Quasiperiodic systems without Cantor-set-like energy bands

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A class of quasiperiodic systems is proposed that does not show the Cantor-set-like energy bands. The general aspects of such systems are investigated.

It has long been believed that an electron in a quasiperiodic system shows a Cantor-set-like energy spectrum.[1–7] However, this is no longer true for a class of quasiperiodic systems that arise from the integrable nonlinear lattices. In this paper, we will show such examples and discuss the general aspects of the theory.

First, we introduce a model that does not provide a Cantor-set-like energy spectrum. Suppose that there is an infinite chain that is constructed by a repetition of the unit cell of N equivalent atoms. Then, let the Hamiltonian for the lattice system be described by

$$H_L=\sum_{n=1}^{N}\left(\frac{1}{2}P_n^2+e^{-(X_{n+1}-X_n)}\right), \tag{1}$$

where X_n is the position of the nth atom and P_n its momentum, i.e., $P_n=dX_n/dt$. This is known as the *periodic Toda lattice* (PTL), since this was first solved by Toda using the knowledge of the elliptic functions.[8] And later it was solved by a so-called *inverse scattering method*, considering a particular methematical wave that is assumed to propagate through the nonlinear lattice system.[9,10] We will regard this scattering wave as a real electron that propagates through the PTL in order to have a definite physical meaning in our problem.

The Hamiltonian for this electron is represented by

$$H_{\text{el}}=\sum_{n=1}^{N}(T_n\psi_{n+1}^{+}\psi_n+\text{c.c.}+V_n\psi_n^{+}\psi_n). \tag{2}$$

This leads to the discrete Schrödinger equation

$$T_n\psi_{n+1}+T_{n-1}\psi_{n-1}+V_n\psi_n=E\psi_n\,, \tag{3}$$

where ψ_n is the wave function and E an energy of the electron. Since the lattice has the periodicity of N, we impose the periodic boundary conditions for the hopping matrix between n and $n+1$ sites, T_n, and the on-site potential V_n, such that $T_{n+N}=T_n$ and $V_{n+N}=V_n$, where for the PTL we have

$$T_n\equiv e^{-(X_{n+1}-X_n)/2}\quad\text{and}\quad V_n\equiv P_n=\frac{dX_n}{dt}. \tag{4}$$

And this periodicity induces the Bloch theorem for the wave functions $\psi_{n+N}=e^{ikN}\psi_n$, or equivalently, the Bloch theorem reads $\psi_n(E)=e^{ikn}U_n(E)$, $U_{n+N}(E)=U_n(E)$.

In this paper, we are concerned with the PTL, in which a stationary lattice distortion exists. In this static limit, we have $V_n=0$ and the wave functions satisfy $\psi_n(-E)=(-)^n\psi_n(E)$, since the energy spectrum is symmetric around $E=0$. Therefore this provides us a model known as the *off-diagonal model* in solid state physics.[11]

When we follow the arguments of the soliton theory, Eqs. (1) and (3) are completely integrable using the *Lax pair formalism*.[8–10] This model was intensively studied by the Russian physicists and mathematicians in the 1980's.[12] However, the relationship between the integrable nonlinear systems and quasiperiodic systems was not so clear until recently. The main purpose of this paper is to draw our attention to this problem from the viewpoint of the usual quasiperiodic systems.

Second, we construct a quasiperiodic potential. Here, we call the hopping matrices the *potentials* because we consider only the static excitations of the PTL. It is well known that the PTL has a particular time-dependent solution called a *cnoidal wave*, which was the first exact solution for it,[8] having stimulated physicists to study the nonlinear lattices for the search of integrable systems.[9,10]

The cnoidal wave solution is given by[8]

$$T_n^2\equiv e^{-(X_{n+1}-X_n)}=1+\omega^2\left\{\text{dn}^2\left[2K\left(\frac{n}{\Lambda}\pm\nu t\right)\right]-\frac{E}{K}\right\}, \tag{5}$$

$$\omega^2\equiv(2K\nu)^2=\frac{1}{1/\text{sn}^2(2K/\Lambda)-1+E/K}. \tag{6}$$

Here $\text{dn}(x)$ [$\text{sn}(x)$] stands for the dn(sn) function in the elliptic functions. K (and $E)\equiv K(\kappa)[E(\kappa)]$ is the complete elliptic function of the first (second) kind, while $\kappa(0\leqslant\kappa\leqslant1)$ is its modulus, and will be defined later. And Λ is the wavelength of the stationary lattice distortion. Since $\text{dn}(x)$ has the following symmetries: $dn(x\pm mK)=\text{dn}(x)[\text{dn}(x+K)]$ for m even (odd); $\text{dn}(x+K)=\kappa'/\text{dn}(x)$, $\kappa'\equiv\sqrt{1-\kappa^2}$, the shortest wavelength is $\Lambda=2$. And due to the fact that $\text{dn}(x+2K)=\text{dn}(x)$, $T_{n+\Lambda}=T_n$ ($V_{n+\Lambda}=V_n$). This means that if $\Lambda>2$, then Λ can be an arbitrary wavelength, including both rational and

