Bandwidths for a quasiperiodic tight-binding model

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A study is made of the spectrum of a class of one-dimensional models that are equivalent to the equation for an electron in a magnet field and a two-dimensional periodic potential. A rigorous lower bound for the measure of the spectrum is derived, and theoretical and numerical arguments are presented to show that this bound is attained in the incommensurate limit. In the case that corresponds to an isotropic system this lower bound is zero, and numerical work shows that the measure has the asymptotic form A/p, where p is the period. The existence of a finite Lyapunov exponent and of a nonzero spectral measure in the incommensurate limit seems to be correlated with the existence of semiclassical open orbits in the problem of an electron in a magnetic field.

I. INTRODUCTION

In a study of the eigenvalue problem

$$V_1 c_{n-1} + 2V_2 \cos(2\pi n\phi + \nu)c_n + V_1 c_{n+1} = Ec_n , \qquad (1.1)$$

where *n* has an infinite range, Aubry and Andre¹ gave numerical evidence that for ϕ irrational the spectrum has measure $4 | V_2 - V_1 |$. For rational values of ϕ the union of the spectrum for all values of v has a measure greater than this, but it tends rapidly towards it as the denominator of ϕ gets larger. Sokoloff² has obtained some results which give a value for the measure of the extended spectrum, for ϕ irrational, lower than $4(V_1 - V_2)$. Since the duality arguments¹ suggest that for $V_1 > V_2$ all states should be extended, there seems to be a conflict, but I show in this paper that $4|V_1 - V_2|$ is a rigorous lower bound for rational values of ϕ . Theoretical arguments suggest that the difference of the spectral measure from this lower bound should be of order $\exp\left[\frac{1}{2}p \mid \ln(V_2/V_1) \mid \right]$, where p is the denominator of ϕ , and numerical results given in Sec. III support this conjecture. At the critical point $V_2 = V_1$, where the self-similar nature of the band structure was studied by Hofstadter,³ the numerical results show a spectral measure proportional to p^{-1} , with a constant of proportionality which asymptotically approaches $9.3300V_2$ for most values of the numerator q of ϕ .

Equation (1.1) has been used to describe the quantum theory of an electron confined to a plane with a periodic potential in the plane and a uniform magnetic field perpendicular to the plane. It arises in two different cases. The first is an s-band tight-binding model in a weak magnetic field,^{4,5} in which case ϕ is the number of flux quanta per unit cell. In the second case the potential is weak compared with the cyclotron energy $\hbar\omega_c$, it oscillates sinusoidally in two directions, and $1/\phi$ is the number of flux quanta per unit cell.⁶

Aubry and André¹ pointed out that Eq. (1.1) satisfies an important duality property. This can be derived by making the substitution

$$c_n = \sum_m d_m \exp[i(K + 2\pi m\phi)n]$$
(1.2)

in Eq. (1.1), in which case an equation for d_m is obtained which is the same as Eq. (1.1) for c_n with V_1 and V_2 interchanged, and v replaced by K. It can also be obtained from the two-dimensional problem by choosing a vector potential in the x direction instead of the y direction. This duality relation has been used to show that the Lyapunov exponent which gives the inverse localization length is equal to

$$1/L = \ln(V_2/V_1) \tag{1.3}$$

for $V_2 > V_1$, for all energies in the energy bands and for ϕ irrational. This can be identified with the inverse localization length in the x direction for the two-dimensional problem—the states are extended in the y direction for $V_2 > V_1$. It is only for the isotropic case $V_1 = V_2$ that the localization length is infinite in both directions.

If the localization length is identified with a correlation length, $V_1 = V_2$ appears like a critical point where the length diverges linearly. This has led me to examine other aspects of the critical behavior, and the linear dependence of the sum of the bandwidths (measure of the spectrum) on both $|V_2 - V_1|$ and p^{-1} gives two more critical exponents that are equal to unity. Tentatively, p has been identified with a finite size in the scaling problem.

In order to verify the association of the vanishing measure of the spectrum with the infinite localization length two slightly different models were examined. The first was the anisotropic triangular lattice, where again it can be shown that the localization length diverges and the spectral measure vanishes at the critical point corresponding to isotropy. The second model has anisotropic nearest-neighbor coupling on a square lattice and isotropic next-nearest-neighbor coupling. From a combination of theoretical and numerical arguments it appears that the localization length is infinite and the spectra measure is zero wherever the isotropic next-nearest-neighbor coupling is dominant. This indicates that the critical region has some sort of stability against weak anisotropy.

