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Robustness of perturbation series at high energies

Martin Kunz

Eidgenössische Technische Hochschule Zürich, 8092 Zürich, Switzerland

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Abstract. Completely integrable Hamiltonians submitted to a smooth perturbation are considered in the high-energy limit. It is shown that certain perturbation series, when suitably truncated, keep their validity even if the perturbation amplitude is much larger then the distance between levels. This is related to the localization of the corresponding eigenfunctions in the space of quantum numbers; such eigenstates are robust against level crossing. They are the natural analogues of classical KAM tori. Moreover, the method can also be used in classically resonant regions.

1. Introduction

The theorem of Kolmogorov, Arnol'd and Moser (KAM) [2, 6, 11] was an unexpected achievement in classical mechanics because simple perturbative methods do not allow one to predict the motion of a system slightly departing from integrability. This problem of 'small divisors' finds its origin in the existence of stochastic trajectories in the perturbed system. Such trajectories exist, however small the perturbation is, so that there is always a dense region in phase space which cannot be described by perturbative methods of any kind.

The situation is quite different in quantum mechanics, since conventional perturbation theory can always be used if the perturbation is small enough[†]; in this sense there is no need for an improved perturbation scheme, like Newton's method in KAM theory. On the other hand, perturbation series cease to converge when the distance between energy levels becomes smaller than the amplitude of the perturbation; now the spacing between levels usually decreases as some inverse power of the energy, which leads to the somewhat paradoxical situation that perturbation theory fails when the perturbation is comparatively the smallest. However, this new problem of small divisors, of a purely quantum origin[‡], should not preclude us from applying the correspondence principle to the perturbed Hamiltonian. According to this principle, and by virtue of KAM theory, it should be possible to describe a large fraction of the perturbed eigenstates by conventional perturbative methods. Equivalently, most eigenstates should remain localized in the lattice of quantum numbers; superposition of several states of this kind would occur only if their energies differ by an amount smaller than their coupling, which is exponentially small.

Of course, there should also exist eigenstates which are more sensitive to the perturbation. However, unlike classical resonant tori, these states should not manifest their 'resonant' character when the perturbation is infinitesimal; this is in accordance with the intuitive idea that quantum eigenstates represent a finite volume of classical phase space.

[†] In quantum mechanics, the effect of classical resonances is strongly attenuated by the curvature of the energy surface.

[‡] Superposition of states close in energy can be interpreted as a consequence of the tunnel effect.

One is therefore led to the conjecture that, for a given perturbation of arbitrary (but sufficiently large) amplitude, two distinct class of eigenstates manifest themselves as the energy is increased: the first and broader class contains eigenstates that are increasingly localized around some point in the lattice of quantum numbers. The second class, by analogy with the classical resonant zones, escapes from perturbative methods at all energies.

A natural approach to this problem consists in constructing semi-classical wavefunctions from quantized KAM tori [4,8,9]. Arnol'd [3] called such wavefunctions *quasi-modes*, because they do not always approximate a true eigenstate. These functions indeed satisfy the stationary Schrodinger equation up to an error ϵ proportional to some power of \hbar (depending on the order of the semi-classical approximation); they may therefore represent a superposition of several eigenstates whose energies lie within an interval of width ϵ .

In the present work, however, we shall focus on the quantum perturbation problem, avoiding both the intricacies of the semi-classical quantization method and KAM perturbation techniques. An elementary method of truncation of the perturbation series is presented, yielding quasi-modes with an error decreasing exponentially with the energy. At high energies this error is much smaller than the average distance between levels, so that most quasi-modes are close to the actual eigenstates. Moreover, this method extends to the most common class of resonance. In some cases it can therefore be used to completely describe the perturbed spectrum.

Our approach is based upon the study of localization properties of eigenstates in the lattice of quantum numbers; this point of view was inspired by the work of Altshuler and Levitov [1] on the scattering of a free particle by a singular periodic potential (the attention of these authors is drawn towards critical states). The spectacular failure of perturbation theory for energy levels corresponding to resonant tori, observed by Kunz and Rezakhanlou in the case of magnetic billards [13], served also as a motivation for this work. In particular, Kunz [7] suggested to look for an analogue of KAM theory in quantum mechanics in the form of a global perturbation theory. Finally, we mention the paper of Percival [12] in which the existence of a regular and an irregular spectrum is conjectured for mixed systems at high energies, on the basis of the correspondence principle.

