SPECTRAL GAPS
FROM
ORDERED
TO
DISORDERED
SYSTEMS

Thesis by

John Florian Lindner

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Foreword

Physics is the mathematical modeling of nature.* Simple, exactly solvable models are important because they provide orientation and intuition in more complicated (and more realistic) unsolvable models. I have examined and have tried to understand the behavior of certain idealized models of disordered systems. Also, I have tried to see—and elucidate—things in a fresh and novel way. During the course of my self-education, I have

> uncovered much;
> recovered (in my own way) things elsewhere known; and
> discovered things heretofore unknown.

If, in my research, my primary motivation is learning, then, in my writing, my primary motivation is teaching. Consequently, I have been (and am) very concerned with the presentation of my research. The unusual graphic style of my thesis reflects the visual nature of my thinking. I don't yet know if this experiment is successful.

I thank Professor Barry Simon for supporting me during the 3 years of my research, and also his students: Bart Huxtable, Kris Odencrantz, Clemens Glaffig, and Askell Hardarsson. I also thank Professor F. Gesztesy for comments and advice. Teaching has been an important and rewarding part of my experience here at Caltech, and in that I have enjoyed the company of Michael Cross, Sam Finn, Steve Frautschi, Bart Huxtable, Randy Kamien, Michael Kovari, Mike Morris, David Politzer, Tom Prince, among others, and especially my many students. I thank my new friends, Steve and Liz. Special thanks is due my family: Florian, Mary, and Jim.

And, of course, K & D.

JL

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* It's also fun.

Abstract

As is well known, the allowed energies of periodic electronic systems and the allowed frequencies of periodic elastic systems form banded sets (at least for certain idealized models). Recent work, by Werner Kirsch and others, demonstrates that this band-gap structure persists in disordered versions of these periodic systems. Here, I extend this result by showing that **for specific "point" interactions, the spectrum of a generic disordered system is the union of the spectra of all possible pure systems formed from it.** This permits the explicit construction of these spectral sets.

This result is the outgrowth of a perspective I call "**growing disorder** ." The idea is to evolve, or "grow," an ordered array (whose spectrum is known) into a disordered array (whose spectrum is sought). The trick is to evolve the spectrum along with it. The approach is very visual, lends itself readily to graphical presentation, and accounts in part for the unconventional but appropriate *look* of this thesis.

The unconventional style also reflects an attempt to make the material easily accessible to a physics audience. It is inspired by the way in which physicists informally communicate ideas, namely, with words and pictures in front of a blackboard. Each page, or set of facing pages, of text and graphics is a unit to be assimilated before proceeding onto the next unit. There is, thus, **no unique path through the thesis**.

An intuitive and straightforward approach, constructive proofs, an informal style, and some ingenuity simply communicate the ideas herein. However, the condensation inherent in the graphical presentation demands significant reader engagement!

A Dialogue

Q: Why is glass transparent? It's always puzzled me. After all, a window pane is just as solid as a wooden desk.

A: True, but since atoms are mostly empty space, and glass and wood are both made of atoms, you might better ask: Why isn't <u>wood</u> transparent?

Q: OK, but what's the difference? Why are some things transparent and others opaque?

A: Quantum theory provides one answer. The allowed electronic energies of a regular solid form bands separated by gaps. At room temperature, roughly, there is an energy below which all levels are filled and above which all are empty. If this energy is in a band, then the solid is opaque. If it's at a band top and the next gap is large, it's transparent.

Q: I don't follow. Why?

A: Consider a visible-light photon. Take its energy to be 1 eV. The photon can interact with the solid only by exciting the top electrons. But if there's a gap of several eV, as is the case, for example, with diamond, then no excitation is possible.

Q: I see—the only allowed excited states are too many eV's away.

A: Yeah, so the photon doesn't interact and passes right through. That's why diamonds are transparent.

Q: Hmm. That's interesting, but glass isn't a regular solid like diamond. It's a disordered solid, akin to a liquid.

A: You're right. And so my simple argument would break down for glass, except that recent work indicates that the electronic band-gap structure of regular solids is quite robust and may persist in disordered solids.

Q: I'd like to hear more....

Short Contents

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Idealized experiments

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Dirac delta: δ

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- Growing array spectrum

Dirac delta-prime: δ'

- Growing array spectrum

Growing disorder

- Example growths

$\sigma(\text{random}) = U\sigma(\text{pure})$

Spectral construction

Long Contents /Overview

The starting point is a series of (computer) experiments involving idealized models (namely, harmonic chains and δ arrays) of selected physical systems that allow parallel mathematical descriptions. The results are interesting, even surprising. The goal is to understand them as simply and as transparently as possible. [pages 1-5]

This understanding has its foundation in history. The relevant previous work is highlighted. The 3 most important results (which concern the spectra of ordered and disordered operators) are first stated and then elucidated by heuristic arguments. [pages 6-10]

The δ is the best-known point interaction. Here, it is defined by, and analyzed in terms of, its effect on wave functions (which are arbitrary superpositions of eigenfunctions). The ordered array (or KP) spectrum is continuously evolved, or grown, from simple limit cases, and is parameterized in a natural way. [pages 11-24]

A related, but less well-known, point interaction is the δ′. While the δ exhibits many canonical features (of more general interactions), the δ′ exhibits some exceptions to those features. [pages 25-31]

A method of obtaining the spectra of disordered arrays is described. The idea is to evolve (continuously or discretely) an ordered array into a disordered array and to evolve the spectrum along with it. Eigenvalue flow crystallizes into spectral trajectories. [pages 32-38]

The above perspective leads to a connection between the spectra of ordered and disordered point interactions, which extends previous work: The spectrum of a "typical" random system is the union of the spectra of all "pure" systems formed from it. This is the central result of the thesis. [pages 39-45]

Finally, these results easily explain the initial spectral experiments by constructing, explicitly and elegantly, the relevant spectra (for both δ arrays and harmonic chains). [pages 46-55]

Idealized Experiments: Elastic Systems

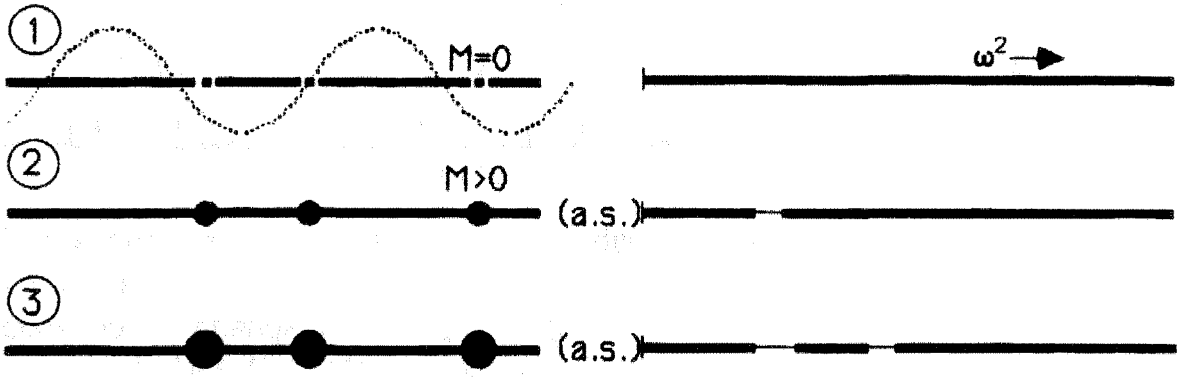
Resonant frequencies of transverse (small) oscillations of a beaded, elastic, massive string.

The experiment is to vary the mass of the beads and monitor the change in the allowed frequencies of transverse oscillation of the beaded string. This is depicted on the facing page (1-3). Notice that M=0 corresponds to an ideal string, which can oscillate at any frequency (1). However, for M>0, gaps appear in the frequency spectrum (2-3).

Resonant frequencies of (longitudinal) oscillations of a beaded, elastic, massless string.

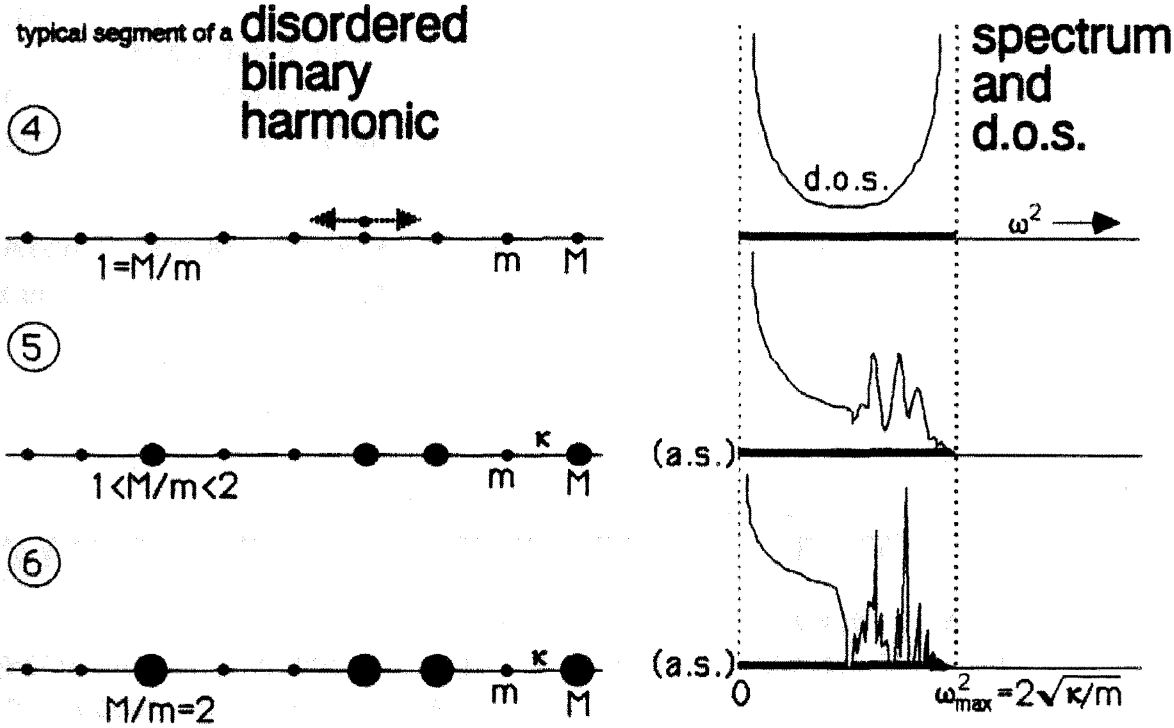
This thesis began right here, with the experiment depicted opposite (4-6). Begin with a "harmonic chain" (of beads connected by "Hooke's law" springs) (4). Being a lumped system, it exhibits a high-frequency cut-off. The density of states or **d.o.s.** is a smooth, continuous function. However, continuously increasing the masses of a selected subset of beads typically has a dramatic effect on the d.o.s.: sharp peaks and valleys appear (5-6). Abruptly, when the heavy beads are twice the mass of the light bead, zeros appear in the d.o.s. (6). (These "zeros" in the d.o.s. widen to gaps in the spectrum, if arbitrarily long runs of light beads are eliminated from the chain.) At still higher mass ratios, many more zeros appear in a complicated and intriguing way. **Where is the structure? What is the pattern governing the appearance of these "valleys" in the d.o.s.?** A formula was known (thanks to [Matsuda◆1964]), but it lacks the elegance of the understanding derived herein and visualized in the frontispiece and endpiece.

typical segment of a selected **beaded** **spectrum** is the set of allowed frequencies



typical segment of a **disordered binary harmonic**

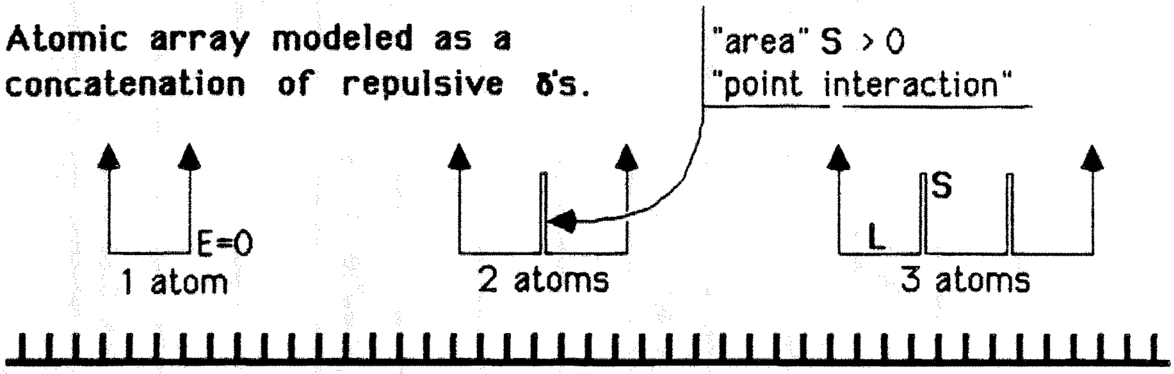
spectrum and d.o.s.



(a.s. = almost surely
= "typically")

Idealized Experiments: Electrons in a Crystal

Atomic array modeled as a concatenation of repulsive δ's.



many atoms form an array

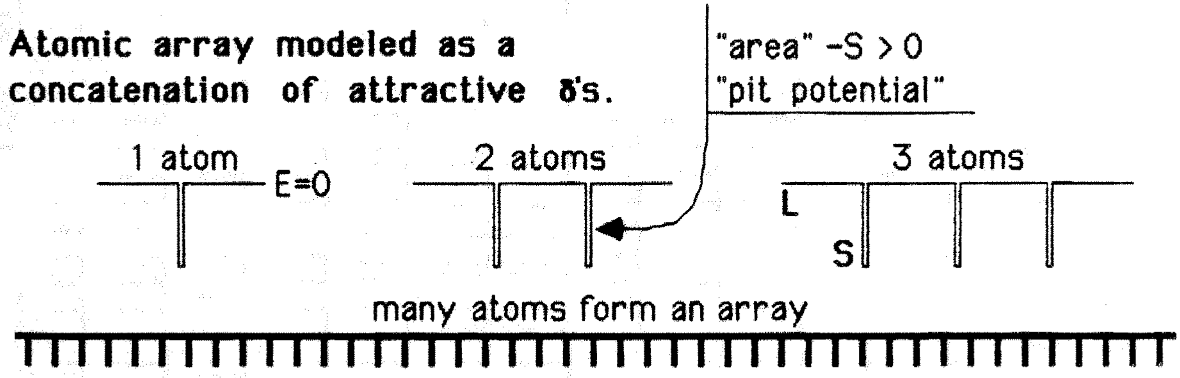
The experiment (1–4, 4–7 & 8–10) depicted on the facing page is to vary the Lengths and Strengths of the array and to examine the consequent change in its <u>spectrum,</u> or set of allowed energies.

Notice that strengthening (2) contracts the spectrum from "below" while lengthening (3) "depresses" it.

Varying lengths (5 & 6) closes infinitely many gaps, but subsequent strengthening (7) opens others (that are not necessarily the same).

Even more interesting, varying strengths (9) typically has no effect at all except, for example, when strengths are alternated strong–weak (10), thereby splitting each band!

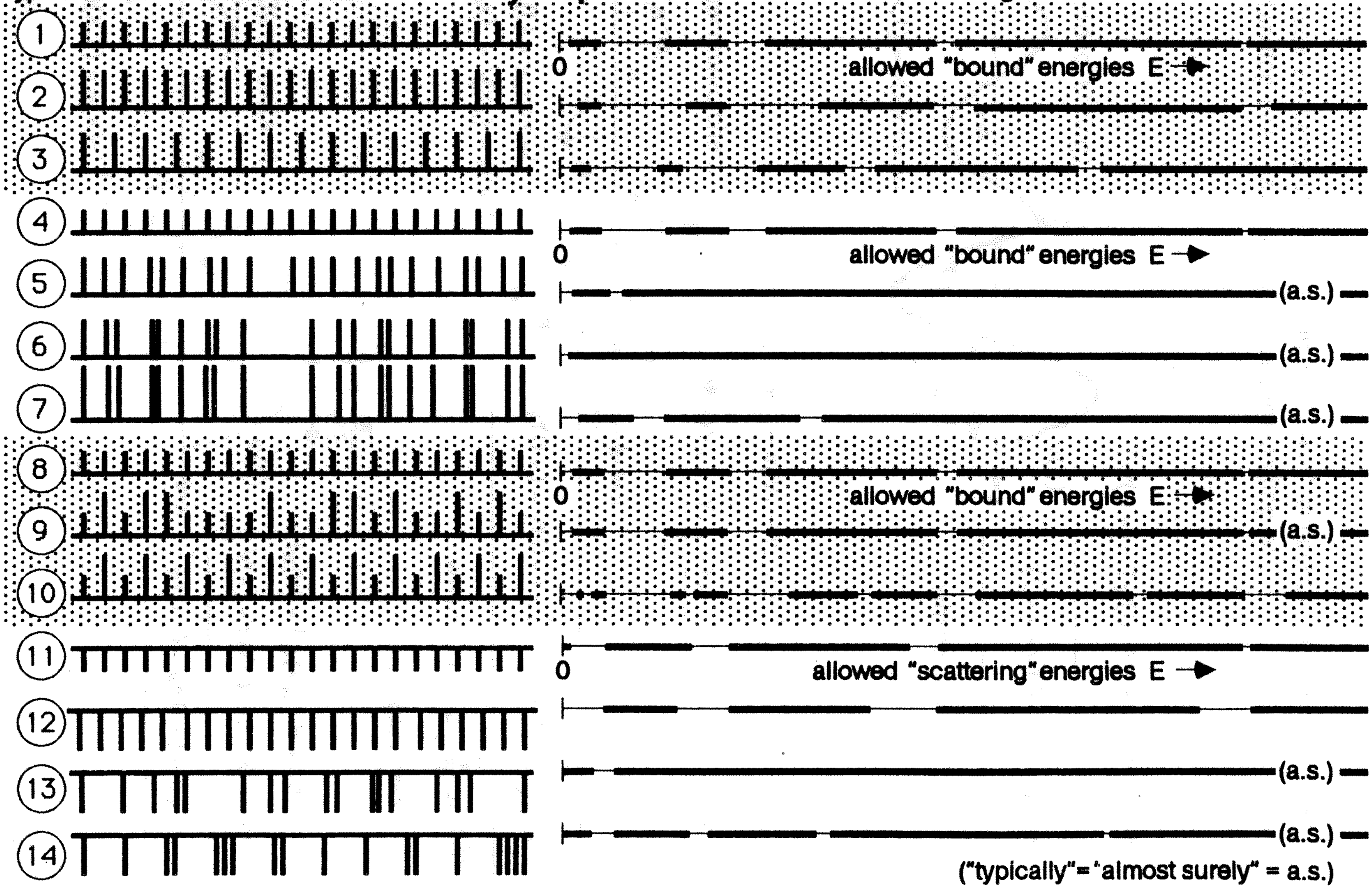
Atomic array modeled as a concatenation of attractive δ's.



The experiment (11–14) depicted on the facing page is (again) to vary the Lengths and Strengths of the array and examine the consequent change in its spectrum.

Notice that strengthening (11) contracts the spectrum from "above." Varying lengths (13 & 14) closes gaps; a <u>continuum</u> of lengths (13) leaves <u>finitely</u> many gaps, while <u>infinitely</u> many gaps remain if the lengths are <u>discretely</u> scattered between, say, 1 of 2 possibilities (14).

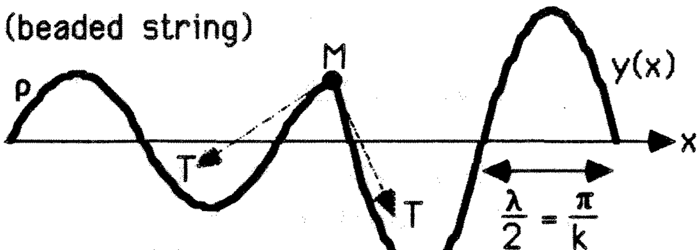
typical section of a selected **atomic array** **spectrum** is the set of allowed energies



These systems share the same “kinky” property, and hence, understanding one (say, the δ) is understanding all.

$$Ty'(0+) - Ty'(0-) = F_\perp = M\ddot{y} = -M\omega^2 y$$

(beaded string)



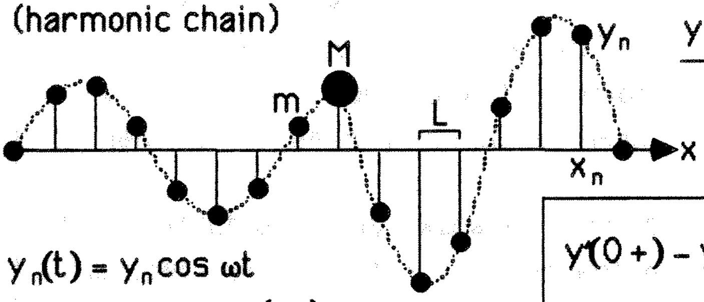
$y(x,t) = y(x)\cos\,\omega t$

$$\boxed{y'(0+) - y'(0-) = -\frac{M\omega^2}{T}y(0)}$$

where $\omega = kc$, $c = \sqrt{T/\rho}$

$$\kappa(y_{n+1} - y_n) - \kappa(y_n - y_{n-1}) = F_\parallel = m_n\ddot{y}_n = -m_n\omega^2 y_n$$

(harmonic chain)



$$\frac{y_{n+1} - y_n}{L} - \frac{y_n - y_{n-1}}{L} = -\frac{m_n\omega^2}{\kappa L}y_n$$

And also,

$$\boxed{y'(0+) - y'(0-) = \left(1 - \frac{M}{m}\right)k\tan\left(\frac{kL}{2}\right)y(0)}$$

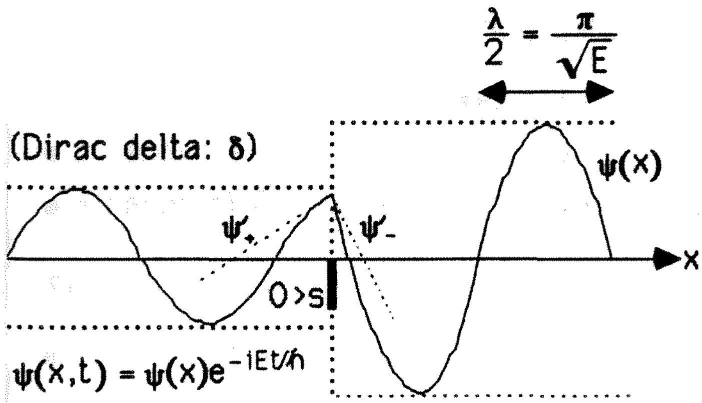
$y_n(t) = y_n\cos\,\omega t$

$(\Delta x)_n = y(x_n) = y(nL) = y_n$

where $\omega = 2\sqrt{\frac{\kappa}{m}}\sin\left(\frac{kL}{2}\right)$

$(L < \lambda/2 \Rightarrow kL < \pi)$.

