Localization by a Potential with Slowly Varying Period

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In order to understand some discrepancies in the recent Letter of Griniasty and Fishman, a study has been made of localization by a one-dimensional potential with slowly varying period. Away from the band center, localization is produced by local regions in which the Bragg condition allows backward scattering, and the result agrees with that obtained from perturbation theory. The localization length increases as the band center is approached in a manner that cannot be obtained directly from perturbation theory. It is shown that rounding errors set an upper bound to the localization length that would be determined from numerical studies of such a problem.

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In a recent paper, Griniasty and Fishman[1] have studied the problem of localization on a one-dimensional lattice with a weak sinusoidal potential whose phase varies as an^{ν}, where n labels the site on the lattice. For $\nu \leq 1$, the eigenstates were found to be extended, and for $\nu \geq 2$ they were localized with a localization length equal to that for a random potential of the same mean square strength. In the case $1<\nu<2$ there was some discrepancy between the analytical results obtained by use of the perturbative theory of Thouless[2] and the numerical results obtained by a direct solution of the recursion relations. In order to find out the reasons for this discrepancy I have studied the problem of the discrete Schrödinger equation with a sinusoidal potential whose period varies slowly in space using different methods. Away from the band center similar results were obtained, but quite different results were found near the band center. An analogous discrepancy in results for the localization length of a random system near the band center was found some years ago by Kappus and Wegner.[3]

Bragg reflection for a slowly varying period.—I study the equation

$$a_{n-1}+[E-2V\cos\phi(n)]a_n+a_{n+1}=0\,, \tag{1}$$

where $|E|<2$, V is small, and $\phi''(n)$ is small for large n. The problem studied by Griniasty and Fishman[1] is of this form for $\nu<2$. Locally the potential is like a periodic potential of the form $2V\cos(k_1 n+\eta)$, where

$$k_1=\phi'(n)(\mathrm{mod}2\pi)\,. \tag{2}$$

The WKB approximation can be used to represent the effects of the potential with slowly varying period. In general, this gives an unimportant modulation of the wave function, but there are resonant regions where Bragg reflection occurs, and there the treatment has to be more careful. In these resonant regions the wave numbers of the running waves, which from the Floquet theorem are known to exist for this periodic potential, are complex, and the periodic potential couples solutions of the form $\exp(\pm\frac{1}{2}ik_1 n+\lambda n)$. Degenerate perturbation theory then gives the energy $E=2\cos k_2$ as an eigenvalue of the matrix

$$\begin{pmatrix} 2\cos(\frac{1}{2}k_1+i\lambda) & Ve^{i\eta} \\ Ve^{-i\eta} & 2\cos(-\frac{1}{2}k_1+i\lambda) \end{pmatrix}. \tag{3}$$

For k_1 close to $2k_2$, this gives

$$\lambda(n)^2=\frac{V^2}{4\sin^2 k_2}-(k_2-\tfrac{1}{2}k_1)^2\,, \tag{4}$$

provided that the right-hand side of this equation is positive. There is a similar formula for k_1 close to $2(\pi-k_2)$.

The integrated growth of the wave through a resonant region is the exponential of

$$\int\lambda(n)dn=\frac{1}{|dk_1/dn|}\int\left[\frac{V^2}{4\sin^2 k_2}-k^2\right]^{1/2}dk=\frac{\pi V^2}{4\sin^2 k_2\,|dk_1/dn|}\,. \tag{5}$$

There are two resonant regions for each change of k_1 or $\phi'(n)$ by 2π, so that the total growth of the wave function when k_1 changes by 2π is

$$\exp\left(\frac{\pi V^2}{2\sin^2 k_2\,|dk_1/dn|}\right). \tag{6}$$

These regions of growth related to strong Bragg scattering are separated by regions in which there is no exponential growth, and so the average rate of growth per site is equal to

$$\bar{\lambda}=\frac{V^2}{4\sin^2 k_2}\,, \tag{7}$$

which is the result obtained by Griniasty and Fishman,[1] and is the same growth rate which would be obtained for a random potential of the same strength. There is in fact a correspondence term by term with the summation of the perturbation-theory result for the localization length by the method of stationary phase in their Eq. (8); each point at which the phase is stationary corresponds to a region of Bragg scattering between degenerate Bloch waves.