In Sec. IV these results are discussed briefly in terms of scaling theory. There is also a discussion of the association between the existence of broadened bands and of a finite localization length at all energies in the bands and

<u>28</u> 4272

BANDWIDTHS FOR A QUASIPERIODIC TIGHT-BINDING MODEL

the existence of open orbits at some energies in the semiclassical theory of the tight-binding models.

II. LOWER BOUND FOR THE SUM OF BANDWIDTHS

If ϕ has a rational value q/p, Eq. (1.1) can be reduced to a finite-matrix problem of order p for the Bloch-wave solutions satisfying

$$c_{n+p} = c_n \exp(iKp) . \tag{2.1}$$

It is obvious that the characteristic equation for E depends on K only through the constant term $-2V_1^p \cos Kp$, and then duality requires that the v dependence should involve only the constant term $-2V_2^p \cos vp$. This implies that the band edges are given by extremal values of the expression

$$-2V_1^p \cos Kp - 2V_2^p \cos vp \quad . \tag{2.2}$$

This means the band edges (for V_1V_2 positive) can be found by considering K=0, v=0 and $K=\pi/p$, $v=\pi/p$. For the sake of symmetry we choose, instead of $v=\pi/p$, the equivalent values $v=\pi$ for p odd and $v=\pi q/p$ for p even.

The solutions for $K = 0, \pi/p$ can be split into those that are odd or even about the two symmetry points n = 0 and p/2. For v=0 and p=2s+1 odd the eigenvalues corresponding to the solutions symmetric about n=0 are given by

$$2V_{2}a_{0} + \sqrt{2}V_{1}a_{1} = E^{+\pm}a_{0},$$

$$\sqrt{2}V_{1}a_{0} + 2V_{2}\cos(2\pi\phi)a_{1} + V_{1}a_{2} = E^{+\pm}a_{1},$$

$$V_{1}a_{n-1} + 2V_{2}\cos(2\pi n\phi)a_{n} + V_{1}a_{n+1} = E^{+\pm}a_{n}, \quad 2 \le n < s$$

$$V_{1}a_{s-1} + 2V_{2}\cos(2\pi s\phi)a_{s} \pm V_{1}a_{s} = E^{+\pm}a_{s},$$

(2.3)

where $a_0 = \sqrt{2}c_0$, $a_n = c_n + c_{-n}$. The solutions antisymmetric about n = 0 are given by

$$V_1 b_{n-1} + 2V_2 \cos(2\pi n\phi) b_n + V_1 b_{n+1} = E^{-\pm} b_n, \quad 1 \le n < s$$
(2.4)

$$V_1 b_{s-1} + 2V_2 \cos(2\pi s\phi) b_s \pm V_1 b_s = E^{-\pm} b_s$$
,

where $b_0 = 0$, $b_n = c_n - c_{-n}$. The top of the highest band is given by the highest eigenvalue E_{s+1}^{++} of Eq. (2.3), and the band gaps are the intervals between the corresponding eigenvalues E_m^{++} and E_m^{--} of Eqs. (2.3) and (2.4). For $v=K=\pi$ the positions of the band edges are simply minus the band edges for v=K=0. Equation (2.4) shows that E^{-+} and E^{--} are the eigenvalues of two symmetric matrices that differ from one another by a positive definite matrix of trace $2V_1$, and so it follows that

$$E_m^{-+} > E_m^{--}, \quad \sum_{m=1}^s (E_m^{-+} - E_m^{--}) = 2V_1 \;.$$
 (2.5)

Similarly, comparison of Eqs. (2.3) and (2.4) shows that, if the 01 element of the matrix whose eigenvalues are E^{++} is replaced by zero, a matrix whose eigenvalues are $2V_2$ and the E^{-+} is obtained. The E^{-+} , which are the zeros of the 00 element of the resolvent of the first matrix, lie between the E^{++} , and the two matrices have the same trace. It follows that

$$E_m^{++} < E_m^{-+} < E_{m+1}^{++} ,$$

$$\sum_{m=1}^{s} (E_m^{-+} - E_m^{++}) + 2V_2 - E_{s+1}^{++} = 0 .$$
(2.6)