(Dirac delta: δ)



$H\psi(x) = E\psi(x)$, $H = -\partial_x^2 + V(x)$

$V(x) = s\delta(x)$, $s < 0 \quad \Rightarrow$

$$\boxed{\psi'(0+) - \psi'(0-) = s\psi(0)}$$

$\psi(x,t) = \psi(x)e^{-iEt/\hbar}$

Historical Highlights

Two historical efforts (one originating in the mathematics community and one in the physics community) presage the work herein.

Physicists have been concerned with the electric (and elastic) properties of solids:

① existence, persistence, and robustness of gaps

- energy (frequency) band-gap structure of periodic solids
    - general theory [Bloch◆1928]
    - specific, solved, model [Krönig/Penney◆1931]
- a gap common to 2 elements is a gap for all their alloys? [Saxon/Hutner◆1949]
- computer experiments (see [Dean◆1972] for a review)
- model-specific sufficient conditions
    - KP alloy [Luttinger◆1951]
    - KP liquid [Borland◆1961]
- general sufficient condition [Hori/Matsuda◆1964]
- general necessary condition [Halperin◆1967]

from which one may extract: $\sigma(\text{random}) \overset{?}{\approx} \bigcup \sigma(\text{periodic})$, where the spectrum σ is the complement of the gaps.

Mathematicians have been concerned with the (spectral) analysis of random (Schrödinger) operators:

② spectrum of periodic and random operators

- $\sigma(\text{periodic})$ is banded (see [Floquet◆1883])
- $\sigma(\text{random}) \overset{\text{a.s.}}{=} \Sigma$ [Pastur◆1980]
- $\sigma(\text{random}) \overset{\text{a.s.}}{=} \overline{\bigcup \sigma(\text{periodic})}$ [Kirsch/Martinelli ◆1982].

……

For KP alloys and liquids (and their analogues),

- $\sigma(\text{random}) \overset{\text{a.s.}}{=} \overline{\bigcup \sigma(\text{pure})}$ [herein].

The history of this subject is well documented in 2 monographs:

> [Hori◆1968] summarizes the work of ①, although there is no mention of [Halperin◆1967]. It emphasizes the "phase theory" method (which features a transfer matrix in polar form) developed and exploited by Hori, Matsuda, and colleagues.

20 years later,

> [Albeverio/Gesztesy/Høegh-Krohn/Holden ◆ 1988] is a comprehensive introduction, synthesis, and summary of point interactions, in the spirit of ②. It is rigorous and up-to-date, although it doesn't subsume the previous monograph.

As a contribution to this history, I'd like to spotlight and compare Hori's fundamental statement with Kirsch's; the 2 are clearly related. [Hori◆1968] states, "If an interval of frequency or energy lies in the spectral gaps for all *constituent regular* systems, it gives a spectral gap of the mixed system [subject to a nontrivial technical hypothesis]." A *constituent regular* system is formed from a given system by infinitely repeating any finite segment of it. Equivalently (but, for comparison, omitting extra hypotheses),

HORI

> The spectrum of a mixed array is contained in the union of the spectra of all arrays formed by infinitely repeating each finite section of the array.

Contrast this with

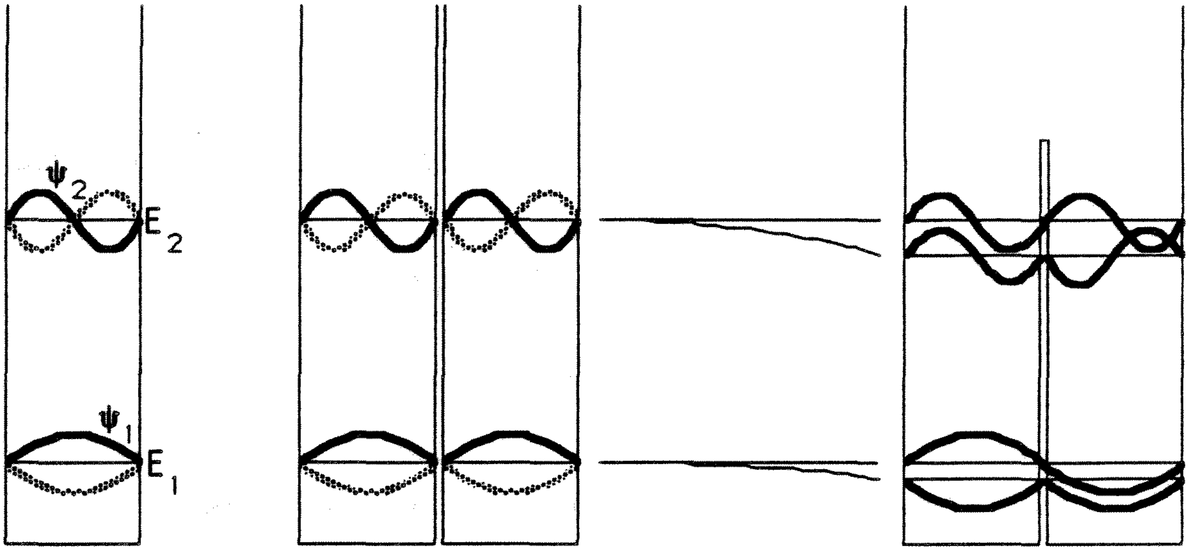
KIRSCH

> The spectrum of a typical mixed array is [contained in] the union of the spectra of all arrays formed by infinitely repeating each finite section of a typical array.

Thus, Hori's statement cannot refer to any particular array but rather, like Kirsch's, must refer to a typical array. (A particular array may, in fact, be quite exceptional—for example, pure.)

σ(periodic) is banded: Why?

This is usually understood as the "collectivization" of atomic levels into bands. Model the atoms as rigid (1-dimensional) boxes and allow them to interact "at a point." The energy level splitting is proportional to the tunneling time (as indicated).

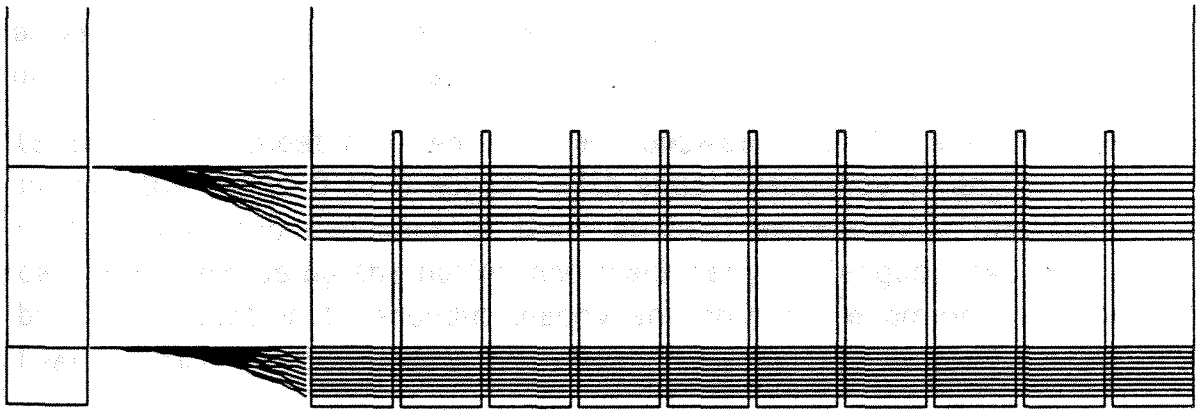


1 isolated atom

2 isolated atoms

2 interacting atoms

In a real crystal of $O(10^{23})$ atoms, a single energy level of an isolated atom broadens into $O(10^{23})$ levels whose spacing is smaller than the typical inverse lifetime of the level and hence whose identity is lost. (Recall, $\Delta E\,\Delta t \gtrsim \hbar$)



1 isolated atom

10 interacting atoms

(It is characteristic of point interactions that the band tops coincide with the energy levels of the isolated atoms.)

$\sigma(\text{random}) \overset{\text{a.s.}}{=} \Sigma$ Why?

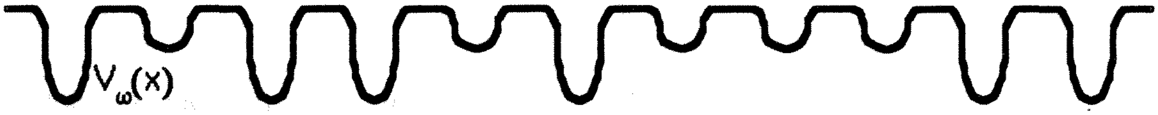
If $H_\omega = -\Delta + V_\omega$ is an "ergodic" Hamiltonian, then its spectrum $\sigma(H_\omega)$ is a fixed set Σ with probability one. This can be understood as a consequence of the "ergodic theorem" or, more simply, by the following argument.

Consider a "random charge configuration":

$$V_\omega(x) = \sum_n q_n(\omega) f(x - nL_0)$$

f(x) = 

$$\mathbf{prob}(q_n = Q) = \frac{1}{2} \qquad \mathbf{prob}(q_n = q) = \frac{1}{2} \qquad Q > q$$



Here's the key: "Almost all" realizations of V_ω are the "same" in that an arbitrarily long segment of a "typical" V_ω can be found (arbitrarily often) in any other "typical" V_ω.

(Similarly, "almost all" real numbers between 0 and 1 are "normal" in that the digits 0 to 9 appear with equal frequency in any sufficiently long sequence of their decimal expansions. This, too, can be proven using the notion and machinery of "ergodicity." For a brief introduction to ergodic theory and physics, examine [Reed/Simon ◆1980].)

Over 20 years ago, [Lifshitz◆1964] coined the term "self-averaging" for the idea that the properties of disordered solids should hold with probability one.

$\sigma(\text{random}) \overset{\text{a.s.}}{=} \overline{\cup\sigma(\text{periodic})}$ Why?

co=cut-off
nbr=**neighbor**
per=**per**iodic

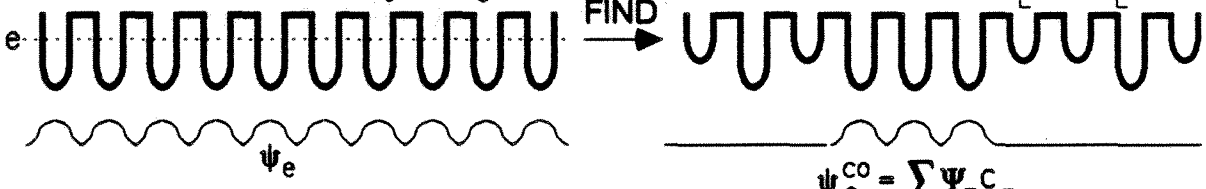
This can be understood by the following arguments.

- show: $\sigma(\text{random}) \supset \cup\sigma(\text{periodic}) \supset \sigma(\text{periodic})$ [Halperin◆1967]
  $e \in \sigma(\text{periodic}) \Rightarrow e \in \sigma(\text{random})$

(hint: FIND arbitrarily long truncated periodic in random)

$h = -\Delta + v \quad h\psi_e = e\psi_e$

(typical random)
$H = -\Delta + V \quad H\Psi_E = E\Psi_E$



$$\psi_e^{co} = \sum_E \Psi_E c_E$$

$$\|(H-e)\psi_e^{co}\| < \varepsilon\|\psi_e^{co}\| \quad \Rightarrow$$

$$(E^{nbr}-e)^2\|\psi_e^{co}\|^2 = (E^{nbr}-e)^2\sum_E |c_E|^2 \le \sum_E (E-e)^2|c_E|^2 = \|(H-e)\psi_e^{co}\|^2 < \varepsilon^2\|\psi_e^{co}\|^2$$

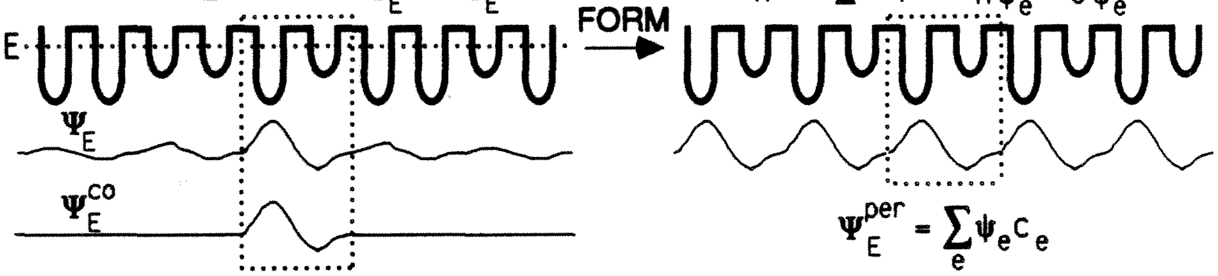
$$\Rightarrow |E^{nbr}-e| < \varepsilon \qquad \text{(and so on)}$$

- show: $\sigma(\text{random}) \subset \cup\sigma(\text{periodic})$
  $E \in \sigma(\text{random}) \Rightarrow E \in \sigma(\text{periodic})$

(hint: truncate random and repeat to FORM periodic)

(typical random)
$H = -\Delta + V \quad H\Psi_E = E\Psi_E$

$h = -\Delta + v \quad h\psi_e = e\psi_e$



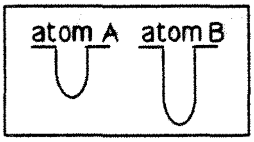
$$\Psi_E^{per} = \sum_e \psi_e c_e$$

$$\|(H-E)\Psi_E^{co}\| < \varepsilon\|\Psi_E^{co}\| \quad \Rightarrow$$

$$\|(h-E)\Psi_E^{per}\| < \varepsilon\|\Psi_E^{per}\| \quad \Rightarrow$$

$$(e^{nbr}-E)^2\|\Psi_E^{per}\|^2 \le \|(h-E)\Psi_E^{per}\|^2 < \varepsilon^2\|\Psi_E^{per}\|^2$$

$$\Rightarrow |e^{nbr}-E| < \varepsilon \qquad \text{(and so on)}$$



The Dirac Delta: δ

Take

$$H\psi(x) = E\psi(x) \qquad H = \frac{p^2}{2m} + V(x) \qquad p = -i\hbar\frac{\partial}{\partial x} \qquad V(x) = s\delta(x) \Rightarrow$$

$$-\frac{\hbar^2}{2m}\psi''(x) + s\delta(x)\psi(x) = E\psi(x)$$

to mean

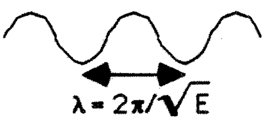
$$\left.\begin{matrix} -\frac{\hbar^2}{2m}[\psi'] + s\psi = 0 \\ [\psi] = 0 \end{matrix}\right\}(x=0),$$

where the "jump" of f(x) at x_0 is

$$[f(x_0)] = f(x_0+) - f(x_0-) = \lim_{\varepsilon\downarrow 0}\left(f(x_0+\varepsilon) - f(x_0-\varepsilon)\right)$$

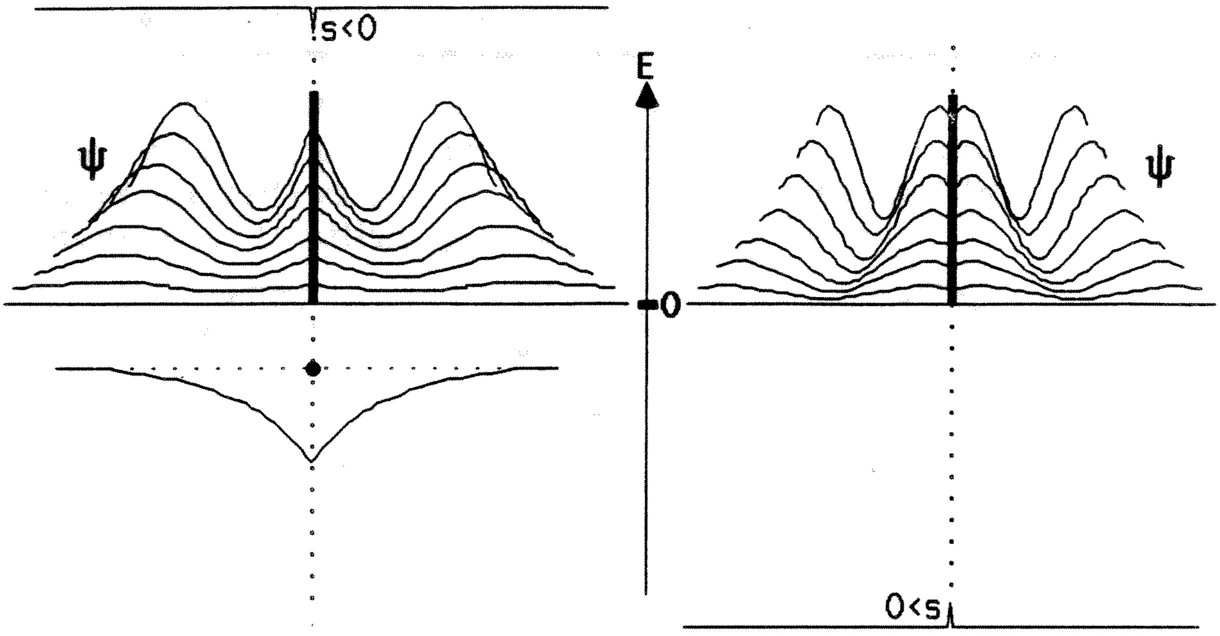
Or, by "renormalizing" the strength s, $s \to \frac{\hbar^2}{2m}s$, take

$$\left.\begin{matrix} [\psi'] = s\psi \\ [\psi] = 0 \end{matrix}\right\}(x=0) \quad \&$$

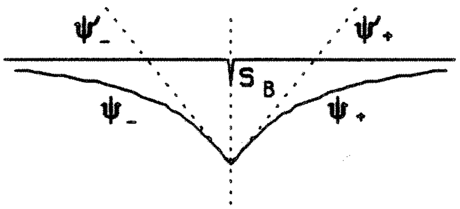


$(x \neq 0)$.

The spectral properties of H are then easily inferred. The <u>eigenfunctions</u> ψ, together with the <u>eigenvalues</u> E (which form the <u>spectrum</u> σ), are indicated below (for fixed strength s).



For each 0<E, it is easy to construct suitable (kinked-sinusoidal) eigenfunctions. For E<0, there is only a single (kinked-hyperbolic) eigenfunction with $s = s_B < 0$, such that



$$\psi_{\pm}(x) = A_{\pm} e^{\mp\sqrt{E}\,x}$$

$$x = 0 \Rightarrow \begin{cases} \psi_- = \psi_+ \\ \psi'_+ - \psi'_- = s_B \psi_\pm \end{cases}$$

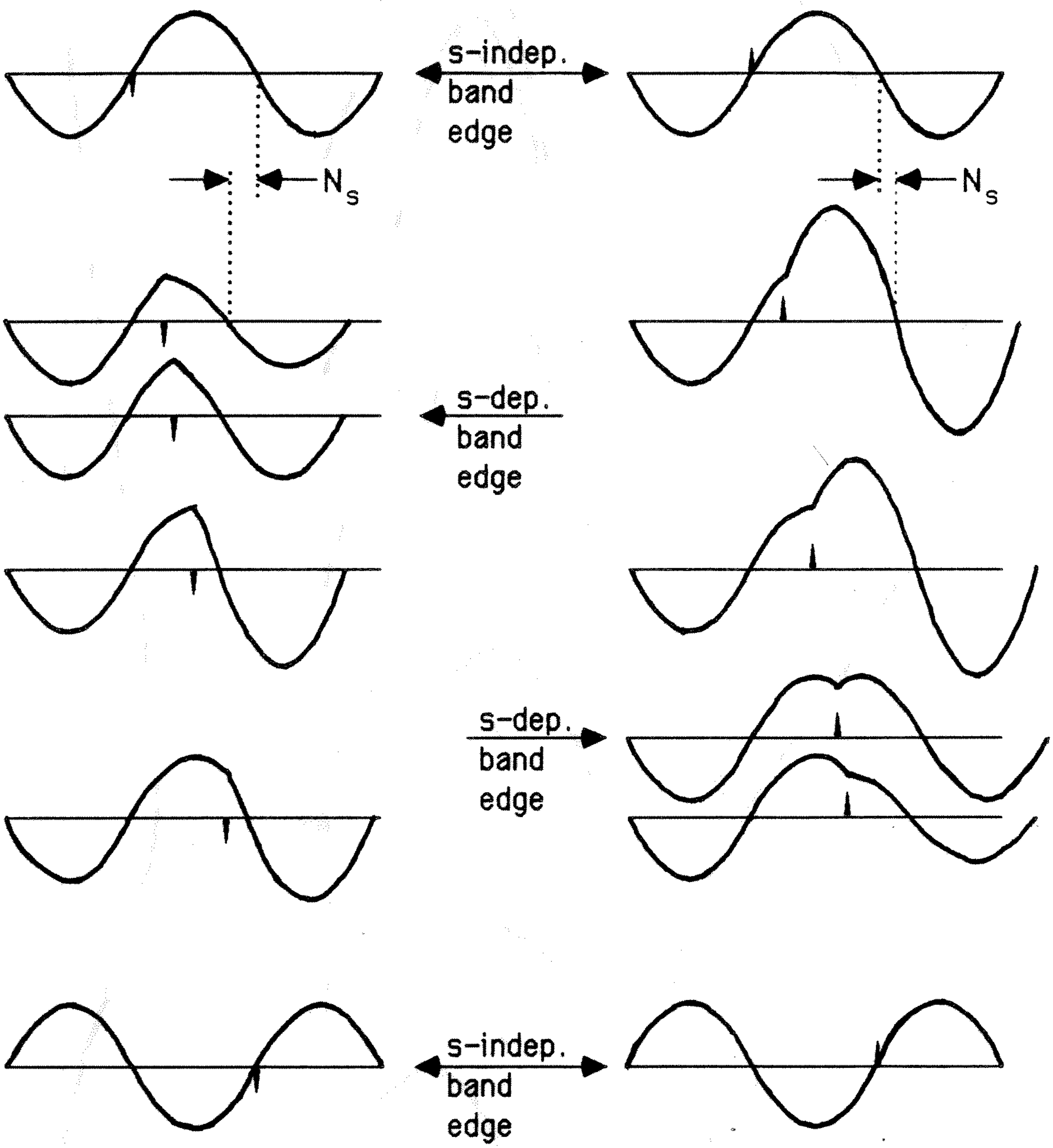
$$\Rightarrow \begin{cases} A_- = A_+ \\ -2\sqrt{E}A_\pm = s_B A_\pm \end{cases}$$

$$\Rightarrow \boxed{s_B = -2\sqrt{-E}} = i2k .$$

s_B sets the strength scale of the model. It is the δ strength needed to bind a particle of energy E. It will appear often in what follows.

