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LETTER TO THE EDITOR

Renormalisation procedure for the quasiperiodic Schrödinger equation

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Abstract. A renormalisation procedure is constructed for the one-dimensional Schrödinger equation with a quasiperiodic potential. The renormalisation transformation has a trivial fixed point describing the behaviour of the system near the unperturbed free motion, and a non-trivial fixed point corresponding to the critical case. A number system of an irrational base is introduced for the scaling of the spectra.

The Bloch theorem applied to a perfect crystal with certain translation invariance states that all the eigenfunctions of electrons are plane waves modulated with functions of the same periodicity. Under an incommensurate perturbation, e.g. created by the Peierls instability, the potential in the crystal becomes quasiperiodic. There is no longer any true translation symmetry and the Bloch theorem cannot be applied. The quasiperiodic potential represents a natural intermediate case between periodicity and randomness. Dinaburg and Sinai [1], proving the existence of quasiperiodically modulated plane wave eigenfunctions for some eigenenergies, have partially extended the Bloch theorem to a quasiperiodic potential.

Here we shall consider a specific simple quasiperiodic model:

$$\frac{d^2\psi}{dx^2}+(\lambda_1\cos 2\pi x+\lambda_2\cos 2\pi\omega x)\psi=E\psi \tag{1}$$

with ω being the inverse golden mean,

$$\omega=(\bar{\omega})^{-1}=\tfrac{1}{2}(\sqrt{5}-1)=[0;1,1,\ldots]=\lim_{n\to\infty}F_n/F_{n+1} \tag{2}$$

where the Fibonacci sequence $\{F_n\}$ satisfies $F_{n+1}=F_n+F_{n-1}$, $F_0=0$, $F_1=1$. We shall construct a renormalisation procedure for the model. By means of the renormalisation transformation it is possible to study the property of the model near the critical amplitudes of the potential where the Bloch-like eigenfunctions begin to disappear.

It is generally believed that by means of renormalisation group methods the numerically observed scaling properties [2, 3] of the spectra and wavefunctions of quasiperiodic Schrödinger operators can be studied most conveniently. There are two main ways of carrying out renormalisation: by a non-perturbative method [3, 4] or by an approximate one [5, 6]. The former, known as exact renormalisation, is based on

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the scaling hypothesis and the procedure of renormalisation is constructed in a functional space. The theory is in quantitative agreement with the numerical observations. The approximate one is not so accurate, but the procedure of renormalisation is constructed in a parameter space, so is much simpler. Furthermore, the method provides a simple physical picture for understanding the existence of the scaling properties. In both cases the exponents that characterise scaling behaviour are related to the eigenvalues of the linearised renormalisation transformation near the fixed points. If under the renormalisation transformation different quasiperiodic Schrödinger operators flow to the same fixed point, then they will share the same scaling behaviour (the so-called universality of the scaling exponents). The methods have been applied to the discrete quasiperiodic Schrödinger equation by using the 'real space decimation' technique [3, 4, 6]. Instead, in this letter, we shall extend a 'momentum space Killing' technique [7] to study the continuous quasiperiodic Schrödinger equation.

For equation (1) the Bloch-like eigenfunctions, if they exist, can be expressed as

$$\psi_k = \exp(\mathrm{i}2\pi kx)\left(1+\sum_{l,m} c_{lm}\exp[\mathrm{i}2\pi(l\omega+m)x]\right). \tag{3}$$

The most important modes are the slow 'near-resonant' ones, i.e. terms with $l\omega+m$ close to zero. These are $l\omega+m=F_{n+1}\omega-F_n\equiv\gamma_n$. We shall focus our attention only on these modes. For convenience, we denote by α_n the Fourier coefficient c_{lm} with $l=F_{n+1}$ and $m=-F_n$, define $\gamma_{-1}=1$ and add the superscript $^{(0)}$ to ψ, λ_1, λ_2, x and E in equation (1).

We first make the transformation of the argument

$$2\pi x^{(0)}=2\pi\theta^{(0)}+e^{(0)}\sin 2\pi\theta^{(0)}$$

where $e^{(0)}$ is a constant. The transformation converts a function periodic in $x^{(0)}$ to one that is periodic in $\theta^{(0)}$ with the same period, and brings equation (1) into the form

