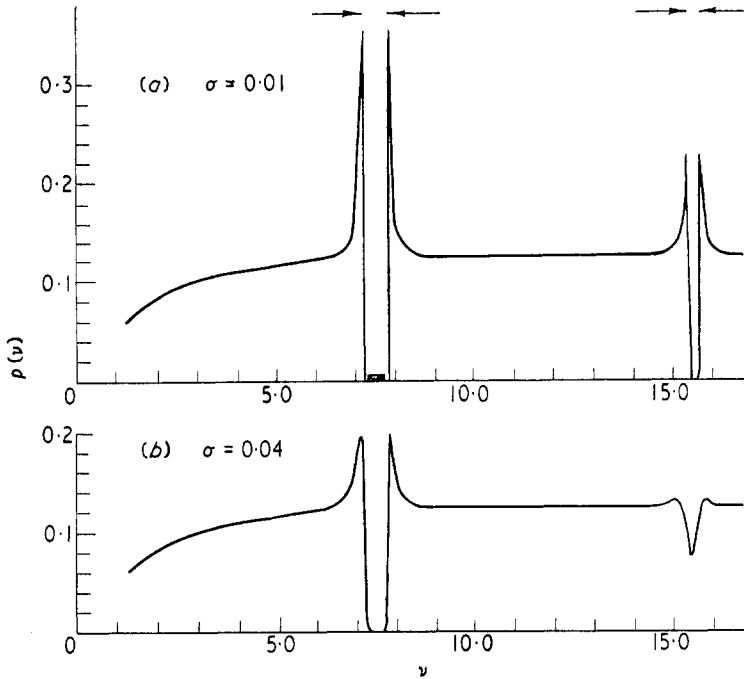


Figure 4. The densities of energy spectrum of the liquid-like Kronig–Penney model calculated by Borland and Bird. (After Borland and Bird 1964.)

The elements of the transfer matrix describing the i th cell of the system are given by (Hori 1968)

$$A_i = \left(1 + \frac{iV}{2k}\right) \exp(ikl_i) \quad (4.4)$$

$$B_i = \frac{iV}{2k} \exp(-ikl_i).$$

The relation between the phases at the i th and $(i+1)$ th cells are therefore given by

$$\exp(i\delta_{i+1}) = \frac{A_i \exp(i\delta_i) + B_i}{B_i \exp(i\delta_i) + A_i} \quad (4.5)$$

according to (2.3). We constructed the sample chains with 10 000 potentials, and calculated the forward and backward phase distribution functions $f(\delta)$ by computing the successive phases by (4.5) and its inverse transformation, respectively. At the same time the degree of localization

$$\begin{aligned} \bar{L} &\equiv \frac{1}{10^4} \sum_{i=1}^{10000} \log |A_i \exp(i\delta_i) + B_i|^2 \\ \text{or} \\ &= \frac{1}{10^4} \sum_{i=1}^{10000} \log |A_i^* \exp(i\delta_i) - B_i|^2 \end{aligned} \quad (4.6)$$

was computed.

The function $f(\delta)$ was calculated as a histogram f_k , $k = 1, 2, \dots, 40$, with the interval $\Delta\delta = 2\pi/40$. For this value of $\Delta\delta$ the sample fluctuation was found to be reasonably small, as may be seen in figure 5, where the forward distributions calculated on two