After this work was completed, the results of Feldman *et al* [5] were brought to my knowledge; these authors studied in detail the Bloch spectrum of a particle on a two- or threedimensional periodic potential. They proved the existence of a stable and an unstable spectrum, the former consisting of pairs of levels that do not cross any other level under the effect of the perturbation. For generic periods of the potential, the stable spectrum is a subset of the density one; in other words, the problem of small divisors affects only a small part of the spectrum. This remarkable result depends on the dimension of the system and the symmetry of the matrix elements of the perturbation. In a sense, the robust and resonant spectra defined in this paper generalize their analysis to cases where small divisors cannot be avoided.

2. Smooth perturbations of quantum integrable systems

2.1. Definitions

As explained in the introduction, the aim of this paper is to investigate the properties at high energies of an integrable Hamiltonian submitted to a smooth perturbation. This sentence can be given a precise meaning in classical mechanics, but this is not so easy in quantum mechanics; our approach is therefore based on the examination of a few motivating examples (see section 4), from which generic features can be recognized. Rather than starting with examples, we shall, however, try to formulate our definitions and results in a general form and then come back to

examples. It should therefore be emphasized that the following definitions only synthesize the main properties of the examples; they are by no means an attempt to characterize all quantum integrable systems, for which no equivalent of the Liouville–Arnol'd theorem is known.

The quantum systems we have in mind in this paper consist in a single, spinless particle submitted to some external field, so that the corresponding classical system is unambiguously defined and consists in an integrable part plus some perturbation.

Our object of study is thus an Hamiltonian $H = H_0 + V$ with discrete spectrum, where H_0 is integrable and V is a smooth perturbation. We shall explain now what we mean by this.

Let v be the dimension of the configuration space; H_0 is an integrable Hamiltonian of dimension v if there exists a complete set of compatible observables A_2, \ldots, A_v with discrete spectrum, such that $[A_i, A_j] = 0$, $[A_i, H_0] = 0$. Now such a definition is not very helpful, since the lack of a quantum Liouville–Arnol'd theorem leaves us without powerful tools such as invariant tori and action-angle coordinates. We must therefore fill this gap with a set of minimal assumptions, that seem reasonable when concrete examples are considered. The description of integrable systems we shall adopt is based on the notion of a *lattice of quantum numbers*: the smoothness of the perturbation will be defined with respect to this lattice. But since the existence and properties of this lattice are guaranteed by no theorem, one must be flexible when trying to characterize it; the right attitude would be to construct explicitly such a lattice for a given Hamiltonian (it is not unique in general) and then check that it has the good properties. This may be a hard task in many cases[†]; note however that the difficulty to construct and analyse explicit integrable Hamiltonians exists in classical mechanics as well.

We now explain what the lattice of quantum numbers is. The eigenstates of H_0 can be labelled in a variety of ways; for instance, if the integer n_i labels the eigenvalues $\cdots < \lambda_{n_i} < \lambda_{n_i+1} < \cdots$ of A_i , $i = 2, \dots, \nu$, and n_1 labels the energy levels in each subspace defined by a fixed value of n_2, \ldots, n_{ν} , then $n = (n_1, \ldots, n_{\nu})$ labels the eigenstates of H_0 (assuming there are no further degeneracies). Let $\Lambda \subset Z^{\nu}$ be the union of all vectors n; we call Λ the *lattice of quantum numbers* defined by H_0 . We immediately note that this definition is not always optimal; for instance if p_1 , p_2 are two commuting operators with discrete spectrum and $H_0 = p_1^2 + p_2^2$, it is simpler (because of degeneracies) to use directly the eigenvalues of p_1 , p_2 rather than the construction above. Finding the good definition of A therefore depends on the explicit form of H_0 ; in what follows we shall assume that A has been chosen so that *n* bears some resemblance to a vector of quantized actions defined by the corresponding classical Hamiltonian $H_0^{\rm cl}$. In this case the matrix elements of a perturbation V can be interpreted, in the semi-classical limit, as Fourier coefficients of $V^{cl}(I, \theta)$, where (I, θ) are the action-angle variables defined by $H_0^{cl}(I)$. For technical convenience, we shall also assume that the volume of the unit cell in Λ , as well as the norm of the shortest vector in the lattice, is >1.