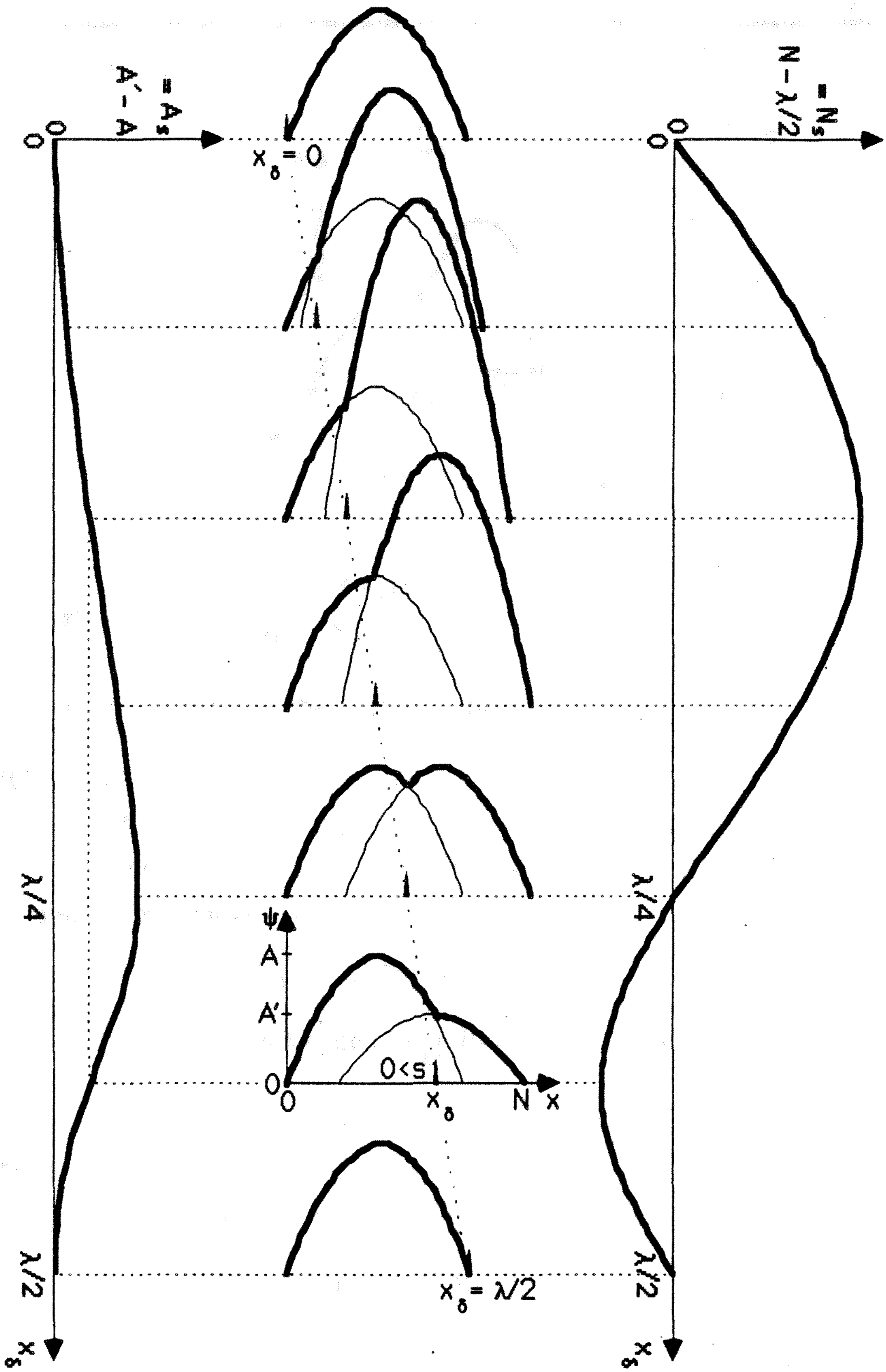
Qualitative Node (or Phase) and Amplitude Shifts: N_s & A_s

It will be important to understand the effect of a δ on the wave function. Below, the sinusoid to the left of the δ is fixed. As the δ moves one half-wavelength, left-to-right, the sinusoid to the right adapts so as to satisfy $[\psi'] = s\psi$.



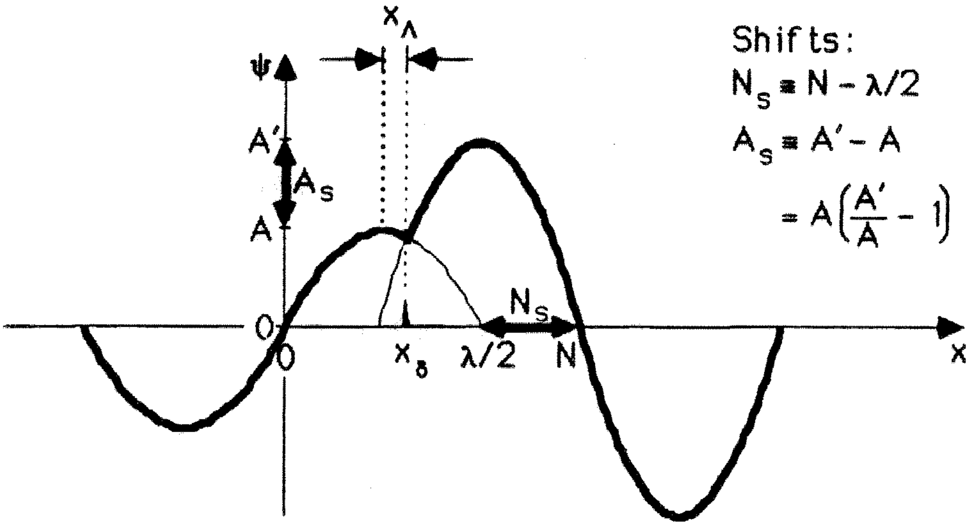
The band edge wave functions are critical to what follows. Here, they are identified by zero amplitude shifts and distinguished by extreme (max or min) node shifts. Compare the s-dependent band edge wave functions. Note how the attractive ($s<0$) δ attracts the nodes, while the repulsive ($s>0$) δ repels them.

Here's a closer look for repulsive δ's. Fix $s > 0$. Fix $\psi(x \le x_\delta)$.



Quantitative Node (or Phase) and Amplitude Shifts: N_s & A_s

Fix $s>0$. Fix $\psi(x \le x_\delta)$.



Shifts:
$N_s \equiv N - \lambda/2$
$A_s \equiv A' - A$
$= A\left(\frac{A'}{A} - 1\right)$

$$\psi(x) = \begin{cases} A\sin kx & x \le x_\delta (\le \lambda/2) \\ -A'\sin k(x-N) & x_\delta \le x \end{cases} \qquad \sqrt{E} = k = \frac{2\pi}{\lambda}$$

Thus, in particular, to the right of the δ,

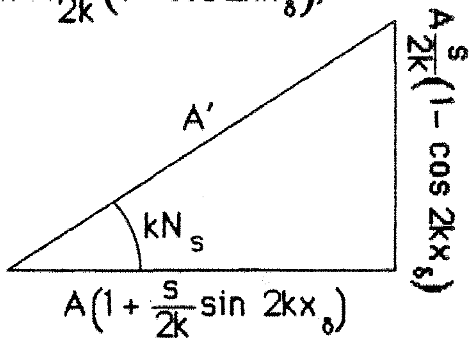
$$\begin{aligned} \psi(x \le x_\delta) &= -A'\sin k(x-N) \\ &= +A'\sin k(x-N_s) \qquad\qquad N_s = N - \lambda/2 \\ &= A'\sin kx \cos kN_s - A'\cos kx \sin kN_s \end{aligned}$$

But also, from above,

$$\begin{aligned} \psi(x \le x_\delta) &= A\sin kx + \frac{s}{k}\psi(x_\delta)\sin k(x-x_\delta) \qquad \psi(x_\delta) = A\sin kx_\delta \\ &= A\left(1+\frac{s}{k}\sin kx_\delta \cos kx_\delta\right)\sin kx - A\frac{s}{k}\sin^2 kx_\delta \cos kx \\ &= \sin kx\, A\left(1+\frac{s}{2k}\sin 2kx_\delta\right) - \cos kx\, A\frac{s}{2k}(1-\cos 2kx_\delta), \end{aligned}$$

where

$$\begin{aligned} A'\cos kN_s &= A\left(1+\frac{s}{2k}\sin 2kx_\delta\right) \\ A'\sin kN_s &= A\frac{s}{2k}(1-\cos 2kx_\delta). \end{aligned}$$



Thus,

$$\frac{A_s}{A} + 1 = \frac{A'}{A} = \sqrt{\left(1 + \frac{s}{2k}\sin 2kx_\delta\right)^2 + \left(\frac{s}{2k}\right)^2\left(1 - \cos 2kx_\delta\right)^2}$$

$$\tan kN_s = \frac{1 - \cos 2kx_\delta}{\frac{2k}{s} + \sin 2kx_\delta}$$

Or, with $s/2k = |\not{s}| = \tan(\hat{s}\pi/2)$,

$$\boxed{\begin{aligned} \frac{A_s}{A} &= -1 + \sqrt{\left(1 + |\not{s}|\sin 2kx_\delta\right)^2 + |\not{s}|^2\left(1 - \cos 2kx_\delta\right)^2} \\ \tan kN_s &= \frac{1 - \cos 2kx_\delta}{\frac{1}{|\not{s}|} + \sin 2kx_\delta} \qquad \text{(for } s>0 \text{ \underline{and} } s<0\text{).} \end{aligned}}$$

The condition for the amplitude to <u>decrease</u> will be important later:

$$0 \geq A_s \iff 1 \geq \frac{A'}{A} > 0 \iff$$

$$1 \geq \left(\frac{A'}{A}\right)^2 = \left(1 + |\not{s}|\sin 2kx_\delta\right)^2 + |\not{s}|^2\left(1 - \cos 2kx_\delta\right)^2$$

$$0 \geq \sin kx_\delta\left(\cos kx_\delta + |\not{s}|\sin kx_\delta\right)$$

$$\sin kx_\delta \geq 0 \implies \underbrace{-\cot kx_\delta}_{} \geq |\not{s}| = \tan\left(\frac{\pi}{2}\hat{s}\right)$$

$$-\cot\left(kx_\Lambda + \frac{\pi}{2}\right) = \tan kx_\Lambda \quad \text{where } x_\Lambda = x_\delta - \frac{\lambda}{4}$$

$$\implies \tan(kx_\Lambda) \geq \tan\left(\frac{\pi}{2}\hat{s}\right), \quad \hat{s} > 0$$

$$\implies \quad kx_\Lambda \geq \frac{\pi}{2}\hat{s} > 0 \quad \text{or} \quad \frac{x_\Lambda}{\lambda/4} \geq \hat{s} > 0\,.$$

And, in general,

$$\boxed{A_s \leq 0 \iff \left|\frac{x_\Lambda}{\lambda/4}\right| \geq |\hat{s}|\,.}$$

For the amplitude to decrease, the distance (in quarter wave lengths) to the nearest maximum must be at least the (normalized) strength $|\hat{s}|$.

Propagation of ψ Through a δ Array: Kinky Sinusoids

$$\left.\begin{array}{l} H\psi = E\psi \\ H = -\Delta + \sum_n s_n \delta(\cdot - x_n) \end{array}\right\} \quad \text{means} \quad \left\{\begin{array}{ll} [\psi] = 0,\ [\psi'] = s_n\psi, & \text{at } x_n \\ \psi = A\sin(\sqrt{E}\,x + \phi), & \text{else} \end{array}\right.$$

Thus, if $0 = s = (\ldots, s_n, \ldots)$,

$$\psi_0(x) = \psi_0(0)\cos kx + \psi_0'(0)\frac{\sin kx}{k} \qquad k \equiv \sqrt{E}$$

magnitude & slope
at origin specify sinusoid

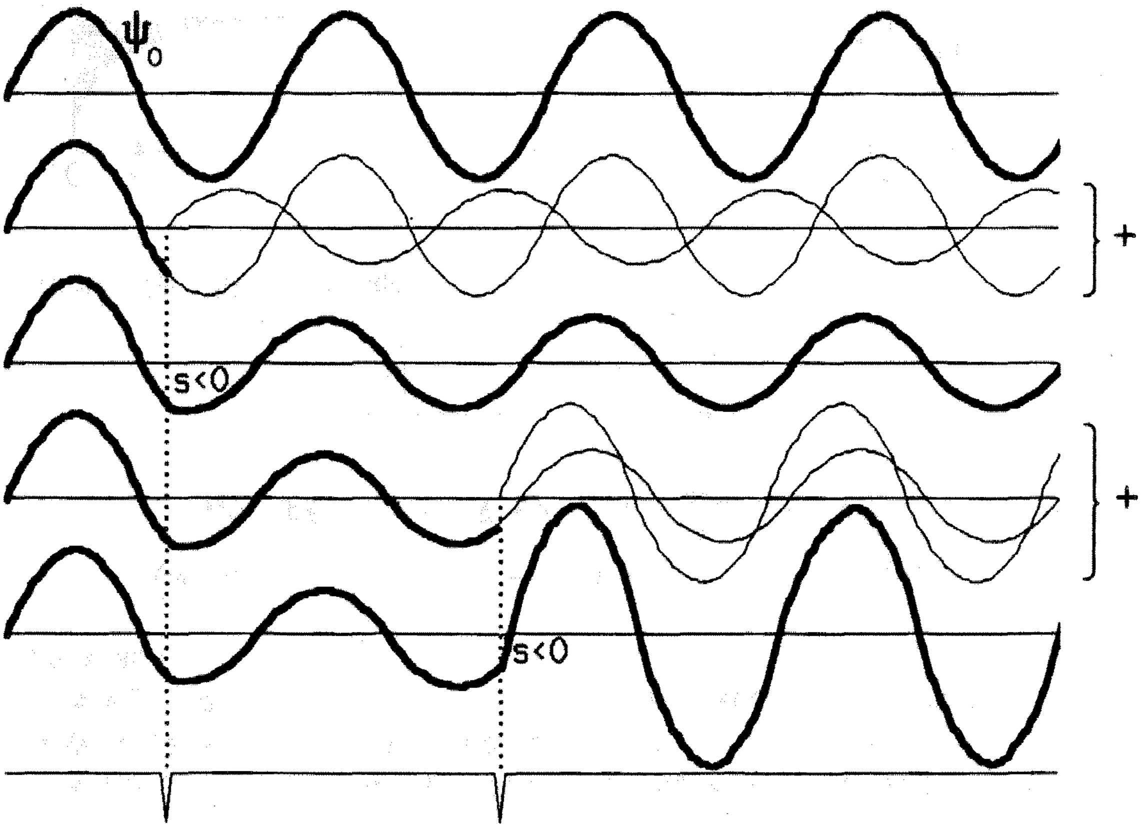
If $s \neq 0$,

$$\psi_s(x) = \psi_0(x) + \sum_{x_n < x} \frac{s_n}{k}\psi_s(x_n)\sin k(x - x_n),$$

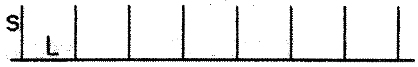
or

$$\psi_s(x < x_{n+1}) = \psi_s(x < x_n) + \frac{s_n}{k}\psi_s(x_n)\sin k(x - x_n),$$

which suggests the following <u>construction</u>.

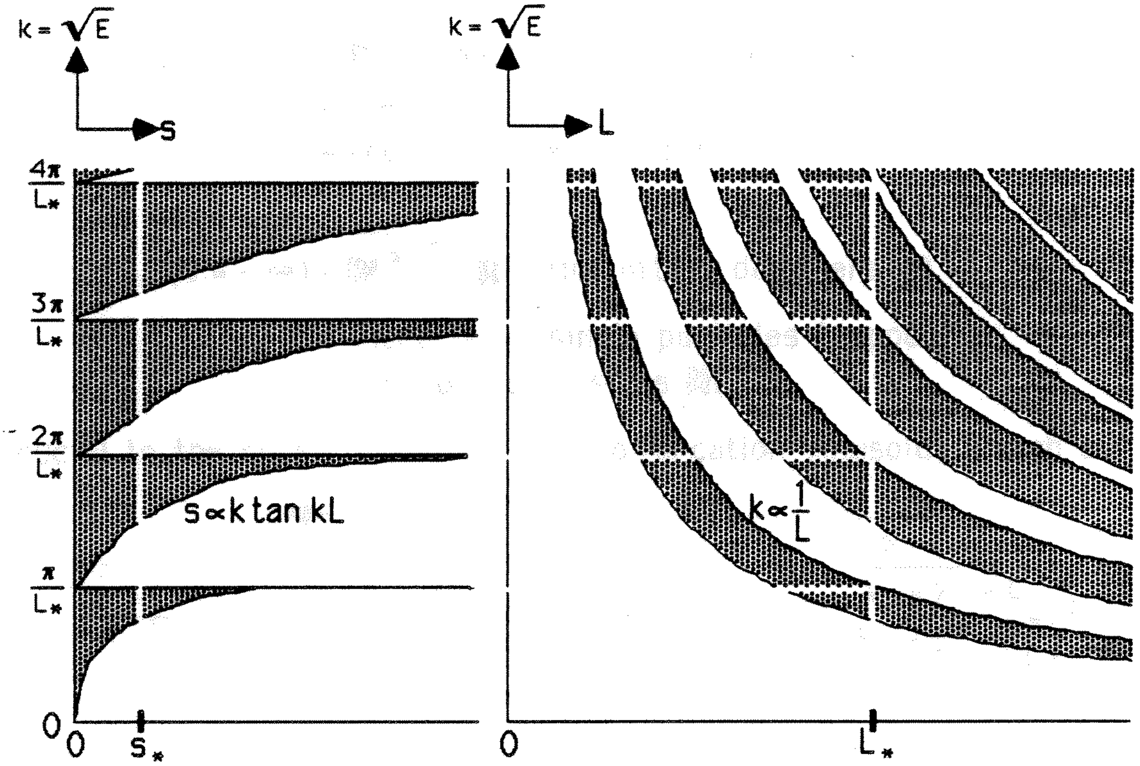


Regular KP models (= pure δ arrays) are characterized by the two parameters, Strength S and Length L:

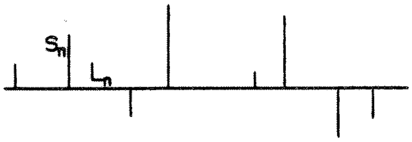


$$H\psi = E\psi \qquad H = -\Delta + V \qquad V = s\sum_n \delta(\cdot - nL).$$

Changes in the parameters s and L change the KP-spectrum in crucially different ways.



Among random KP models,



$$H\psi = E\psi \qquad H = -\Delta + V \qquad V = \sum_n s_n\delta(\cdot - x_n)$$

(where s_n & $L_n = x_{n+1} - x_n$ are randomly chosen),

there are

- KP "liquids," where the strength is fixed and the lengths vary (*à la* a "snapshot" of a liquid) and
- KP "alloys," where the strengths vary and the length is fixed.

GROWING an ORDERed δ Array

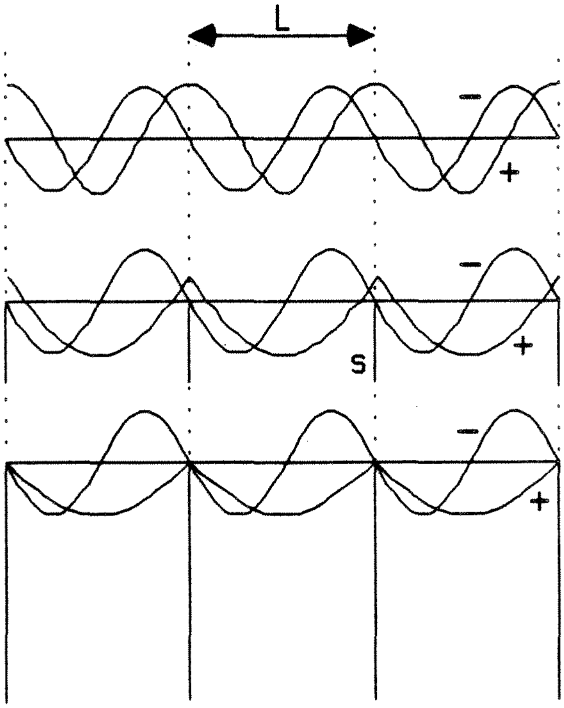
The next three pages construct the δ array (=KP) spectrum in a novel way. The idea is to "grow" the spectrum σ for arbitrary δ strength s from the extreme cases s=−∞,0,+∞, by continuously changing s and observing the consequent changes in the sinusoidal (or hyperbolic) wave functions.