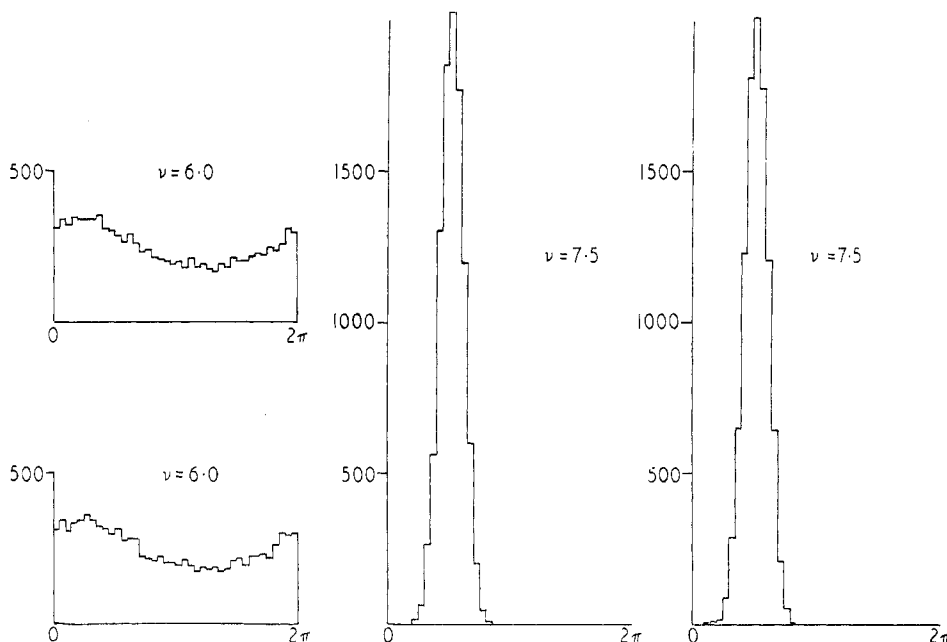
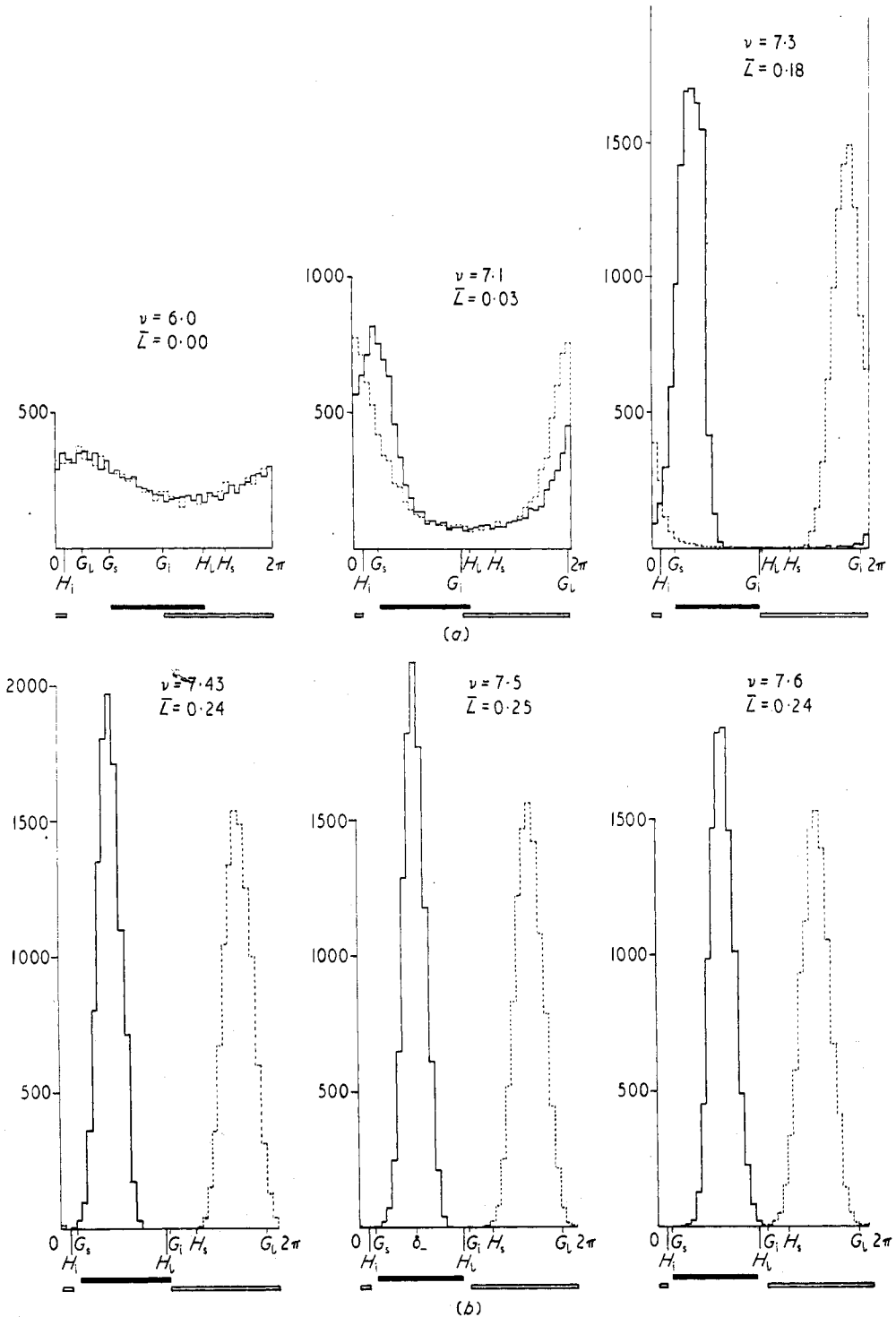


