PHYSICAL REVIEW B VOLUME 28, NUMBER 12 15 DECEMBER 1983

Wave functions at a mobility edge: An example of a singular continuous spectrum

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(Received 12 August 1983)

An incommensurate model is solved for Liouville-number commensuration, intermediate between the rational and the usual irrational case. The spectrum is singular continuous. The states are sparse at infinity with a hierarchic structure. The spread of a wave packet is oscillatory on any given time scale, the amplitude of oscillation increasing with the time scale.

There is much current interest in the quantum mechanics of particles at a mobility edge, i.e., at the value of a parameter such that the wave functions are "between" conducting and insulating (i.e., between extended and localized), and for which the spectrum is between point and continuous. Such a spectrum is called singular continuous. This is an exotic situation mathematically.[1] It is therefore worthwhile to study a solvable example. Not surprisingly, the example we produce is one of a mobility edge in an incommensurate potential, which is more tractable than the case of random systems, and is of interest in its own right.[2] There are just a few known examples with physical interpretation suspected of possessing such a spectrum, which are at all tractable, even numerically.[3]

We have earlier[4] proposed and solved an incommensurate potential problem with two periods whose ratio is denoted by α. It is representative of a larger class of models[5] for which the density of states is known exactly.[6] The states of the model are extended (Bloch states) when α is rational, and are localized when α is "sufficiently" irrational. In fact, for almost all α, the states are exponentially localized with a characteristic scale $1/\gamma$ independent of α. Here we concentrate on a set of special values of α, a subset of the so-called Liouville numbers, which "interpolate" between the rationals and "irrationals" and for which the states are not necessarily normalizable. When α is a Liouville number the states and spectrum exhibit a variety of structures that depend on the particular number. This ranges from states which have a definite center and decay in a more or less arbitrary way at $\pm\infty$ to states which are not largest at a single center, and increase at infinity.

The states have in common a great increase in "sparseness" as spatial infinity is approached, that is, there are peaks in the wave function whose height may become large or small, but the peaks are more and more spread apart at large distances. The local density of states has an infinite hierarchy of points of accumulation, with each level consisting of self-similar accumulation points.

The model is

$$T_m u_m + \sum_r W_r u_{m+r} = E u_m \quad . \tag{1}$$

Here u_m is the amplitude on the mth lattice site, $W_r = W^*_{-r}$ is the hopping matrix element, $E \equiv -W_0$ is the energy eigenvalue, $T_m = \tan[\omega - \tau m)/2]$, and ω and τ are parameters with $\tau = 2\pi\alpha$. We showed earlier[4] that it is convenient to use a representation in which E is a parameter and ω the eigenvalue. In this representation

$$u(\theta) = u^{\pm}(\theta)/[1 \pm iW(\theta)]$$

and

$$u^+(\theta) = e^{i\omega} e^{-iV(\theta)} u^+(\theta - \tau) \quad , \tag{2}$$

where $W(\theta)$, and $u(\theta)$ are Fourier series transforms of W_m, and u_m, respectively, and

$$e^{-iV(\theta)} \equiv [1 + iW(\theta)]/[1 - iW(\theta)] \quad .$$

If α is irrational, Eq. (2) shows that $|u^+|$ is constant on a dense set of θ in the interval $(0, 2\pi)$. If $|u^+|$ is continuous, it is constant for all θ, and therefore u^+ (and u) can be normalized and possesses a point spectrum. Then $u^+ = e^{i\nu\theta} e^{-i\phi(\theta)}$, with ν an integer and $\phi(\theta) = \phi(\theta + 2\pi)$, and Eq. (2) implies (in terms of the Fourier transform of V)

$$\phi(\theta) = \sum_{m \neq 0} V_m e^{im\theta}/(1 - e^{-im\tau}) \quad . \tag{3}$$

The congruence $\omega \equiv V_0(E) + \nu\tau(\mathrm{mod}\, 2\pi)$ determines E in terms of ω, ν or, alternatively, determines ω for fixed E, ν.