$$\begin{aligned}[][\mathrm{d}/\mathrm{d}\theta^{(0)}]^2\psi^{(0)}&+\{\lambda_2^{(0)}J_0(\omega e^{(0)})\cos 2\pi\omega\theta^{(0)}\\ &+\lambda_2^{(0)}[J_0(\omega e^{(0)})e^{(0)}+J_1(\omega e^{(0)})]\cos 2\pi(\omega-1)\theta^{(0)}\}\psi^{(0)}\\ &=\{E^{(0)}-\lambda_1^{(0)}[e^{(0)}J_0(e^{(0)})+J_1(e^{(0)})]\}\psi^{(0)}-2\pi e^{(0)}\sin 2\pi\theta^{(0)}\,\mathrm{d}\psi^{(0)}/\mathrm{d}\theta^{(0)}\\ &\quad-[\lambda_1^{(0)}J_0(e^{(0)})-2e^{(0)}E^{(0)}]\cos 2\pi\theta^{(0)}\psi^{(0)}\end{aligned}$$

where J_ν are the Bessel functions and we have dropped all the higher-order terms. We now split $\psi^{(0)}$ into two parts $\varphi^{(0)}$ and $\psi^{(1)}=\psi^{(0)}-\varphi^{(0)}$ in such a way that

$$\mathscr{L}^{(1)}\psi^{(1)}\equiv\gamma_0^2[\mathrm{d}/\mathrm{d}x^{(1)}]^2\psi^{(1)}+(\lambda_1^{(1)}\cos 2\pi x^{(1)}+\lambda_2^{(1)}\cos 2\pi\delta_1 x^{(1)})\psi^{(1)}=E^{(1)}\psi^{(1)} \tag{4a}$$

$$\begin{aligned}\mathscr{L}^{(1)}\varphi^{(0)}=E^{(1)}\varphi^{(0)}&-\{2\pi e^{(0)}\sin 2\pi\theta^{(0)}\,\mathrm{d}/\mathrm{d}\theta^{(0)}\\ &+[\lambda_1^{(0)}J_0(e^{(0)})-2e^{(0)}E^{(0)}]\cos 2\pi\theta^{(0)}\}\psi^{(0)}\end{aligned} \tag{4b}$$

with the notation

$$\delta_m=\gamma_m/\gamma_{m-1}\qquad x^{(1)}=\delta_0\theta^{(0)}=\omega\theta^{(0)}\qquad E^{(1)}=E^{(0)}-\lambda_1^{(0)}[e^{(0)}J_0(e^{(0)})+J_1(e^{(0)})]$$
$$\lambda_1^{(1)}=\lambda_2^{(0)}J_0(\omega e^{(0)})\qquad \lambda_2^{(1)}=\lambda_2^{(0)}[J_0(\omega e^{(0)})e^{(0)}+J_1(\omega e^{(0)})].$$

Assume that at step m we have

$$\begin{aligned}\mathscr{L}^{(m)}\psi^{(m)}\equiv\gamma_{m-1}^2&[\mathrm{d}/\mathrm{d}x^{(m)}]^2\psi^{(m)}\\ &+(\lambda_1^{(m)}\cos 2\pi x^{(m)}+\lambda_2^{(m)}\cos 2\pi\delta_m x^{(m)})\psi^{(m)}=E^{(m)}\psi^{(m)}\end{aligned} \tag{5a}$$

$$\mathscr{L}^{(m)}\varphi^{(m-1)} = E^{(m)}\varphi^{(m-1)} - [\gamma_{m-2}^2 2\pi e^{(m-1)}\sin 2\pi\theta^{(m-1)}\,\mathrm{d}/\mathrm{d}\theta^{(m-1)} + (\lambda_1^{(m-1)}J_0^{(m-1)} - 2e^{(m-1)}E^{(m-1)})\cos 2\pi\theta^{(m-1)}]\psi^{(m-1)} \tag{5b}$$

$$\psi^{(m-1)} = \psi^{(m)} + \varphi^{(m-1)} \tag{5c}$$

where $J_\nu^{(m)} = J_\nu(e^{(m)})$. The transformation

$$2\pi x^{(m)} = 2\pi\theta^{(m)} + e^{(m)}\sin 2\pi\theta^{(m)} \tag{6}$$

converts equation $(5a)$ to the same form as equations (5) with $m+1$ taking the place of m and with the new notation

$$\tilde{J}_\nu^{(m)} = J_\nu(\delta_m e^{(m)}) \qquad x^{(m+1)} = \delta_m\theta^{(m)} \qquad E^{(m+1)} = E^{(m)} - \lambda_1^{(m)}(J_1^{(m)} + e^{(m)}J_0^{(m)}) \tag{7a}$$

and

$$\lambda_1^{(m+1)} = \lambda_2^{(m)}\tilde{J}_0^{(m)} \qquad \lambda_2^{(m+1)} = \lambda_2^{(m)}(\tilde{J}_0^{(m)}e^{(m)} - \tilde{J}_1^{(m)}). \tag{7b}$$

In the above derivation we have used the property

$$\theta^{(m)} \sim x^{(m)} = \delta_{m-1}\theta^{(m-1)} \sim \delta_{m-1}\delta_{m-2}\ldots\delta_0\theta^{(0)} = \gamma_{m-1}\theta^{(0)} \tag{7c}$$

and have kept only the near-resonant modes.