In classical mechanics, KAM theorem applies only if the perturbation V^{cl} is a smooth function of (I, θ) . From a quantum standpoint, it is reasonable to define a smooth perturbation V as an operator whose matrix elements decrease exponentially with the distance between lattice points in Λ . More precisely, we assume the existence of two positive functions $\tilde{V}_0(n)$, $\tilde{\alpha}(n)$ such that for all $n, m \in \Lambda$

$$|\langle \boldsymbol{n}|\boldsymbol{V}|\boldsymbol{m}\rangle| \leqslant \tilde{V}_0(\boldsymbol{n}) \mathrm{e}^{-\tilde{\alpha}(\boldsymbol{n})|\boldsymbol{n}-\boldsymbol{m}|} \tag{1}$$

(we use Dirac's bra-ket notation for states and scalar products throughout the paper). The important point is that the lattice Λ allows for the definition of a *distance* between eigenstates of H_0 (the Euclidean distance in \mathbf{R}^{ν}); this distance leads in turn to the notion of a smooth perturbation.

[†] For example, the study of a particle in a disc involves a deep understanding of the asymptotic behaviour of Bessel functions.

The lattice Λ must possess another important property: the energy $E_n = \langle n | H_0 | n \rangle$ must depend smoothly on n (at least for large quantum numbers). By this we mean that it must be possible to expand E_{n+k} in a Taylor series in terms of k, so that the first few terms give an accurate approximation for substantially large k. This requirement is essential for defining robust states and resonant gaps (see next section). Again, only explicit examples can tell to what extent this requirement is fulfilled. Simple counter-examples can be found if, for instance, the dimension of Λ is smaller than ν .

We conclude this section by defining some auxiliary functions that will be used throughout this paper. Observe that in many cases Λ is not truly a lattice, i.e., Λ is only a subset of the 'full' lattice Λ_c generated by all vectors \boldsymbol{n} . The following functions depend only on Λ_c and on the variable α :

$$C_1(\alpha) = \sum_{n \in \Lambda_1} e^{-\alpha |n|}$$
⁽²⁾

$$C_2(\alpha) = \sum_{n \in \Lambda_c} e^{-\frac{1}{2}\alpha\sqrt{|n|}}$$
(3)

$$C_{3}(\alpha) = \max_{m \neq 0} \left(\sum_{j \ge 0} \sum_{n \in \Lambda_{c}, n \cdot m \le 0} e^{-\alpha |jm-n|} \right)$$
(4)

$$C_4(\alpha) = \max_{r \ge 0} \left(e^{\alpha r/2} \sum_{|n| \ge r} e^{-\alpha |n|} \right)$$
(5)

$$C_5(\alpha) = \left(\frac{12(2\nu+4)}{\alpha e}\right)^{2\nu+4}.$$
 (6)

Notice that all these functions are bounded from above by some power of α .

2.2. Resonant gaps and robust states

The basic technique we shall use to avoid small divisors is to restrict the perturbation series to a finite region of the lattice of quantum numbers. The smoothness of the perturbation will then imply that the perturbative state is exponentially localized in this region: this is enough to insure that the approximation is accurate. We therefore now examine the *local* properties of the lattice Λ .