- The spectra of the limit cases are

$$\begin{aligned}\sigma(s=0) &= \mathbb{R}^+ \quad \text{(doubly degenerate)}\\ &= \sigma(-\Delta)\\ &= \text{energies of a free particle}\end{aligned}$$

$$\begin{aligned}\sigma(s=\pm\infty) &= \overline{\left(\mathbb{N}\frac{\pi}{L}\right)^2} = \mathbb{R}^+ \quad \text{(infinitely degenerate)}\\ &= \text{energies of single particles trapped in rigid boxes of sizes } \mathbb{N}L.\end{aligned}$$

- Crucial to the construction are the "bifurcation sinusoids," such as



$\boxed{s=0}$

$\lambda_+ = \lambda_- = L$

$E_+ = E_- = \left(\frac{\pi}{L}\right)^2$

$\boxed{-\infty > s > 0}$

$\lambda_+ > \lambda_-$

$E_+ < E_-$

$\boxed{s \gtrsim -\infty}$

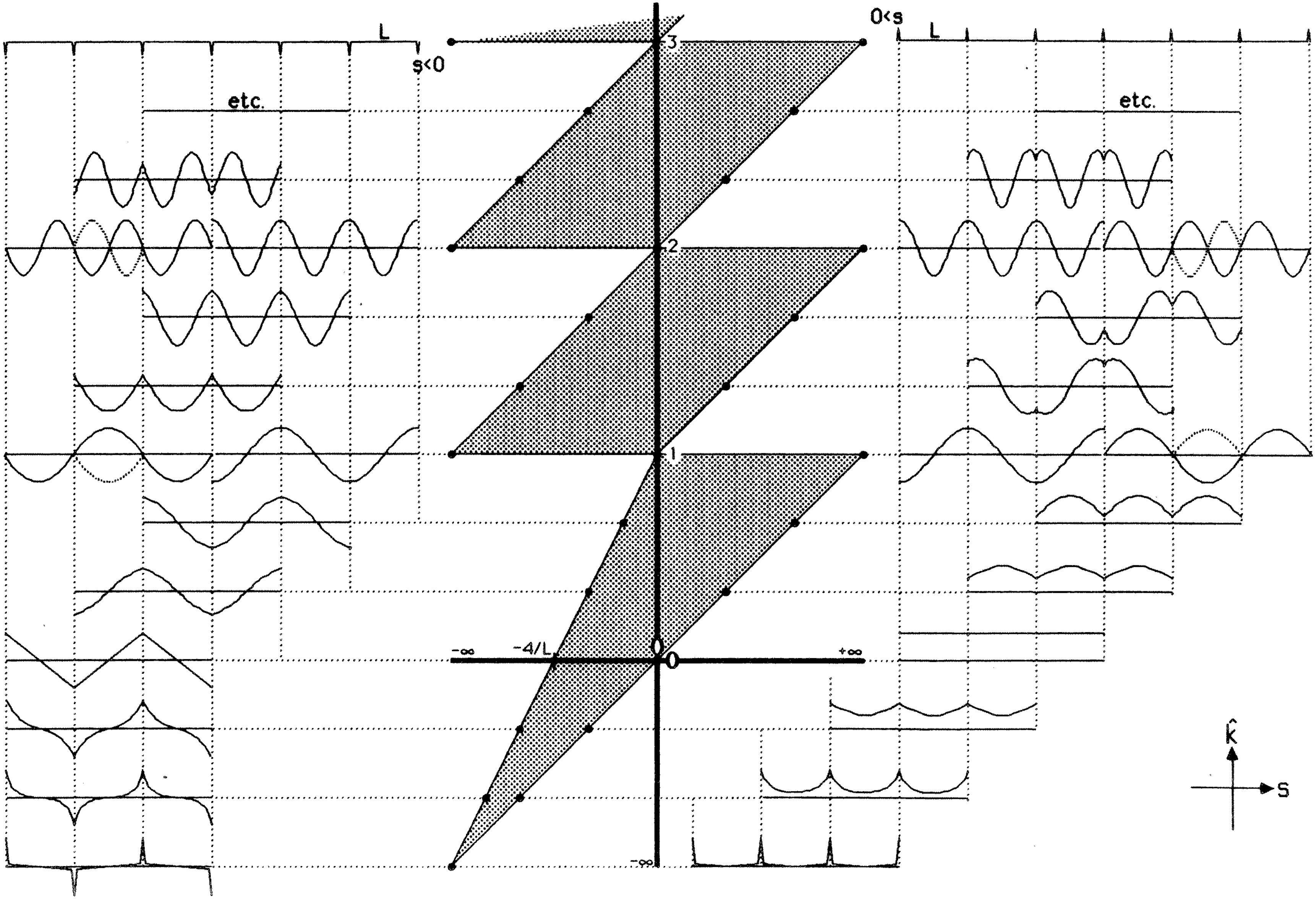
$2L = \lambda_+ > \lambda_- = L$

$\left(\frac{\pi}{L}\right)^2 = E_+ < E_- = \left(\frac{2\pi}{L}\right)^2.$

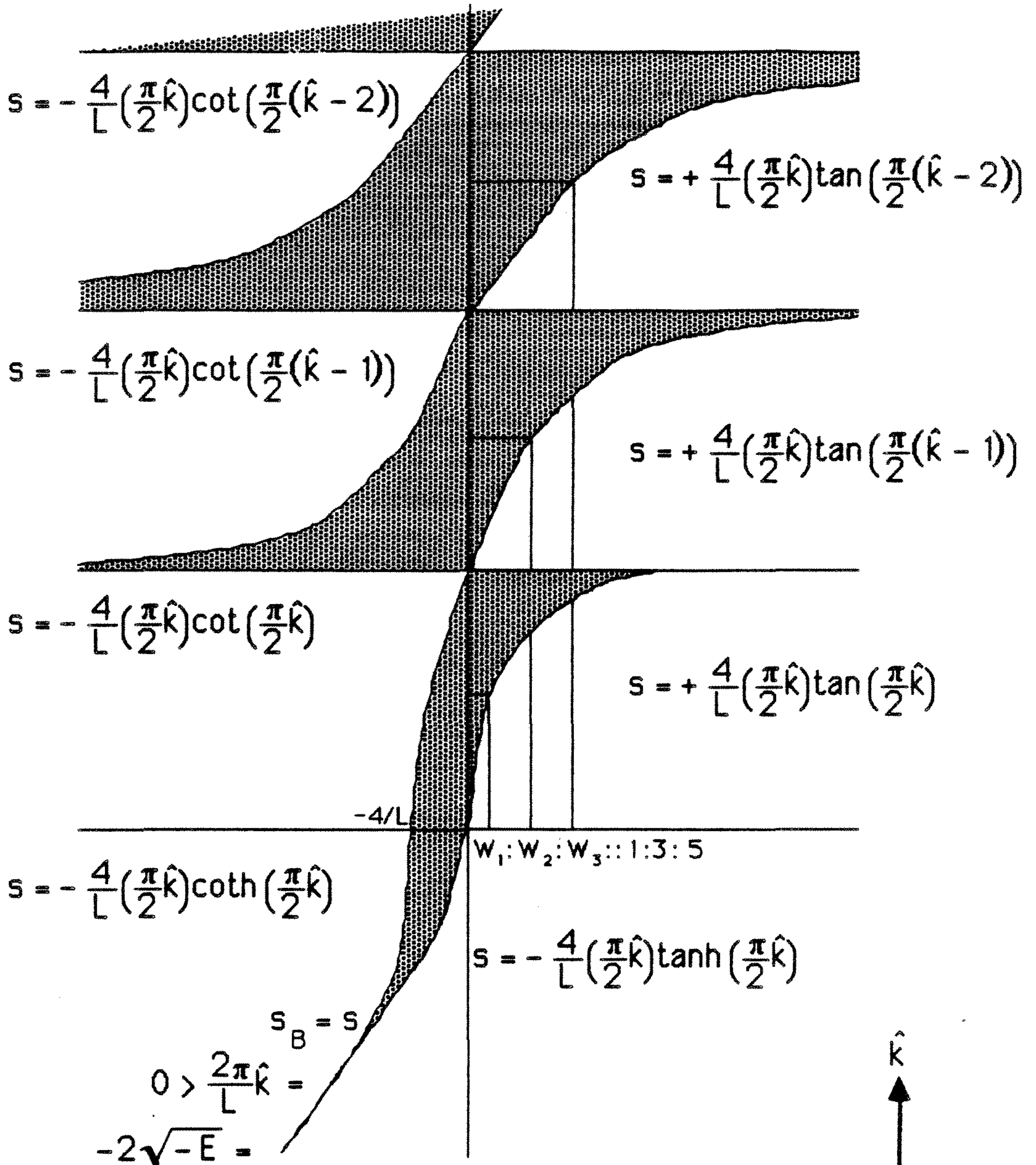
- It is convenient to work with the dimensionless wave number

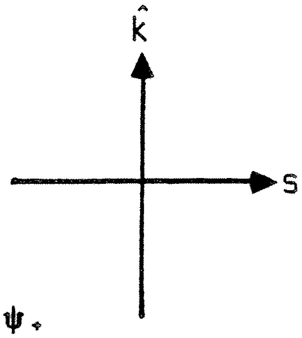
$$\hat{k} \equiv \frac{L}{\pi} \times \begin{cases} +\sqrt{+E} & E > 0\\ -\sqrt{-E} & E < 0.\end{cases}$$

Band Edge Wave Functions "Grown" From Limit Sinusoids and Resulting Schematic Spectrum

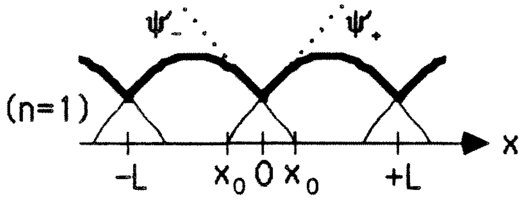


Exact Bands from Form of Band Edge Wave Functions





Sample s-dependent band edge calculation:



$$x_0 + L + x_0 = n\frac{\lambda}{2} \Rightarrow kx_0 = n\frac{\pi}{2} - \frac{kd}{2}$$

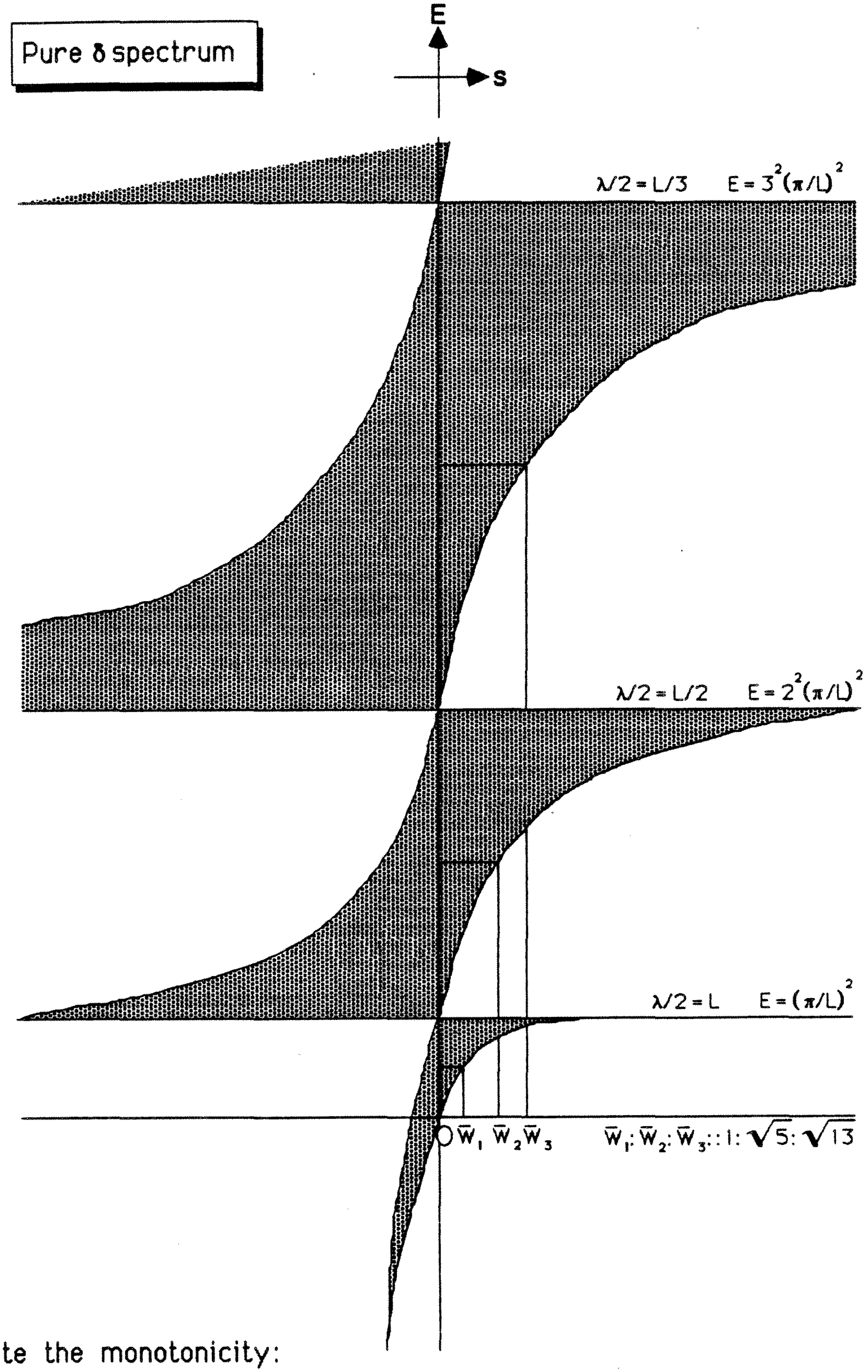
$$\psi_\pm = A\sin k(\pm x + x_0)$$

$\underline{x = 0}$

$$\Rightarrow \begin{cases} \psi_- = \psi_+ \\ \psi'_+ - \psi'_- = s\psi_\pm \end{cases}$$

$$\Rightarrow \begin{cases} \psi_\pm = A\sin kx_0 \\ 2kA\cos kx_0 = sA\sin kx_0 \end{cases}$$

$$\Rightarrow s = 2k\cot kx_0 = \pm\frac{4}{L}\left(\frac{\pi}{2}\hat{k}\right)\binom{\tan}{\cot}\left(\frac{\pi}{2}\hat{k}\right)$$



Note the monotonicity:

$\sigma(s^\infty) \subset \sigma(s_0^\infty)$ for $0 < s_0 < s < \infty$ or $-\infty < s < s_0 < 0$ and $E > 0$.

Natural Parameters Describing a Pure δ Array

- parameterize E by $\hat{k}$

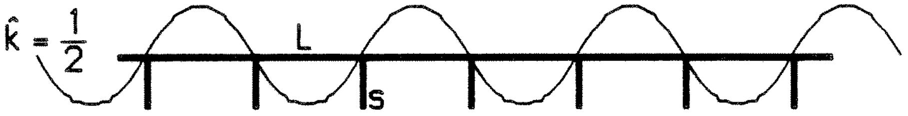
For E>0, the [real part of the] KP wave functions are "kinky sinusoids" and hence define a local wavelength $\lambda = 2\pi/k = 2\pi/\sqrt{E}$. Also, in a pure δ array, there is only a single length scale, the separation L. These suggest defining the dimensionless wave number

$$\hat{k} \equiv \frac{L}{\pi}\sqrt{E} = \frac{L}{\pi}k = \frac{L}{\lambda/2} \qquad (E > 0).$$

Note that

$$0 \to \hat{k} \to 1 \iff 0 \to E \to \left(\frac{\pi}{L}\right)^2$$

and so on. Geometrically, for E>0, $\hat{k}$ is the number of half-wavelengths (or "lobes") in a length L. For example,



- parameterize s by $\hat{s}$

A natural strength scale is set by the strength needed to form a bound state of energy E<0:

$$s_B = -2\sqrt{-E} < 0$$

Generalize this to E>0 and parameterize the dimensionless ratio s/s_B by

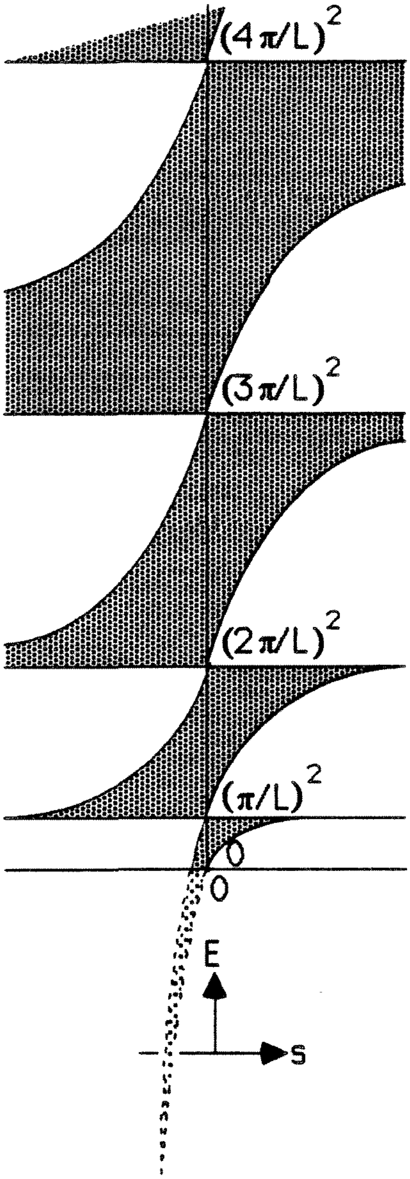
$$\tan\left(\frac{\pi}{2}\hat{s}\right) \equiv \frac{s}{|s_B|} = \frac{s}{2\sqrt{E}} = \frac{s}{2k} \quad \text{where } s_B \equiv i2\sqrt{E}\,.$$

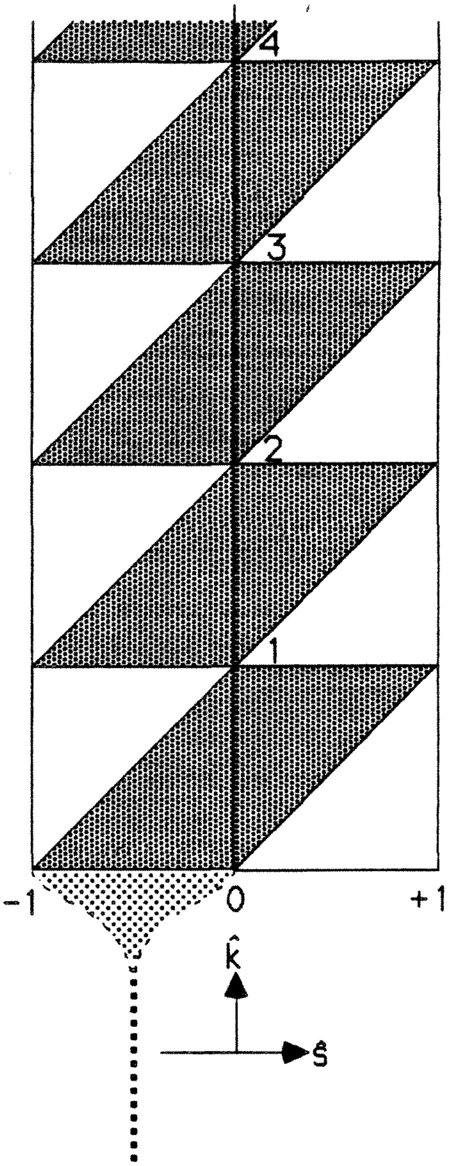
Note that

$$-1 \to \hat{s} \to +1 \iff -\infty \to s \to +\infty\,.$$

Note also that $\hat{s}$ depends on E.

Natural coordinates $(\hat{s},\hat{k})$ simplify the display of the $(0<E)$ spectrum.





In the $(\hat{s},\hat{k})$ representation, each "Brillouin zone" $(n \leq \hat{k} < n+1,\ n \in \mathbb{N})$ appears identical and both band edges are straight lines.

