Physica 124A (1984) 535-542
North-Holland, Amsterdam



# ON THE STATIONARY SCHRÖDINGER EQUATION WITH A QUASI-PERIODIC POTENTIAL

Jürgen MOSER and Jürgen POSCHEL

Mathematik, ETH-Zürich, CH-8092 Zürich, Switzerland

We consider the stationary Schrödinger equation

$$Ly = -y'' + q(x)y = \lambda y \tag{1}$$

on the real line, where q is a real, quasi-periodic potential. Our aim is to extend the result of Dinaburg and Sinai about the existence of Floquet type solutions--or extended states--to the resonant case and to obtain a large number of spectral gaps, which are generically open.

Let us briefly recall the case of a periodic potential q. If q is periodic, then the spectrum of L is an infinite sequence of closed bands tending to infinity. Between these bands lie the spectral gaps, which may degenerate so that adjacent bands touch.

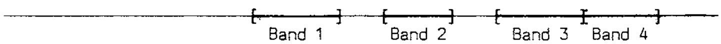


Figure 1

In addition, by Floquet theory, there is for all $\lambda$ a basis of solutions

$$e^{wx}p_1 \ , \ e^{-wx}p_2 \ , \quad 2w \notin i\omega\mathbb{Z}$$

except at the endpoints of spectral gaps, where one has the basis

$$e^{wx}(p_1 + \varepsilon x p_2), \quad e^{wx}p_2 \quad , \quad 2w \in i\omega\mathbb{Z} \ ,$$

and where $\varepsilon = 0,1$ depending on whether the gap is degenerate or not. The functions $p_1, p_2$ are periodic with the same period $\ell$ as the potential q, and $\omega = 2\pi/\ell$ is the basic frequency of q (see ref. 8). In particular, if a gap is degenerate, than all solutions are periodic with twice the period of q. This case is referred to as "coexistence of periodic solutions".

For a general almost periodic* potential q, the spectrum is less well

*For almost periodic functions and their frequency module, see e.g. ref. 4.

Presented at the VIIth INTERNATIONAL CONGRESS ON MATHEMATICAL PHYSICS, Boulder, Colorado, 1983.

known, and a Floquet representation is usually not available.[9,15] However, as was shown in ref. 5, the Floquet exponent

$$w = w(\lambda)$$

can still be defined as a holomorphic function of $\lambda$ on the upper half plane $\mathrm{Im}\,\lambda > 0$. Its imaginary part is the so called rotation number $\alpha$ for q. This rotation number extends continuously to the real line $\mathrm{Im}\,\lambda = 0$, where it can be defined by

$$\alpha(\lambda) = \lim_{x\to\infty} \frac{1}{x} \arg(\phi'(x,\lambda) + i\phi(x,\lambda)) \quad ,$$

choosing any real solution $\phi$ of (1).

The following important properties of $\alpha$ were also shown in ref. 5. On the real line, $\alpha$ is a nonnegative, monotone increasing and unbounded function, which increases precisely on the spectrum $\sigma(L)$ of L. That is,

$$\mathrm{supp}\, d\alpha = \sigma(L) \ .$$

Moreover, if I is an interval of constance in $\mathbb{R}\setminus\sigma(L)$, then

$$2\alpha(\lambda) \in M \ , \quad \lambda \in I \quad ,$$

where $M = M(q)$ is the frequency module of q.

The last property is often referred to as the "gap labelling theorem;" it tells us, where we have to look for spectral gaps. It can be used to show that for a limit-periodic potential q, the spectrum is generically a Cantor set, by opening up all possible spectral gaps.[2,11] But this case is easy, since a limit-periodic potential is the uniform limit of periodic potentials.

We are going to consider quasi-periodic potentials q. They can be written in the form

$$q(x) = Q(\omega x) \ , \quad \omega = (\omega_1,\dots,\omega_d) \in \mathbb{R}^d \quad ,$$

where $Q = Q(\theta_1,\dots,\theta_d)$ is a continuous function of period $2\pi$ in all d variables. The frequency module of q is the set

$$M = \{(j,\omega) \ , \quad j \in \mathbb{Z}^d \} \ ,$$

where $(j,\omega) = j_1\omega_1 + \dots + j_d\omega_d$ . We will suppose that the function Q is in fact real analytic, and indicate this by writing

$q \in \mathcal{Q}^a(\omega)$ .