Suppose that we are given two functions of the quantum numbers $\tilde{R}(n)$, $\tilde{\delta}_1(n)$ (typically increasing as some power of the energy) with the following property: for all n' such that $|n' - n| < \tilde{R}(n)$, $\tilde{R}(n) < 2\tilde{R}(n')$. For any couple $\{m, -m\} \subset \Lambda$, we define a *resonant gap* G_m

$$G_m = \{ n \in \Lambda : m \leq 4\tilde{R}(n) \text{ and } \min_{k=\pm 1} |E_{n+km} - E_n| < 2\tilde{\delta}_1(n) \}.$$
(7)

We say that *n* is a *robust* state if the ball

$$B_{\tilde{R}} = \{ n' \in \Lambda : |n - n'| < R(n) \}$$

$$\tag{8}$$

has an empty intersection with all resonant gaps. These definitions correspond qualitatively to their classical analogues: a quantum resonant gap G_m is created when two lattice points n, n + m are almost tangent to the energy surface, so that $m \cdot \partial_n E \sim 0$. If we interpret quantum numbers as quantized classical actions, this tangency condition exactly corresponds to the resonance condition for classical tori. In this analogy, robust states correspond to quantized KAM tori. Moreover, since $|\partial_n E|$ usually grows as some power of E, resonant gaps (when suitably defined) fill only a small fraction of the space of quantum numbers. This fact, which rests on the assumption that E_n is a smooth function of n, is at the basis of the present work. Since most difficulties in the analysis are related to resonant gaps, it is necessary to describe their structure in more detail. Let m be a primitive vector in the lattice; it is convenient to define a *maximal resonant gap* as

$$\bar{G}_m = \bigcup_{j \in \mathbb{Z}} G_{jm}.$$
(9)

Now consider a subset Ω of the maximal gap \bar{G}_m , of diameter smaller than \tilde{R} , having an empty intersection with all other resonant gaps. In this region, the local structure of Λ can be described as the product of a one-dimensional 'resonant' lattice and a $(\nu - 1)$ -dimensional 'robust quasi-lattice'[†]. More precisely, we can define *resonant chains*

$$C_n = \{s \in \Omega : s = n + jm, j \text{ integer}\}$$
(10)

and write

$$\Omega = \bigcup_{n \in \Omega_0} C_n \tag{11}$$

where Ω_0 is a set defined so that two points in Ω_0 never belong to the same chain; we call n the *centre* of the chain and m the *resonant vector*. Since all chains in Ω intersect no other gap than \bar{G}_m , their spectra do not overlap; more precisely, the distance between two levels belonging to different chains is $>2\tilde{\delta}_1$.

Chains can be continued until they reach robust points. In the following, the centre will be defined as the point of minimal energy in the chain (assuming that the energy surface is convex). For each resonant chain C_n , we also define a function $\kappa_n(x)$ as follows: if |jm| > x then $|E_{n,j} - E_{n,j-1}| > \kappa_n(x)$, where $E_{n,j} = E_{n+jm}$.

The analysis of resonant gaps is simplified if we take into account the following fact: if the curvature of the energy surface varies sufficiently slowly, then the spectrum of a resonant chain is close to the spectrum of a free particle on a circle. This lead us to make the following hypothesis about H_0 (assumed to be valid throughout sections 3.3 and 3.4).

Curvature assumptions. Let E_0 , J be two constants depending on the integrable Hamiltonian H_0 only. For any chain C_n of resonant vector m such that $E_n > E_0$, the following conditions hold:

(1) If j > J and j > j' > 0 (or j < -J and j < j' < 0) then $E_{n,j} - E_{n,j'} > 0$. (2) If j > J and j' < 0 then $|E_{n,j} - E_{n,j'}|$ is minimal when $|j + j'| \le 1$. (3) If |j| > J, then $|E_{n,j} - E_n| < 2|j|\kappa_n(m(|j| - 2))$.

These assumptions are related to the almost constancy of the curvature through the following argument: if we expand the energy $E_{n+jm} = E_{n,j}$ in a Taylor series, discarding terms of third and higher order, we have

$$E_{n,j} = E_n + jm \cdot \partial_n E + \frac{1}{2}j^2m^t \cdot \partial_n^2 E \cdot m + \cdots .$$
⁽¹²⁾

Since n is the centre of the chain, the energy surface is almost tangent to m at n; geometrical arguments show indeed that there is usually a lattice point n such that

$$|\partial_n E \cdot m| \leqslant \frac{m^2}{2\rho} |\partial_n E| \tag{13}$$

[†] This decomposition can be thought of as a quantum counterpart to the foliation of the classical resonant torus by a one-parameter family of invariant tori.

