Spectra and gap amplification for systems with two widely different incommensurate periodicities

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We derive analytically the spectrum for the Schrödinger equation for quasiperiodic systems with two length scales: one large "macroscopic" scale [e.g., $a\cos(2\pi x/\lambda)$] and one small "microscopic" scale [e.g., $v\cos(2\pi x)$]. The phase diagram includes regimes with exponentially narrow gaps due to the slowly varying potential, regimes where the rapidly varying potential amplifies these narrow gaps, and regimes with exponentially narrow "Landau bands." The full "devil's-staircase" spectrum with gaps at wave vectors $q=m\pi+n\pi/\lambda$ develops in a hierarchical manner as a increases. The results apply to systems with superlattices, to celestial orbits with two periodic perturbations, to systems with slowly varying lattice distortions, and, in particular, to quasi-one-dimensional magnets such as bis(tetramethyltetraselenafulvalene) perchlorate [$(TMTSF)_2ClO_4$] in magnetic fields, where our findings may provide insight into the experimentally observed cascade of phase transitions.

I. INTRODUCTION

Most nondissipative problems in physics reduce to the determination of eigenstates. The nature of these eigenstates depends heavily on the symmetry of the system. For a quantum system, periodicity leads to Bloch functions. Randomness may lead to Anderson localized states. Incommensurability in general produces a spectrum including infinities of gaps,[1] the "devil's staircase." The study of the spectra and eigenstates for systems with incommensurate periodicities has been a fascinating area of study for mathematicians and physicists for quite some time.[2] The eigenstates may either be localized or extended. Here, we are interested in a region of the spectrum which has previously been largely unexplored, namely the case where one potential is sizable but slowly varying while the second potential has very small amplitude but a rapid spatial variation (see Fig. 1). The spectrum is explored at energies larger than either of the potentials. This situation applies, for instance, to superlattice structures; to lattice distortions induced by a sonic wave; to the problem of stability of periodic orbits with respect to periodic perturbations, such as the orbits forming Saturn's rings;[3] and to quasi-one-dimensional conductors in magnetic fields.[4] In an Appendix we discuss the application of our results to the latter case in detail. Moreover, the study of this comparatively simple case leads to insight into the problem of the development of the full devil's-staircase spectrum as the strength of the slowly varying potential increases.

The incommensurate system has gaps at wave vectors $q=n\pi+m\pi/\lambda$ (where λ is the ratio between the two periods), but the sizes of these gaps depend decisively on the strengths and the relative periodicity of the two potentials. The long-wavelength term [e.g., $a\cos(2\pi x/\lambda)$] taken by itself produces gaps with a very small interlevel distance π/λ [see Fig. 1(a)]. The eigenfunctions are given by Mathieu's equation, and only the gaps for small energies, $q^2<a$, are noticeable, whereas all gaps at higher energies above the barrier a are exponentially narrow and thus unobservable. The wave functions are well approximated by quasiclassical solutions in this regime. The spectrum is rather dull: a continuous spectrum above and narrow bands below the potential, and a nontrivial spectrum may arise only in the vicinity of the top of the barrier. Similarly, the rapidly varying potential [e.g., $v\cos(2\pi x)$] alone produces widely separately gaps at $q=n\pi$ [see Fig. 1(b)]. Naively, one might expect that the gap spectrum caused by the combination of a weak, rapidly varying potential and a stronger, slowly varying potential [see Fig. 1(c)] would simply be a superposition of the spectra produced by the two potentials taken separately, i.e., that the introduction of the rapidly varying potential into Mathieu's equation would introduce a simple gap at $q=\pi n$, since the effect of the potential $a\cos(2\pi x/\lambda)$ is weak at this high energy. This is not so. We shall demonstrate that the strength of one potential combines with the periodicity of the other to produce highly nonperturbative results. We shall see that the spectrum of the slow potential is highly sensitive to a very weak potential with rapid variation, and this leads to a dramatic amplification of gaps and eventually to a whole hierarchy of gaps.

The process by which the hierarchy develops is the subject of this paper. It will be seen that for small values of the parameter a the energy gaps are confined to branches around the gaps produced by the fast potential (see Fig.

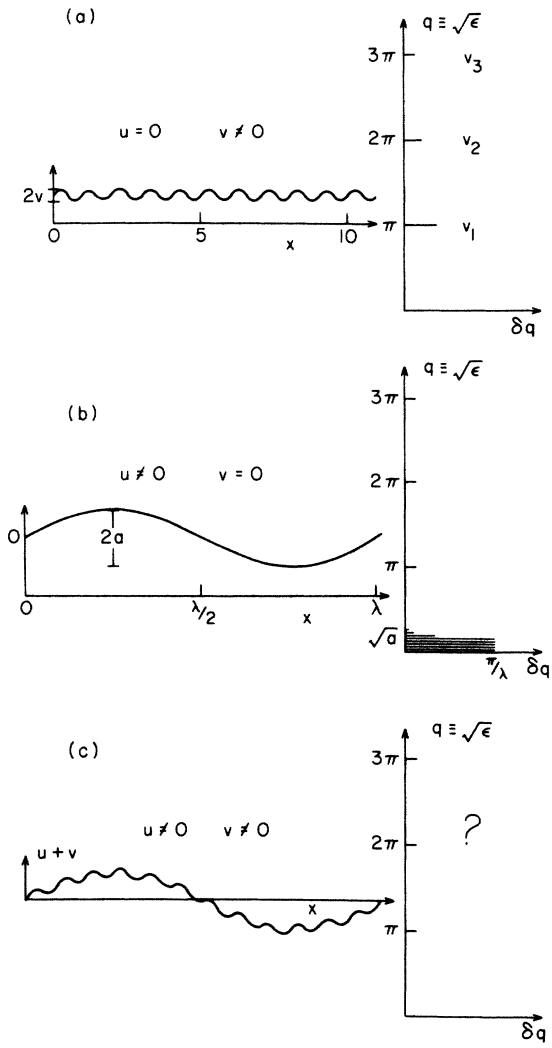

FIG. 1. (a) Rapidly varying periodic potential and the corresponding spectrum, with gaps at $q=\pi n$. (b) Slowly varying periodic potential and the corresponding spectrum with dense gaps only at energies low compared with a. (c) Double-periodic potential to be considered here. The spectrum is shown in Figs. 2, 3, 5, and 6.

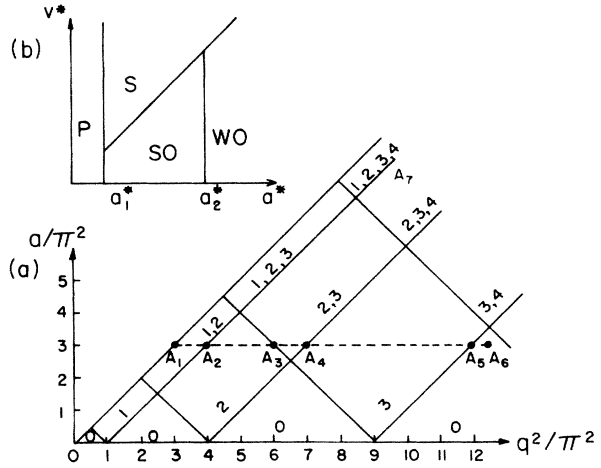

FIG. 2. Phase diagram for the Schrödinger equation (1.1) (schematic). (a) Branch structure for $v\to 0$. The numbers indicate the n's of the branches of type-A gaps. Regions with no type-A gaps are indicated with 0. When $\lambda\to\infty$ the boundaries become infinitely sharp phase transitions. A change in energy from A_6 to A_1 leads to variations in the number of branches as discussed in the text. (b) Regions with different behavior for the total gap width $\delta q_{\rm tot}$. P: conventional perturbative regime, $\delta q\approx |v_n|/\pi$. S: saturated, insulating region with $\eta=1$, and $\delta q_{\rm tot}\approx(a)/\pi n$. SO: strong oscillations of gap width vs $a\lambda$. WO: weak oscillations. Axis: $a^*=16\pi n a\lambda$, $v^*=(v_n\lambda)^2$. Characteristic points: $a_1^*=32\pi^3 n^2$, $a_2^*=16\pi^3 n^2(2\pi n\lambda)^{1/2}$.