These two results can be combined to give the sum of all band gaps (for both K = v = 0 and $K = v = \pi$) as

$$2\sum_{m=1}^{s} |E_{m}^{++} - E_{m}^{--}|$$

$$\leq 2\sum_{m=1}^{s} (|E_{m}^{++} - E_{m}^{-+}| + |E_{m}^{-+} - E_{m}^{--}|)$$

$$= 2E_{s+1}^{++} - 4V_{2} + 4V_{1}. \qquad (2.7)$$

Since the extremals of the band are at $\pm E_{s+1}^{++}$ this shows that the sum of the bandwidths is greater than or equal to $4(V_1 - V_2)$. Duality immediately shows that it is also greater than or equal to $4(V_2 - V_1)$.

For large values of p and $V_2 > V_1$ the nonzero value of the Lyapunov exponent would lead one to expect very little interference between the effect of changing the 01 element of matrix from $\sqrt{2}V_1$ to zero in going from E^{++} to E^{-+} and the effect of changing the *ss* element by $2V_1$, since eigenvectors should be localized and should not have appreciable amplitudes at two sites *s* apart. This suggests that for large p and $V_2 > V_1$ the sum of bandwidths is given by

$$W = 4(V_2 - V_1) + O((V_1 / V_2)^{p/2}).$$
(2.8)

The rapid approach to the limiting value is in agreement with the numerical results of Aubry and André,¹ while the numerical work described in Sec. III gives a more detailed confirmation of this conjecture.

For even values of p the argument is very similar. The only difference is that for v=0 the equations have offdiagonal terms at each end which are either $\sqrt{2}V_1$ or zero, while for $v=\pi q/p$ the equations have diagonal terms $\pm V_1$ at each end.

It is possible to generalize this argument to a limited number of other interesting systems. Firstly,

$$2V_1 \cos[\pi(n-\frac{1}{2})\phi+\nu/2]c_{n-1}+2V_2 \cos(2\pi n\phi+\nu)c_n +2V_1 \cos[\pi(n+\frac{1}{2})\phi+\nu/2]c_{n+1}=Ec_n \quad (2.9)$$

gives the spectrum for an electron in an anisotropic triangular tight-binding lattice. The spectrum in the isotropic case $V_1 = V_2$ was calculated by Claro and Wannier.⁷ Secondly,

$$\{V_{1}+2V_{3}\cos[2\pi(n-\frac{1}{2})\phi+\nu]\}c_{n-1} + 2V_{2}\cos(2\pi n\phi+\nu)c_{n} + \{V_{1}+2V_{3}\cos[2\pi(n+\frac{1}{2})\phi+\nu]\}c_{n+1} = Ec_{n} \quad (2.10)$$

represents an electron in a square tight-binding lattice with anisotropic coupling to nearest-neighbor sites and isotropic coupling V_3 to next-nearest-neighbor sites. In both cases the same equations can be obtained for a strong magnetic field and a weak periodic potential of the appropriate form. The dependence on K of the characteristic equations for the Bloch waves is obtained by taking the

4273

product of off-diagonal terms, and the v dependence can then be deduced from the rotational properties of the lattice. For the triangular lattice this gives a term

$$2V_2^p \cos(pv) \pm 4V_1^p \cos(\frac{1}{2}pv) \cos(\sqrt{3}pK/2) , \qquad (2.11)$$

while for the square lattice it gives

$$4V_{3}^{p}\left[-\cosh\left[p\cosh^{-1}\frac{V_{2}}{2V_{3}}\right]\cos(p\nu) -\cosh\left[p\cosh^{-1}\frac{V_{1}}{2V_{3}}\right]\cos(pK) + (-1)^{p+q}\cos(p\nu)\cos(pK)\right].$$
(2.12)

For V_2 greater than V_1 and $2V_3$ these expressions are dominated by the leading term for large p, so the extremals are found for v=0 and π/p , just as for expression (2.2). For finite p the effect of restricting attention to these values of v can only be to underestimate the sum of bandwidths, so it still gives a lower bound for the measure of the spectrum.

