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LETTER TO THE EDITOR

Hierarchical spectra in systems with incommensurate potentials

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Abstract. The energy spectrum of a potential consisting of an array of barriers is obtained by solving the Schrödinger equation. The barriers have the same height and constant separation, but their widths are incommensurately modulated. The hierarchical band splittings obey the same rules which were derived earlier for the tight-binding Aubry model. We have also demonstrated their equivalence to Hofstadter's rules which were derived by Stinchcombe and Bell recently.

The spectral properties of systems with incommensurate potentials have been extensively studied by many authors [1-17] using the one-dimensional Harper equation [18] or the equivalent Aubry model [19]:

$$H(Q)=\sum_{n=-\infty}^{\infty}[E(Q,n)a_n^{\dagger}a_n+t(a_{n+1}^{\dagger}a_n+a_{n-1}^{\dagger}a_n)] \tag{1}$$

where $E(Q,n)=V\cos(Q2\pi n)$ and Q is an irrational number. In more general form, the site energy $E(Q,n)$ contains a phase ϕ and has the form $E(Q,n)=V\cos(Q2\pi n+\phi)$. However, Sinai [20] has shown that, except for the possible introduction of some special states in the gaps, ϕ does not change the spectrum of $H(Q)$. One explicit example is the existence of the zero-eigenenergy state if $\phi=\pm\pi/2$ [21]. Therefore, almost all existing works on the Aubry model ignored the phase ϕ.

The spectrum of (1) is characterised by the hierarchical band splittings which had previously been suggested [22] to arise from the continued fraction representation of Q. Yet the correct rules of hierarchical band splittings were established later by Hofstadter [23] through his extensive numerical calculations to identify two principal gaps which split each existing band into one centre subband and two outer subbands. Recently, Stinchcombe and Bell [17] have derived these rules with a degenerate perturbation method.

Although the model Hamiltonian (1) has its intrinsic theoretical interest and importance, in order to compare theoretical predictions with experimental data, one must consider a three-dimensional model with the incommensurate modulation of potential along one crystal axis. Recent calculation of the optical transmission coefficient based on such a three-dimensional model reproduced very well the measured spectrum of Rb_2ZnBr_4 [24]. Another class of materials in which modulation of potential along one crystal axis can be realised is semiconductor superlattices [25]. But for semiconductor superlattices, the tight-binding Hamiltonian [26] cannot describe properly the electronic properties. Instead, we should solve the Schrödinger equation with a modulated potential. Some early work along this line used an extremely

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simplified potential consisting of delta-function barriers with their positions and/or strengths modulated incommensurately [27-30]. Based on the free-electron model there have been theoretical investigations on the plasma excitations in semiconductor superlattices [31, 32] and the result suggested its possible experimental confirmation by Raman scattering.

In this letter we study the spectrum of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x). \tag{2}$$

The potential consists of an array of barriers and can be expressed as

$$V(x)=\begin{cases}0 & \text{for } x_n \leqslant x \leqslant x_n+d \\ U>0 & \text{for } x_n+d \leqslant x \leqslant x_n+d+b+A\cos(Q2\pi n)=x_{n+1}\end{cases} \tag{3}$$

where n is an integer between $-\infty$ and ∞. All barriers have the same height and the separation between two adjacent barriers is a constant d. However, the widths of barriers are incommensurately modulated by $A\cos(Q2\pi n)$ over a constant width b. One limiting case of $V(x)$ is an array of delta-function barriers with constant separation but with strength modulated according to $A\cos(Q2\pi n)$. It is shown [28] that this limiting case can be mapped onto the Aubry model Hamiltonian (1), except that the amplitude V is now energy dependent. Consequently, as the modulation strength A increases, the eigenfunctions of the corresponding Schrödinger equation do not exhibit an energy-independent transition from all extended states to all localised states [30]. Such an energy-independent transition localised to an extended transition is characteristic of the tight-binding Aubry Hamiltonian [33].

On the other hand, the symmetry properties of the tight-binding Hamiltonian (1) are the same as the symmetry properties of the potential (3). Therefore, the hierarchical band splittings of the Aubry Hamiltonian (1) should be identical to the hierarchical band splittings of the Schrödinger equation (2). This is indeed the conclusion of our numerical calculation. Before presenting our numerical result, let us first briefly outline the rule of band splittings, which is determined entirely by the symmetry of the Hamiltonian $H(Q)$ of (1) [16].