Then q is clearly real analytic in x. But note that the converse is false in general: q may be analytic, while Q is only continuous.[5]

Since we are going to deal with small divisor problems, we impose on $\omega$ the small divisor conditions

$$|(j,\omega)| \geq \Omega^{-1}(|j|) \ , \quad |j| = |j_1| + \ldots + |j_d| \neq 0 \ ,$$

where $\Omega$ is a not too rapidly increasing approximation function. For instance,

$$\Omega(s) = ce^{s/\log^{1+\varepsilon} s} \quad , \quad s \geq s_0$$

with $c \geq 1$, $\varepsilon > 0$ will do.[13] The set of all $\omega$ satisfying this condition is denoted by $\mathcal{SD} = \mathcal{SD}(\Omega)$.

Dinaburg and Sinai constructed Floquet type solutions--or extended states--of (1) for rotation numbers $\mu$ , which are badly approximable by the resonances $\frac{1}{2}(j,\omega)$ in the spectral gaps. Precisely, they considered the set

$$\mathcal{N} = \mathcal{N}(\Omega) = \{\mu \in \mathbb{R}: \ |\mu - \tfrac{1}{2}(j,\omega)| \geq \Omega^{-1}(|j|) \ , \quad j \in \mathbb{Z}^d \} \ .$$

This is a Cantor set, whose complement is small in measure.

Theorem 1:[3,13] Suppose $q \in \mathcal{Q}^a(\omega)$ and $\omega \in \mathcal{SD}$. If $\mu \in \mathcal{N}$ is sufficiently large, then equation (1) possesses two linearly independent solutions of the form

$$e^{i\mu x}\chi \ , \ e^{-i\mu x}\bar{\chi} \ , \quad \chi \in \mathcal{Q}^a(\omega)$$

for $\lambda = \alpha^{-1}(\mu)$ .

This result gives rise to a Cantor set contained in the upper part of the spectrum, in fact, in the absolutely continuous spectrum. But it does not imply, that this part is a Cantor set.

We will derive a similar result for resonant rotation numbers $\mu = \frac{1}{2}(k,\omega)$. Again, we have to impose a nonresonance condition, restricting ourselves to the set

$$\mathcal{R} = \mathcal{R}(\Omega) = \{\mu = \tfrac{1}{2}(k,\omega): \ |\mu - \tfrac{1}{2}(j,\omega)| \geq \Omega^{-1}(|j|) \ , \quad k \neq j \in \mathbb{Z}^d \} .$$

This set is disjoint from $\mathcal{N}$ and not empty for suitable $\Omega$, as we will show later.

Now, a rotation number $\mu \varepsilon \mathcal{R}$ corresponds to a (possibly collapsed) spectral gap, whose endpoints lie in the spectrum $\sigma(L)$.

Theorem 2:[12] Suppose $q \varepsilon \mathcal{Q}^a(\omega)$ and $\omega \varepsilon \mathcal{SD}$. If $\mu \varepsilon \mathcal{R}$ is sufficiently large, then the interval

$$[\lambda_-, \lambda_+] = \alpha^{-1}(\mu)$$

is either collapsed to a point, in which case (1) has two linearly independent solutions

$$e^{i\mu x}\chi \ , \quad e^{-i\mu x}\overline{\chi} \ , \quad \chi \varepsilon \mathcal{Q}^a(\omega) \quad , \tag{2}$$

or has positive length, in which case (1) has two linearly independent solutions

$$e^{i\mu x}(\chi_1 + x\chi_2) \ , \quad e^{i\mu x}\chi_2 \quad , \quad \chi_1, \chi_2 \varepsilon \mathcal{Q}^a(\omega)$$

at each endpoint of $[\lambda_-, \lambda_+]$ .

Thus, the spectral gaps corresponding to large rotation numbers in $\mathcal{R}$ behave exactly like the gaps for periodic potentials.

The collapse of a gap in the above theorem is exceptional. In this case, according to (2), the squares of all solutions are quasi-periodic, and in fact, in $\mathcal{Q}^a(\omega)$ , since $2\mu = (k,\omega)$. This situation is in general unstable under perturbations. Indeed, by a simple variation of an argument in [11], arbitrarily small, generic perturbations in $\mathcal{Q}^a(\omega)$ open up such a spectral gap. Applying this argument repeatedly to all collapsed gaps, we obtain the

Addendum to Theorem 2: All the gaps provided by the above theorem can be opened up by arbitrarily small perturbations in $\mathcal{Q}^a(\omega)$.

The same arguments also apply to the situation described in Theorem 1. But here, the squares of all solutions are in $\mathcal{Q}^a(\omega, 2\mu) \supsetneq \mathcal{Q}^a(\omega)$, and the perturbation has to be chosen in $\mathcal{Q}^a(\omega, 2\mu)$. Thus, opening up one gap increases the frequency module, and the argument can not be iterated.