Figure 5. Sample fluctuations in the calculated forward phase distributions at $\nu = 6.0$ and $\nu = 7.5$ for $\sigma = 0.04$.

different sample chains are shown for $\nu = 6.0$ and $\nu = 7.5$. (See also figure 6, where the distribution on another different sample is shown for each of these ν values.) There are no remarkable differences in the curves for different sample chains. It is to be noted that, for $\nu = 7.5$, we obtained a few scattered intervals where f_k had very small values (1–3). However, the δ values responsible always occurred among the first fifteen δ 's to be computed. This means that the small values of f_k in these scattered intervals have been brought about by the end effect, and must be regarded as spurious as far as one is investigating the spectral properties of very long (ideally infinite) chains. The histograms in figure 5 are the ones which were obtained by discarding such spurious f_k values. The same remark applies to every curve in the following figures which are completely concentrated in a narrow sub-interval of $(0, 2\pi)$.

Figure 6 shows the forward and backward phase distributions and the values of the degree of localization calculated for several energies around the first gap in the case of $\sigma = 0.04$. The forward and backward distributions are indicated by the full and broken curves respectively. The values of \bar{L} calculated had considerable sample fluctuations, but almost all of them were consistent to two decimal places, and in the figure only the consistent parts are shown. The thick black and white bars indicate the intervals $\text{III}L^{(4)}$ for the forward and the backward transfers, respectively.