where ρ is the radius of curvature of the curve defined as the intersection of the energy surface with the plane spanned by $\partial_n E$ and m. On the other hand, if $\partial_n E \cdot m = 0$ then

$$\boldsymbol{m}^{t} \cdot \partial_{n}^{2} \boldsymbol{E} \cdot \boldsymbol{m} = |\partial_{n} \boldsymbol{E}| \frac{\boldsymbol{m}^{2}}{\rho}$$
(14)

so that usually

$$|\boldsymbol{m}\cdot\partial_{\boldsymbol{n}}\boldsymbol{E}| < \frac{1}{2}\boldsymbol{m}^{t}\cdot\partial_{\boldsymbol{n}}^{2}\boldsymbol{E}\cdot\boldsymbol{m}.$$
(15)

Since the quadratic term is always dominant, the spacing between levels in the chain increases (linearly) with |j|. Actually, two levels can be close to each other, but they correspond in this case to nearly opposite sites (for instance j and -j).

3. Quasi-modes

The simplest strategy to avoid small divisors in the perturbation series is to eliminate the corresponding terms by a suitable truncation; the resulting approximation is accurate enough if it satisfies the stationary Schrodinger equation up to an error much smaller than the average distance between levels (quasi-mode). The description of integrable systems sketched in the previous section suggests that such an approximation can be obtained by considering a finite region in the lattice of quantum numbers and diagonalizing the corresponding (finite dimensional) Hamiltonian; the accuracy of the resulting approximation is then directly related to its *localization* in the lattice.

This section is organized as follows: we first give a precise definition of quasi-modes and then explain why they provide really accurate approximations of the true eigenstates. Then we construct quasi-modes in the simplest case, i.e. quasi-modes localized around robust lattice points; the corresponding exact states are the natural analogues of KAM tori in classical mechanics. Finally, we apply the same method to single resonances: the construction is not limited to the neighbourhood of robust points, but it ultimately depends on the localization of the approximation.

The localization lemma given in the appendix is the main technical tool used in this section.

3.1. Definition and properties

Consider an integrable Hamiltonian H_0 of dimension ν and a smooth perturbation V. Let B_r be a ball of radius r in the lattice Λ of quantum numbers; we write H_r , V_r the restrictions of $H = H_0 + V$, V to the subspace spanned by states in B_r and we define

$$\alpha = \min_{s \in B_r} \tilde{\alpha}(s) \tag{16}$$

$$V_0 = \max_{s \in B_c} \tilde{V}_0(s). \tag{17}$$

We say that $|q\rangle$ is a *quasi-mode* of the Hamiltonian $H = H_0 + V$ if $|q\rangle$ is a normalized eigenstate of H_r and if there exists a function $C_0(\alpha)$, bounded from above by some power of α , such that for any $n \in \Lambda$, $n \notin B_r$

$$|\langle q|V|n\rangle| \leqslant C_0 V_0 \exp\left(-\alpha \left(\frac{\sqrt{r}}{8} + d_n\right)\right)$$
(18)

where $d_n = \operatorname{dist}(n, B_r)$.

Quasi-modes have the following simple property:

$$|(H - H_r)|q\rangle|^2 = \left|\sum_{n \notin B_r} |n\rangle \langle n|V|q\rangle\right|^2$$

$$\leqslant C_0^2 V_0^2 e^{-\alpha \sqrt{r}/4} \sum_{n \notin B_r} e^{-2\alpha d_n}$$

$$\leqslant \text{constant} \times C_0^2 V_0^2 \frac{r^{\nu-1}}{\alpha} \left(1 + O\left(\frac{1}{\alpha r}\right)\right) e^{-\alpha \sqrt{r}/4}$$

$$= \epsilon(V_0, \alpha, r)$$
(19)

therefore, if $H_r |q\rangle = E_q |q\rangle$

$$|(H - E_q)|q\rangle|^2 \leqslant \epsilon.$$
⁽²⁰⁾

Thus if ϵ is small, quasi-modes are almost solutions of the stationary Schrödinger equation. Our definition of quasi-modes is indeed meaningful if $\alpha \sqrt{r}$ grows as some power of the energy: in this case ϵ decreases exponentially with some power of *E*.