The argument goes through with little alteration. In Eqs. (2.3) and (2.4), V_1 is replaced by one of the more complicated expressions from Eqs. (2.9) or (2.10), and similarly in Eq. (2.5), V_1 is replaced by $|2V_1 \cos[\frac{1}{2}(\pi q + \nu)]|$ or by $|V_1 + 2V_3 \cos(\pi q + \nu)|$, where ν is 0 or π . The final result is that the sum of bandwidths is bounded below by

$$4(V_2 - V_1) \tag{2.13}$$

for the triangular lattice, and by

$$4V_2 - 4\max(V_1, 2V_3) \tag{2.14}$$

for the square lattice.

The duality argument can again be used to get the localization length. The cofactors that come into the Aubry-André¹ calculation are the coefficients of $\exp(ipK)$ in Eqs. (2.11) and (2.12). It is convenient for the triangular lattice to consider three different coupling constants in the three directions so that the rotational symmetry can be used; the Lyanpunov exponent for this lattice is $\ln V_2/V_1$. For the square lattice, with $2V_3 < V_1 < V_2$, the exponent is

$$\ln[V_2 + (V_2^2 - 4V_3^2)^{1/2}] - \ln[V_1 + (V_1^2 - 4V_3^2)^{1/2}], \quad (2.15)$$

with $V_1 < 2V_3 < V_2$ it is

$$\ln[V_2 + (V_2^2 - 4V_3^2)^{1/2}]/2V_3 , \qquad (2.16)$$

and with $V_1 < V_2 < 2V_3$ it is zero. Because the exponent is nonzero the lower bound (2.13) should be attained in the incommensurate limit for $V_1 < V_2$ in the triangular lattice. The lower bound (2.14) for the square lattice should be attained for $2V_3 < V_2$.

It is interesting to note that as $2V_3$ approaches V_2 the sum of bandwidths tends to zero and the Lyanpunov exponent tends to zero even though the square symmetry is broken by unequal values of V_2 and V_1 . The argument presented here does not allow anything to be said about the bandwidths in the case $V_1 < V_2 < 2V_3$, where the exponent is also zero, but numerical results described in Sec. III support the conjecture that in this case the sum of bandwidths is of order p^{-1} , and so tends to zero in the incommensurate limit.

III. NUMERICAL RESULTS

Since the band edges for the square lattice can be found from the eigenvalues of tridiagonal matrices of the forms given by Eqs. (2.3) and (2.4), or the corresponding equations for even values of p, there is no difficulty in generating extensive results with a modest use of computer time. For the isotropic square lattice with nearest-neighbor coupling ($V_1 = V_2$, $V_3 = 0$) a complete set of results were obtained for $p \le 20$, and scattered results for larger values of p up to about 400. In this case the results fell into such a regular pattern that little gain was expected from more extensive results or larger values of p.

The conjecture that the total bandwidth should tend to zero as some negative power of p was confirmed, and it was established that the exponent of p is unity with rather high precision (of the order of one part in 10⁵). This value of the exponent seems to be demanded by Hofstadter's observation that the diagram of energy bands as a function of ϕ is self-similar.³ Furthermore, if the sum of bandwidths is W(q/p), the limiting value of pW appears to be independent of the way in which q varies as p tends to infinity (with one possible exception which is discussed below). The limiting value is given by

$$\lim_{p \to \infty} pW(q/p) = 9.3300V_1 .$$
 (3.1)

For even p the value of pW(q/p) is above the limit, and for odd p it is below the limit in all cases that have been examined. For even values of p the distance from the limit is about twice as far as it is for corresponding odd values. The speed of approach to the limit does depend on the manner in which q varies. Two of the most favorable cases are q = 2 for odd p and $q = \frac{1}{2}p - 1$ for even p, and there the convergence is roughly quadratic, while for q = 1the convergence is so slow that the limiting value is doubtful. Some values of pW(q/p) are shown in Table I.

The behavior for q = 1 (or equivalently q = p - 1) appears anomalous. My best extrapolations of those systematic results give limits of 9.42 for even p and 9.29 for odd p, with deviations of order $p^{-1/2}$, but these extrapolations are not reliable. It may be more than a coincidence that the average of $pW(1/p)/V_1$ for an even value of p and the two neighboring odd values of p is very close to the limiting value 9.3300. In each of the two cases shown in Table I the difference is of order one part in 10⁵.