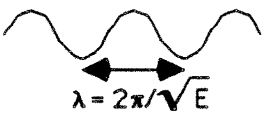
The Delta-Prime: δ'

Take

$$H\psi(x) = E\psi(x) \qquad H = \frac{p^2}{2m} + V(x) \qquad p = -i\hbar\frac{\partial}{\partial x} \qquad V(x) = s\delta'(x)$$

to mean

$$\left.\begin{array}{l} [\psi] = s'\psi' \\ [\psi'] = 0 \end{array}\right\} (x=0) \quad \&$$



$(x \neq 0)$,

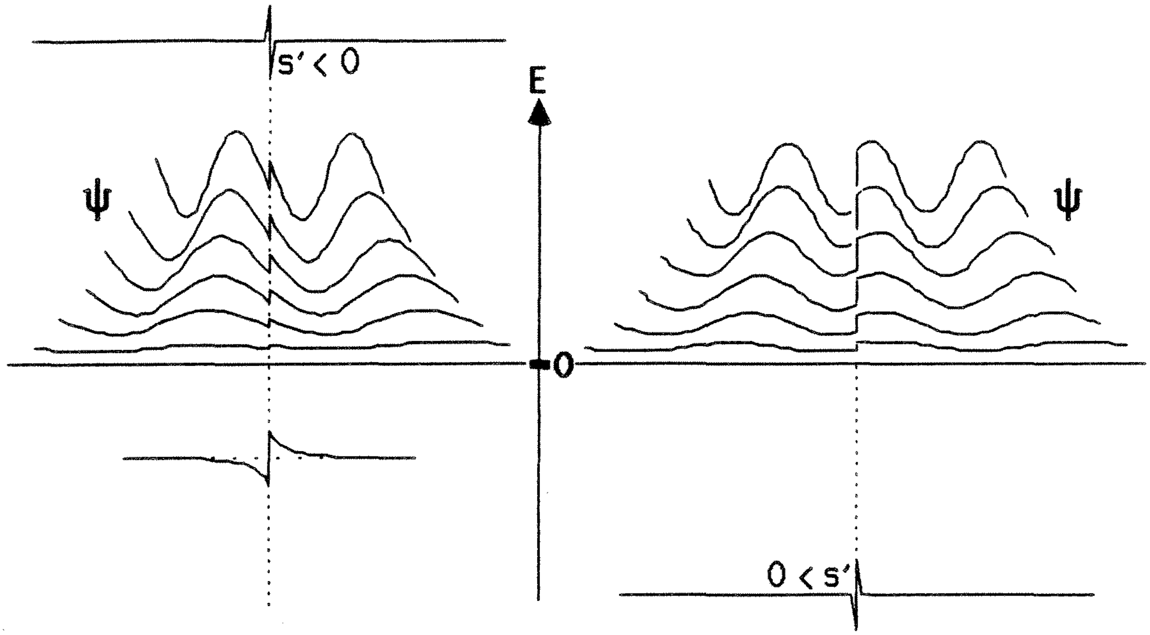
where the "jump" of f(x) at x_0 is

$$[f(x_0)] \equiv f(x_0+) - f(x_0-) = \lim_{\varepsilon \downarrow 0} \left(f(x_0+\varepsilon) - f(x_0-\varepsilon)\right).$$

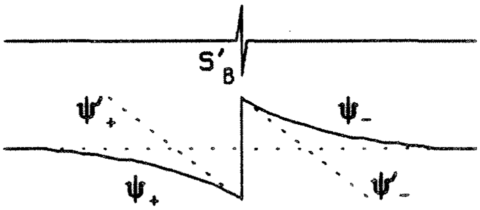
The spectral properties of H are then easily inferred. The eigenfunctions ψ, together with the eigenvalues E (which form the spectrum σ), are indicated on the next page (for fixed s′).

REMARKS:

- The δ' can <u>not</u> be understood as the "derivative" of the δ and hence can <u>not</u> represent a "point dipole." (According to [Gesztesy◆1988], the early intuition that motivated its name proved incorrect.)
- An exhaustive and rigorous analysis of the δ' can be found in [Gesztesy/Holden◆1987].



For each 0<E, it is easy to construct suitable (broken-sinusoidal) eigenfunctions. For E<0, there is only a single (broken-hyperbolic) eigenfunction with $s' = s'_B < 0$, such that



$$\psi_\pm(x) = A_\pm e^{\mp\sqrt{E}\,x}$$

$$x = 0 \Rightarrow \begin{cases} \psi'_- = \psi'_+ \\ \psi_+ - \psi_- = s'_B \psi'_\pm \end{cases}$$

$$\Rightarrow \begin{cases} \sqrt{-E}\,A_- = -\sqrt{-E}\,A_+ \\ \pm 2A_\pm = +s'_B A_\pm \sqrt{-E} \end{cases}$$

$$\Rightarrow \boxed{s'_B = -\frac{2}{\sqrt{-E}}} = i\frac{2}{k}\,.$$

s'_B sets the strength scale of the model. It is the δ' strength needed to bind a particle of energy E.

Propagation of ψ Through a δ' Array: Broken Sinusoids

$$\left.\begin{array}{l} H\psi = E\psi \\ H = -\Delta + \sum_n s'_n \delta'(\cdot - x_n) \end{array}\right\} \quad \text{means} \quad \left\{\begin{array}{l} [\psi] = s'_n \psi' \cdot [\psi'] = 0, \text{ at } x_n \\ \psi = A \sin(\sqrt{E}\, x + \phi), \text{ else} \end{array}\right.$$

Thus, if $0 = s' = (\dots, s'_n, \dots)$,

$$\psi_0(x) = \underbrace{\psi_0(0)\cos kx + \psi'_0(0)}\frac{\sin kx}{k} \qquad k \equiv \sqrt{E}$$

magnitude & slope
at origin specify sinusoid

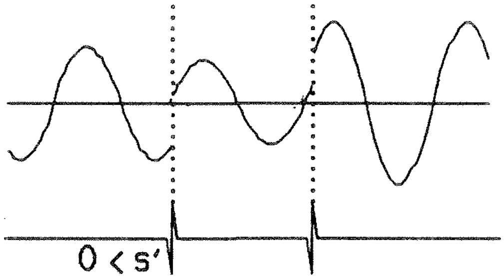
If $s' \neq 0$,

$$\psi_{s'}(x) = \psi_0(x) + \sum_{x_n < x} s'_n \psi'_{s'}(x_n) \cos k(x - x_n),$$

or

$$\psi_{s'}(x < x_{n+1}) = \psi_{s'}(x < x_n) + s'_n \psi'_{s'}(x_n) \cos k(x - x_n),$$

which facilitates the construction of solutions like:



REMARK: The above δ' solution $\psi_{s'}$ may be obtained by differentiating the corresponding δ solution ψ_s (see above) and exchanging primes and unprimes:

$$\psi' \text{ of } \delta \equiv \psi \text{ of } \delta'$$

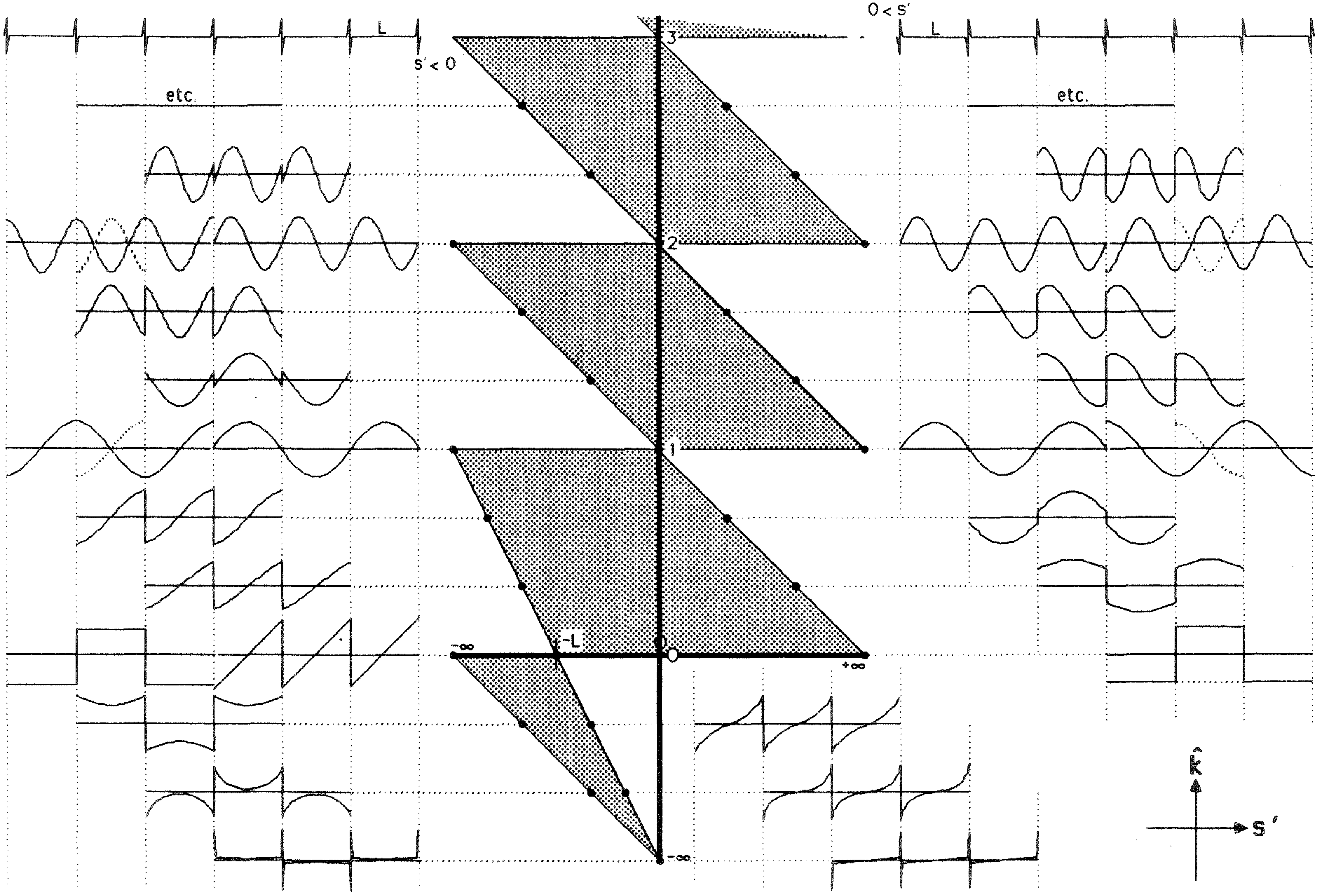
GROWING an ORDERed δ' Array

In the following pages the spectrum of a pure δ' array is constructed by "growing" it from obvious limit cases. The procedure is the same as that used for the pure δ array (see above), but the construction reveals several unexpected features of the spectrum. In particular, note

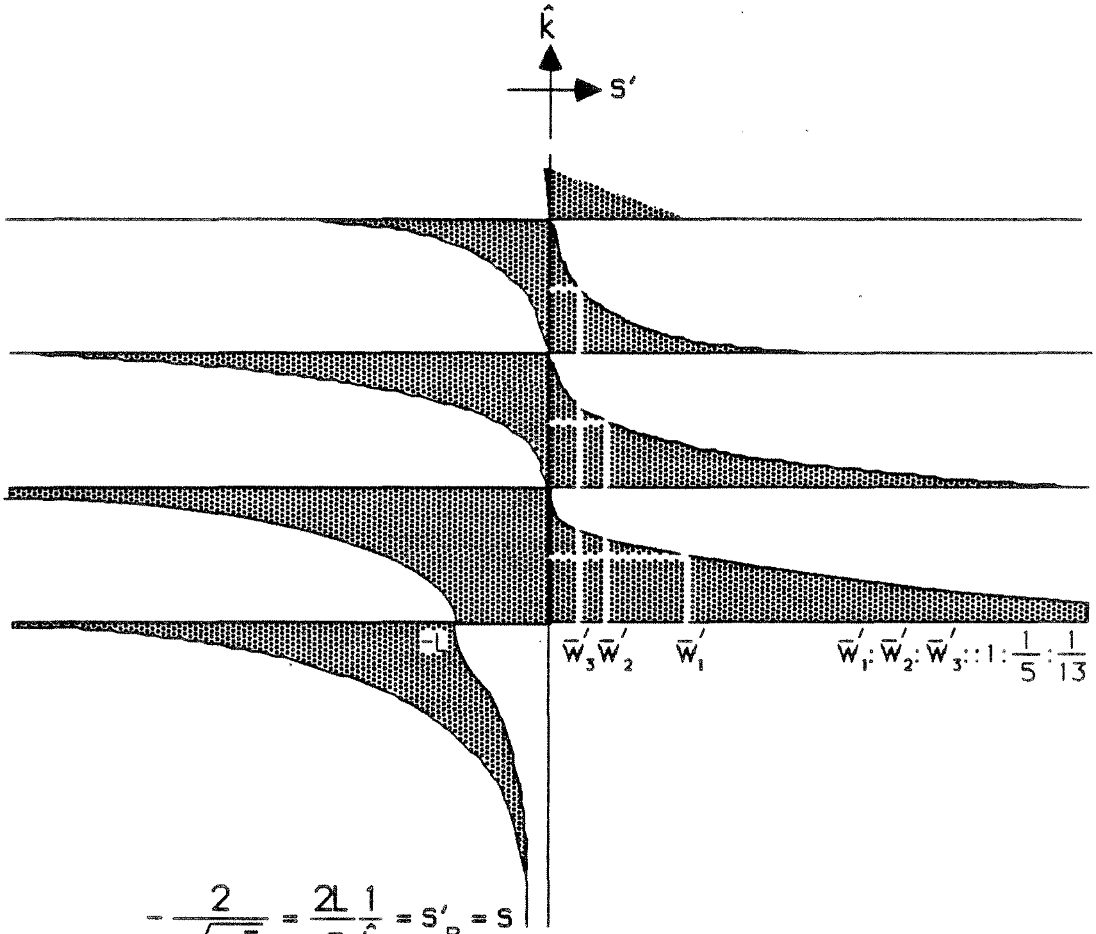
- the unusual behavior of the band "widths," and
- how eigenfunction degeneracy closes the first gap.

$$\left(\text{Also, recall that} \quad \hat{k} \equiv \frac{L}{\pi} \times \begin{cases} +\sqrt{+E} & E > 0 \\ -\sqrt{-E} & E < 0 . \end{cases} \right)$$

Band Edge Wave Functions "Grown" From Limit Sinusoids and Resulting Schematic Spectrum

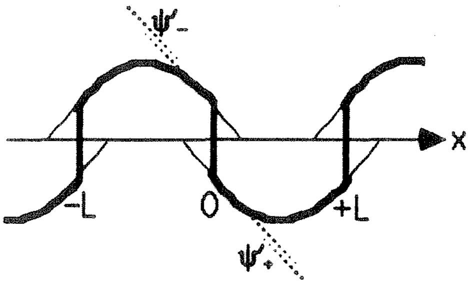


Exact Bands from Form of Band Edge Wavefunctions



$$-\frac{2}{\sqrt{-E}} = \frac{2L}{\pi}\frac{1}{\hat{k}} = s'_B = s$$

Sample s′-dependent band edge calculation:

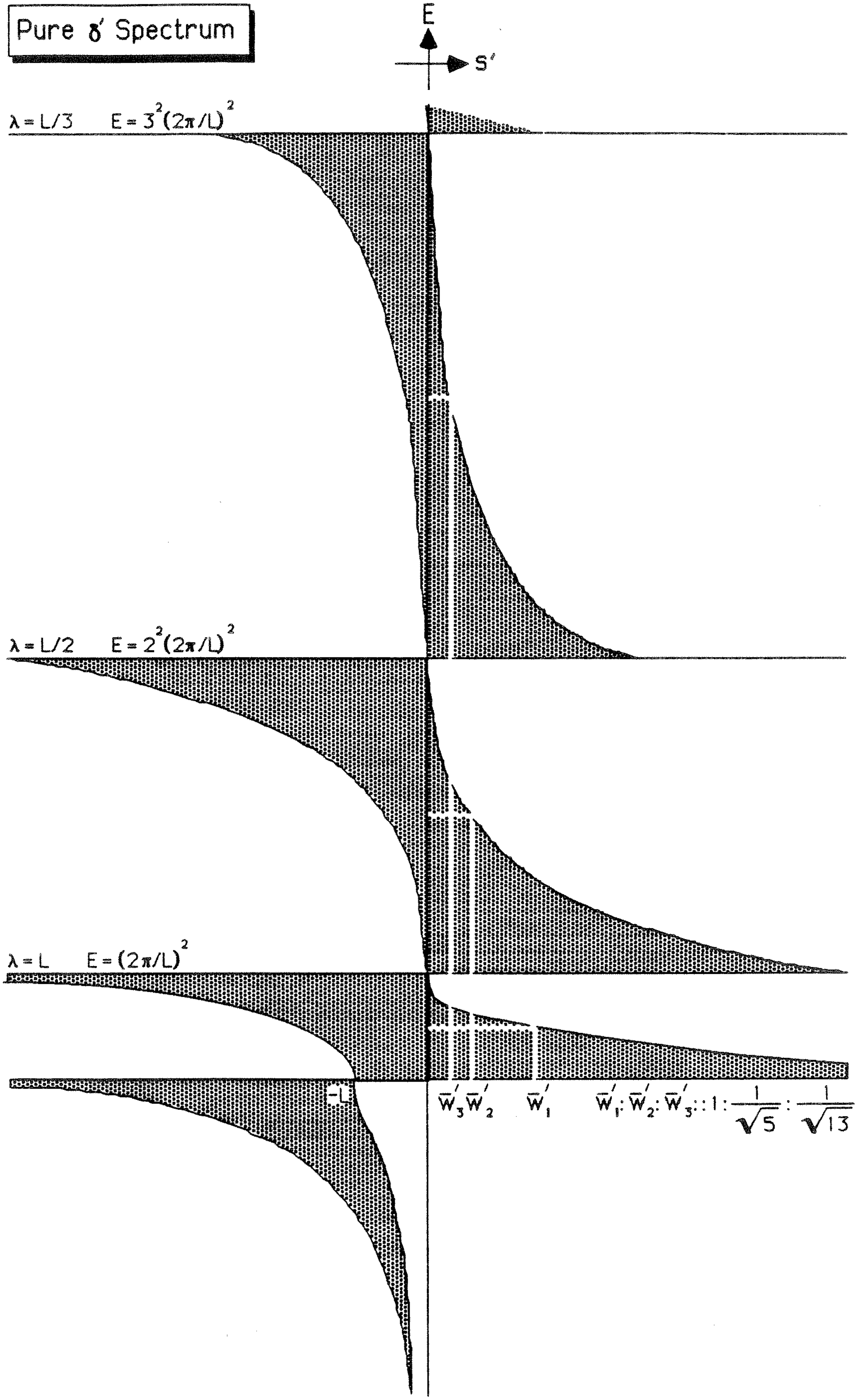


$$\psi_\pm = \mp A\cos k\left(x \mp \frac{L}{2}\right)$$

$$x = 0 \Rightarrow \begin{cases} \psi_+ - \psi_- = s'\psi'_\pm \\ \psi'_+ = \psi'_- \end{cases}$$

$$\Rightarrow \begin{cases} -2A\cos\frac{kL}{2} = -s'kA\sin\frac{kL}{2} \\ \psi'_\pm = -kA\sin\frac{kL}{2} \end{cases}$$

$$\Rightarrow s' = \frac{2}{k}\cot\frac{kL}{2} = L\frac{\cot\left(\frac{\pi}{2}\hat{k}\right)}{\left(\frac{\pi}{2}\hat{k}\right)}$$


Pure δ' Spectrum
E
S'
λ = L/3   E = 3²(2π/L)²
λ = L/2   E = 2²(2π/L)²
λ = L   E = (2π/L)²
-L
W̄'₃ W̄'₂
W̄'₁
W̄'₁: W̄'₂: W̄'₃ : : 1 : 1/√5 : 1/√13

GROWING DISORDER

As a first step to understanding the spectra of disordered sytems, many authors have studied the effects of defects on otherwise ordered systems (see, for example, [Bacon/Dean/Martin◆1962]). Qualitative descriptions of such spectra are easily obtained by the technique of "growing disorder." This heuristic perspective has guided my thinking throughout my research and made possible my major results. It is described below in detail but briefly, the idea is to transform an ordered array (whose spectrum is known) into a disordered array (whose spectrum is sought). The trick is to transform its spectrum along with it.

There follows:

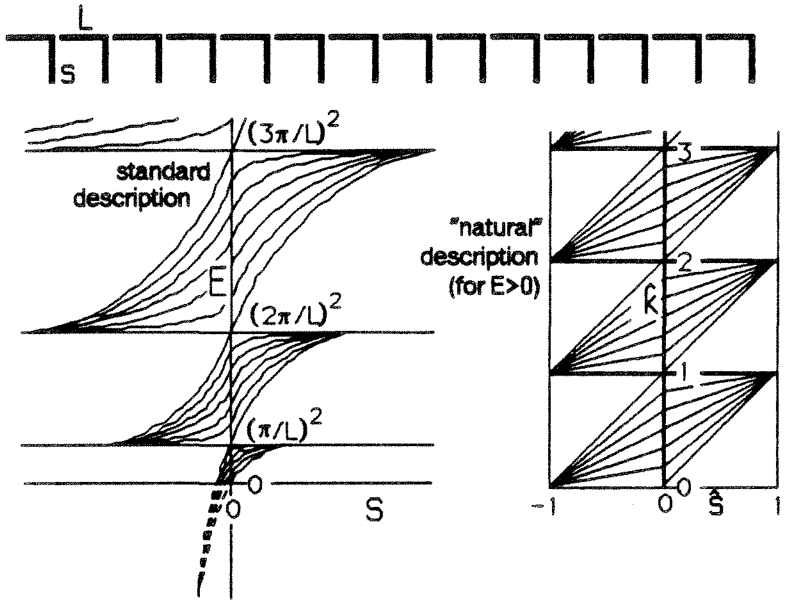
- an introduction to "spectral trajectories" (or "modal curves")
  (and a side-by-side comparison
  of the δ array
  and
  the harmonic chain)

- a set of rules constraining spectral trajectories
  (which account for their usefulness)

- two illustrations
  (one each of
  continuous
  and
  discrete
  growth).

Consider a pure δ array and its spectrum.