We now adopt a particular choice for V, that corresponding to a W_r of finite range. Then $W(\theta)$ as a function of the complex variable $z = e^{i\theta}$ has no singularity except at the origin. Thus V is analytic in an annulus $e^{-\gamma} < |z| < e^{\gamma}$ determined by the zero of $(1 - iW)$ nearest the unit circle. This structure implies that, asymptotically, $|V_m| \propto e^{-\gamma m}$. It follows from Eq. (3) that, provided there is no complication with an infinite subsequence of the denominators becoming small, ϕ is analytic in the same annulus as is V. Then from Eq. (2) it has a dense set of singularities on the circles $|z| = e^{\mp\gamma}$, i.e., it is a lacunary function.[7] Given this analytic structure, it is easy to show that asymptotically $(1/m)\ln u_m \rightarrow -\gamma$.

If α is irrational, the denominators never vanish, but may become very small. Their smallness depends on how well α is approximated by a rational m/n. More precisely, if $|m\alpha - n| \ll 1$, the denominator $|1 - e^{-im\tau}| \sim 2\pi |m\alpha - n|$. This must be compared with V_m.

To study this we use the continued fraction representation[8] of α:

$$\alpha = \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cdots}} \quad . \tag{4}$$

The "elements" of α the a_i are positive integers. The truncations of the continued fraction define a sequence of rational numbers p_n/q_n, the convergents of α. The denominators q_n can be determined from the a_i's by well-known recursion relations $q_{n+1}=a_{n+1}q_n+q_{n-1}$. Only for n/m a convergent can a denominator be very small, since otherwise $|m\alpha-n|>1/2m$. The inequalities for convergents,

$$\frac{1}{q_k(a_{k+1}+2)}<|q_k\alpha-p_k|<\frac{1}{q_ka_{k+1}} \quad , \tag{5}$$

show that small denominators are associated with large elements. For almost all α, the right side of (5) may be replaced by $q_k^{-1-\epsilon}$ for all but a finite number of k and any $\epsilon>0$. The exceptional α are the Liouville numbers, of which we consider a subclass for which an infinite subsequence of a_{k+1}'s are of order $e^{\gamma q_k}$. In particular, we imagine there is a subsequence of the q_k (denoted Q_j) which have particularly small denominators in (3) with all the other denominators large enough not to need special treatment. Using $V_{(j)}$ for V_{Q_j}, we let

$$2V_{(j)}/(1-e^{-i\tau Q_j})\equiv iA_je^{i\eta_j} \quad .$$

For all m other than these the ϕ_m decrease as mV_m. Thus we may write $\phi=\phi'+\phi^c$, where $\phi'=\sum'\phi_me^{im\theta}$ and the sum is over $m\neq Q_j$. This function is analytic as discussed earlier and is essentially ϕ for a nearby, more typical α. On the other hand

$$\phi^c(\theta)=-\sum A_j\sin(Q_j\theta+\eta_j)$$

may not exist, depending on the behavior of the A_j's.

The A_j's may be chosen arbitrarily in the sense that a Liouville number can be found (in fact, one in every open set of reals) which, to arbitrary accuracy, gives rise to a predetermined and completely arbitrary sequence of nonnegative A's, with possibly a finite number of exceptions. The Q's are not so arbitrary, but because of the recursion relation must grow rapidly with j, at minimum, in this case as an iteration of exponentials.

Since ϕ^c is undefined for some sequences A_j we resort to considering a sequence of "noble" irrational numbers $\alpha^{(j)}$ which approach the Liouville number α. The first $j+1$ elements of $\alpha^{(j)}$ are the same as those of α, with the remaining elements unity. The sequence of A_i for $\alpha^{(j)}$ coincides with that of α for $i\leq j$, but terminates there. For this case, then, ϕ^c is well defined, being a finite series.

We study the wave function in the position representation. Let the wave function for $\alpha^{(j)}$ be $u^{(j)}$. Then it can be shown that

$$u_m^{(j)}=\sum_{n_j}u_{m-n_jQ_j}^{(j-1)}J_{n_j}(A_j) \quad . \tag{6}$$

Here $J_n(A)$ is a Bessel function of the first kind, times a conceptually unimportant phase factor $e^{in_j\eta_j}$. Thus

$$u_m^{(j)}=\sum_{n_1}\sum_{n_2}\cdots\sum_{n_j}u'_{m-n_1Q_1-n_2Q_2-\cdots-n_jQ_j}J_{n_1}(A_1)\cdots J_{n_j}(A_j) \quad . \tag{7}$$

Here $u'=e^{-i\phi'}$. In this derivation we have not noted the dependence of u' on j since it is weak (as is that of the $u^{(i)}$ with $i<j$).