2), and each branch can be labeled by the n of the appropriate "fast" gap. We argue[5] that it is this bunching of strong gaps which is responsible for the cascade of phase transition observed in organic conductors such as bis(tetramethyltetraselenafulvalene) perchlorate [$(TMSTSF)_2ClO_4$] as the magnetic field is varied.[6,7] Since these branches are limited by well-defined boundaries we shall speak of these branches as energy spectrum "phases" in a phase diagram in, for instance, q-a space (Fig. 2). Since there are no (observable) gaps outside the branches one may introduce an order parameter for these transitions which measures the local relative amount of gaps inside the branches. As the strength a of the slow potential increases, the various branches start to overlap, and eventually the whole devil's-staircase spectrum will develop. The order parameter has a kink when phase boundaries cross.

Our approach is analytical, in contrast to most work on the general case with comparable periodicities of the two potentials,[2] which has been purely numerical. We specifically take advantage of the exponential narrowness of the gaps for the limit that we consider, $\lambda\gg 1$, $q^2\gg a$. The quasiclassical nature of the Bloch wave functions outside these gaps is sufficient to allow us to construct analytical solutions to the Schrödinger equation. We derive a simple formula which is convenient both for general analysis and for the actual calculation of the spectrum. The approach is demonstrated for the case of a one-dimensional Schrödinger equation, but it may be generalized to higher dimensions and to various other eigenstate problems in electrodynamics, hydrodynamics, acoustics, astronomy, etc. Possibly, it may even lead to insight into the development of chaos and strange attractors through the overlap of bands.

To be more specific, let us consider the double-periodic Schrödinger equation

$$\psi''+[q^2-u(x)-v(x)]\psi=0\,, \tag{1.1}$$

where $u(x+\lambda)=u(x)$ and $v(x+1)=v(x)$. Suppose $q^2>u+v$, and $q\approx\pi$. Our findings are as follows. First, assume $w\equiv\max(v)\ll 1/\lambda$ and increase $a\equiv\max(u)$. When $a\ll 1/\lambda$ the largest ("type-A") gaps are at $q\approx n\pi$, n integer. Much smaller "type-B" gaps are at $q\approx n\pi+m\pi/\lambda$, with nonzero integer m. These gaps decrease exponentially with m. When $a\gg 1/\lambda$ then a number $N_A\approx a\lambda/\pi^2$ of the type-B gaps (with $|m|<N_A/2$) change into type-A gaps and become observable. At certain values of a of order π^2 the branches corresponding to

different n's merge. Only then does the intergap distance react to the incommensurability (or commensurability) of the periods. Of course, a potential $(u+v)$ with a total period Λ yields a spectrum with intergap distance $\Delta=\pi/\Lambda$, and when λ is irrational then $\Lambda\to\infty$. However, most of these dense gaps are type-B gaps at $n\pi+m\pi/\lambda$ generated by remote n's and play absolutely no role.

Thus, in the vicinity of A_6 in Fig. 2 there are "unobservable" type-B gaps, between A_5 and A_4 there is a one-branch region with periodic type-A gaps, between A_4 and A_3 there is a two-branch region with gaps at $2\pi+m\pi/\lambda$ and $3\pi+m\pi/\lambda$, between A_3 and A_2 there is again a one-branch region, and between A_1 and A_2 there is another two-branch region. The point A_7 is in a three-branch region with $n=2,3,4$.

Now fix $a\gg\lambda^{-1}$ and increase w. When $w\gg(a/\lambda)^{1/2}$ the gaps fill essentially the whole branch of width a/π and the space left for the intergap bands is approximately equal to $\exp(-w^2\lambda/4\pi a)$. This limit may correspond to orbits around Saturn perturbed by the slow potential from the Sun and a fast potential from one of the moons, Mimas, and the resulting empty branch may explain the Cassini division of Saturn's rings, not explainable by the fast perturbation alone. In the case of anisotropic conductors in magnetic fields these bands are regularly spaced "Landau levels." The effect of a macroscopic $\lambda\to\infty$ is most remarkable. In this case the condition above for w can be fulfilled even for an infinitesimal w, which thus causes exponentially small gaps $\Delta q\approx(a/2q^2)^{\lambda}$ to blow up to fill the whole interval of width a/q (see Fig. 6). The system changes from being completely "metallic" with no gaps to completely "insulating" with only gaps. It is as if the effective potential combines the strength of v with the larger period of u. When $\lambda\to\infty$ the boundaries of the various branches become infinitely sharp.

The remaining part of the paper is organized as follows. In Sec. II the qualitative nature of the Schrödinger spectrum is demonstrated by means of perturbation theory starting from the quasiclassical solutions for $v=0$. Section III presents the derivation of a general formula for the wave function and energy spectra. Sections IV and V demonstrate the strength of this formula by applying it to two special limits. Section IV derives a systematic perturbation theory in v^2 and the results in Sec. II are recovered in a rigorous way. Section V deals with the most remarkable limit where λ becomes macroscopic, and the gaps fill out completely the n branches in Fig. 2. Section VI summarizes our results for the spectra. The reader who is interested in the results rather than the specific technical details may proceed directly to Sec. VI which should be self-contained. In an Appendix our results are applied to the case of magnetic-field-induced phase transitions in highly anisotropic organic conductors, and it will be shown how the oscillations of Hall resistance, etc., can be understood in terms of the oscillations of the gaps as described in Sec. VI.

II. PERTURBATIVE DERIVATION OF SPECTRUM WITH HIERARCHY OF GAPS

Although we shall derive a general formula for the spectrum in Sec. III, much can be learned about the structure of the phase diagram and the origin of the hierarchy of gaps from perturbative methods. First, consider the Schrödinger equation

$$\psi''+[\epsilon-V(x)]\psi=0 \tag{2.1}$$

with the simplest double periodic potential

$$V(x)=a\cos(2\pi x/\lambda)+v\cos(2\pi x)\ . \tag{2.2}$$

Suppose $\epsilon=q^2$ and let us first apply perturbation theory with respect to the total potential in Eq. (2.2). The general pth-order perturbation term is of the form

$$V_p=V(q_1-q_2)V(q_2-q_3)\cdots V(q_p-q_{p+1})\ , \tag{2.3}$$

where the matrix elements $V(q)$ are given as

$$V(q)=(1/L)\int_0^L[a\cos(2\pi/\lambda)+v\cos(2\pi x)]\exp(iqx)dx\ , \tag{2.4}$$

which is nonzero only for $q=\pm2\pi/\lambda$ or $q=\pm2\pi$, so the general term in Eq. (2.3) is different from zero only when

$$q_1-q_{n+1}=(q_1-q_2)+(q_2-q_3)+\cdots+(q_p-q_{p+1})=2\pi m/\lambda+2\pi n\ , \tag{2.5}$$

where $m+n=p$. Hence gaps are opened in the energy spectrum at

$$q=\pi n+\pi m/\lambda\ , \tag{2.6}$$

since the wave vector (2.5) connects degenerate states for the unperturbed spectrum $\epsilon=q^2$ only for these values of q. The widths of these gaps are $\delta q=v^n a^{|m|}$. When $\lambda\gg1$ (and $a,v\ll1$), the major gaps are located in the vicinity of $q\approx\pi n$. For a fixed n, the largest gaps are those at $m=0$. Denote these gaps as type-A gaps. They are the generators of closely spaced ($\Delta q=\pi/\lambda$) type-B gaps with nonzero m. These gaps are decreasing exponentially with m. When $|m|>\lambda$ the gaps generated by different n's are found in the same q region and react to the commensurability of π and π/λ. The gaps which penetrate into a foreign region near an n which is different from that of the generator are extraordinary small, $\delta q\approx a^{\lambda}=\exp(\lambda\ln a)$. These gaps may be denoted as "type-C" gaps. In the more general case where the total potential is

$$V=a\cos(2\pi/\lambda)+\sum_p v_p\cos(2\pi px)\ , \tag{2.7}$$

the widths of the gaps become $\delta q\approx v_n a^m$, where v_n quickly decreases with n. If $v(x)$ is analytical then the decrease is exponential. The implications of this are obviously as before for Eq. (2.2). In practice, when $\lambda\gg1$ one has periodic bands with width approximately equal to π related to the rapidly varying potential, and only near the edges are there narrow gaps, periodically situated at distances $\Delta q\approx\pi/\lambda$.