A few calculations have also been made for $V_1 \neq V_2$. In Fig. 1 some bands are compared for $V_1 = V_2$ and $0.5V_2$. The results support the form for the sum of bandwidths given in expression (2.8). Various sequences of values of ϕ were studied for $V_1 = 0.5V_2$ and $0.9V_2$. In all cases the results fairly rapidly approached an apparent limit of the form

$$W(q/p) \sim 4(V_2 - V_1) + \alpha p^{-1} V_2 (V_1/V_2)^{p/2}$$
, (3.2)

but the coefficient α varies from one sequence to another.

TABLE I. Values of pW(q/p) for selected values of q/p, for the square lattice with $V_1 = V_2 = 1$, $V_3 = 0$.

q/p pW(q/p)	$\frac{89}{233}$ 9.329 01	$\frac{144}{377}$ 9.329 87	$\frac{70}{169}$ 9.329 80	$\frac{169}{408}$ 9,330,03	$\frac{2}{199}$ 9 329 89	99 200 9 330 11	$\frac{2}{399}$ 9 329 96	199 400 9 330 01
q/p pW(q/p)	$\frac{1}{47}$ 9.1784	$\frac{1}{48}$ 9.6312	¹ / ₄₉ 9.1806	$\frac{1}{199}$ 9.2334	$\frac{1}{200}$ 9.5225	$\frac{1}{201}$ 9.2337	5.025 50	

For example, for $V_1=0.5V_2$ the sequence q=2, p=15,17,19,21 gave $\alpha=7.16$, while the sequence $\frac{7}{16}, \frac{9}{20}, \frac{11}{24}, \frac{13}{28}, \frac{15}{32}$ gave $\alpha=7.73$. Other sequences examined were too short to show convergence, but suggested values of α in the range from 7 to 9. For $V_1=0.9V_2$ the sequence q=2, p=15,25,35,45,55,65,75,85 gave $\alpha=9.66$, while the sequence $\frac{23}{48}, \frac{27}{56}, \frac{31}{64}$ gave 9.68. It is clear that the general form of these results is in agreement with what is expected, but it does not appear that α has a value independent of q as it seems to for $V_1=V_2$.

Some calculations were also carried out for the square lattice with next-nearest-neighbor coupling given by Eq. (2.10). The most interesting region for this model is $2V_3 > V_2 > V_1$, since the localization length is infinite there despite the anisotropy, and the lower bound (2.14) gives no information. In this region the extremals of (2.12) are at $v=0,\pi/p$ and $K=0,\pi/p$; all four stationary points were found for each band and the highest and lowest were used to determine the band edges. Some results were obtained for $V_3=10V_1=5V_2$ and for $V_3=2V_1=V_2$. A selection of the values of $pW(q/p)/V_3$ is shown in Table II. The results are scattered and do not follow any obvious pattern. It seems likely that the sum



FIG. 1. Energy bands for a sequence of values for ϕ approximating $(\sqrt{5}-1)/2$ for (a) $V_1/V_2=1$ and (b) $V_1/V_2=0.5$. Arrows show the positions of the narrowest gaps.

of bandwidths is tending to zero at least as fast as p^{-1} in this case also.

IV. DISCUSSION

There is some analogy between the behavior of the system described by Eq. (1.1) and a system displaying critical phenomena. The localization length calculated by Aubry and André¹ is analogous to a correlation length which diverges linearly as V_2/V_1-1 tends to its critical value, zero. The value of p can be taken as analogous to the length in a finite-size-scaling theory, since it gives the distance up to which an incommensurate system with irrational ϕ is approximated by the commensurate system. The sum of bandwidths W for infinite p tends linearly to zero with V_2/V_1-1 . Finite-size-scaling theory suggests that, for fixed p, W should not depend much on the correlation length ξ when ξ is much larger than p. Finite-size scaling therefore gives

$$W = (V_2 - V_1) f(\xi/p) , \qquad (4.1)$$

and so f must be linear in ξ/p where ξ is too large to be important, and so, close to the critical point, W is proportional to p^{-1} .

Some tests of the finite-size-scaling relation (4.1) are possible. Since ξ^{-1} is $\ln(V_2/V_1)$ it is possible to compare $W/(V_2-V_1)$ for two different values of V_2/V_1 that give the same value of $p \ln(V_2/V_1)$. This was done for q = 2 in the two cases $V_2/V_1=0.9$ and 0.5705, where the logarithms differ by a factor of 5. Reasonable agreement between the values for q = 2, p = 55,65,75,85 in the first case and q = 2, p = 11,13,15,17 in the second case was obtained. The scaling cannot be exact, or the values of α defined by Eq. (3.2) would be proportional to $(1 - V_2/V_1)/$ $\ln(V_2/V_1)$, and there are considerable discrepancies from this, but the scaling may be good near the critical point.