Behavior near the band center.—The arguments presented in the previous section cannot be readily applied in the neighborhood of the band center, since lowest-order Bragg scattering does not then simply connect a pair of nearly degenerate states. When k_1 is close to π, changes in the wave number by either k_1 or $2\pi - k_1$ connect nearly degenerate states, so that a long sequence of states must be considered. In fact, the band structure of the periodic or quasiperiodic system is quite different when k_1 is close to π. Instead of having a pair of well-defined energy gaps each of width $2V$, as is given by Eq. (3), there is a gap around zero of width $4V$ which is penetrated by a number of narrow energy bands [see Eq. (11) below].

The quasiperiodic case, with $k_1/2\pi$ irrational, can be studied as a limit of the periodic case $k_1/2\pi = q/p$ rational. There is a recent review of the quasiperiodic case by Sokoloff.[4] For the purposes of our discussion the most important results for the quasiperiodic case were those obtained by Aubry and André[5] using the duality transformation that transforms Eq. (1) for $\phi(n) = k_1 n + \eta$ into an equation of the same structure for the amplitudes of the Bloch waves. From this it was deduced that the Lyapunov exponent λ is zero in the spectrum for $V < 1$; the exponent is of course positive in the gaps outside the spectrum.

It is clear that $E = 0$ cannot lie in a finite band gap for any value of k_1. For $k_1/2\pi = q/p$ with p odd, symmetry about $E = 0$ shows that one of the p energy bands must be centered on $E = 0$; it can also be shown that for p even there are two bands touching there. Since any irrational k_1 can be approximated arbitrary closely by a rational, there must be points in the spectrum arbitrarily close to $E = 0$, and the exponent must be zero.

It is also known[6] that the total measure of the spectrum is $|4(1-V)|$, so that the sum of the total widths of the gaps is equal to $4V$ plus the increase in distance between the extremal band edges. The increase in distance between the band edges can be calculated by perturbation theory easily when k_1 is close to π, and it is approximately V^2; so we know that the sum of the gap widths is still of order $4V$.

Two methods were used to study the band structure for $\kappa = \pi - k_1$ close to zero. Direct numerical studies were made for periodic systems, with values of κ of the form π/p, and then most of the systematic results were derived by analytical arguments. If the substitution $b_n = \sqrt{2}\cos[(2n-1)\pi/4]a_n$ is made in Eqs. (1) and (2), the equation

$$b_{n+1} + [(-1)^n E - 2V\cos(\kappa n + \eta)]b_n - b_{n-1} = 0 \quad (8)$$

is obtained. A further substitution $b_n = f(n) + (-1)^n g(n)$, where f and g are slowly varying, gives the differential equations

$$\begin{aligned} f' &\approx V\cos(\kappa x + \eta) f - Eg/2 , \\ g' &\approx -V\cos(\kappa x + \eta) g + Ef/2 . \end{aligned} \quad (9)$$

In this continuum approximation the value of η is irrelevant, and so it is set equal to $-\pi/2$ for convenience. The function g can be eliminated from Eq. (9) to get

$$-f'' + V^2\sin^2(\kappa x) f - V\kappa\cos(\kappa x) f = E^2 f/4 . \quad (10)$$

This is a Schrödinger equation, and in the neighborhood of the minima of the potentials it is like a harmonic oscillator with energy levels

$$E^2 = 8nV\kappa . \quad (11)$$

These indeed give the centers of the bands observed for the periodic system, and their widths should be calculable by the calculation of the tunneling rate between the potential minima for Eq. (10).

For $E = 0$ the solutions of Eq. (9) are

$$\begin{aligned} f(x) &= A\exp[-(V/\kappa)\cos(\kappa x)] , \\ g(x) &= B\exp[(V/\kappa)\cos(\kappa x)] . \end{aligned} \quad (12)$$

For nonzero E the equations can be expanded in powers of E, which gives

$$\begin{pmatrix} f(\pi/\kappa) \\ g(\pi/\kappa) \end{pmatrix} \approx \begin{pmatrix} 1 - \frac{1}{2}[(E\pi/\kappa) I_0(2V/\kappa)]^2 & -(E\pi/\kappa) I_0(2V/\kappa) \\ (E\pi/\kappa) I_0(2V/\kappa) & 1 - \frac{1}{2}[(E\pi/\kappa) I_0(2V/\kappa)]^2 \end{pmatrix} \begin{pmatrix} f(-\pi/\kappa) \\ g(-\pi/\kappa) \end{pmatrix} , \quad (13)$$

where I_0 is a modified Bessel function. This transfer matrix gives the limits of the energy band centered at $E = 0$ as

$$E_B = \pm 2\kappa/\pi I_0(2V/\kappa) , \quad (14)$$

which agrees with the results which I obtained numerically. Outside this central energy band it gives rise to a Lyapunov exponent

$$\lambda \approx \frac{\kappa}{\pi}\cosh^{-1}\left[\frac{\pi E}{2\kappa} I_0\left(\frac{2V}{\kappa}\right)\right] . \quad (15)$$