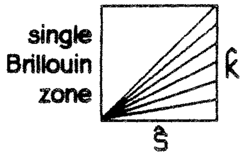
$(E,s) \rightarrow (\hat{k},\hat{s})$

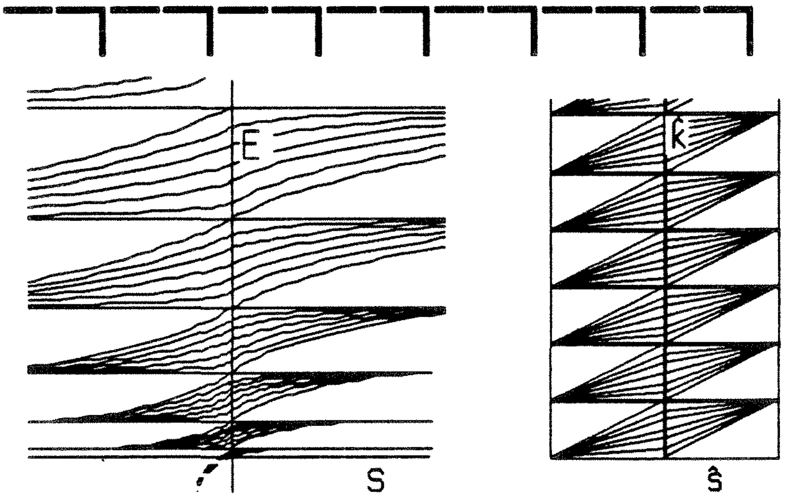


$$\hat{k} = L\frac{|s_B|}{2\pi} = \frac{L}{\pi}\sqrt{E}$$

$$\frac{s}{|s_B|} = \tan\left(\frac{\pi}{2}\hat{s}\right)$$

$$|s_B| = 2\sqrt{E} = 2k = \frac{4\pi}{\lambda}$$

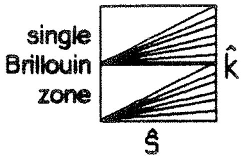




or

$$s = 2\sqrt{E}\tan\left(\frac{\pi}{2}s\right)$$

with E>0



The curves above are lines of constant integrated density of states. If the potential array is finite and consists of N δ's, then there are N such <u>spectral trajectories</u>. The nth one from the bottom is the nth energy level of the array as a function of the δ strength s:

$$H(s)\psi(s)=E(s)\psi(s).$$

$\psi(s)$ and $E(s)$ exist for each s, and ψ and E at a first s flow smoothly to ψ and E at a second s. This can be construed to follow from the <u>quantum adiabatic theorem</u>, which says, to paraphrase: In the limit of "slow" change, once in an eigenstate, always in an eigenstate.

and Harmonic Chains

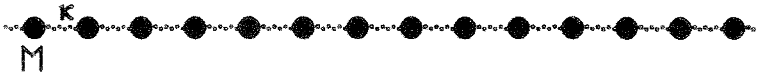
Consider a harmonic chain and its spectrum.

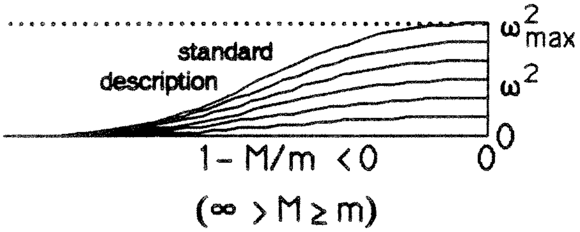
$$\left(\omega, \frac{M}{m}\right) \rightarrow (\hat{k}, \hat{M})$$

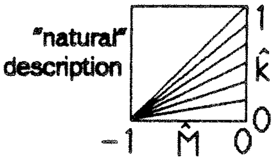
$$\omega = \omega_{max} \sin\left(\frac{\pi}{2}\hat{k}\right)$$

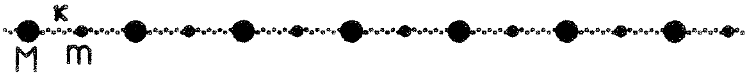
$$1 - \frac{M}{m} = \left(\left(\frac{\omega_{max}}{\omega}\right)^2 - 1\right) \tan\left(\frac{\pi}{2}\hat{M}\right)$$

where $\omega_{max} = 2\sqrt{\frac{\kappa}{m}}$





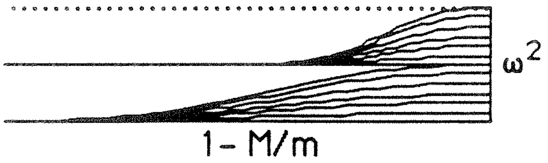


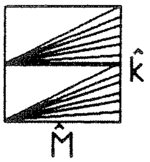


or

$$1 - \frac{M}{m} = \frac{\tan\left(\frac{\pi}{2}\hat{M}\right)}{\tan\left(\frac{\pi}{2}\hat{k}\right)}$$

where M/m>1

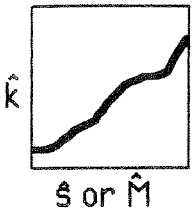




The curves above are lines of constant integrated density of states. If there are N masses in the chain, then there are N such <u>spectral trajectories</u>. Each trajectory is also a curve of constant <u>action</u>:

$$\text{action} = (\text{"area" of phase space orbit}) = \oint p\,dq \propto \frac{E}{\omega} = \frac{\text{energy}}{\text{frequency}}.$$

The action is an <u>adiabatic invariant</u>: "Slowly" changing the mass ratio M/m changes the energy E and frequency ω such that their ratio E/ω remains constant. (Note the classical-quantum correspondence.)



A spectral trajectory
(or "modal curve")
is constrained by
four simple rules.

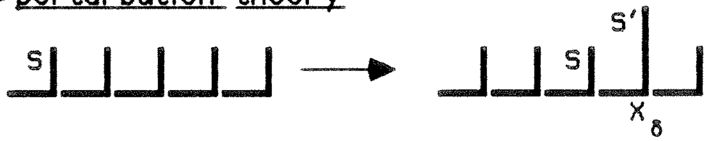
limit cases
- $\hat{s} = 0$ (free particle)
- $\hat{s} = \pm 1$ ($s = \pm \infty$) (disjoint, rigid, boxes)

ψ & λ $\left(\Rightarrow \hat{k} = \frac{L}{\pi}\sqrt{E}\right)$ are obvious

growth lemmas
- monotonicity
  - nondecreasing $\hat{s} > 0$
  - nonincreasing $\hat{s} < 0$
- increasing [decreasing] δ strength(s)
  either
  unperturbs a trajectory
  or
  raises [lowers] it,
  the change being bounded by
  the original next higher [lower] trajectory

The growth lemmas are suggested by the following ideas.

- perturbation theory

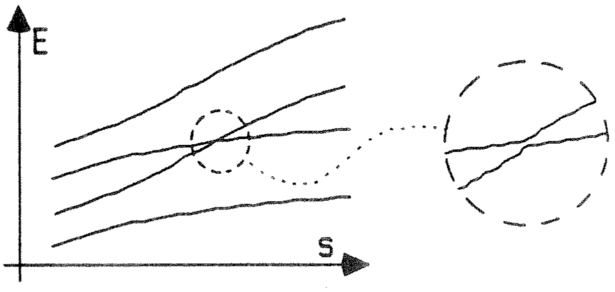


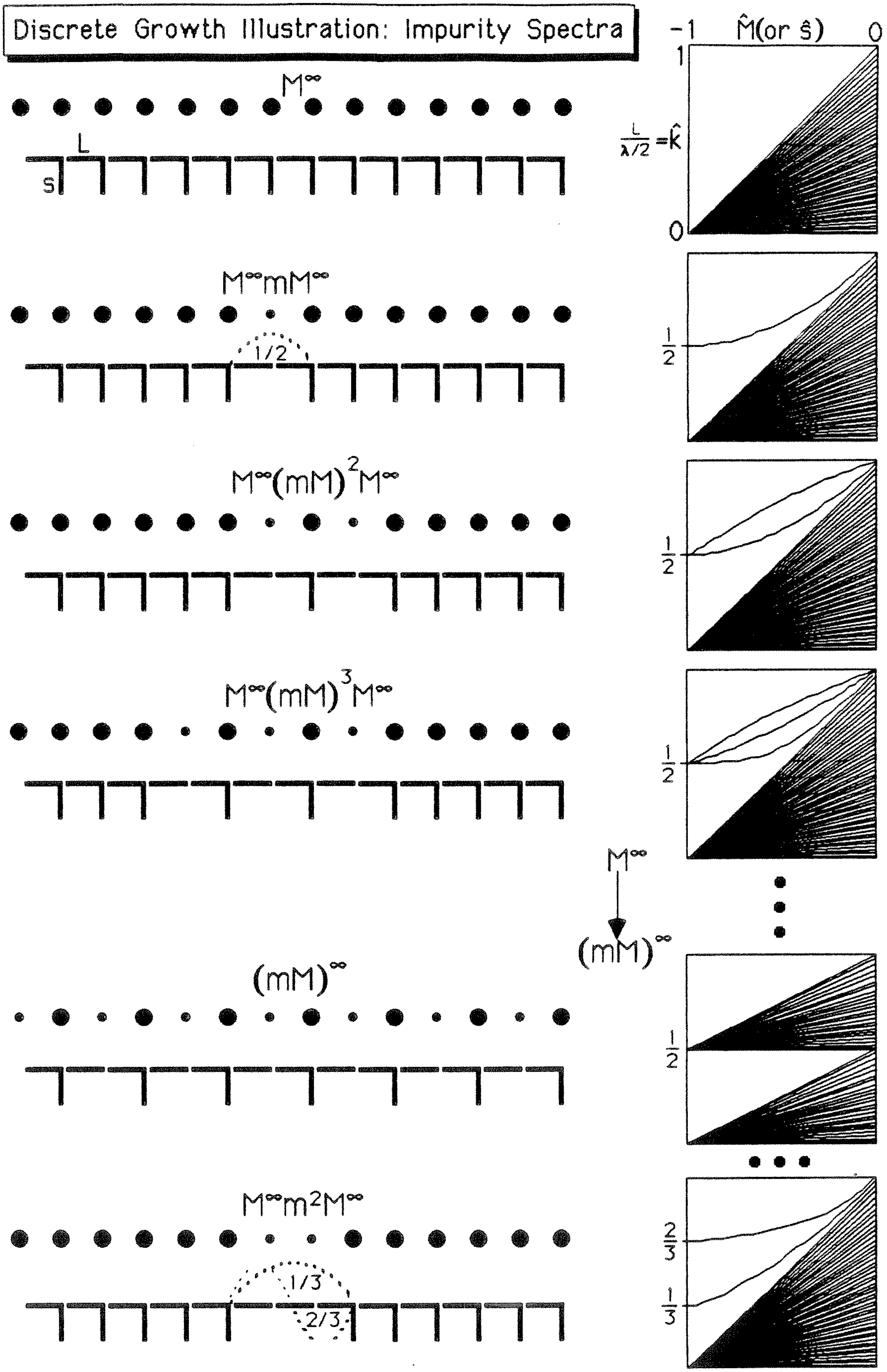
$$H' = H + W$$

$$E' \sim E + \langle\psi|W|\psi\rangle = E + \Delta s\,|\psi(x_\delta)|^2$$

where $\Delta s \equiv s' - s$

- level repulsion
  The eigensolutions of a (finite) 1-dimensional array are "unique" (=nondegenerate) and hence there is no crossing of levels.





Discrete Growth Illustration: Impurity Spectra

Continuous Growth Illustration

Consider a KP liquid and its spectrum (see facing page). Imagine slowly increasing the δ strength s from 0 to ∞. The eigenenergies must increase (or remain unchanged), but they cannot cross (as they are nondegenerate). Hence, they flow *en masse* to higher energies. The flow is nonuniform. The eigenenergies bunch up in some places and thin out in others. Eventually, the flow "chokes off" as zeros appear in the density of states. Then the opening of gaps tears the spectrum apart.

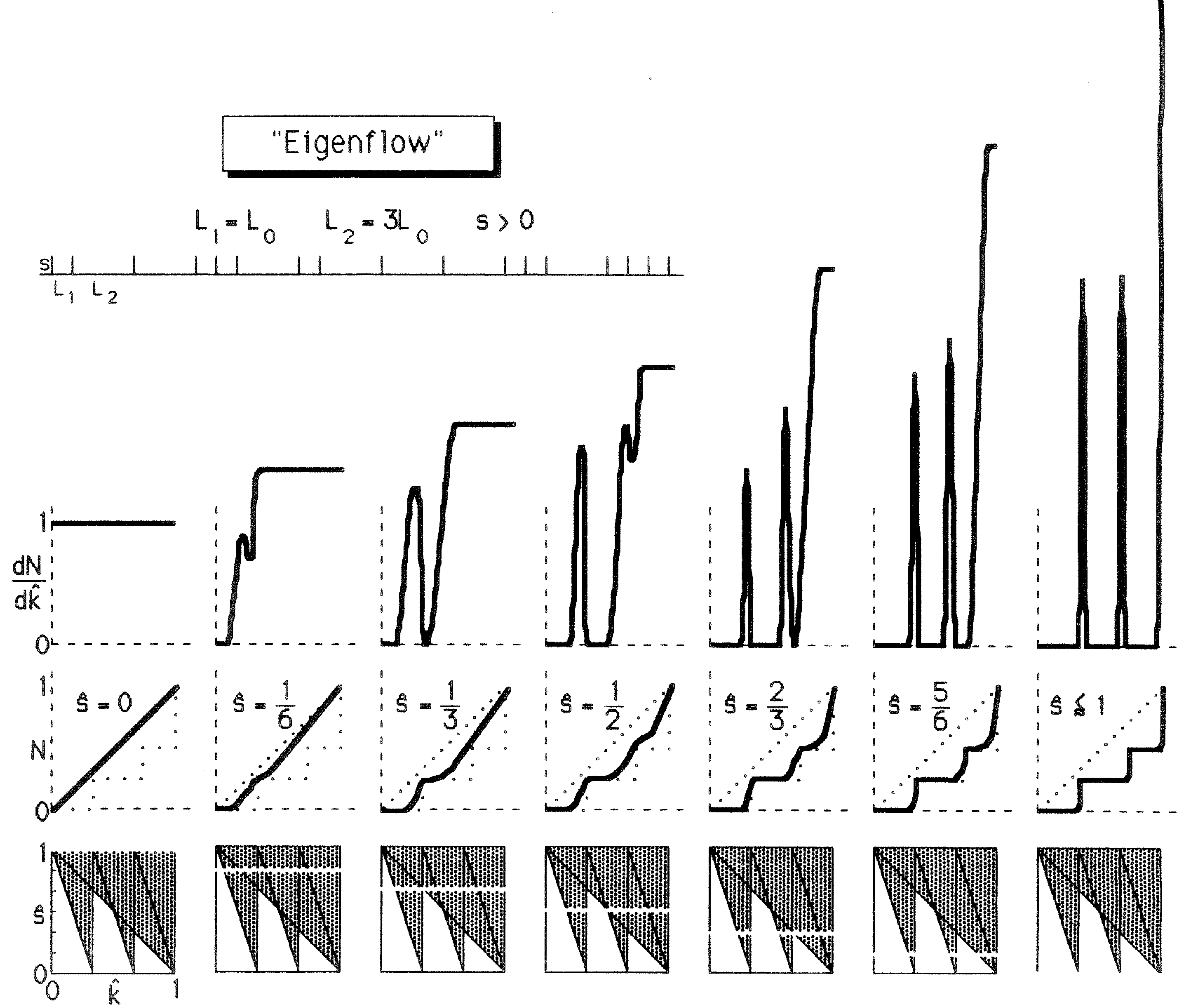
(The <u>integrated density of states</u> for a finite array is

$$N_L(E) \equiv \begin{pmatrix}\text{number of states}\\ \text{with energy} \leq E\end{pmatrix}/L \sim \begin{pmatrix}\text{number of}\\ \text{zeros of } \psi_E\end{pmatrix}/L.$$

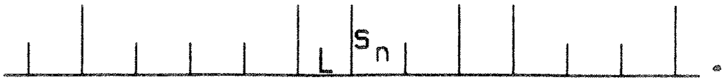
For an infinite array,

$$N(E) \equiv \lim_{L\uparrow\infty} N_L(E).$$

The limit is known to exist and to be a.s. a nonrandom continuous nondecreasing function (see [Pastur◆1980]). The <u>density of states</u> is simply dN/dE, where it exists.)


"Eigenflow"
$L_1 = L_0$ $L_2 = 3L_0$ $s > 0$
s
L_1 L_2
$\frac{dN}{d\hat{k}}$
1
0
N
1
0
$\hat{s}$
1
0
0
$\hat{k}$
1
$\hat{s} = 0$
$\hat{s} = \frac{1}{6}$
$\hat{s} = \frac{1}{3}$
$\hat{s} = \frac{1}{2}$
$\hat{s} = \frac{2}{3}$
$\hat{s} = \frac{5}{6}$
$\hat{s} \lesssim 1$

Consider a KP-alloy:



($s_n > 0$ or $s_n < 0$ & $E > 0$)

The spectrum of a typical mixed-strength, fixed-length δ array is the union of the spectra of all possible pure δ arrays formed from it.

$$\boxed{\sigma(\text{mixed-strength}) \overset{\text{a.s.}}{=} \overline{\bigcup \sigma(\text{fixed-strength})}}$$

Why?

Key: s-independent band edge ψ

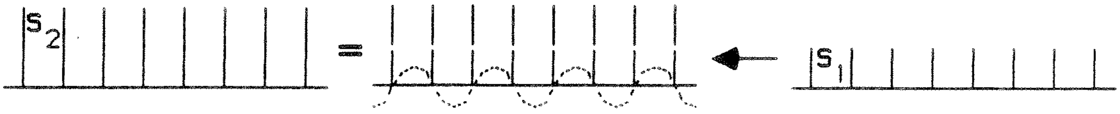
Know: $\sigma(\text{random}) \overset{\text{a.s.}}{=} \overline{\bigcup \sigma(\text{periodic})} \supseteq \overline{\bigcup \sigma(\text{pure})}$

Need show: $\sigma(\text{random}) \subseteq \overline{\bigcup \sigma(\text{pure})}$

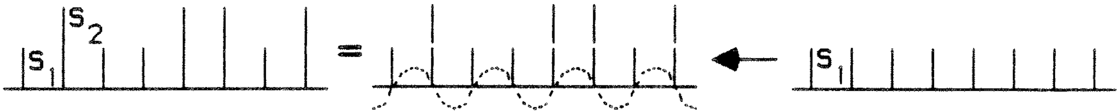
In fact: $\sigma(\text{random}) \subseteq \sigma(s^{\infty}_{\min}) = \overline{\bigcup \sigma(\text{pure})}$ where $s_{\min} \equiv \min_n \{s_n\}$

Idea: "Grow" the random array from the $s^{\infty}_{\min}$ array, and "grow" the spectrum along with it.

This is illustrated below with repulsive δ's.



$\sigma(s_2^\infty) \subset \sigma(s_1^\infty)$

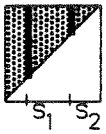


$\sigma(\text{random}) \subseteq \sigma(s_1^\infty)$

$s_2 > s_1 = s_{min} = \min\{s_1, s_2\}$

The spectrum contracts under these continuous transformations as the growth of the repulsive δ's raises the energies of some of the wave functions but not through the energies of the s-independent band edge wave functions that don't "feel" them.

The first illustration above can be understood as the aforementioned monotonicity of $\sigma(s^\infty)$ with s.



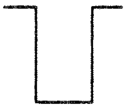
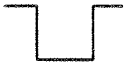
The second is the insight that clinches the result.

REMARKS:

- The conclusion is actually

$$\sigma(\{s_n\}) \overset{a.s.}{=} \sigma(s^\infty_{min}), \text{ where } s_{min} = \min_n\{s_n\},$$

which can be found in [Kirsch/Martinelli◆1982]. (Although it is the above, new, formulation that generalizes; see below.) Thus, for example, altering a fraction of the δ strengths in an array doesn't (typically) alter the spectrum!

- The above argument hinges on the point nature of the interaction. In fact, the result is false for the next simplest interaction, namely, the "finite square wells"  and  . See [Kerner◆1954].

- However, there are generalizations:
  - [Gesztesy/Holden/Kirsch◆1988] handles arrays of mixed attractive and repulsive δ's, $s \lessgtr 0$.
  - [Kirsch/Martinelli◆1982] considers generalized interactions, $\delta \to f$.

- The argument implies $\sigma(\text{mixed}) \subset \bigcup \sigma(\text{fixed})$

$$\Leftrightarrow E \in \sigma(\text{mixed}) \Rightarrow E \in \bigcup \sigma(\text{fixed})$$

$$\Leftrightarrow E \notin \bigcup \sigma(\text{fixed}) \Rightarrow E \notin \sigma(\text{mixed})$$

$$\Leftrightarrow E \in \bigcap \rho(\text{fixed}) \Rightarrow E \in \rho(\text{mixed}) \text{ where } \rho = \sigma^c = \mathbb{R} - \sigma.$$

Essentially, this is the seminal conjecture of [Saxon/Hutner◆1949].

- An <u>atypical</u> realization of "random" is s^∞_2. But $\sigma(s^\infty_2) \not\supseteq \sigma(s^\infty_1)$ <u>and</u> $s_2 > s_1$. Hence, the "a.s." in $\sigma(\text{random}) \overset{as}{\supseteq} \sigma(\text{pure})$.

Consider a <u>KP-liquid</u> :

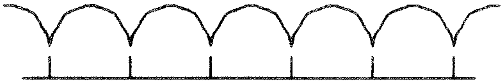
($s > 0$ <u>or</u> $s < 0$ & $E > 0$)

The spectrum of a typical mixed-length, fixed-strength δ array is the union of the spectra of all possible pure δ arrays formed from it.

$$\boxed{\sigma(\text{mixed-length}) \overset{\text{a.s.}}{=} \overline{\bigcup \sigma(\text{fixed-length})}}$$

<u>Why ?</u>

Key: s-dependent band edge ψ



Know: $\sigma(\text{random}) \overset{\text{a.s.}}{=} \overline{\bigcup \sigma(\text{periodic})} \supseteq \overline{\bigcup \sigma(\text{pure})}$

Need show: $\overline{\bigcup \sigma(\text{periodic})} \subseteq \overline{\bigcup \sigma(\text{pure})}$

$\Longleftarrow \quad \sigma(\text{periodic}) \subseteq \overline{\bigcup \sigma(\text{pure})} \quad (\forall \text{ periodic})$

$\Longleftarrow \quad E \in \sigma(\text{periodic}) \Rightarrow E \in \sigma(\text{pure}) \ (\forall E)\ (\forall \text{ periodic})\ (\exists \text{ pure})$

Idea: For fixed E, state with highest s is an s-dependent band edge. The argument below demonstrates, by explicit construction, that a point in the spectrum of any periodic liquid is contained in the spectrum of a pure array.