Now suppose that a increases such that $a\gg1/\lambda$, but v remains sufficiently small that it can still be considered a perturbation. Then the perturbation theory must start from the wave functions of Eqs. (2.1) and (2.2) with $v=0$:

$$\phi''+(q^2-u)\phi=0\ . \tag{2.8}$$

The solutions are Bloch functions,

$$\phi=\exp(-i\kappa x)u^{\kappa}(x),\quad u^{\kappa}(x)=u^{\kappa}(x+\lambda)\ , \tag{2.9}$$

where κ and $-\kappa$ are degenerate quasi wave vectors. The matrix-element coupling states κ and κ' due to an arbitrary potential $v(x)=v(x+1)$ are

$$\begin{aligned} v^{(\kappa\kappa')}&\approx(1/\Lambda)\int_0^{\Lambda}\phi^{\kappa}(x)\phi^{-\kappa'}(x)v(x)dx \\ &=(1/\Lambda)\int_0^{\Lambda}\exp[i(\kappa-\kappa')x]v(x)u^{\kappa}(x)u^{-\kappa'}(x)dx \\ &=(1/\Lambda)\int_0^{\Lambda}\exp[i(\kappa-\kappa')x]\sum_{\mu}v_{\mu}\exp(2\pi i\mu x)(u^{\kappa}u^{\kappa'})_{\nu}\exp(2\pi i\nu x/\lambda)dx\ , \end{aligned} \tag{2.10}$$

where Λ is the total period of $u+v$. Clearly, $v^{(\kappa\kappa')}$ is nonzero only when $\kappa-\kappa'=2\pi n+2\pi m/\lambda$ and, reasoning as before, we realize that gaps will be located at

$$\kappa=n\pi+m\pi/\lambda\ . \tag{2.11}$$

In the quasiclassical approximation the quasi wave vector for the eigenfunction with energy q^2 is

$$\kappa=(1/\pi)\int_0^{\pi}(q^2-a\cos x)^{1/2}dx\ . \tag{2.12}$$

The gap width $\delta\kappa$, to first order in v, becomes

$$\delta\kappa\approx(2/\Lambda)\left|\int_0^{\Lambda}\phi_{\kappa}v\bar{\phi}_{-\kappa}dx\right| \tag{2.13}$$

with κ given by (2.12). Assuming λ to be irrational we find

$$\begin{aligned} \delta\kappa&=(2/\lambda)\left|v_n\int_0^{\lambda}\exp(-2\pi imx/\lambda)u^2(x)dx\right| \\ &=(2/\lambda)\left|v_n\int_0^{\lambda}\exp(2\pi inx)\phi_{\kappa}^2(x)dx\right|\ , \end{aligned} \tag{2.14}$$

where v_n is the nth Fourier component of v. Equations (2.11)—(2.14) will be derived from a general nonperturbative theory in Sec. III. The exact Bloch solutions to (2.8) may be presented in the form

$$\phi=(1/\sqrt{\rho})\exp(-iS/2)\ , \tag{2.15}$$

$$S=2\int_{x_0}^{x}\rho_1dx_1,\quad \rho_1=\rho(x_1) \tag{2.16}$$

where the function ρ is the solution to the equation

$$\rho^2-\tfrac{1}{4}(\ln\rho)'^2+\tfrac{1}{4}(\ln\rho)''=q^2-u\ . \tag{2.17}$$

Notations such as $\rho_2=\rho(x_2)$, $\psi_{\Lambda}\equiv\psi(x+\Lambda)$ are used throughout the paper. Choose a point x_0 according to

$$\rho(x_0)\equiv\langle\rho\rangle=\kappa=(1/\lambda)\int_0^{\lambda}\rho_1dx_1\ . \tag{2.18}$$

Such a choice of x_0 is always possible since $\rho-\langle\rho\rangle$ must change sign. The leading approximation to ρ is the quasiclassical expression[9]

$$\rho\approx(q^2-u)^{1/2}\ . \tag{2.19}$$

Substituting (2.15) and (2.16) into (2.13) yields

$$\delta\kappa=(2/\lambda)\left|v_n\int_0^{\lambda}(1/\rho)\exp\left[2i\int_0^{x}r_1dx_1\right]dx\right|\ , \tag{2.20}$$

where $r=\rho-\pi n$. When $\left|\int_0^{x}(\rho_1-\pi n)dx_1\right|\gg1$ then the WKB method is applicable. With exponential accuracy only the points x^* where $r=0$ are important, i.e., only the points defined by

$$\rho^*(x^*)=\pi n\ . \tag{2.21}$$

Such turning points exist only when

$$(q^2-a)^{1/2}<\pi n<(q^2+a)^{1/2}\ , \tag{2.22}$$

which can be fulfilled only in the interval (q^+,q^-) where

$$(q^{\pm})^2=(n\pi)^2\pm a \tag{2.23}$$

and $a=\max(u)$. This equation defines the phase-transition lines in Fig. 2. If $u(x)=u(-x)$, a simple calculation gives the width of type-A gaps in this interval,

$$\begin{aligned} \delta\kappa&=(2v_n/\lambda\rho^*)\,|\pi^{-1}d\rho^*/dx^*|^{-1/2} \\ &\quad\times\left|\cos\left[2\int_0^{x^*}r_1dx_1+\pi/4\right]\right|\ , \end{aligned} \tag{2.24}$$

and the number of gaps N_A in this interval is given by Eq. (2.23), i.e.,

$$N_A\approx a\lambda/\pi^2n \tag{2.25}$$

and the widths of these gaps are

$$\delta\kappa\approx v_n(qa\lambda)^{-1/2}\,|\cos[(a\lambda/2\pi q)-m\pi/2-\pi/4]|\ . \tag{2.26}$$

Outside the interval defined by Eq. (2.23) the WKB points (2.21) disappear and $\delta\kappa$ decreases exponentially with m. These are the type-B gaps. For $u=a\cos(\pi x/\lambda)$ the gaps can be calculated explicitly,

$$\delta\kappa=v_n\,|J_m(a\lambda/2\pi q)|\ , \tag{2.27}$$

and qualitatively the results follow from the peroperties of the Bessel functions. We stress, however, that the results above are valid for any periodic potential.

For large enough a the equation $\rho(x)=\pi n$ can be fulfilled for more than one integer value of n; this gives rise to overlap of two or more type-A regimes as shown in Fig. 2. The overlap between n and n' takes place when $a\approx\frac{1}{2}\pi^2(n'^2-n^2)$. Only then does the system react to the incommensurability of the two periods, and the full spectrum[1] develops in a stepwise manner as a function of a as more and more bands overlap.