This formula is easy to study since at most one term in the sums is appreciable: u_m is relatively large only when the subscript of u_r' is of order γ^{-1}. The subscript satisfies this condition only when m is close to one of the points $n_1Q_1+n_2Q_2+\cdots+n_jQ_j$. However, the Bessel function factors suppress the value of the wave function for $n_k\gg A_k$ and $Q_{k+1}\gg A_kQ_k$. Thus a peak near the origin is repeated about A_1 times at successive distances Q_1; this whole structure is again repeated A_2 times at distances Q_2, and so on. This structure is much like that found numerically in Ref. 3, but the scales Q_j increase here much more rapidly, as an iteration of exponentials rather than exponentially. (Exponential growth also occurs in our model for the choice $V_m\propto 1/m$, α an ordinary irrational.) Figure 1 shows such a function, with the scale of Q_j artificially reduced to make possible the plot.

Note that $u^{(j)}$ is normalized to unity. If the maximum value of (7) vanishes as j becomes infinite, then the limiting wave function is not normalizable. Let $|J_n(A_k)|$ be maximum for $n=m_k$. Then, if the infinite product $\prod|J_{m_k}(A_k)|>0$, the wave function is normalizable. The product is positive if and only if $\sum A_k^2<\infty$, i.e., ϕ^c is square integrable. If the A's approach zero, the height of the largest peak at distance $\sim Q_j$ is A_j times smaller than that at zero, so there are Liouville numbers for which the wave function decays at infinity, and which may or may not be normalizable. Conversely, the peaks of the function may grow at infinity (as can be seen by taking all the A's to be near a zero of J_0). Although the decay or growth as a function of k may be a power law, or exponential, or even faster, the behavior as a function of distance is very slow, since Q_k increases rapidly.

We turn now to the spectrum and discuss the local integrated density of states (the spectral measure with respect

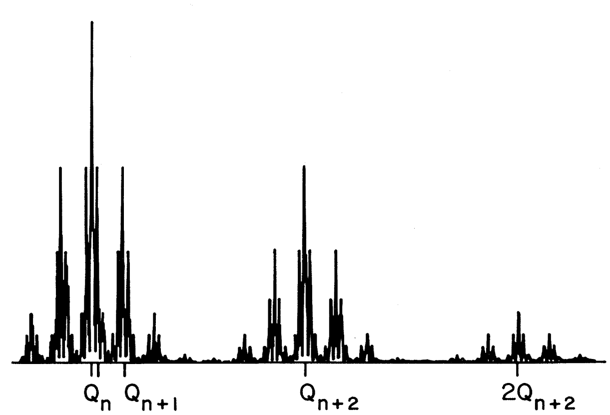

FIG. 1. Absolute square of a wave function, $A_i=1$, which is symmetric about the highest peak, at the origin. The Q_j artificially are made to increase "only" exponentially. The heights of the peaks at Q_j remain constant with j in this case.

to site m)

$$\mu_m(\omega) = \int^{\omega} d\omega' \sum_{\nu} |u_m^{\nu}|^2 \delta(\omega' - \omega_\nu) \quad ,$$

with $\mu(\omega + 2\pi) - \mu(\omega) = 1$. If the spectrum is point, the wave functions are localized and there are a finite number of significant points of increase in μ. Thus $d\mu/d\omega$ vanishes except at a discrete and disjoint set of points. In the extended case, the sum over ν is replaced by an integral over a continuous variable, (θ_0), and μ increases continuously over bands of energies.