Since these numerical results show that for the isotropic case the measure of the spectrum tends to zero as p goes to infinity, there can be no analytic local density of states, so the spectrum has no absolutely continuous part in the incommensurate limit.

The q independence of the limit of pW(q/p) and its numerical value are intriguing observations for which I have no explanation. Further questions are raised by the quantity α defined by Eq. (3.2); it does seem to have a weak dependence on q and its value is not entirely in accord with the predictions of finite-size scaling.

The model given by Eq. (2.10) has some interesting and

TABLE II. Value of pW(q/p) for the square lattice with next-nearest-neighbor coupling V_3 and isotropy broken by a weaker nearest-neighbor coupling. In (a) the coupling constants are $V_3=1$, $V_1=0.1$, and $V_2=0.2$, and in (b) they are $V_3=1$, $V_1=0.5$, and $V_2=1$.

(a)	q / p	5 12	<u>12</u> 29	<u>29</u> 70	8 21	<u>13</u> <u>34</u>	21 55	$\frac{12}{41}$	<u>29</u> 99
	pW(q/p)	10.60	6.63	3.22	6.54	4.71	2.29	5.13	2.86
(b)	q/p pW(q/p)	$\frac{2}{45}$ 8.55	$\frac{2}{55}$ 6.20	$\frac{2}{65}$ 8.81	$\frac{2}{75}$ 6.86	$\frac{2}{85}$ 3.68	$\frac{23}{48}$ 4.10	$\frac{27}{56}$ 1.65	$\frac{31}{64}$ 2.55

unexpected features, which can be clarified by comparison with the semiclassical theory of electron motion in a magnetic field.^{8,9} In the semiclassical theory the magnetic field drives electrons around contours of constant $E(\vec{k})$. Important distinctions exist between electron orbits, which surround minima of $E(\vec{k})$, hole orbits, which surround maxima, and open orbits. The energy ranges in which the three types of orbits occur can be found by examining the stationary points of $E(\vec{k})$. For example, the tight-binding model described by Eq. (2.10) has energies given by

$$E(\overline{\mathbf{k}}) = 2V_1 \cos k_1 a + 2V_2 \cos k_2 a$$
$$+ 4V_3 \cos k_1 a \cos k_2 a . \tag{4.2}$$

For $0 < 2V_3 < V_1 < V_2$ this has a maximum at $k_1 = k_2 = 0$, a minimum at $k_1 = k_2 = \pi/a$, and two inequivalent saddle points at $(\pi/a,0)$ and $(0,\pi/a)$. There are orbits open in the k_1 direction for

$$-2V_1+2V_2-4V_3 > E > 2V_1-2V_2-4V_3$$

Similarly for $0 < V_1 < 2V_3 < V_2$ there are open orbits for

$$-2V_1+2V_2-4V_3>E>-2V_1-2V_2+4V_3.$$

In the region $2V_3 > V_2 > V_1 > 0$ in which V_3 dominates there are maxima at (0,0) and $(\pi/a,\pi/a)$, minima at $(0,\pi/a)$ and $(\pi/a,0)$, and four equivalent saddle points at $k_1a = \pm \cos^{-1}(-V_2/2V_3)$, $k_2a = \pm \cos^{-1}(-V_1/2V_3)$, so there are no open orbits except at this singular value of the energy. When these results are compared with the theoretical analysis which leads to Eqs. (2.14) and (2.16), and with the numerical results in Sec. III, it can be seen that the existence of a band of semiclassical open orbits corresponds to a finite localization length in one direction (and therefore, from duality, states which are extended in the perpendicular direction) at *all* energies in the spectrum, and to a spectrum of nonzero width in the commensurate limit. When there is no band of open orbits, but only a singular energy, then the localization length is infinite in both directions, and the width of the spectrum tends to zero, as one might expect for the quantization of closed orbits. These relations between the nature of the orbit, the width of the spectrum, and localization have been discussed by a number of authors.^{10–13}

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