The irrational number Q can be expressed as a continued fraction

$$Q=[\mu_1,\mu_2,\mu_3,\dots]=\cfrac{1}{\mu_1+\cfrac{1}{\mu_2+\cfrac{1}{\mu_3+\dots}}} \tag{4}$$

where μ_i are positive integers. To make the outline simple and clear, we consider a special class of quadratic irrational numbers $\{Q(\mu);\ \mu=1,2,\dots\}$ defined as

$$Q\equiv Q(\mu)=[\mu,\mu,\mu,\dots]=\frac{1}{\mu+Q(\mu)}\equiv\frac{1}{\mu+Q}. \tag{5}$$

For this class of Q, the site energy of (1) can be written as

$$E(Q,n)=E\left(\frac{1}{\mu+Q},n\right)=V\cos\left(\frac{2\pi n}{\mu+Q}\right). \tag{6}$$

If Q is a rational number ν/N (for fractional μ), we have $E(Q,n)=V\cos(2\pi\nu n/N)$ and the initial spectrum of $H(Q)$ splits into N subbands. Let N_t be the total number

of eigenstates in the initial spectrum. Then the number of eigenstates in each subband is simply N_t/N. If Q is a quadratic irrational number, the rules of hierarchical band splittings [16] are as follows.

(i) For even μ, the initial spectrum splits into μ equivalent subbands and one non-equivalent subband. The non-equivalent subband lies at the centre and contains Q^2N_t eigenstates. In each of the remaining μ equivalent subbands the number of eigenstates is QN_t. Every subband then continues to split in the same fashion as the initial spectrum.

(ii) For odd μ and $\mu \geq 3$, the initial spectrum splits into μ equivalent subbands and one non-equivalent subband, just as the previous case of even μ. However, one equivalent subband overlaps with the centre non-equivalent subband and the total number of eigenstates in these two overlapped subbands is $QN_t + Q^2N_t$. The splitting of the overlapped subbands produces one centre subband containing Q^3N_t eigenstates and $\mu + 1$ outer subbands, each of which has Q^2N_t eigenstates. Now all subbands are separated from each other, and every one of them continues to split in the same fashion as the initial spectrum.

(iii) For $\mu = 1$, the initial spectrum can be considered as the two centre overlapped subbands in the previous case (ii). The first split produces one centre non-equivalent subband and two outer equivalent subbands. This pattern of splitting repeats itself when the centre non-equivalent subband splits again. However, each outer equivalent subband continues to split into $\mu + 1 = 2$ subbands. The ratio of the numbers of eigenstates in these two subbands is 1 to Q.

It can be shown that the above rules yield the same hierarchical band splittings as those obtained from Hofstadter's rules [23] which were derived recently by Stinchcombe and Bell [17]. However, in this letter we will only demonstrate their equivalence when we discuss our numerical results.

Now we will calculate the spectrum of the Schrödinger equation (2). In any region $\xi_1 \leq x \leq \xi_2$ where the potential $V(x)$ is constant (either $V(x) = 0$ or $V(x) = U$), the eigenfunction is simply

$$\psi(x) = A \exp(ikx) + B \exp(-ikx) \tag{7}$$

where $k = \{2m[E - V(x)]\}^{1/2}/\hbar$. Since $\psi(x)$ = and $\psi'(x) \equiv d\psi(x)/dx$ are continuous everywhere, we readily obtain

$$\begin{pmatrix} \psi(\xi_2) \\ \psi'(\xi_2) \end{pmatrix} = \begin{pmatrix} \cos k(\xi_2 - \xi_1) & (1/k)\sin k(\xi_2 - \xi_1) \\ -k \sin k(\xi_2 - \xi_1) & \cos k(\xi_2 - \xi_1) \end{pmatrix} \begin{pmatrix} \psi(\xi_1) \\ \psi'(\xi_1) \end{pmatrix}. \tag{8}$$

Using this recursion relation, the eigensolutions of the Schrödinger equation (2) can be derived by counting the nodes of $\psi(x)$ throughout the system [34].