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irrational ones, and the physical meaning of $1/\Lambda$ becomes the density of solitons in the infinite chain. To obtain the static lattice distortion, either we can substitute $t=0$ in Eq. (5) or we can Galilean transform the coordinate system to eliminate t in the argument. Therefore, the above potentials are quasiperiodic, in general. In this way, this class of potentials derived from the integrable nonlinear lattices provides a class of new quasiperiodic systems.

We now prove that the above quasiperiodic potentials are the consequence of the energy bands that are not belonging to the Cantor-set types. This assertion seems to contradict the usual belief on the quasiperiodic systems. Let us consider this point.

Suppose there is no nonlinear excitation on the Toda lattice. In this case, $T_n=1$ and $V_n=0$. Therefore the solution of the Schrödinger equation is trivial: $\psi_n=e^{ikn}$, $k=2\pi/\lambda$ for λ being the electronic wavelength and $E=2\cos k$ ($-\pi<k<\pi$, the Brillouin zone). If we regard that the unit cell has N equivalent atoms, by the Bloch theorem, it results to the Brillouin zone reduced to $-\pi/N<k<\pi/N$, and the energy spectrum has $N-1$ accidental degeneracies at $k_j=\pm(\pi/N)j$ ($j=1,...,N-1$) in the extended zone scheme.

A long time ago, Peierls considered that if a lattice distortion is introduced in such a situation, those degeneracies are removed by the degenerate perturbation method, so as to have $N-1$ band gaps.[13] But this is no longer true if one considers a lattice distortion on an integrable nonlinear lattice, although we have been led to believe that the Peierls' classic idea is relevant to obtain the Cantor-set-like energy bands in a quasiperiodic system. Because of the inverse scattering method, first we assume a finite number of energy bands, and second we construct both the quasiperiodic potentials and the wave functions by using the concept of the *Jacobi inversion method*.[8-10] Therefore, there is no room to enter the Cantor-set-like energy bands into this problem.

Consider the cnoidal wave case.[8] In this case, only one gap appears in $E>0$ (in $E<0$) region at $k=\pm\pi/\Lambda$ [$k=\pm\pi(1-1/\Lambda)$], if and only if the wavelength of the cnoidal wave satisfies the commensurability condition: $\Lambda=N/M$ (M, N are relatively prime numbers with $1\leqslant M<N$). Therefore, we have only three energy bands in the spectrum for an electron. Let us assume that our band edges are characterized by the three parameters λ_1, λ_2, and λ_3, such that the three energy bands are given by (See Fig. 1.)

$$-\lambda_3\leqslant E\leqslant-\lambda_2,\quad -\lambda_1\leqslant E\leqslant\lambda_1,\quad \text{and}\quad \lambda_2\leqslant E\leqslant\lambda_3. \tag{7}$$

Let us consider the discrete Schrödinger equation. If the energy E is thought of as a real variable, there are two independent real solutions: $\phi_1(n)$ and $\phi_2(n)$, satisfying the initial conditions: $\phi_1(0)=1$, $\phi_1(1)=0$, and $\phi_2(0)=0$,

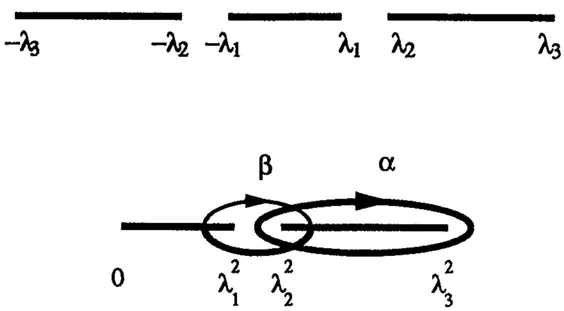

FIG. 1. The energy band and the contours are drawn.