We now make the ansatz for the solution to equation $(5b)$:

$$\varphi^{(m)} = \exp(\mathrm{i}2\pi kx)[\alpha_m\exp(\mathrm{i}2\pi\theta^{(m)}) + \alpha_{-m}\exp(-\mathrm{i}2\pi\theta^{(m)})] \tag{8}$$

which 'kills' slow modes one by one. Correspondingly, we make the approximation

$$\psi^{(m)} = \exp(\mathrm{i}2\pi kx) + \varphi^{(m)}. \tag{9}$$

From equations (8), (9) and $(5b)$ we find the equations for α_m, α_{-m} and $e^{(m)}$:

$$2\pi^2 e^{(m)}\gamma_{m-1}[(k-\gamma_{m-1})\alpha_{-m} - (k+\gamma_{m-1})\alpha_m] + \tfrac{1}{2}(\lambda_1^{(m)}J_0^{(m)} - 2e^{(m)}E^{(m)})(\alpha_m + \alpha_{-m}) = 0 \tag{10a}$$

$$[E^{(m+1)} + 4\pi^2(k\pm\gamma_{m-1})^2]\alpha_{\pm m} = -e^{(m)}E^{(m)} + \tfrac{1}{2}\lambda_1^{(m)}J_0^{(m)} \pm 2\pi k e^{(m)}\gamma_{m-1} \tag{10b}$$

which approximately result in

$$\alpha_{\pm m} = \mp e^{(m)}E^{(m)}/8\pi^2 k\gamma_{m-1} \tag{11a}$$

$$\lambda_1^{(m)} = 4\pi^2\gamma_{m-1}^2 e^{(m)} \tag{11b}$$

where we have used the property $J_0^{(m)} \sim 1$ for small $e^{(m)}$ and $\gamma_m = (-1)^m\omega^{m+1} \xrightarrow{m\to\infty} 0$ to keep only the leading terms. Equations $(11b)$ and $(7b)$ constitute the renormalisation transformation.

From the above discussion we see that in every step of iteration the transformation (6) separates the lowest mode (i.e. the mode corresponding to γ_m with the smallest m) from the higher modes to obtain equations for φ and ψ, respectively. The equations for φ and ψ retain the same form at every step, so the original equation reduces to a map in the parameter space. The simple form of the transformation (6) and the fact that the wavefunction is mainly determined by the modes corresponding to the

Fibonacci numbers allow us to work in a parameter space with a very small dimensionality. In this way we can relate the energy spectrum to the 'naked' one (i.e. $-4\pi^2k^2$) to write (see equation (7a))

$$E = E^{(0)} = E^{(\infty)} + \sum_{m=0}^{\infty} \lambda_1^{(m)}(J_1^{(m)} + e^{(m)}J_0^{(m)})$$

$$= -4\pi^2k^2 + \sum_{m=0}^{\infty} \lambda_1^{(m)}(J_1^{(m)} + e^{(m)}J_0^{(m)}) \tag{12}$$

and from equation (7c) we obtain the wavefunction

$$\psi = \psi^{(\infty)} + \sum_{l=0}^{\infty} \varphi^{(l)}$$

$$= \exp(\mathrm{i}2\pi kx)\left(1 + \sum_{m=0}^{\infty} \alpha_m \exp(\mathrm{i}2\pi\gamma_{m-1}x) + \alpha_{-m}\exp(-\mathrm{i}2\pi\gamma_{m-1}x)\right). \tag{13}$$

We now investigate the property of the renormalisation transformation. For simplicity, we make the approximation $\tilde{J}_0^{(m)} \sim 1$, $\tilde{J}_1^{(m)} \sim \delta_m e^{(m)}/2$, and introduce a new variable $r^{(m)} = \lambda_2^{(m)}/\lambda_1^{(m)}$. It can be seen from the renormalisation transformation that

$$\begin{aligned} r^{(m+1)} &= (1-\delta m/2)e^{(m)} \\ e^{(m+1)} &= \bar{\omega}^2 e^{(m)} r^{(m)} \end{aligned} \tag{14}$$