We have used a system of 10^5 barriers in our numerical calculation. The separation d between two adjacent barriers is our unit of length and the unit of energy is $(1/2m)(\hbar/d)^2$. To detect the hierarchical band splittings, it is sufficient to consider an initial spectrum (the spectrum of a periodic potential without incommensurate modulation, $A = 0$) consisting of only one single band. This single-band initial spectrum can be achived if we set the barrier height $U = 6$ and the barrier width $b = 1$. These parameter values are chosen for the convenience of numerical calculation without qualitative influence on the pattern of hierarchical band splittings.

For given values of the irrational number Q and the modulation amplitude A, we have derived the spectrum for the potential (3). We have used many different values

of Q and A and all results confirm the above-mentioned rules of hierarchical band splittings. One example of our calculation is shown in figure 1 for $A = 0.8$ and $Q = (\sqrt{5}-1)/2$ (the golden mean). This value of Q is simply the quadratic irrational number $Q = 1/(\mu + Q)$ with $\mu = 1$. The three columns 1, 2 and 3 on the left of figure 1 represent three stages of bond splittings. Each vertical bar indicates a subband with band edges marked by the two numbers at the ends. At each stage of band splittings, the numbers (either 1 or Q) at the left side of the vertical bars are the relative numbers of eigenstates in these subbands. The actual numbers of eigenstates in the three subbands at the first stage of band splittings are Q^2N_t, Q^3N_t and Q^2N_t, where N_t is the total number of eigenstates in the initial spectrum. The pattern of hierarchical band splittings in figure 1 clearly follows the above-stated rules.

Let us modify the assignment of subbands when the two outer bands of stage 1 continue to split. From stage 2 to stage 3, we ignore the splittings of the two subbands, each of which contains relatively Q eigenstates. Then, the hierarchical band splittings are shown on the right of figure 1. This modified pattern follows the Hofstadter's rules [23] which have been derived recently by Stinchcombe and Bell [17].

We would like to point out that the spectrum in figure 1 is not symmetric at any stage of band splitting. In the original derivation [16] of the rules of hierarchical band splittings, the electron-hole symmetry of the tight-binding Hamiltonian (1) was considered in order to determine if there is overlap between the non-equivalent subband and one of the equivalent subbands. For the potential $V(x)$ given by (3), our numerical results indicate that, even for very large values of the modulation amplitude A, the

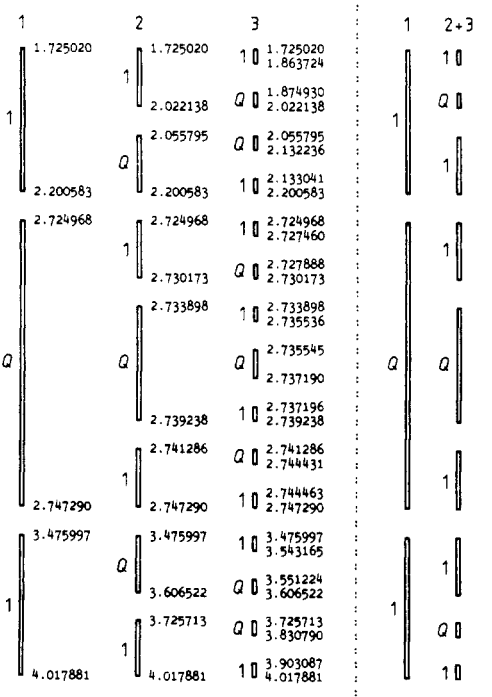

Figure 1. Hierarchical band splittings for $Q = (\sqrt{5}-1)/2$ (corresponding to $\mu = 1$) and the modulation amplitude $A = 0.8$. Each vertical bar represents a band with band edges marked by numbers at the ends. After each band splitting, the relative numbers of eigenstates in subbands (either 1 or Q) are indicated at the left of the bars.

condition of overlap of subbands which was derived for the Aubry Hamiltonian [16] is still valid for the present problem.

Finally, we must emphasise that one should not make theoretical predictions of novel properties of modulated semiconductor superlattices which result only from the structure of hierarchical band splittings. Because these materials are three dimensional, the hierarchical band splittings along one particular direction in the reciprocal space will be hidden under the overall three-dimensional band structure. In this respect, a more general theoretical model is required [24].

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