When this is averaged over κ in the range $0 < \kappa < \pi$ for

small E it gives

$$\bar{\lambda} \approx \frac{2V^2}{\pi^2 \ln[(4V/E)(\kappa_E/V\pi)^{1/2}]}, \tag{16}$$

where κ_E is the value of κ that solves Eq. (14) for $E_B = E$.

The Lyapunov exponent is therefore zero for the incommensurate periodic potential at $E=0$, and there are a number of other regions where it is zero in a neighborhood of width $4V$ of this point. One cannot expect perturbation theory to work well for the Lyapunov exponent in such a region, since perturbation theory will not give the rapid variations which are associated with the vanishing values in the energy bands. Equation (16) shows that the average Lyapunov exponent is reduced in this region by a factor of order $\ln(V/E)$.

Effect of rate of variation of period.—In the previous section it was assumed that the wave number of the potential variations was so slow that the Lyapunov exponent could be calculated by taking the potential to be periodic and averaging over the wave number k_1. There is, however, some dependence of the exponent on the rate of variation ϕ'' when E is close to zero. For a potential of the form $2V\cos(\frac{1}{2}an^2)$, where a and E are small, the main contributions to the Lyapunov exponent will come from regions where an is close to an odd multiple of π. In such a region, Eqs. (9) and (10) can be adapted with small modifications. At $E=0$ the analogy to Eq. (9) is

$$f' \approx \pm V\cos(\tfrac{1}{2}ax^2+\eta), \tag{17}$$

whose solution is

$$f = \exp\{\pm V(\pi/a)^{1/2}[C((a/\pi)^{1/2}x)\cos\eta - S((a/\pi)^{1/2}x)\sin\eta]\}, \tag{18}$$

where C and S are Fresnel integrals. Since C and S change by unity through the origin, the function f increases by a factor

$$\exp[V(\pi/a)^{1/2}|\cos\eta - \sin\eta|] \tag{19}$$

each time an passes through an odd multiple of π. When this expression is averaged over η it leads to an average exponent per site

$$\bar{\lambda} \approx \frac{V}{\pi}\left(\frac{2a}{\pi}\right)^{1/2}, \tag{20}$$

provided that each individual factor (19) is much larger than unity; this is equivalent to the condition that Eq. (20) should be less than $V^2/4$.

Discussion.—The method used in the first section should be accurate for small values of V except for the region $|E| < 2V$, and so the perturbative result obtained by Griniasty and Fishman[1] should be correct except for this region, and their numerical results seem to confirm this. In this region close to the band center the exponent should be reduced by the logarithmic factor given in Eq. (16). At the band center the rate of variation of the period is the most important factor, and Eq. (20) can be used to study the effect of this. For curve b of Fig. 1 in Ref. 1, I find that this equation predicts 0.32 for $\gamma/\tilde{\gamma}$ where $N=10^7$, and 0.16 where $N=10^8$. These numbers are quite close to the plotted values.

Even when the rate of variation of the period is vanishingly slow a numerical calculation at zero energy would give a finite value of the Lyapunov exponent, because rounding errors would accumulate in certain regions, where the width of the energy bands given in Eq. (14) is comparable with the rounding error, or, equivalently, where the excursions in the values of f or g given by Eq. (12) are of this magnitude. For rounding errors of 2^{-52} (for IBM double precision) this would give a calculated average Lyapunov exponent of order $V^2/26\ln 2\pi^2$, which is considerably lower than any value reported in Ref. 1 for $v>1$.

A closely analogous situation exists for random systems. It was shown by Kappus and Wegner[3] that the localization length in the band center is 9% longer than is given by the perturbative argument[2] used by Griniasty and Fishman.[1] It was subsequently shown by Derrida and Gardner[7] that there are similar anomalies in higher orders of perturbation theory at all rational points in the band. In a recent paper Bovier and Klein[8] have shown that formal perturbation series exist at both rational and irrational points in the spectra, but the series differ in their higher-order terms. It seems likely that the same situation exists for the slowly varying potential studied in this paper.

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