We very briefly indicate the proof of Theorem 2. Equation (1) is written in the form

$$\begin{pmatrix} y \\ y' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ Q(\theta)-\lambda & 0 \end{pmatrix} \begin{pmatrix} y \\ y' \end{pmatrix} , \qquad \theta' = \omega ,$$

which in suitable complex coordinates $z = \binom{z_1}{z_2}$ becomes

$$z' = \begin{pmatrix} i\sqrt{\lambda} & 0 \\ 0 & -i\sqrt{\lambda} \end{pmatrix} z + P(\theta,\lambda)z \quad , \quad \theta' = \omega \quad , \tag{3}$$

where P has trace 0 and is small for large $\lambda$. We consider this as a perturbation of a family of rotations, which we try to transform back in to a system with constant coefficients. The effect of the small divisors occurring is controlled by a rapidly converging iteration scheme, as it was done in refs. 1,3,7,10, and 13.

The linearized equation for the transformation I+U we are looking for is

$$\partial U + [C,U] = P \quad , \quad \partial = \sum_{\nu=1}^{d} \omega_\nu \partial_{\theta_\nu} \quad ,$$

where $C = C(\lambda)$ is a real 2x2-matrix with constant coefficients and eigenvalues $\pm w$ , $\operatorname{Im} w = \mu$ .

The main difference to the proof of Theorem 1 lies in the null space of the linear operator $\partial+[C,.]$. In the nonresonant case $\mu \varepsilon N$, the null space is only 1-dimensional and can be compensated for by adjusting the parameter $\lambda$ [3,13]. But in the resonant case $\mu \varepsilon R$, this null space has dimension 3 and can be identified with the Lie algebra $s\ell(2,\mathbb{R})$ of real matrices with trace 0. This null space can not any more be compensated for by a single parameter.

The Lie algebra $s\ell(2,\mathbb{R})$ contains the cone $\mathcal{C} = \{C: \det C = 0\}$, which separates $s\ell(2,\mathbb{R})$ into two open regions, the stable ($\det C > 0$) and unstable ($\det C < 0$) one. The unperturbed system corresponds to a curve $C(\lambda)$ in $s\ell(2,\mathbb{R})$ for $-\delta<\lambda-\lambda_0<\delta$ , which passes through the vertex of $\mathcal{C}$ for $\lambda = \lambda_0$ and otherwise lies in the stable region. After perturbation, such a curve, $C_*(\lambda)$, will in general not any more pass through the vertex of $\mathcal{C}$, but will partially lie in the unstable region. This geometrical fact corresponds to the opening of a gap under perturbation. It also shows the exceptional character of a collapsed gap. (See Fig. 2.)

The iterative construction finally yields a $\lambda$-interval $[\lambda_-,\lambda_+]$ and a family of transformations $S(\theta,\lambda)$ , $\lambda_- \leq \lambda \leq \lambda_+$ , with determinant 1 and coefficients in $\mathcal{Q}^a(\omega)$, which transform (3) into the differential equation

$$z' = i(\beta+\mu)z + be^{i(k,\omega)}\bar{z} \quad , \quad \theta' = \omega \quad \left(\mu = \tfrac{1}{2}(k,\omega)\right) \tag{4}$$

and its complex conjugate, where $\beta \varepsilon \mathbb{R}$, $b \varepsilon \mathbb{C}$ depend continuously on $\lambda$ and satisfy $|\beta| \leq |b|$, equality holding exactly at the endpoints of $[\lambda_-,\lambda_+]$. This

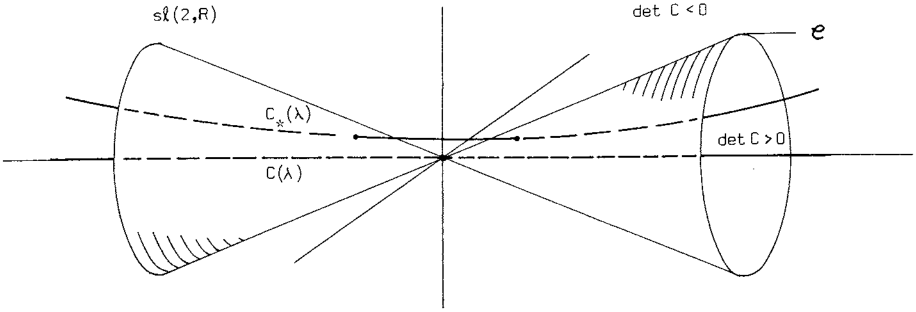


Figure 2

way, we actually obtain a continuous family of Floquet solutions over the spectral gap up to its endpoints.