The width $\delta\kappa$ oscillates with $a\lambda$, and the period of the oscillations correspond to $\Delta N_A=2\pi$ (Fig. 3). For Z_n

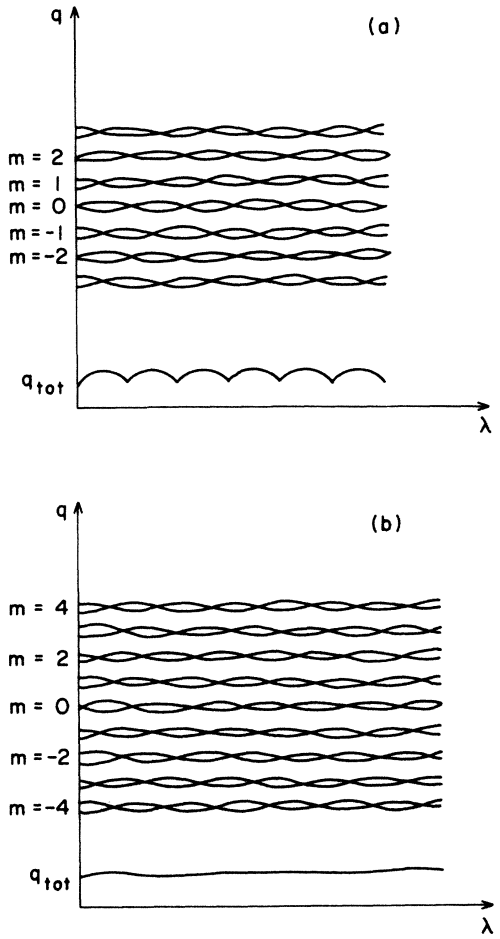

FIG. 3. Oscillation of gaps within one n branch in the (a) SO regime of Fig. 2 with strong oscillations of the total width and in the (b) WO regime where the total width has weak oscillations.

$=2\pi^5 n^3/a^2\lambda > 1$ the phase $a\lambda/2\pi q$ in (2.26) varies little as a function of m in the interval (2.23) [see Fig. 5(b)], so the total width oscillates strongly with $a\lambda$. For $Z_n < 1$ the phase depends on m (through the m dependence of q) and the gaps for different m are "out of phase" leading to weak oscillations in the total width. Regimes with various behavior for the total width are shown in Fig. 2. Figure 3 shows the gap structure as a function of $a\lambda$ for different m in the two cases $Z > 1$ and $Z < 1$.

The applicability of perturbation theory is related to δq being small compared with the intergap distance π/λ. Indeed, later we shall see that the condition for perturbation theory to be applicable is

$$X_n = v_n \mid \pi n a/\lambda \mid^{-1/2} \ll 1 . \tag{2.28}$$

This condition may be met even when $a \approx \pi^2$ and different branches merge. Since v_n usually decreases exponentially with n, this condition is fulfilled even for moderately large n. The oscillations remain as long as $Y_n = a\lambda/2\pi q > 1$, and since this quantity decays only as $1/n$ the oscillations die out at much larger n.

When λ increases, the branch merging yields "phase transitions" in the energy spectrum. A possible "order parameter" is the density of gaps $\eta(q) = dq_{\rm tot}/dq$, where $q_{\rm tot}$ is the total gap below q. Its average over the "infinitesimal" interval $\Delta q \approx \pi/\lambda$ is a measure of the degree to which the system is insulating. $\eta = 0$ corresponds to a metallic system since there is no gap; when $\eta = 1$ the gaps fill up everything and the system is insulating. When branches merge, η has a kink. The width of the phase boundary goes to zero when $\lambda \to \infty$, and the phase transition in the energy spectrum becomes sharp.

The most remarkable of the results derived above is the increase of the gap width from $\delta q \approx a^{\lambda}$ to $\delta q \approx v_n$. In order to understand this, consider the simplest potential (2.2). First suppose $v = 0$. For high energies $\epsilon \equiv q^2 > a$ there are classical turning points $u(x) = \epsilon$ only at complex $x = \pm i x^*$ where

$$a \cos(2\pi i x^*/\lambda) = a \cosh(2\pi x^*/\lambda) = q^2 , \tag{2.29}$$

$$x^* = (\lambda/2\pi)\operatorname{arccosh}(q^2/a) \approx (\lambda/4\pi)\ln(q^2/a) . \tag{2.30}$$

The gaps as determined by the transfer matrix are proportional to the reflection coefficient R at the barrier:

$$R \approx \exp\left[-2q \int_{-x^*}^{x^*} [q^2 - a\cosh(2\pi x/\lambda)]^{1/2} dx\right]$$

$$\approx (a/2q^2)^{\lambda q/\pi} , \tag{2.31}$$

yielding exponential small gaps. When $q^2 > a$, even a very small v significantly changes the turning point $x = ix^*$,

$$a \cos(2\pi i x^*/\lambda) + v \cos(2\pi i x^*) = q^2 . \tag{2.32}$$

If $v \gg R$ the solution to (2.32) becomes

$$x^* \approx (1/2\pi)\operatorname{arccosh}[(q^2 - a)/v] \tag{2.33}$$

and consequently the reflection rate R is greatly increased and the gap strongly amplified.

Until now we have considered only high energies $q^2 > a$. If $a > q^2$ and $v = 0$ then the quasiclassical solutions reduce to tight binding, and the bands become exponentially narrow since the classical turning points become real and the reflection rate $R \approx 1$. The positions of these bands are given by Bohr's quantization rule

$$\int_{-\tilde{x}}^{\tilde{x}} [\epsilon - u(x)]^{1/2} dx = (n + \tfrac{1}{2})\pi, \quad u(\tilde{x}) = u(-\tilde{x}) = \epsilon , \tag{2.34}$$

where ϵ is the dimensionless energy. Naturally, the wide gaps at $q^2 < a$ are little affected by small v. Thus the impact is only important when $q^2 > a$, which is precisely the case considered in this paper.

III. ANALYTICAL ESTIMATES FOR GENERATION SOLUTIONS TO SCHRÖDINGER EQUATION

The perturbative approach of Sec. II provided significant insight into the structure of the phase diagram for the Schrödinger equation, including the stepwise development of the full spectrum as the strength of the slow potential increases. However, in order to deal with the most interesting case where λ becomes very large and the gaps fill up the interior of the n branches (see Fig. 2), one must go beyond perturbation theory. In this section we derive a

simple general formula for the spectum. The results of Sec. II follow in a more rigorous way as a special case of this approach.

Consider a general case of the equation

$$\psi''+(q^2-V)\psi=0, \quad V=u+v \tag{3.1}$$

where $V(x+\Lambda)=V(x)$, $u(x+\lambda)=u(x)$, $\Lambda=\lambda\lambda_1$, and $q\approx\pi$. The only specific feature of Eq. (3.1) is two different length scales. Suppose that for a specific solution ψ one knows the three complex values $\psi_\Lambda/\psi_0=\psi(x_0+\Lambda)/\psi(x_0)$, $(\ln\psi_0)'$, and $(\ln\psi_\Lambda)'$ at a certain point x_0. This is sufficient to allow us to determine the quasi wave vector $K(q)$ of Eq. (3.1). A Bloch-function solution $\psi_B(x+\Lambda)=\exp(iK\Lambda)\psi_B(x)$ can be expressed in terms of ψ and its complex conjugate $\bar{\psi}$ as $\psi_B=\alpha\psi+\beta\bar{\psi}$. Continuity of ψ_B and its derivative ψ_B' implies

$$\begin{aligned}\alpha\psi_\Lambda+\beta\bar{\psi}_\Lambda&=\exp(iK\Lambda)(\alpha\psi_0+\beta\bar{\psi}_0)\ ,\\ \alpha\psi_\Lambda'+\beta\bar{\psi}_\Lambda'&=\exp(iK\Lambda)(\alpha\psi_0'+\beta\bar{\psi}_0')\ .\end{aligned} \tag{3.2}$$

A nontrivial solution (α,β) exists only when the determinant

$$\begin{vmatrix}\psi_\Lambda-\exp(iK\Lambda)\psi_0 & \bar{\psi}_\Lambda-\exp(iK\Lambda)\bar{\psi}_0\\ \psi_\Lambda'-\exp(iK\Lambda)\psi_0' & \bar{\psi}_\Lambda'-\exp(iK\Lambda)\bar{\psi}_0'\end{vmatrix}=0\ . \tag{3.3}$$

Accounting for current conservation

$$j=2\,\mathrm{Im}(\psi_0\bar{\psi}_0')=2\,\mathrm{Im}(\psi_\Lambda\bar{\psi}_\Lambda') \tag{3.4}$$

one obtains the dispersion relation

$$\cos(K\Lambda)=\mathrm{Re}((\psi_\Lambda/2\psi_0)\{1-[\ln\psi_\Lambda/(\psi_0\bar{\psi}_0)^{1/2}]'/i\,\mathrm{Im}(\ln\bar{\psi}_0)'\})\ . \tag{3.5}$$