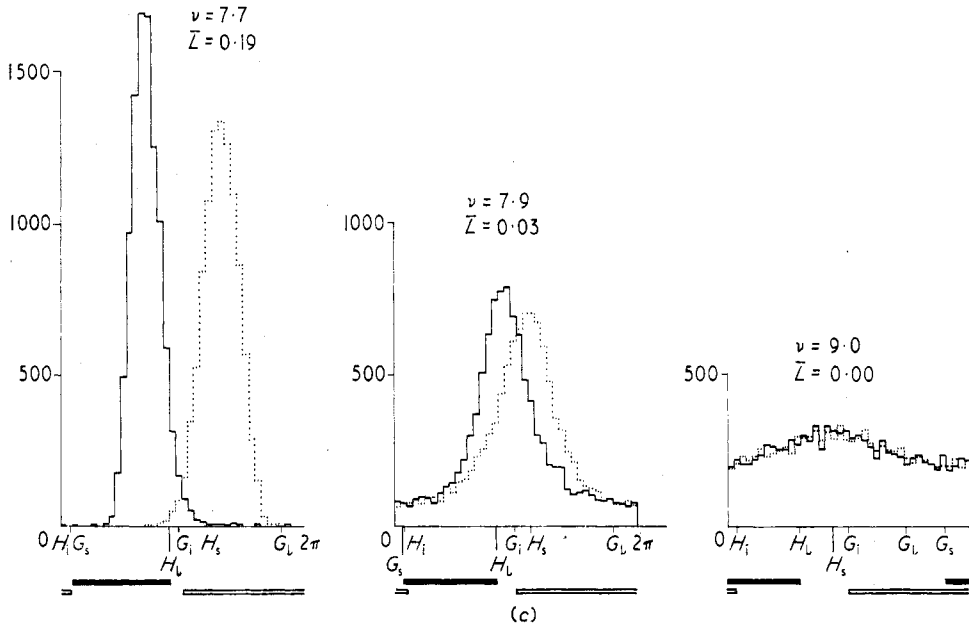


Figure 6. The values of the degree of localization \bar{L} and the forward and the backward phase distributions calculated for $\sigma = 0.04$ at the energies around $\nu = 7.5$. The broken lines indicate the backward distributions. The horizontal black and white bars indicate the intervals $\Pi L^{(4)}$ for the forward and the backward transfers, respectively. G_1 and H_1 indicate the values of G and H respectively for the backward transfer. (For the backward transfer these values were found to be almost independent of l , the separation.) G_s and H_s indicate the values of G and H for the shortest separation for the forward transfer. G_l and H_l indicate the values of G and H for the longest separation for the forward transfer.

At $\nu = 6.0$ the distributions are rather concentrated in the interval $\Pi S^{(4)}$, but since the value of \bar{L} is positive, though small, one should consider that the effect of the randomness expected in the preceding section is already coming into play. As the energy increases, the tendency for $f(\delta)$ to be concentrated in the L regions becomes rapidly strong. At $\nu = 7.1$ the peak of each distribution lies approximately at the edge of the interval $\Pi L^{(4)}$, and at $\nu = 7.3$ most of the area under the histogram is on $\Pi L^{(4)}$. At the same time the distributions become rapidly peaked, and each distribution becomes almost confined within a relatively narrow interval. As a consequence, the overlapping of the forward and the backward phase distributions becomes rapidly small. At $\nu = 7.43$ the distributions become completely non-overlapping. This state of complete non-overlapping lasts until $\nu = 7.6$. Then the whole situation begins to change in just the reverse direction: the distributions begin to overlap again, then become broader and broader. The situations at $\nu = 7.7$, $\nu = 7.9$ and $\nu = 9.0$ are quite similar to those at $\nu = 7.3$, $\nu = 7.1$ and $\nu = 6.0$, respectively.

From figure 4 it is seen that the interval from $\nu = 7.43$ to $\nu = 7.6$ corresponds to the empirical gap found by Borland and Bird. This implies that the calculated gap can be explained as an interval where the two distributions are non-overlapping, in spite of the fact that not all of the transfer matrices are hyperbolic. It is to be noted, however, that the interval (7.43, 7.6) seems to be somewhat narrower than the calculated gap. This presumably means that a very small overlapping of the phase distributions, which occurs on both sides of the interval (7.43, 7.6), does not give rise to a numerically perceivable spectral density. Moreover, we may well suspect that also in the interval (7.43, 7.6) the non-overlapping is really not complete. To examine this, we calculated at some energies in this interval the phase distributions on several different sample chains. It was found that a few distributions were accompanied by a non-spurious tail, which may give rise to a very

slight overlapping. Thus it is highly probable that the non-overlapping found above is not genuine, but merely so slight that it does not bring about any numerically detectable spectral density. It can be concluded, therefore, that the empirical gaps are the intervals throughout which the phase distributions are almost non-overlapping, such that the spectral density is extremely small. In other words, these gaps are quasi-gaps.