We remark that the existence of Floquet solutions on the open resolvent set $\rho(L) = \mathbb{C}\setminus\sigma(L)$ is well known, see for instance refs. 6 and 14. Precisely, one has

Theorem 3: If $q \in \mathcal{Q}^a(\omega)$ and $\omega \in \mathcal{SD}$, then for all $\lambda \in \rho(L)$ there are two linearly independent solutions

$$e^{wx}\chi_1 \ , \ e^{-wx}\chi_2 \ , \quad \chi_1, \chi_2 \in \mathcal{Q}^a(\omega) \quad , \quad w = w(\lambda)$$

of equation (1).

This is also proven in ref. 12.

We finally consider the distribution of the set $R$ on the real line. Let $R'$ be the set of all its cluster points. It is easy to see that

$$R'(\Omega) \subset N(\Omega) \quad .$$

But it is not so easy to see that the set is not empty. We are indebted to Peter Sarnak and Walter Craig for proving to us that under very mild growth conditions on the approximation function $\Omega$, one in fact has the inclusion

$$R'(\Omega) \supset N(\Omega/3) \quad . \qquad (5)$$

Thus, $R'$ and hence $R$ cover the real line with increasing density as one approaches infinity.

The inclusion (5) has several important consequences. First, any sufficiently large point in the Dinaburg-Sinai set $\alpha^{-1}[N]$ is a cluster point of generically open spectral gaps. Hence, at these points, the spectrum is "locally a Cantor set", and the Dinaburg-Sinai set lies in the boundary of the spectrum.

Second, the closure of the set of all gaps of Theorem 2 leaves out a set of only small measure, which tends to zero as one approaches infinity.

Finally, we even recover Theorem 1 from Theorem 2. Using uniform estimates and a suitable normalization, we show that the family of transformations $S(\theta,\lambda)$ leading to (4) is continuous on the closure of all spectral gaps corresponding to rotation numbers in $R$. At any cluster point $\lambda_*$ of gaps the transformation $S(\theta,\lambda_*)$ then transforms (3) into a system (4), which yields the Floquet solutions of Theorem 1.

## REFERENCES


1) V I Arnold, Proof of a theorem by A N Kolmogorov on the invariance of quasi-periodic motions under small perturbations of the Hamiltonian. Russ. Math. Surveys 18, 5 (1963) 9-36.

2) J Avron and B Simon, Almost periodic Schrödinger operators I. Limit periodic potentials. Commun. Math. Phys. 82 (1981) 101-120.

3) E I Dinaburg, Ya G Sinai, The one-dimensional Schrödinger equation with a quasi-periodic potential. Funct. Anal. Appl. 9 (1975) 279-289.

4) A Fink, Almost periodic differential equations. Lecture Notes in Mathematics 377 (Berlin, Heidelberg, New York, 1974).

5) R A Johnson, J Moser, The rotation number for almost periodic potentials, Commun. Math. Phys. 84 (1982) 403-438.

6) R A Johnson, G R Sell, Smoothness of spectral subbundles and reducibility of quasi-periodic linear differential systems. J. Diff. Eq. 41 (1981) 262-288.

7) A N Kolmogorov, On the conservation of conditionally periodic motions under small perturbations of the Hamiltonian. Dokl. Akad. Nauk SSSR 98 (1954), 527-530.

8) W Magnus and S Winkler, Hill's equation, (Interscience, 1966).

9) V M Millionscikov, Proof of the existence of irregular systems of linear equations with quasiperiodic coefficients, Diff. Equ. 5 (1969) 1475-1478.

10) J Moser, Convergent series expansions for quasi-periodic motions. Math. Ann. 169 (1967) 136-176.

11) J Moser, An example of a Schrödinger equation with almost periodic potentials and nowhere dense spectrum. Comment. Math. Helv. 56 (1981) 198-224.

12) J Moser and J Pöschel, An Extension of a result by Dinaburg and Sinai for quasi-periodic potentials. Preprint, ETH-Zürich, 1983.

13) H Russmann, On the one-dimensional Schrödinger equation with a quasi-periodic potential. Annals of the New York Acad. Sci. 357 (1980) 90-107.

14)R J Sacker and G R Sell, A spectral theory for linear differential systems, J. Diff. Eq. 27 (1978) 320-358.

15)R E Vinograd, A problem suggested by N P Erugin. Diff. Equ. 11 (1975) 474-478.