The region of q where $|\,\mathrm{Re}(\,)\,|>1$ belongs to the gap. To calculate a specific solution we introduce

$$\psi=\phi\chi, \quad \chi_0=1, \quad \chi_0'=0\ , \tag{3.6}$$

where ϕ is the solution to (3.1) for $v=0$. In general, ϕ is given by Eqs. (2.15)–(2.17). Let us again choose x_0 such that (2.18) is fulfilled. Everywhere, except for the small gaps, ψ is a Bloch function $\psi(x+\lambda)=\exp(i\kappa\lambda)\psi(x)$ with wave vector $\kappa=\langle\rho\rangle$. When $q^2>|u|$ these gaps are exponentially small and will be ignored, and the equations derived will be accurate outside the gaps. The solutions can easily be generalized for the region inside the gaps. Inserting Eq. (3.6) into (3.1) we obtain

$$\chi''+2(\phi'/\phi)\chi'=v\chi\ . \tag{3.7}$$

The solution to this equation is

$$\chi=1+\int_{x_0}^{x}v_1\phi_1^2\chi_1dx_1\int_{x_1}^{x}dx_2/\phi_2^2\ . \tag{3.8}$$

Now ϕ from (2.15) is substituted into (3.8), and accounting for $\int S'\exp(iS)dx=\exp(iS)$ one obtains

$$\chi=1+i\int_0^x[\sigma_1-\exp(iS)\Phi_1]\chi_1dx_1\equiv1+i\hat{N}\chi\ , \tag{3.9}$$

where

$$\Phi=\sigma\exp(iS), \quad \sigma=v/S'=v/2\rho\ , \tag{3.10}$$

so χ is given by the operator $\hat{N}$ defined by (3.9):

$$\chi=(1-i\hat{N})^{-1}\ . \tag{3.11}$$

Equation (3.6) with χ given by Eq. (3.8) is substituted into Eq. (3.5):

$$\cos(K\Lambda)=\mathrm{Re}[\exp(-i\kappa\Lambda)H_\Lambda]\ , \tag{3.12}$$

where

$$\begin{aligned}H_\Lambda&=1+i\int_{x_0}^{x_0+\Lambda}\sigma_1\chi_1dx_1\\ &=1+i\int_{x_0}^{x_0+\Lambda}\sigma_1(1-i\hat{N})^{-1}dx_1\equiv1+iA_\Lambda\ .\end{aligned} \tag{3.13}$$

Our goal is to derive an equation for H. We introduce another quantity B:

$$B=\int_{x_0}^{x}\bar{\Phi}_1(1-i\hat{N})^{-1}dx_1\ . \tag{3.14}$$

A simple transformation employing $(1-iN)^{-1}=1+iN(1-iN)^{-1}$ and Eqs. (3.9) and (3.10) yields

$$\begin{aligned}A&=\gamma+i\int_{x_0}^{x}\sigma_1A_1dx_1-i\int_{x_0}^{x}\Phi_1B_1dx_1\ ,\\ B&=\int_{x_0}^{x}\Phi_1dx_1+i\int_{x_0}^{x}\bar{\Phi}_1A_1dx_1-i\int_{x_0}^{x}\sigma_1B_1dx_1\ ,\end{aligned} \tag{3.15}$$

where

$$\gamma=\int_{x_0}^{x}\sigma_1dx_1\ . \tag{3.16}$$

By Eqs. (3.16) and (3.17), $A_0=B_0=0$. The derivatives of Eqs. (3.15) are

$$\begin{aligned}a'&=\sigma\exp(-i\gamma)-iQb\ ,\\ b'&=\bar{Q}\exp(-i\gamma)+i\bar{Q}a\ ,\end{aligned} \tag{3.17}$$

where

$$\begin{aligned}a&=A\exp(-i\gamma), \quad b=B\exp(i\gamma)\ ,\\ Q&=\Phi\exp(-2i\gamma)\ .\end{aligned} \tag{3.18}$$

Using (3.18) and (3.16) we can rewrite (3.17):

$$a=-i-i\Omega b, \quad b=i\Omega[a-i\exp(-i\gamma)]\ , \tag{3.19}$$

where the operator Ω is defined by

$$\Omega f=\int_{x_0}^{x}Q_1f_1dx_1\ . \tag{3.20}$$

Finally, Eq. (3.18) gives

$$a=i\exp(i\gamma)-i(1-\Omega\bar{\Omega})^{-1} \tag{3.21}$$

and, by means of Eqs. (3.18) and (3.13),

$$H_\Lambda=\exp(i\gamma_\Lambda)[-2i\sin\gamma_\Lambda+\exp(i\gamma_\Lambda)(1-\Omega\bar{\Omega})_\Lambda^{-1}]\ . \tag{3.22}$$

Assume that q and v are chosen in such a way that $\gamma_\Lambda=0$.[10] Then

$$H_\Lambda=(1-\omega)_\Lambda^{-1},\quad \omega=\Omega\bar{\Omega}\ . \tag{3.23}$$

Accounting for the definition of ω through Eqs. (3.10), (3.18), (3.20), and (3.23), one obtains the following simple equation for H:

$$H''-(\ln Q)'H'=|Q|^2H,\quad H_0=1,\quad H_0'=0\ . \tag{3.24}$$

This is the equation that we aimed for. By inserting solutions of (3.24) into (3.12) one can obtain the spectrum of the Schrödinger equation. In the next sections the efficiency of this equation will be demonstrated.

IV. EXACT RESULTS TO LEADING ORDER IN v: SUCCESSIVE APPROXIMATIONS

Let us first consider a small periodic v:

$$v(x+1)=v(x),\quad v\ll\sqrt{a/\lambda}\ . \tag{4.1}$$

Band edges correspond to

$$K_g\Lambda=\nu\pi,\quad \nu \text{ integer}\ . \tag{4.2}$$

When $v\to 0$ then $K\to\kappa$ since H to be inserted in (3.12) goes to 0. So choose

$$\kappa\Lambda=K\Lambda+\tilde{g},\quad \kappa_g\Lambda=\nu\Lambda+g \tag{4.3}$$

and introduce $\kappa\Lambda=\tilde{\kappa}$, $K\Lambda=\tilde{K}$. Suppose

$$H_\Lambda=1+\tilde{h}+i\tilde{l}\ , \tag{4.4}$$

where $\tilde{h}$ and $\tilde{l}$ are real. By inserting (4.4) into (3.12) and using (4.3), the wave vectors $\tilde{q}_\pm$ at the gap edges can be related to $\tilde{h}$ and $\tilde{l}$. One finds

$$g_\pm=(1+\dot{h}\pm D^{1/2})/(1+\ddot{h}-2\dot{l})\ , \tag{4.5}$$

$$D=(1+\dot{h})^2+2h(1+h-\ddot{h}-2\dot{l})\ , \tag{4.6}$$

where $\dot{h}=(d\tilde{h}/dg)_{g=0}$, etc. According to (4.3) the gap in κ is given by

$$\delta\kappa=(1/\Lambda)(g_+-g_-)\approx 2D^{1/2}/\Lambda\ . \tag{4.7}$$

By means of Eqs. (3.23), (3.20), and (3.18), one can reduce the calculations to successive approximations of $H_\Lambda=(1-\omega)^{-1}=1+\omega+\omega^2+\cdots$. This is very convenient since the terms decrease with v^2 (ω proportional to v^2), and each approximation reduces to a multiple integral. Start with the leading approximation

$$D\approx 2h=2\,\mathrm{Re}\,\omega_\Lambda\ . \tag{4.8}$$

By Eqs. (3.20) and (3.18),

$$D\approx 2\,\mathrm{Re}\int_{x_0}^{x_0+\Lambda}Q_1dx_1\int_{x_0}^{x_1}Q_2dx_2\ . \tag{4.9}$$