from which we obtain

$$e^{(m+1)} = \bar{\omega}^2(1-\delta m/2)e^{(m)}e^{(m-1)}. \tag{15}$$

Therefore, the mapping (14) has two fixed points $(r_0, e_0) = (0, 0)$ and $(r^*, e^*) = (\omega^2, 2\omega^2/(2-\omega))$. Near the fixed point (r^*, e^*), by introducing the new variables $(P, Q) = (\ln r - \ln r^*, \ln e - \ln e^*)$, the two eigenvalues of the tangent mapping can easily be determined to be

$$\lambda_s = -\omega \qquad \lambda_u = 1 + \omega = \bar{\omega}$$

which means that the fixed point is hyperbolic. At certain initial values λ_1 and λ_2, the iteration (14) will bring (r, e) to the fixed point (r^*, e^*), and form the stable manifold of the mapping. When λ_1 and λ_2 correspond to a point below the stable manifold in the r–e space, the iteration will finally bring (r, e) to $(0, 0)$, and the system is then essentially equivalent to the unperturbed free motion. The behaviour of the system near the fixed point (r^*, e^*) is mainly described by its unstable eigenvalue λ_u. An important straightforward result is the fact that, from equation (11a), we have near the fixed point on the stable manifold

$$\alpha_{\pm m}\gamma_m = \text{constant}.$$

In the above we consider only the reciprocal golden mean incommensurability. However, from the derivation of the renormalisation equations one can see that the same asymptotic behaviour is shared by all 'noble' irrational numbers—those whose continued fraction ends in an infinite string of ones. Since these numbers are dense on the real axis, they can be used to approach any given irrational number. For a direct extension of the discussed procedure to a general irrational number $g = [a_0, a_1, a_2, \ldots]$ with the convergents $\{p_m/q_m\}$, it is necessary to redefine $\gamma_m = q_m g - p_m$, replace the transformation (6) with

$$x = \theta + e \sin b\theta$$

and determine the constant b from a_i. The fact that all noble irrational numbers share the same asymptotic behaviour of the renormalisation transformation is the universality in incommensurability.

From the derivation of the renormalisation transformation one can also see that if the quasiperiodic potential contains more, but finite, terms of the form $\cos[2\pi(m + n\omega)x + \phi]$ with m, n being integers and ϕ a phase constant, then the fixed points of the renormalisation map and the eigenvalues on these points are unchanged. This is the universality in potential components. Combining this with the universality in incommensurability, we can add to the potential more terms that include periodicity of the noble numbers.

In the above discussion the role played by the 'quasimomentum' k has been almost ignored. However, it is essential to the understanding of the scaling of the spectra. To sketch how the role of k can be considered let us introduce a number system of an irrational base. The reciprocal golden mean ω satisfies the relation $\omega^2 + \omega = 1$ or $\omega^{n+1} + \omega^n = \omega^{n-1}$. Like the usual binary system of base 2 we can construct a new number system with the irrational base ω. Any given number $\alpha \in (0, 1)$ can be expressed in terms of powers of ω as $\alpha = \Sigma_{i\in N} a_i \omega^i$ with all a_i being integer 0 or 1. We thus have the representation $\alpha = \langle a_1, a_2, \ldots \rangle$. As an example we can write $\frac{1}{4} = \langle \overline{0, 0, 1, 0, 0, 0} \rangle$, a representation of cycle 6. The representation is unique except for the ambiguity $\langle \ldots, 0, 1, 1, \ldots \rangle = \langle \ldots, 1, 0, 0, \ldots \rangle$. We can define the one on the RHS as standard. (Note the ambiguity in the binary system $\ldots, 0, \overline{1} = \ldots, 1.$) In our representation system the sum of any two successive powers of ω recovers the preceding one, so the system can be regarded as second order, while in the same sense the binary system is first order. Once we find the ω representation for the quasimomentum k, then, recalling the relation $\omega^n = (-1)^{n-1}(F_n\omega - F_{n-1}) = (-1)^{n-1}\gamma_{n-1}$, we see that every digit 1 in the ω representation of k will produce extra 'mode-mixing'. If we take the case of $k = \frac{1}{4}$ as an example, a six-step renormalisation map should be constructed and k shifted after every six steps. There is then another universality in that different quasimomentums with the same ending in the ω representation share the same asymptotic behaviour in the renormalisation iteration. The method is tractable for those quasimomentums ending with a short cycle in the ω representation. The one-step version we discussed earlier is good mainly for $k \sim 0$. After the fixed points of the renormalisation map are determined, the scaling properties of the spectra can be readily obtained.

The details of the above discussion, the justification and improvement of approximations and investigations of the critical scaling properties and other related problems will be presented later.

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