We take $m = 0$ and study the neighborhood of $\omega = \omega_0 (= 0)$ for α Liouville. The frequencies are $\omega_\nu = \nu\tau \bmod 2\pi$, so only for $|\nu\alpha - m| << 1$ will ω_ν be near zero. But these are precisely those values $\nu = Q_j$ for which u_0^{ν} is relatively large. We see that μ has jumps at a sequence of points a distance $1/Q_k$ from the origin which is a point of accumulation of the local spectrum. Moreover, each of the points of the sequence, corresponding to $\nu = Q_{k-1}$, is itself a point of accumulation of the sequence $\nu_j = Q_{k-1} + Q_j$ for $j \geq k$, and each of these points in turn is a point of accumulation. In short, the spectrum is a sort of inverse image of the wave function, and there is a precise self-similarity in that each line of the spectrum is surrounded by its entourage of accumulating satellite lines, and the shape of the entourage for one point is asymptotically proportional to the shape of all the others. The points (near $\omega = 0$) in the support of μ_0 can be written $\omega[\sigma] \approx \sum \sigma_j / Q_{j+1}$, where $\sigma = (\sigma_1, \sigma_2, \ldots)$ and σ_j is an integer of maximum magnitude of order A_j. The set $\{\sigma\}$ is uncountable but of zero Lebesgue measure. The *spectrum* is uninteresting. It is the closure of the union of the support of all μ_n, i.e., all $|\omega| \leq \pi$. Further study shows that $d\mu/d\omega = 0$ almost everywhere (and thus μ is *singular)* but μ is nevertheless *continuous,* having no finite jumps. Each jump which is finite for $\alpha = \alpha^{(j)}$ is split up into an infinite number of subjumps for $j \to \infty$.

The spectrum in E (for fixed ω) is similar, except that, since γ depends on E, there is a critical energy E_c such that $\sum A_j(E)^2 < \infty$, for $|E| > E_c$. This mobility edge in *energy* separates the pure point and the singular continuous parts of the spectrum. It is presumably not generic.

We next consider the spreading in time of a wave packet initially localized at $m = 0$. A simple formula[9] gives the expectation of m^2 as a function of integer time[10] t, namely,

$$S(t) = \sum m^2 V_m^2 \sin^2(mt\tau/2)/\sin^2(m\tau/2) \quad . \tag{8}$$

The sum may be expressed as $S = S' + S^c$, where

$$S^c = \sum Q_k^2 A_k^2 \sin^2(\pi Q_k \alpha t)$$

and S' is an almost periodic function whose maximum value is of order $\gamma^{-2} \sum V_m^2$. S^c has hierarchical behavior. Consider $t \leq Q_k$. Then, since $|Q_k\alpha - P_k| \sim 1/Q_{k+1}$, the kth term is of order $t^2 Q_k^2 V_{(k)}^2$. This is very small, so that for fixed t the sum converges (as it should, since we now deal with a physical quantity). Assume first that $A_k Q_k$ grows powerfully. As t increases, successive terms of the sum become important, with the last important term by far the largest. Once a term becomes large, it dominates for a long time, except, of course, that it oscillates *very* many times back to zero on a scale very slow compared with earlier scales, before the next term at long last becomes large. The development of S_r is thus rather schizophrenic. It oscillates for a long time, as if localized, then escapes ballistically (as t^2) as if in a periodic potential which, in turn, is finally revealed as the start of a period of oscillation on a vastly larger scale. This agrees nicely with an interpretation of Simon[1] (and an example of Pearson[11]) who argues that the particle thinks it is moving in a periodic potential for a while but eventually gets reflected because things are not quite periodic. It then moves to an even further distance and is reflected again, and so on *ad infinitum.*

One may want[9] to find the dependence of the envelope function $Q_k^2 A_k^2$ on time scale Q_{k+1}. One possibility is for the A_k to grow rapidly with Q_k, say, as $e^{\beta Q_k}$. Then $Q_k^2 A_k^2 \sim (Q_{k+1})^{2\beta/(\beta+\gamma)}$, power-law behavior.[9] However, this is not generic, except in the sense that the maximum rate of growth is t^2.

Note that nothing special happens in the physical quantity $S(t)$ as the eigenstates become normalizable. Not until $A_k Q_k \sim 1/\sqrt{k}$ is the spread of the particle limited. This change of behavior therefore occurs when the heights of the peaks in the wave function decay as a power of the distance, even though as a function of peak number k they decay dramatically.

We have produced a picture of the wave functions, spectrum, and wave-packet propagation for a model problem in which the states are neither exponentially localized nor regularly extended. A variety of exotic behavior interpolating between these two extremes is possible. We have provided a readily studied example which may help to build up intuition on the mathematical problems associated with the physical problem of the mobility edge.

ACKNOWLEDGMENTS

This work was supported in part by the NSF under Grants No. DMR 79001172-A02, No. DMR 7908819, the Center for Theoretical Physics, and the U.S.-Israel Binational Science Foundation. We also acknowledge support of the Computer Center of the University of Maryland.

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[9]M. V. Berry (unpublished).

[10]This "time" is not that of the original representation, which is cumbersome to deal with. Asymptotically, the behavior is much the same.

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