Introduce

$$F=\int_{x_0}^{x}Q_1dx_1,\quad Q=F'\ . \tag{4.10}$$

Then

$$D=2\,\mathrm{Re}\left[\int_{x_0}^{x_0+\Lambda}F_1'\bar{F}_1dx_1\right]=|F_\Lambda|^2\ ; \tag{4.11}$$

in the leading approximation, by Eqs. (2.15), (2.16), (3.18), and (3.10),

$$D\approx\left|\int_{x_0}^{x_0+\Lambda}v\phi^2dx\right|^2\ ; \tag{4.12}$$

and $d\kappa$ given by Eq. (4.7) becomes

$$\delta\kappa\approx(2/\Lambda)\left|\int_{x_0}^{x_0+\Lambda}v\phi^2dx\right|\ . \tag{4.13}$$

Since $\phi^2=\phi^{(+)}\bar{\phi}^{(-)}$, where $(+)$ and $(-)$ denote the quasi wave vectors κ and $-\kappa$, Eq. (4.13) is identical with (2.13). Suppose $\lambda=\Lambda/\lambda_1$ where Λ and λ_1 are irreducible, and

$$v(x)=\sum_{n=-\infty}^{\infty}v_n\exp(-2\pi inx)\ . \tag{4.14}$$

Then

$$\int_{x_0}^{x_0+\Lambda}v\phi^2dx=\tfrac{1}{2}\sum_{n=-\infty}^{\infty}v_nJ_n\ , \tag{4.15}$$

where

$$J_n=\int_{x_0}^{x_0+\Lambda}\exp\left[2i\int_{x_0}^{x}r_1dx_1\right]dx/\rho,\quad r=\rho-\pi n\ . \tag{4.16}$$

Since $\rho(x)=\rho(-x)$ then

$$\begin{aligned}J_n&=\sum_{\mu=0}^{\lambda_1-1}\int_{x_0+\mu\lambda}^{x_0+(\mu+1)\lambda}\cdots\\&=\sum_{\mu=0}^{\lambda_1-1}\exp[2i(\kappa-\pi n)\mu\lambda]\\&\quad\times\int_{x_0}^{x_0+\lambda}\exp\left[2i\int_{x_0}^{x}\rho_1dx_1\right]dx/\rho\ .\end{aligned} \tag{4.17}$$

By Eq. (4.3), $\kappa=\nu\pi/\Lambda$. Therefore $J_n\neq 0$ only when

$$\kappa-n\pi=\pi m/\lambda,\quad m \text{ integer} \tag{4.18}$$

[cf. Eq. (2.11)]. In this case

$$J_n=\lambda_1\int_{x_0}^{x_0+\lambda}\exp\left[2i\int_{x_0}^{x}\rho_1dx_1\right]dx/\rho\ , \tag{4.19}$$

and eventually the gaps given by Eq. (4.15) become

$$\delta\kappa_n=\lambda^{-1}\left|v_n\int_0^{\lambda}\exp\left[2i\int_0^{x}r_1dx_1\right]dx/\rho\right|\ , \tag{4.20}$$

which is identical to Eq. (2.20). Hence, we recover Eq. (2.23) for the width of the type-A bands and Eq. (2.26) for the size of the gaps. We have thus demonstrated that the results of Sec. III appear as special limiting cases of the general formalism. Further approximations of D to higher order in v can be obtained by decomposing $\exp(-2i\gamma)$ in Q. For values of κ other than those given by Eq. (4.18) the gaps decap exponentially with $q\lambda$; these are the type-B gaps.

V. GENERAL CASE

Until now we have considered v to be a small parameter where successive approximations as laid out in Sec. IV converge quickly. A necessary condition for this approach to be valid is that the gap $\delta\kappa$ is small compared with the smallest intergap distance π/λ. In the case where $a\lambda\gg 1$ [where $a=\max(u)$] this condition reads

$$v/\sqrt{qa\lambda}\ll\pi/\lambda\ \text{ or }\ v(\pi na/\lambda)^{-1/2}\ll\pi\ , \tag{5.1}$$

since $q \approx \pi n$. Now consider an arbitrary v in the case where $a\lambda \gg 1$ and, for simplicity, $u(x)=u(-x)$. Then WKB reasoning similar to that in Sec. IV reveals that in any ω^n term in the expansion for H defined by Eq. (3.23) one may replace Q in the expression (3.20) defining the operator Ω by

$$Q \rightarrow (v_n/2\rho^*)\exp\left[2i\int_{x_0}^{x}(\rho_1-\pi n)dx_1\right], \tag{5.2}$$

where again ρ^* is the WKB point (2.21). Now Eq. (3.24) for $\kappa=\pi n$ reduces to

$$H''-2irH'=\omega^2 H, \quad H_0=1, \quad H_0'=0, \tag{5.3}$$

$$r=\rho-\pi n, \quad \omega=|v_n/2\rho^*|, \quad \rho^*=\pi n. \tag{5.4}$$

Substituting

$$H \approx \exp\left[i\int \eta_1 dx_1\right] \tag{5.5}$$

into Eq. (5.3) one obtains an equation for η:

$$-\eta^2+i\eta'+2r\eta=\omega^2. \tag{5.6}$$

In the leading quasiclassical approximation, η' is neglected. Then

$$\eta=r\pm(r^2-\omega^2)^{1/2}. \tag{5.7}$$

Since $r^*=\rho^*-\pi n=0$, Eq. (5.7) has classical turning points [in contrast to the imaginary turning points entering (2.29)] at $x_\pm$ where

$$r_\pm=\pm\omega. \tag{5.8}$$

Near these points, which are at the boundaries of a classically inaccessible barrier, the quasiclassical approximation becomes inapplicable. Near the barrier one can expand r,

$$r \approx r^*+r^{*'}(x-x^*)=\rho^{*'}(x-x^*), \tag{5.9}$$

and Eq. (5.3) reduces to

$$H''-2i\rho^{*'}yH'=\omega^2 H, \quad y=x-x^*. \tag{5.10}$$

The transformation

$$H=\int \exp(iyz)H(z)dz \tag{5.11}$$

along a properly chosen contour leads to

$$(zH)'+(i/2\rho^{*'})(z+\omega^2/z)(zH)=0, \tag{5.12}$$

implying

$$H \propto z^{-1}\exp[(i/2\rho^{*'})(\tfrac{1}{2}z^2+\omega^2\ln z)]. \tag{5.13}$$

This knowledge of H allows for the matching of different quasiclassical regions separated by barriers by means of the transfer matrix between consecutive regions and thus for determination of H_Λ and the gaps. The resulting general formulas are slightly transparent so we shall now restrict ourselves to the extreme case where the classically unavailable region is large and the tunneling through it weak (tight-binding case). In order to obtain a physically transparent picture, substitute

$$H=E\exp\left[i\int_{x_0}^{x} r_1 dz_1\right] \tag{5.14}$$

into Eq. (5.3). Then

$$E''+(r^2+ir'-\omega^2)E=0. \tag{5.15}$$

Note that the potential in this equation involves only the period λ, not Λ, which explains why the gaps occur at intervals π/λ rather than π/Λ. To have an idea of the solution, keep (as usual in the leading quasiclassical approximation) only r and drop r'. This is valid when

$$\omega^2 \approx (v_n/\pi n)^2 \gg |r'| \approx a/\lambda. \tag{5.16}$$

This is essentially the regime defined by Eq. (5.1) where the perturbative method is not applicable. The two approaches are thus quite complementary. Then

$$\begin{aligned} &E''+(r^2-\omega^2)E=0, \\ &E_0=1, \quad E_0'=ir_0=-i\langle r\rangle. \end{aligned} \tag{5.17}$$