$\phi_2(1)=1$, respectively. Here $\phi_1(n)$ [$\phi_2(n)$] is an $(n-2)$th- [$(n-1)$th]-order polynomial in E. Let us convert the Schrödinger equation into the form of the transfer matrix: $\Psi_{n+1}=M_{n+1,n}\Psi_n$ with

$$M_{n+1,n}=\begin{pmatrix} \dfrac{E-V_n}{T_n} & -\dfrac{T_{n-1}}{T_n} \\ 1 & 0 \end{pmatrix}$$

and

$$\Psi_n=\begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}. \tag{8}$$

We can calculate the trace of the N multiplication of the transfer matrices, $M_N(E)$ in terms of $\phi_1(N)$ and $\phi_2(N)$ [and $\phi_1(N+1)$ and $\phi_2(N+1)$]. We now have $\Delta_N(E)\equiv\mathrm{Tr}\,M_N(E)=\phi_1(N)+\phi_2(N+1)$ that is, in general, an Nth-order polynomial in E and $\det M_N(E)\equiv\phi_1(N)\phi_2(N+1)-\phi_1(N+1)\phi_2(N)=1$.

If $|\Delta_N(E)|\leqslant 2$, then E lies in an allowed energy. And if $|\Delta_N(E)|>2$, then E lies in a forbidden energy. The latter case is always provided if we consider a particular energy μ_j ($j=1,...,g$; where g is the number of band gaps in the spectrum) that are the zeros of $\phi_1(N+1,\mu_j)=0$ and always lie in the jth band gap, because $\Delta_N(E=\mu_j)=\phi_1(N)+1/\phi_1(N)>2$. This set of the special energies is called the *auxiliary spectrum* in the soliton theory and labels all the band gaps in the spectrum.[8-10]

Following the arguments of the soliton theory,[8-10] the wave function is represented by

$$\psi_n^*(E)\psi_n(E)=\frac{T_0}{T_n}\frac{\phi_1(N+1|n-1)}{\phi_1(N+1)}$$

$$=\prod_{j=1}^{g}\frac{E-\mu_j(n-1)}{E-\mu_j(0)}. \tag{9}$$

Here $\phi_1(n|r)$ and $\phi_2(n|r)$ are the corresponding two independent solutions of the Schifted Schrödinger equation: $T_{n+r}\psi_{n+1}(r)+T_{n-1+r}\psi_{n-1}(r)+V_{n+r}\psi_n(r)=E\psi_n(r)$, such that $\phi_1(0|r)=1$, $\phi_1(1|r)=0$, and $\phi_2(0|r)=0$, $\phi_2(1|r)=1$, respectively. And $\phi_1(N+1|n-1)$ $[\phi_1(N+1)]$ has the g zeros $\mu_j(n-1)[\mu_j(0)]$ for $j=1,...,g$.

We remark the following: In the most general case, g is equivalent to the number of the atoms in the unit cell minus one, i.e., $g=N-1$.[14] This corresponds to the case where all degeneracies are removed by the lattice distortion. However, in the nonlinear lattice case it is not necessary to impose this restriction. Here g can be less than $N-1$. This is due to the fact that some degeneracies still remain in the case of nonlinear excitations.

For our present case of the static cnoidal wave, $g=2$, since we have only two band gaps in the spectrum, and because only two degeneracies are removed, while the others are not. And from the symmetry of the wave function for the off-diagonal model, it must be an even function in E. Thus we can get the wave function

$$\psi_n^*(E)\psi_n(E)=\frac{E^2-\mu_1^2(n-1)}{E^2-\mu_1^2(0)}, \qquad (10)$$

where $\mu_1(n-1)$ and $\mu_1(0)$ lie in the band gap $[\lambda_1,\lambda_2]$. Equation (10) can be converted to the form of the elliptic function by means of the use of a parameter $z(E^2)$, which is defined in the following:

$$\omega\equiv dz\equiv\frac{c_1\,dE}{\sqrt{R(E^2)}}, \qquad (11)$$

where

$$R(E^2)\equiv\Delta_N(E)^2-4=(E^2-\lambda_1^2)(E^2-\lambda_2^2)(E^2-\lambda_3^2). \qquad (12)$$

Here c_1 is determined by the two integrals: $\int_\alpha\omega=1$ and $\int_\beta\omega=\tau$, where α is a contour surrounding the band $[\lambda_2,\lambda_3]$ in the upper sheet and β is a contour surrounding the band gap $[\lambda_1,\lambda_2]$, starting from λ_1 to λ_2 in the lower sheet and going back from λ_2 to λ_1 in the upper sheet. (Fig. 1.) And after some calculation we get $\tau=(\kappa')/K(\kappa)$, $\kappa'\equiv\sqrt{1-\kappa^2}$, and $\kappa\equiv(\lambda_3/\lambda_2)\times\sqrt{(\lambda_2^2-\lambda_1^2)/(\lambda_3^2-\lambda_1^2)}$. Using this τ we can define the elliptic function $\theta_3(v,q)\equiv\Sigma_m q^{m^2}e^{2\pi imv}$, $q\equiv e^{i\pi\tau}=\exp\{-\pi K(\kappa')/K(\kappa)\}$. Then $z(\mu_1^2(n-1))[z(\mu_1^2(0)]$ becomes the zero of $\theta_3(z(\mu_1^2(n-1))-\alpha_{n-1},q)=0[\theta_3(z(\mu_1^2(0))-\alpha_0,q)=0]$, where z_0 is a constant defined by $z_0\equiv\int_{\infty}^{\infty'}\omega$ and $\alpha_{n-1}\equiv(n-1)z_0+\alpha_0$, with α_0 a constant.[12] Therefore, if one uses the Cauchy theorem for analytic functions and the integration by parts, after taking the logarithm of the wave function $\log[\psi_n^*(E)\psi_n(E)]$, then one can obtain