It was also found that at the energies around $\nu = 15.5$ the concentration in the L regions becomes strongest in the midst of the gap of the regular chain, but here it is not sufficient to make the distributions almost non-overlapping. Hence no quasi-gap appears.

Similar calculations were also carried out for the case of $\sigma = 0.01$. At the energies around $\nu = 7.5$ it was found that the general characteristic is completely similar to that for $\sigma = 0.04$. The almost complete non-overlapping takes place in the interval (7.22, 7.8), which is only very slightly narrower than the gap predicted numerically by Borland and Bird. The only important difference is that in the interval (7.30, 7.71) the widths of the distributions become much narrower than in the case of $\sigma = 0.04$. This is natural because this interval is the true spectral gap predicted phase-theoretically, and the phase distributions must there be really non-overlapping. At the energies around $\nu = 15.5$, the situation was found to be much the same as for $\nu = 7.5$ and $\sigma = 0.04$.

In figure 6 it is clearly demonstrated that the value of the degree of localization L increases very rapidly with the increase of the concentration of the phase distribution in the L regions. Thus it is seen that the strong localization of the wave functions is intimately connected with the appearance of the quasi-gaps, through the strong concentration of the phase distributions.

5. Conclusions

It has been shown that the gaps in the spectrum of the liquid-like Kronig-Penney model, which were found numerically and which lie outside the gaps predicted phase-theoretically, just correspond to the energy intervals in which the forward and backward phase distributions are almost non-overlapping. Inasmuch as such a non-overlapping is a consequence of the strong concentration of the phase distributions in the L regions, which leads to the strong localization of wave functions, this gives a natural explanation of the fact that the eigenfunctions are always strongly localized near the edges of these energy gaps.

The characterization of the spectral gaps or quasi-gaps as the intervals in which the phase distributions are completely or almost completely non-overlapping will be useful for investigating the gap problems in other one-dimensional systems as well as in the higher-dimensional systems, although in the latter the argument may become much more involved. It will also be possible to relate the spectral density to the degree of overlapping of the phase distribution. This will be of value especially in the investigation of the behaviour of the spectrum near the gaps.

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Appendix

In this paper it was unnecessary to worry about either the ergodicity or the uniqueness of the phase distribution function, because the phase distributions on sample chains were calculated directly. In the analytical discussions, however, one is obliged to consider the ensemble phase-density function in place of the sample phase distribution, on the assumption of ergodicity. It will be of some value, therefore, to give a brief discussion on the ergodicity and the uniqueness of the phase distribution.

That the phase distribution function has the ergodic property is almost evident from the fact already mentioned in the text that, except for relatively small sample fluctuations, all the histograms calculated on the different sample chains coincide well with one another. The fact that the ensemble phase-density function calculated by Roberts and Makinson (1962) has the form very similar to our histogram also supports this conclusion.

In order to confirm this point further, we calculated, for some energies, two series of the successive phases $\delta_i^{(1)}$ and $\delta_i^{(2)}$ on the same sample chain by starting from two different initial phases ($\delta_1^{(1)} \neq \delta_1^{(2)}$). By comparing the values $\delta_2^{(1)}, \delta_3^{(1)}, \dots, \delta_{101}^{(1)}, \delta_{9902}^{(1)}, \delta_{9903}^{(1)}, \dots, \delta_{10001}^{(1)}$ with $\delta_2^{(2)}, \delta_3^{(2)}, \dots, \delta_{101}^{(2)}, \delta_{9902}^{(2)}, \dots, \delta_{10001}^{(2)}$, it was found that for the energies around a gap the difference between $\delta_i^{(1)}$ and $\delta_i^{(2)}$ decreases very quickly with the increase of i , while for the energies distant from the gaps the phase forgets its initial value much more slowly. In any case, however, the phase does forget its initial value. Thus it can well be expected that for every energy there exists a unique phase-density function which closely represents the phase distribution on the individual sample chain.

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