This may be seen as an effective Schrödinger equation with zero energy and potential energy $U=\omega^2-r^2=(v_n/\rho^*)^2-(\rho-\pi n)^2$. Hence, since $\rho \approx q$ the quantity $\epsilon-U$ (which was $q^2-u>0$ in the absence of v) is lowered by an amount corresponding to $\Delta q=\pi n$. This allows the effective potential U to become positive for a certain range of x, such that the system is in the strong-coupling or tight-binding regime. *The reduction of the effective energy is responsible for the gap amplification.* This is illustrated graphically in Fig. 4, which shows the transformation of the effective potentials due to v_n in the regime

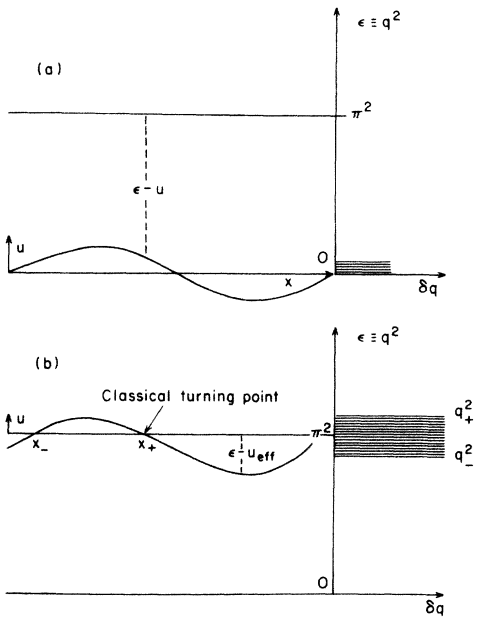

FIG. 4. Schematic representation of the "energy reduction" due to the rapid potential v. (a) In the absence of v, $\epsilon \approx (\pi n)^2 \gg u$ and the gaps are exponentially small around these high energies. (b) In the presence of v ($w \gg \sqrt{a/\lambda}$) the effective $\epsilon-u$ is reduced by an amount corresponding to $\Delta q=\pi n$ bringing the system into the strong-coupling regime, with classical turning points x_+ and x_-. The tunneling between these points makes the bands exponentially narrow: There are regions of width a/λ around πn which are essentially completely filled with gaps (see Fig. 6).

$v_n \gg (a/\lambda)^{1/2}$.

The effective Schrödinger equation (5.17) can be written in an interesting Hermitian form

$$\begin{bmatrix} r+\hat{p} & \omega \\ \omega & r-\hat{p} \end{bmatrix} \bar{E}=0 , \tag{5.18}$$

where $\hat{p}=-id/dx$, $\bar{E}=(E,F)$. The Schrödinger equation is thus equivalent to a two-branch problem with linearized dispersion in the absence of the coupling $\omega \propto v$, in complete analogy with the usual equation for the Peierls interaction where Eq. (5.18) corresponds to orbits at $q \approx \pi n$ and $q \approx -\pi n$, which interact via ω. The Hermitian form of (5.18) guarantees real eigenvalues. The dispersion relation is given in terms of E_Λ as can be seen by inserting (5.14) into (3.12) and using $\kappa = \langle \rho \rangle$ together with the definition of r, $r=\rho-\pi n$:

$$\mathrm{Re}E_\Lambda = (-1)^{n\Lambda}\cos(K\Lambda) . \tag{5.19}$$

Clearly, this condition can be met only in the allowed bands of (5.17). In the tight-binding case the bands are exponentially narrow. Their width δq is

$$\delta q \propto \exp\left[-2\int_{x_-}^{x_+}(\omega^2-r_1^2)^{1/2}dx_1\right] , \tag{5.20}$$

and they are situated according to the Bohr quasiclassical quantization rule

$$\int_{x_+}^{2\pi/\lambda-x_-}(r_1^2-\omega^2)^{1/2}dx_1 \approx m\pi+\tfrac{1}{2} . \tag{5.21}$$

By Eqs. (5.8) and (5.9)

$$x_\pm = x^* \pm \omega/|\rho^{*'}| , \tag{5.22}$$

where $\omega/|\rho^{*'}| \approx v\lambda/a \ll \lambda$. Using Eq. (5.9) in the barrier we obtain from Eq. (5.20)

$$\delta q \approx \exp(-\pi\omega^2/|\rho^{*'}|) = \exp(-\pi v_n^2/4\rho^{*2}|\rho^{*'}|) . \tag{5.23}$$

Thus, the bands are exponentially narrow despite the fact that the energy is much higher than either of the potentials [Fig. 1(c)], so that naively one might have expected narrow gaps. This may be our most important result. The exponent is large and negative in the regime where the approximation (5.16) holds. The line $v_n\lambda \approx 2\pi n\sqrt{a\lambda}$ separates the regions of narrow gaps and exponentially narrow bands, i.e., it separates the S (saturated) region from the WO (weak-oscillation) and SO (strong-oscillation) regions in Fig. 2(b).

VI. SUMMARY

This section summarizes the results of our calculations mainly for the type-A gaps. Consider for simplicity $u=a\cos(2\pi x/\lambda)$ and $|v_n| \ll 1$. The spectrum in the vicinity of $q=\pi n$ is related to the parameters

$$X_n = v_n(\pi n a/\lambda)^{-1/2}, \quad Y_n = a\lambda/2\pi^2 n , \quad Z_n = 2\pi^5 n^3/a^2\lambda . \tag{6.1}$$

The parameter X must be small for perturbation theory to hold, the parameter Y is a measure of the importance of the slowly varying field in determining the gap structure, and the parameter Z must be large for the phase of the gaps in Eq. (2.12) to have no other m dependence within the n branches than the one given by the trivial $m\pi/2$ phase.

(1) $Y_n < 1$. In this case a is unimportant. The only type-A gap is at $q=\pi n$, and the gap width is $\delta q \approx v_n/\pi n$ [Fig. 5(a)].

(2) $Y_n > 1$. $X_n < 1$ [Figs. 5(b), 5(c), and 3]. There are type-A gaps in an interval

$$q_+ - q_- = [(\pi n)+a]^{1/2} - [(\pi n)-a]^{1/2} \approx a/\pi n . \tag{6.2}$$

The gaps are at $\kappa_A \equiv \pi n + \pi m/\lambda$ so there are $N_A = a\lambda/\pi^2 n$ gaps. The branches of type-A gaps are shown in Fig. 2. The quasi wave vector κ is given by Eq. (2.12):

$$\kappa = 1/\pi \int_0^\pi (q^2 - a\cos x)^{1/2}dx . \tag{6.3}$$

The widths of the gaps are given by Eq. (2.26) which for $q \approx \pi n$ reads

$$\delta\kappa = v_n(qa\lambda)^{-1/2}|\cos(Y - m\pi/2 - \pi/4)| . \tag{6.4}$$

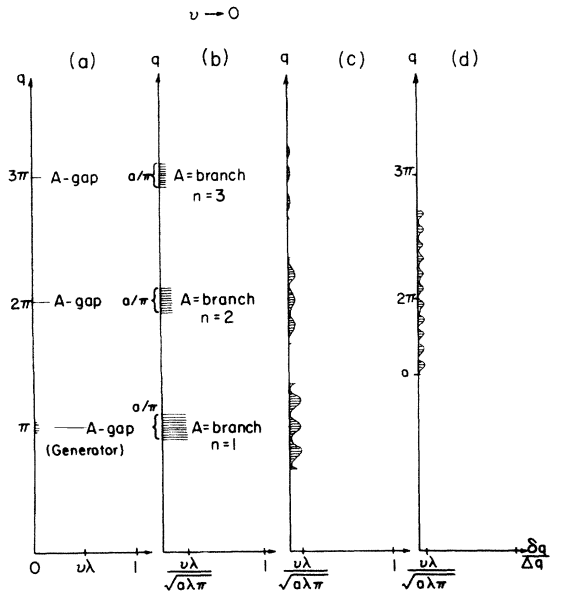

FIG. 5. Development of spectrum for fixed small v as a increases. The vertical axis indicates gap positions and the lengths of the horizontal lines show the widths of the gaps relative to the intergap spacing, $\delta q/\Delta q = \lambda\delta q/\pi$. Note the decrease in the maximal gap width as a increases. For simplicity we have shown only every second gap with, for instance, m even in Eq. (2.26). The intervening gaps are shifted by a phase $\pi/2$. (a) $Y<1$, $X<1$. Only gaps at πn are important. (b) $Y>1$, $X<1$, and $Z>1$. Gaps oscillate as a function of $a\lambda$, but for fixed $a\lambda$ the gap width does not depend on q inside the n branches. The total width δq_{tot} thus oscillates vs $a\lambda$ as demonstrated in Fig. 3(a) (SO regime in Fig. 2). (c) $Y>1$, $X<1$, and $Z<1$. Gaps oscillate vs q inside the n branches, so the total gaps have weak oscillations as shown in Fig. 3(b) (WO regime in Fig. 2). In between the gaps shown there are phase-shifted gaps which are large when the gaps shown are small and vice versa. (d) Same as (c) but overlapping branches.