$$\psi_n^*(E)\psi_n(E)=\frac{\theta_3(z(E^2)-\alpha_{n-1},q)}{\theta_3(z(E^2)-\alpha_0,q)}. \qquad (13)$$

Since $\psi_n^*(E)$ is nothing but the complex conjugate of $\psi_n(E)$, finally we get

$$\psi_n(E)=e^{ik(E)n}U_n(E), \qquad (14)$$

where

$$U_n(E)\equiv\sqrt{\frac{\theta_3(z(E^2)-\alpha_{n-1},q)}{\theta_3(z(E^2)-\alpha_0,q)}} \qquad (15)$$

and

$$e^{ik(E)}\equiv\frac{\theta_3(z(E^2)+z_0,q)}{\theta_3(z(E^2)-z_0,q)}. \qquad (16)$$

On the other hand, using the same theta function θ_3, the nonlinear lattice distortion is given by[8-10,12]

$$T_n^2=e^{-(X_{n+1}-X_n)},$$

$$X_n\equiv S_n-S_{n+1},\quad S_n\equiv\theta_3\left(\frac{2K(\kappa)n}{\Lambda}+\delta,q\right), \qquad (17)$$

where δ is a constant. In this way we can obtain the exact wave function for an electron on the PTL with a static cnoidal wave.

We now discuss the relationship between energy E and wave number k, which gives a so-called *dispersion relation*.[11,13] This dispersion relation is represented as a multivalued function with respect to the wave number k. We can recognize this problem in solid state physics as a *uniformization problem* in mathematics.[15]

The uniformization problem is the following: Suppose we have an algebraic relation $F(E,k)=0$ that gives the multivaluedness of E on k. Is there any way to describe both E and k in terms of a parameter z such that both $E=E(z)$ and $k=k(z)$ become single-valued functions with respect to z?[16]

The answer to our problem is yes. From Eq. (11) we get inversely the relationship between E and z as $E^2=E^2(z)$. And from $R(E^2)=\Delta^2(E)-4$, we find that $\Delta(E)=E^3-\gamma^2E$, where 0, $\pm\gamma$ are the three band centers in the spectrum. Since $dk=d\Delta/\sqrt{R(E^2)}$, we get

$$\begin{aligned}k(z)&=\int_{-\infty}^{E}\frac{d\Delta}{\sqrt{R(E^2)}}\\&=\int_{-\infty}^{E}\frac{3E^2-\gamma^2}{\sqrt{R(E^2)}}dE\\&=\int_{-\infty}^{z(E^2)}(3E^2(z)-\gamma^2)dz,\end{aligned} \qquad (18)$$

where we have the energy band condition $\int_{\lambda_2}^{\lambda_3}dk=2\pi/\Lambda$ and the energy gap condition: $\int_{\lambda_1}^{\lambda_2}dk=0$. In this way both E and k are uniformized (parametrized) by a parameter z. Then, eliminating z from both, finally one can obtain the dispersion relation.[17]

In conclusion, we have discussed an example of the quasiperiodic systems that do not show Cantor-set-like energy bands. Such systems naturally arise from the integrable nonlinear lattices when we have nonlinear excitations. These nonlinear excitations are the consequence of a finite number of energy bands, from which one can construct both the quasiperiodic potentials and the exact wave functions for an electron on the lattice, using the Jacobi inversion method. In this context, to obtain dispersion relation is regarded as a uniformization problem in mathematics. Finally, we would like to mention that the above theory is applicable to more general cases, where the number of band gaps exceeds two.[8-10,12,14]

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[16] For example, consider a circle equation $x^2+y^2=1$. If y is regarded as a function of x, it is a double-valued function $y = \pm\sqrt{1-x^2}$ for $|x|<1$. However, one can uniformize it as $x=\cos z$ and $y=\sin z$ using a parameter z.

[17] The details will be published elsewhere.