For any spectral point (s, k) in the s-k plane of a given periodic liquid, here is constructed an s-dependent band edge wave function that passes at greater s, and hence below, (s, k), and thereby defines a spectral "wedge" containing (s, k).

Fix E (hence λ). Choose s>0. Pick a point in the spectrum of the liquid. The (real part of) corresponding wave function is a kinky sinusoid. (In the drawing, vertical lines ⇒ δ's and horizontal lines ⇒ amplitudes.)

- **LOCATE** a "local maximum" = interval characterized by "amplitude of (center) sinsuoid is <u>at least</u> that of adjacent sinuoids". (Why? Consider ψ as $s\uparrow\infty$.)

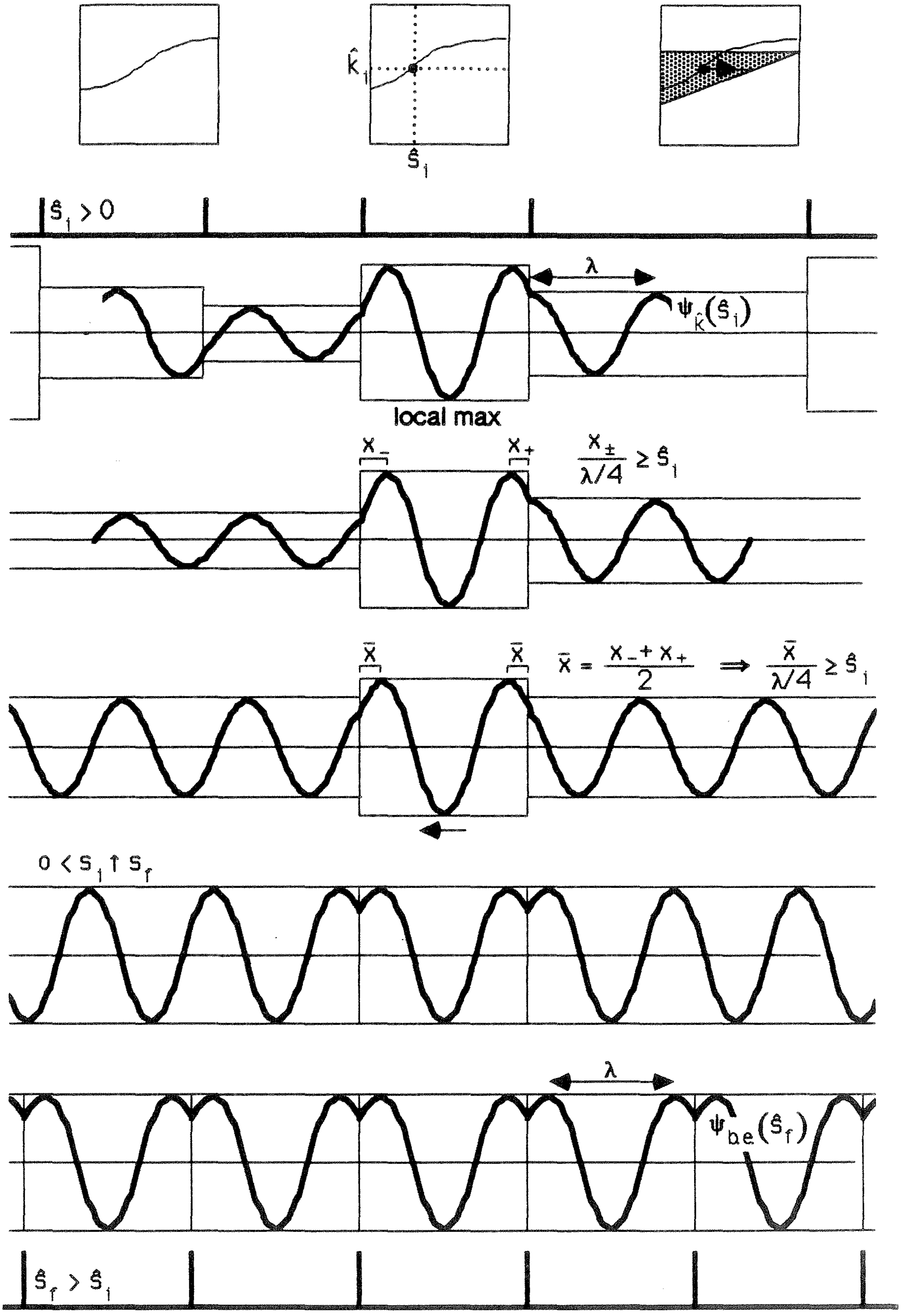
- **FREE** it and its adjacent sinusoids from the array. Only 2 δ's and 2 kinks remain. At both δ's, the condition for negative amplitude shift is satisfied (see above).

- **SYMMETRIZE** by translating the center sinusoid. Adjacent sinusoids adapt so that the adjacent amplitudes
  - equalize at an
  - amplitude <u>not greater than</u> the center amplitude

  as the condition for negative amplitude shift is still satisfied.

- **EQUALIZE** the adjacent amplitudes by increasing s (and hence deepening the kinks), while holding the center sinusoid fixed.

- **REPLICATE** the center cell. The result is an s-dependent band edge wave function
  - of a pure component of the liquid
  - that passes the chosen spectral point at greater s.


$\hat{k}_1$
$\hat{s}_1$
$\hat{s}_1 > 0$
λ
$\psi_{\hat{k}}(\hat{s}_1)$
local max
x_-
x_+
$\frac{x_\pm}{\lambda/4} \geq \hat{s}_1$
$\bar{x}$
$\bar{x}$
$\bar{x} = \frac{x_- + x_+}{2} \Longrightarrow \frac{\bar{x}}{\lambda/4} \geq \hat{s}_1$
$0 < s_1 \uparrow s_f$
λ
$\psi_{be}(\hat{s}_f)$
$\hat{s}_f > \hat{s}_1$

REMARKS:

- This result is new. A similar argument should work for the δ' model.
- Since the spectrum is a closed set, and an infinite union of closed sets need not be closed, it may be necessary to close the union of pure spectra when forming the generic random spectrum. That is why there is a closure in the statement,

$$\sigma(\text{random}) \overset{\text{a.s.}}{=} \overline{\bigcup \sigma(\text{pure})} .$$

- For the binary harmonic chain (which is, of course, an "alter ego" of the attractive s<0 KP liquid), the "pure components" are chains that I call "lightweights." They are of the form,

$$(Mm^n)^\infty \text{ where } n \in \{0, 1, 2, \ldots\}.$$

Periodic with one heavy mass-per-unit cell, this family of chains systematically lightens to an all-heavy chain and systematically "heavies" to an all-light chain. The lightweights are fundamental constituent chains in that any mixed chain is a concatenation of lightweight chains.

$$\cdots MMmMmMMMmmmMmMm \cdots \equiv \cdots (M)(Mm)^2(M)^2(Mm^3)(Mm)^2 \cdots$$

Spectral Construction

On the following pages, the spectra of various δ arrays and/or harmonic chains (including those of the initial experiments) are constructed simply from the spectra of their pure components.

The construction utilizes the major result:

$$\overline{\bigcup \sigma(\text{fixed-length})} \overset{\text{a.s.}}{=} \sigma(\text{mixed-length}).$$

Special attention is given to the complementary "resolvent" or "gap" sets.

Construction Guideline

① $L_0 \quad s > 0$

As a warm-up, and to introduce the style of presentation, here is a pure array, its spectrum (="bands"), and its complement (="gaps"). The complement is presented twice, once in $(\hat{s},\hat{k})$ and once in (s,E). Gaps open only at $s=0$.

② $L_1 = L_0 \quad L_2 = 2L_0 \quad s > 0$

Two simplest commensurate lengths. Gaps open at 2 values of s.

③ $L_1 = 2L_0 \quad L_2 = 3L_0 \quad s > 0$

Two commensurate lengths. Gaps open at 4 values of s.

④ $L_1 = L_0 \quad L_2 = \sqrt{2}L_0 \quad s > 0$

Two incommensurate lengths. Gaps open at infinite values of s. Compare with (5).

⑤ $L \in [L_0, \sqrt{2}L_0] \quad s > 0$

A continuum of lengths. Only 3 gaps! Compare with (4).

⑥ $L_1 = L_0 \quad L_2 = 2L_0 \quad L_3 = 3L_0 \quad s < 0$

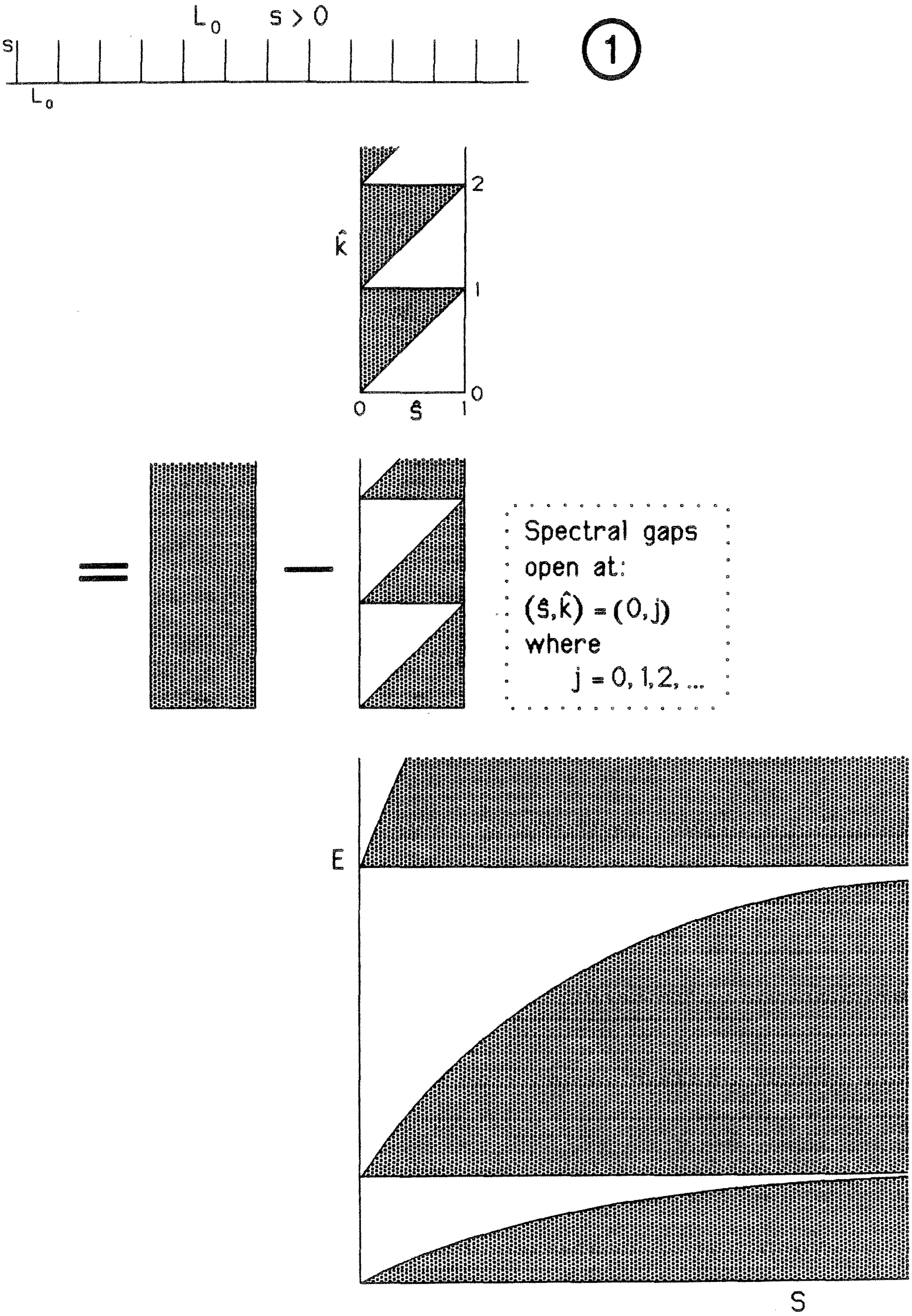
or $M \geq m$ & **no more than 3 consecutive m's anywhere in the chain**

Finite gaps. Compare with (7). The spectral complement is presented twice, once in $(\hat{s},\hat{k})$ or $(\hat{M},\hat{k})$ and once in $(M/m, \omega^2)$.

⑦ $L_n = nL \quad (n \in \mathbb{N}) \quad s < 0$

or $M \geq m$

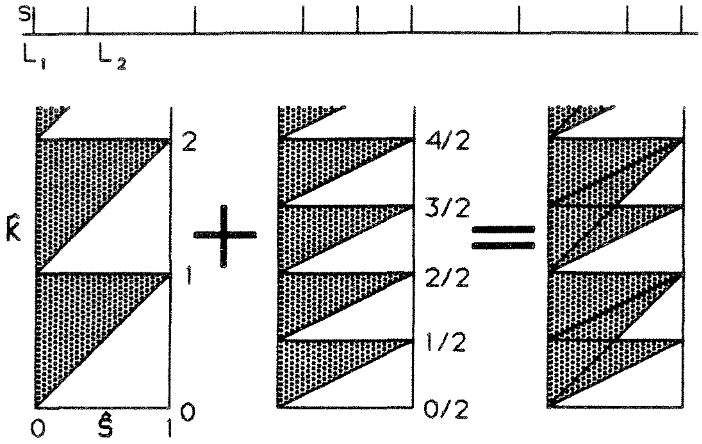
Infinitesimal gaps. Compare with (6).

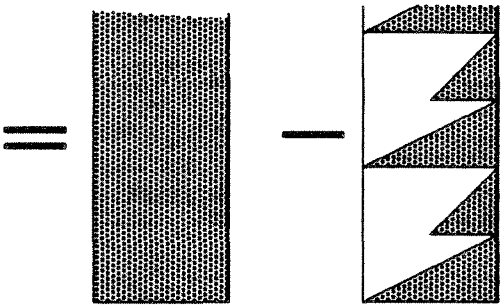


①

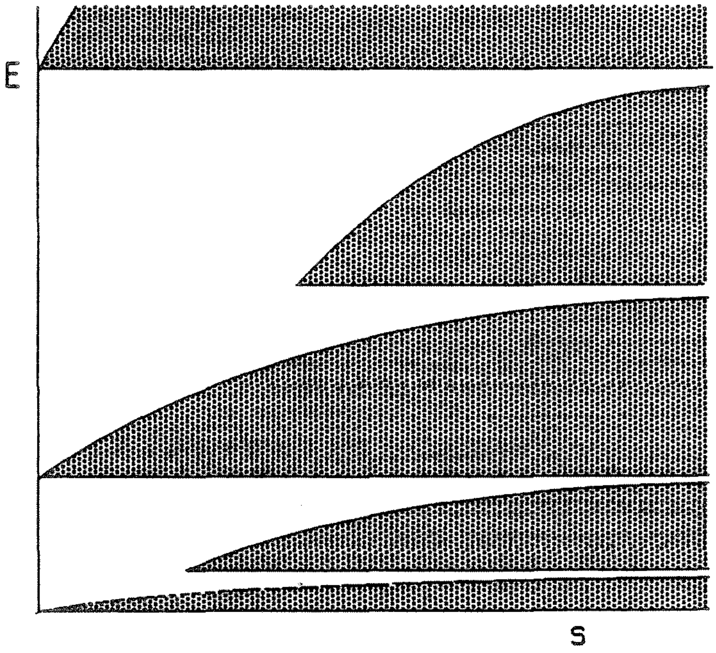
Spectral gaps open at: $(\hat{s},\hat{k}) = (0,j)$ where $j = 0, 1, 2, \ldots$

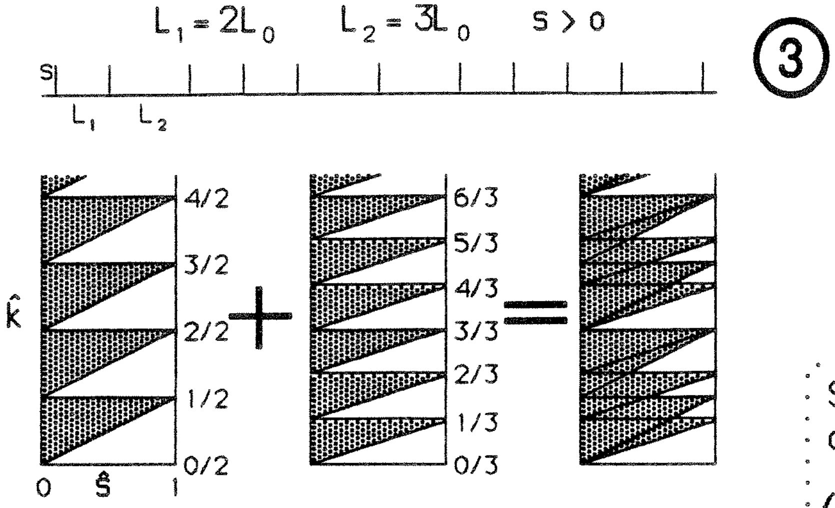
$L_1 = L_0 \quad L_2 = 2L_0 \quad s > 0$ ②

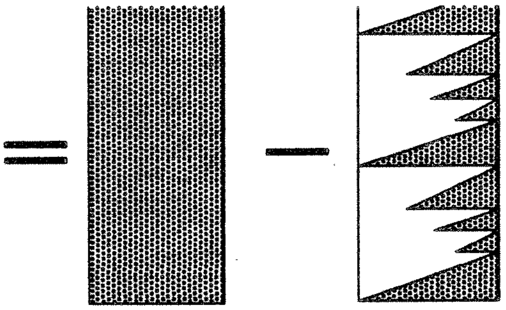




Spectral gaps
open at:
$(\hat{s},\hat{k}) = (0,j)$ &
$= \left(\frac{1}{2}, j+\frac{1}{2}\right)$
where
$j = 0, 1, 2, \ldots$





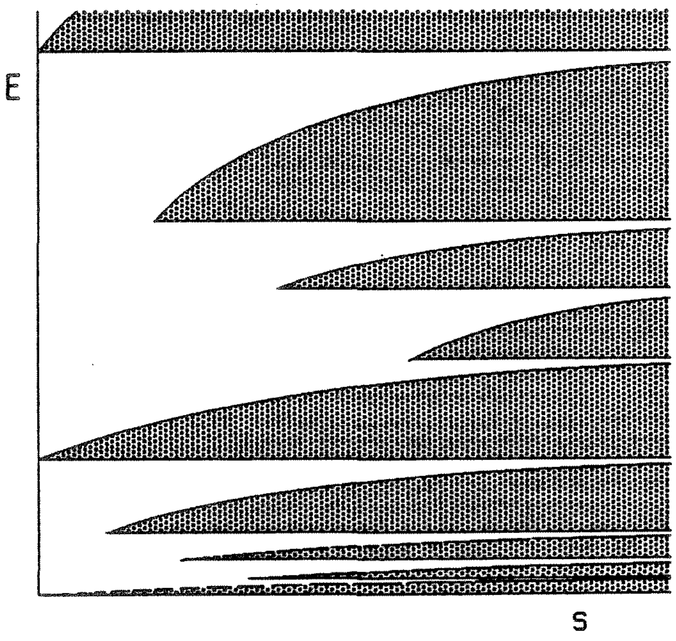


Spectral gaps open at:

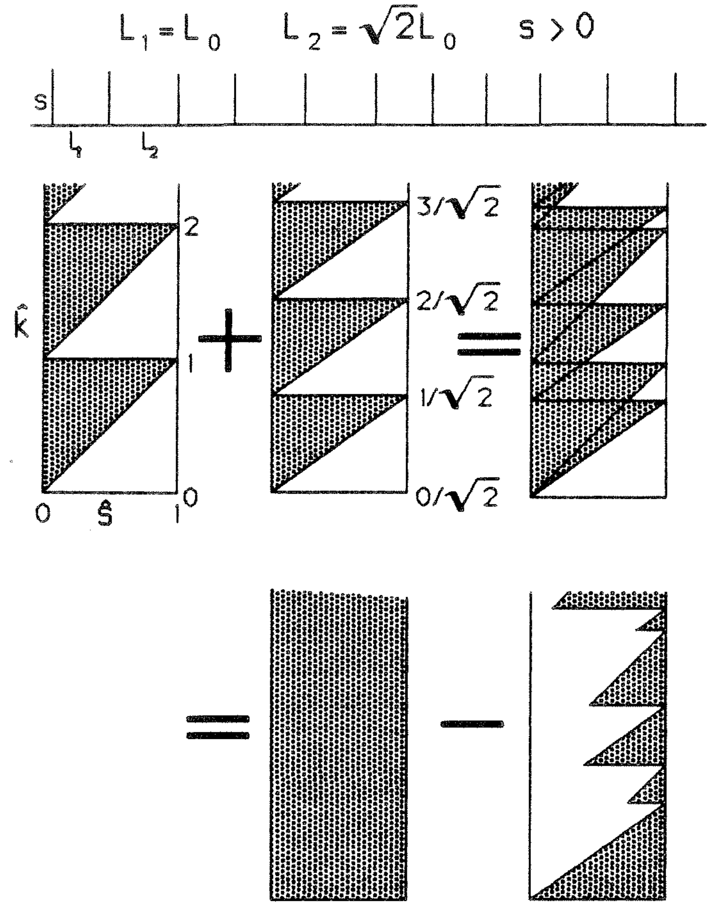
$$(\hat{s},\hat{k}) = (0, j)\ \&$$
$$= \left(\frac{1}{3}, j + \frac{2}{3}\right)\ \&$$
$$= \left(\frac{1}{2}, j + \frac{1}{2}\right)\ \&$$
$$= \left(\frac{2}{3}, j + \frac{1}{3}\right)$$

where

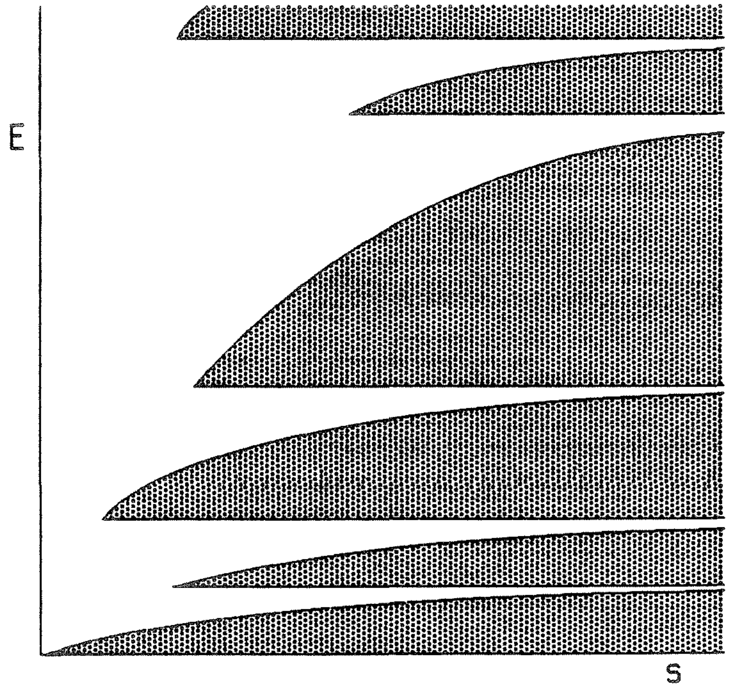
$j = 0, 1, 2, \ldots$



④

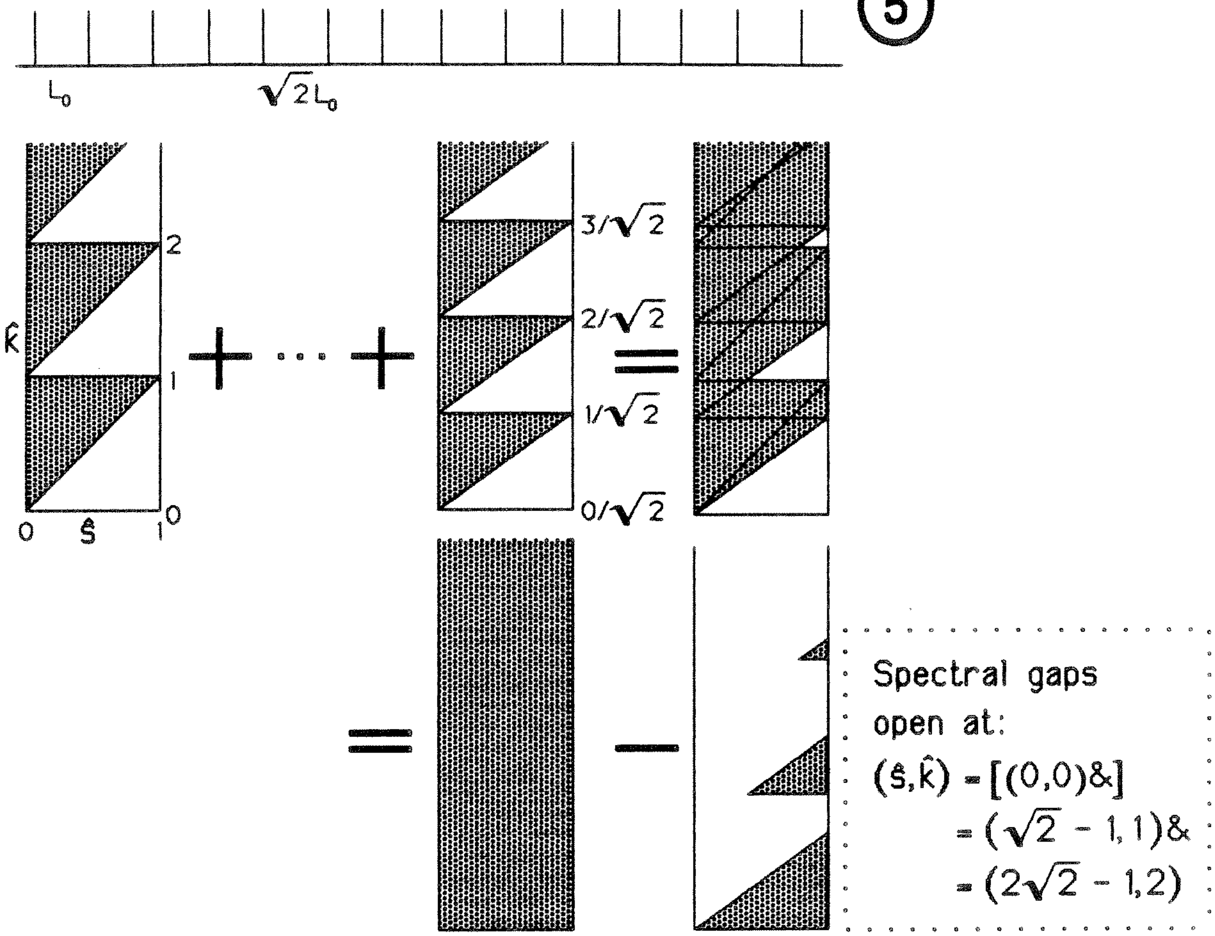


Spectral gaps
open at:
$(\hat{s},\hat{k}) = (j\sqrt{2} (\mathrm{mod}\ 1), j)$ &
$= \left(j\frac{1}{\sqrt{2}} (\mathrm{mod}\ 1), j\frac{1}{\sqrt{2}}\right)$
where
$j = 0, 1, 2, \ldots$

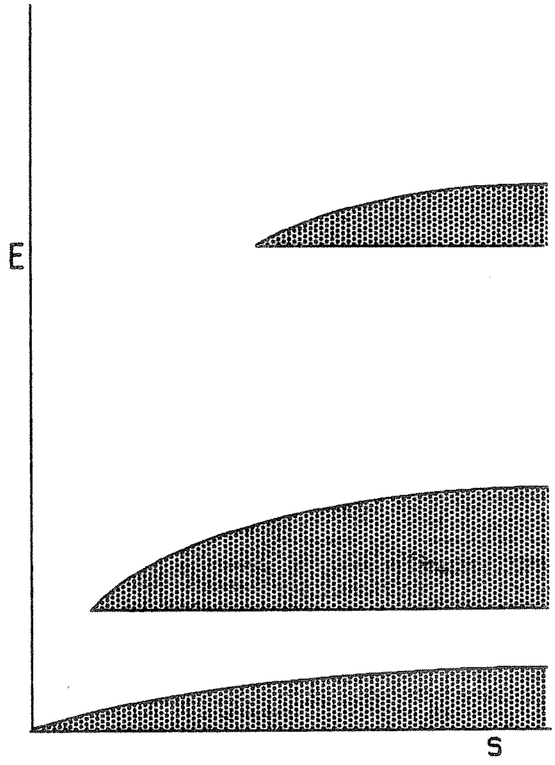


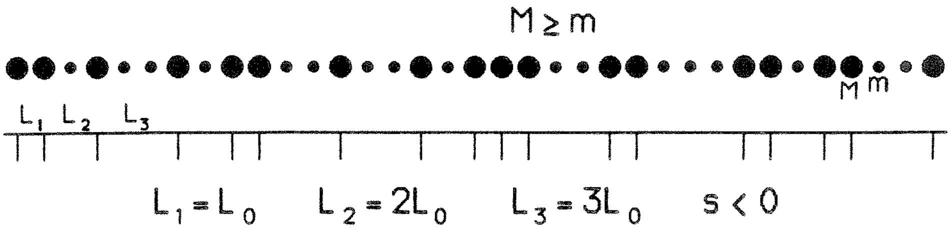
$L \in [L_0, \sqrt{2}L_0] \quad s > 0$

⑤

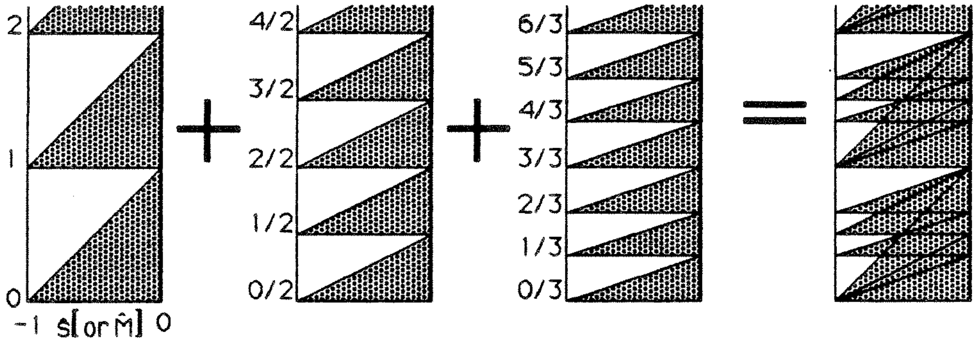


Spectral gaps open at:
$(\hat{s},\hat{k}) = [(0,0)\&]$
$= (\sqrt{2}-1, 1)\&$
$= (2\sqrt{2}-1, 2)$





⑥



Spectral gaps
open at:

$(\hat{s}\ [\text{or } \hat{M}], \hat{k}) = (0, j+1)\ \&$

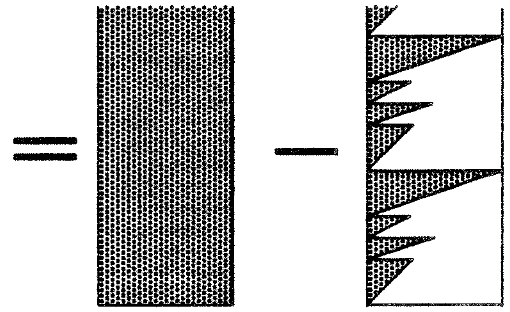
$= \left(-\frac{1}{2}, j+\frac{1}{2}\right)\ \&$

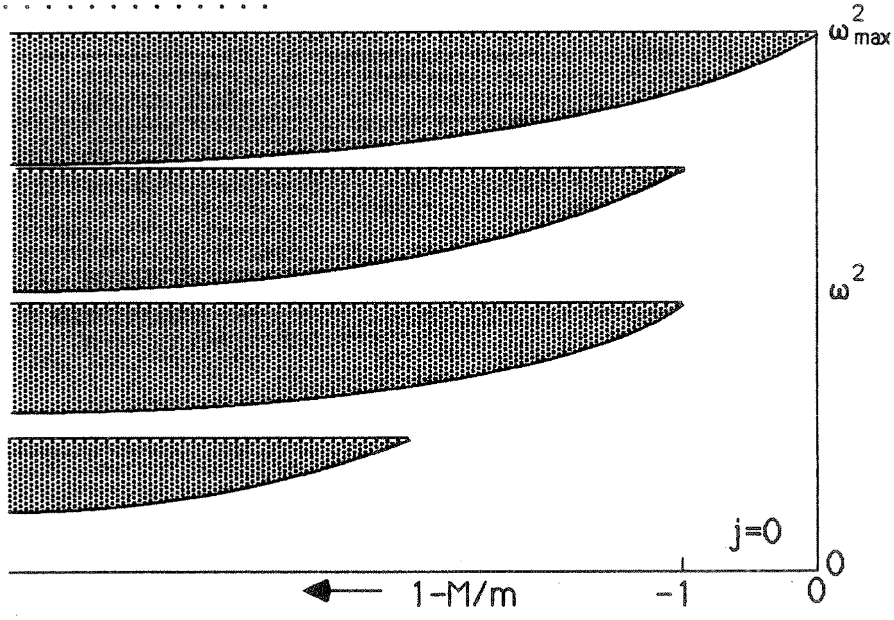
$= \left(-\frac{2}{3}, j+\frac{1}{3}\right)\ \&$

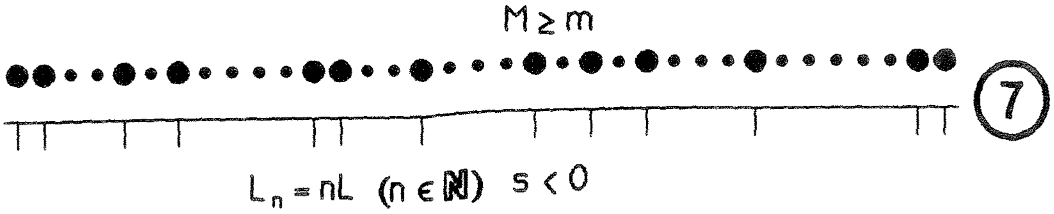
$= \left(-\frac{2}{3}, j+\frac{2}{3}\right)$

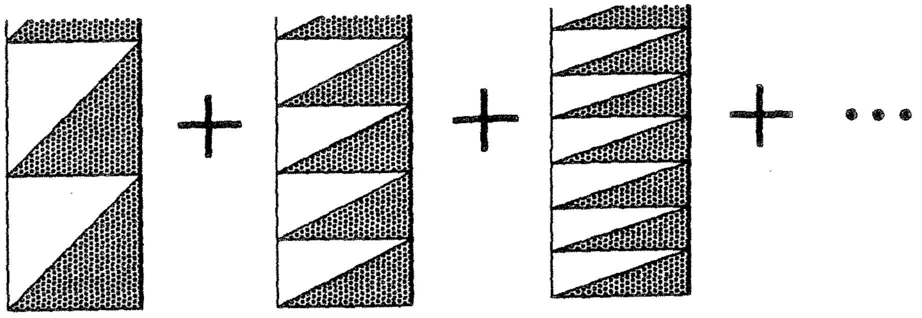
where

$j = [0], 1, 2, \ldots$

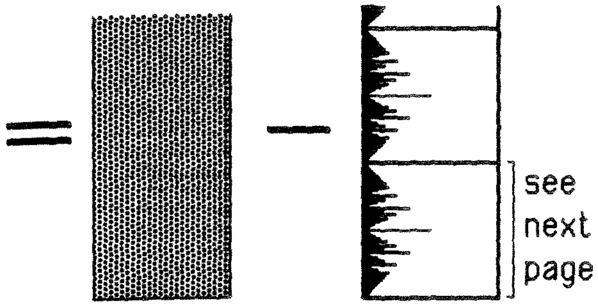


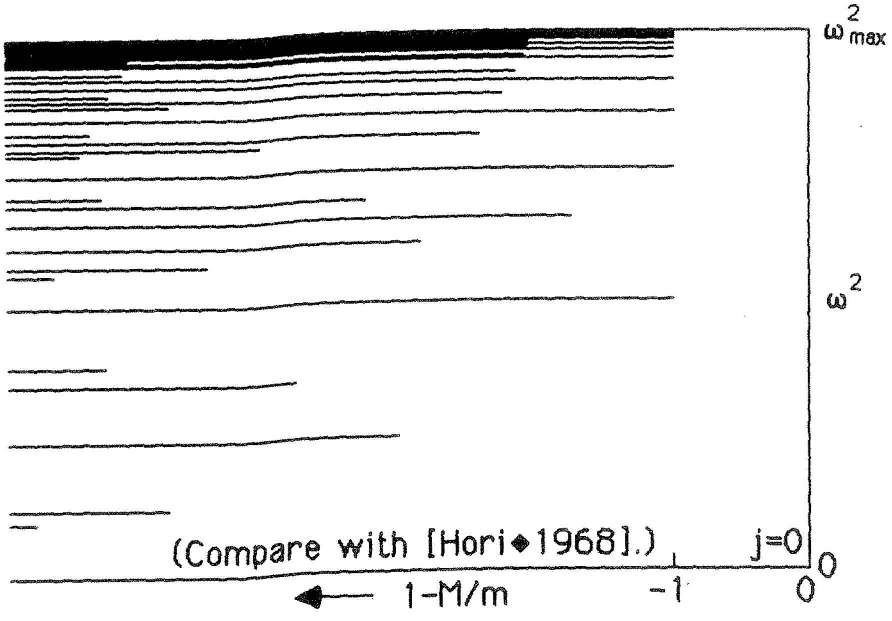






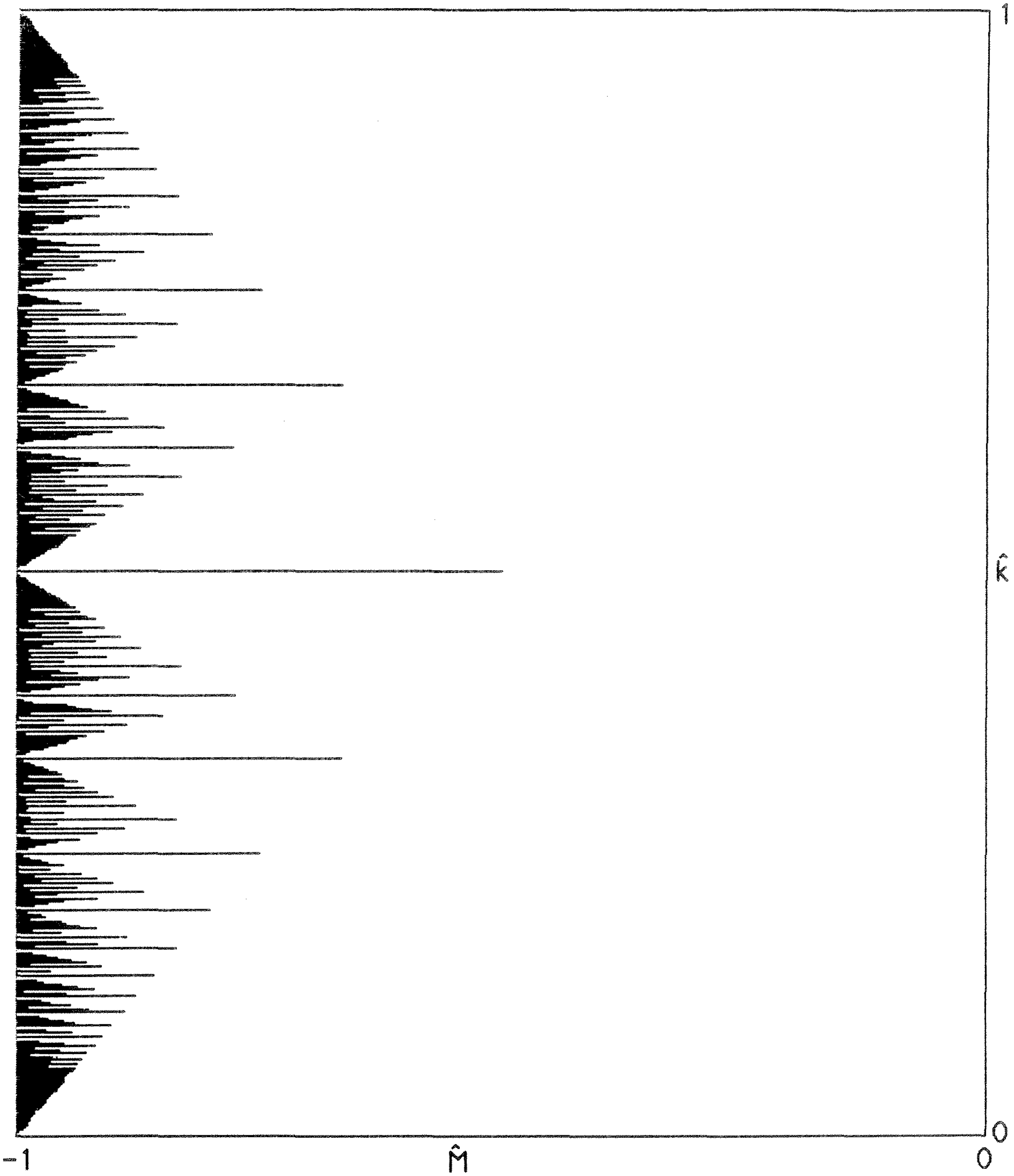
Spectral "gaps"
open at:
$(\hat{s}[\text{or } \hat{M}], \hat{k}) = \left(-1 + \frac{1}{q}, \frac{p}{q} + j\right)$
where
$j = [0], 1, 2, \ldots$
and $\frac{p}{q}$ is irreducible.





(Compare with [Hori◆1968].)

$$\omega = \omega_{\text{max}} \sin\left(\frac{\pi}{2}\hat{k}\right) \qquad 1-\frac{M}{m} = \left(\left(\frac{\omega_{\text{max}}}{\omega}\right)^2 - 1\right)\tan\left(\frac{\pi}{2}\hat{M}\right) \qquad \omega_{\text{max}} = 2\sqrt{\frac{\kappa}{m}}$$



This is the elegant structure underlying the intricate way in which density-of-states zeros (or spectral "gaps") appear as the binary harmonic chain mass ratio is varied. **Each line represents a density-of-states zero**. The intricacy, but not the elegance, was observed in one of the initial experiments.

Afterword

I began 3 years ago wondering if there was any simple structure underlying the complicated appearance of zeros in the density of states of the binary harmonic chain. I found it, but in so doing my research had to encompass the famous Saxon-Hutner conjecture concerning the robustness of spectral gaps in ordered and disordered systems (on the physics side) and Kirsch's elegant expression relating the spectra of ordered and disordered systems (on the mathematics side) and, indeed, to extend them.

Although this success is satisfying, the thesis contains some loose ends. In particular,

- It does not address the special case of hyperbolic wave functions (involving attractive δ's and negative energies);
- It does not consider mixed attractive/repulsive δ arrays;
- It does not consider generalizations to nonpoint interactions.

With respect to the latter point:

> Using transfer matrix techniques it is easy to show that, for a fixed energy, an arbitrary (1-dimensional) potential well can be characterized by 3 parameters, "strength," "extent," "location," and hence can be represented by a δ. There follow several Saxon-Hutner-type results for arbitrary potential wells.
>
> Also, the results herein should hold for sufficiently small energies (= sufficiently large wavelengths) if the point interactions are replaced by arbitrary potential wells of sufficiently small width. (Specifically, if the widths are much smaller than the free particle wavelength, then the wells appear pointlike to the particle.)

Finally, while there is hope that the results herein generalize (to more realistic models), the techniques do not (except in broad outline).

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