The widths oscillate with $a\lambda$. The period corresponds to $\Delta N_A = 2\pi$. Within each branch, the gaps depend on m since the phase $a\lambda/2\pi q$ in Eq. (2.26) depends on m through q. For $Z > 1$, the variation of the phase is small in the interval (6.2) so all gaps with even m and all gaps with odd m are in phase. Consequently the *total* width $\delta q_{\rm tot}$ oscillates with $a\lambda$:

$$\delta q_{\rm tot} = (aX/2\pi^2 n)[\,|\cos(Y-\pi/4)| + |\sin(Y-\pi/4)|\,] . \quad (6.5)$$

For $Z < 1$, Y depends on m in the interval, and the oscillations of the individual gaps are out of phase. This leads to weak oscillations of the total width (see Fig. 3). When n increases, v_n usually decreases exponentially, so the limit considered here is fulfilled at least for moderately large n.

(3) $Y > 1$. $X > 1$. In this case λ is the largest parameter. The bands between the type-A gaps shrink to become exponentially small:

$$\delta q \approx (\pi/\lambda)\exp(-X^2) . \quad (6.6)$$

The band positions oscillate with X. The effective gap width is the total interval (6.2), i.e., it is v independent even for very small $v \ll a$ (Fig. 6). Branches corresponding to n and $n' > n$ merge when $q_+^n = q_+^{n'}$, i.e., when $a = \frac{1}{2}\pi^2(n'^2 - n^2)$. The region $q^2 > a$ corresponds to strong coupling (tight binding) and exponentially narrow bands.

Computer experiments[11] verify all the conclusions above.

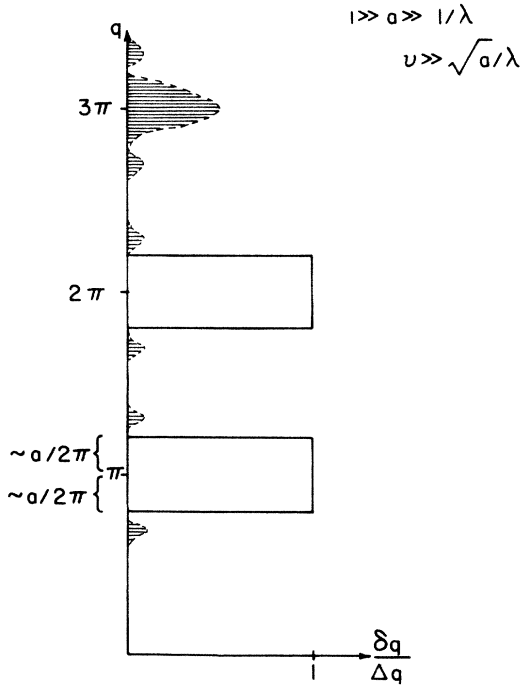

FIG. 6. Spectrum when $\lambda \to \infty$ ($Y > 1$, $X > 1$). There are wide effective gaps independent of v. Inside these gaps there are extremely narrow bands (Landau levels) with distance π/λ. The gaps thus fill up essentially the whole branch of width a/π.

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APPENDIX: APPLICATION TO QUASI-ONE-DIMENSIONAL METALS IN MAGNETIC FIELDS

In Secs. I–VI we studied the spectrum of the Schrödinger equation for an incommensurate system in the case where one potential, u, is sizable but very slowly varying while the second potential, v, has very small amplitude but is rapidly varying. The spectrum was explored at energies much larger than either potential. This case arises in the context of quasi-one-dimensional metals in a magnetic field, and our results may provide insight into the cascade of phase transitions which have been observed in the organic metals $(TMTSF)_2ClO_4$ and $(TMTSF)_2PF_6$ as the field is varied.[6–8]

An anisotropic two-dimensional metal with open orbits can be represented by an electron dispersion that is free-electron-like in one direction and tight binding in another,

$$E(k_x,k_y) = \hbar^2 k_x^2/2m - 2t_b\cos(k_y b) , \quad (A1)$$

where $4t_b$ is the transverse bandwidth. The Fermi surface is open for $E_F > 4t_b$. In the presence of a perpendicular magnetic field the dispersion can be found by making the Landau-Peierls substitution $k \to -i\nabla - eA/c$. Choosing the Landau gauge, we arrive at Mathieu's equation:

$$\psi'' + [q^2 - a\cos(\pi x/\lambda)]\psi = 0 , \quad (A2)$$

where $q^2 = 2mE/\hbar^2$, $a = 4mt_b\hbar^2$, and $\lambda = c\hbar/eHb$. In the relevant materials[6–8] $E_F \approx 1500$ K, $4t_b \approx 300$ K, and accessible magnetic fields introduce a wavelength of $\lambda \approx 10^4$ Å. As we noted in Sec. II [Fig. 1(b)], the gaps produced by the cosine potential are large for $q^2 < a$ and decay exponentially for energies $q^2 > a$. Thus, the slowly varying potential has little effect on the spectrum in the vicinity of the Fermi energy. However, the magnetic field has changed the spectrum from two dimensional, and several authors[12–14] have noted that such a system should be unstable with respect to the usual one-dimensional distortions, Peierls's transitions or spin-density wave. Conventionally, the distortion is introduced by adding a potential of the form $v = v_0\cos(2k_F x)$, and we arrive at an equation of the form (1.1) and we can apply the results that we have derived for the spectrum of this equation.

The region of interest is the first set of gaps ($n = 1$) in Fig. 2, since $k_F \approx \pi$, $E_F \approx \pi^2$, and the physical system corresponds to a range $q_- \leftrightarrow q_+$ which is narrow compared with the distance π between branches since $4t_b \ll E_F$. In the absence of a potential $v(x)$ the natural periodicity in a magnetic field is given by $\lambda k_F/2\pi = $ integer or

$E_F/h\omega' =$ integer where $\omega' = eHk_F b/mc$. In the presence of the $v(x)$ potential the periodicity is given by $a\lambda/2\pi q$ or $4t_b/h\omega'$ from Eq. (2.26). *This reduction in periodicity is comparable to what is experimentally observed for the Hall effect, etc., in a magnetic field.*

Rather than a single gap, the spectrum contains sizable gaps over the entire region $4t_b$ around E_b. If one looks at only one of the gaps, then the expectation is that the magnetic-field-induced transition temperature is reduced to zero periodically with the magnetic field. This was the original result of Ref. 12. The presence of the $m\pi/2$ term in the argument of the cosine in Eq. (2.26) indicates that when a particular gap is close to zero, there is an adjacent gap which is close to maximum. *Thus a simple change of the wave vector with a small amount can reintroduce a sizable gap at E_F. This can explain the series of transitions, with no intervening normal state, which is seen experimentally.*

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[10]This can always be done by renormalization of q and v to $\tilde{q}$ and $\tilde{v}$ according to

$$q^2 - v = \tilde{q}^2 - \tilde{v}, \quad \int_0^{\Lambda} \tilde{v}_1 dx_1/\rho_1 = 0 .$$

If

$$\int_0^1 v_1 dx_1 = \int_0^{\lambda} u_1 dx_1 = 0$$

then the renormalization corrections are exponentially small.

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