The usual definition of quasi-modes [4,8,9] is based upon semi-classical approximations and yields an error ϵ proportional to some power of \hbar . In our case, the interesting point is the exponential decrease of ϵ : if $\epsilon^{1/4}$ becomes much smaller than the average distance between energy levels, then most quasi-modes can be considered as very good approximations of the exact eigenstates[†]. Let E_q be the quasi-energy associated with a quasi-mode q; let us write $|\lambda\rangle$ the exact eigenstates of H, with eigenvalues E_{λ} . We can expand

$$|q\rangle = \sum_{\lambda} c_{\lambda} |\lambda\rangle. \tag{21}$$

But we have seen that

$$|(E_q - H)|q\rangle|^2 = \sum_{\lambda} |c_{\lambda}|^2 |E_q - E_{\lambda}|^2 \leqslant \epsilon$$
(22)

so that

$$\epsilon \ge \sum_{|E_q - E_\lambda|^2 \ge \sqrt{\epsilon}} |c_\lambda|^2 |E_q - E_\lambda|^2$$

$$\ge \sqrt{\epsilon} \sum_{|E_q - E_\lambda|^2 \ge \sqrt{\epsilon}} |c_\lambda|^2 = \sqrt{\epsilon} |q - q_\epsilon|^2$$
(23)

where q_{ϵ} is the projection of q on the subspace $|E_{\lambda} - E_q|^2 < \sqrt{\epsilon}$. We have thus proved that $|q - q_{\epsilon}|^2 \leq \sqrt{\epsilon}$, $|q_{\epsilon}|^2 \geq 1 - \sqrt{\epsilon}$. In particular, there exists an eigenvalue E_{λ} such that $|E_{\lambda} - E_q| < \epsilon^{1/4}$ and if it is unique, then $|q_{\epsilon}\rangle \propto |\lambda\rangle$. If there are several such eigenvalues, then of course the quasi-mode does not necessarily represent an eigenstate, but a linear superposition of almost degenerate eigenstates.

It is interesting to consider quasi-modes in a continuous range of perturbation amplitudes $0 \leq V_0 \leq \overline{V}_0$: it is only when the quasi-energy E_q belongs to a cluster of exponentially close eigenvalues that the quasi-mode q represents a mixing of the corresponding eigenstates; otherwise, q itself is (with exponential accuracy) an eigenstate. Now the formation of such clusters (for a given eigenvalue) occurs only at certain values of V_0 . Moreover, quasi-modes and quasi-energies keep their identity before and after this 'collision' of levels. In other words, this

[†] It is assumed in our reasoning that the level spacing distribution of the *perturbed* system is smooth. This distribution is unsmooth, for instance, for a free particle in a square box; it would be interesting to know if such large degeneracies can also occur in mixed systems.





Figure 1. Robustness of quasi-modes against level crossing.

approximation method can be applied well beyond the range of validity of usual perturbation theory, namely before *and after* the crossing of levels[†].

Of course, this raises the question of the significance of quasi-modes under an adiabatic change of V_0 . We start with $V_0 = 0$ and slowly increase the amplitude V_0 . The initial state of the system is the eigenstate $|n\rangle$. Assume that the timescale T of the adiabatic change satisfies $1/\Delta E \ll T \ll 1/\epsilon$, where ΔE is the average distance between levels and ϵ is roughly proportional to the coupling between quasi-modes. As we shall see in the next section, a quasi-mode $|q\rangle$ can often be associated to an eigenstate $|n\rangle$ of H_0 ; standard arguments imply then that the adiabatic evolution of $|n\rangle$ is given by the corresponding quasi-mode $|q\rangle$. This is indeed obvious as long as the corresponding quasi-level E_q meets no other energy level (because $1/\Delta E \ll T$); on the other hand, if E_q meets some other level, the system 'jumps' to stay on E_q (see figure 1): this is because the time T is much smaller than the coupling $1/\epsilon$ (recall that remaining continuously on the same level would imply a complete change of the physical state at every 'avoided crossing'). The quantum number n can therefore be used to label eigenstates even if many level crossings have already occurred.

3.2. KAM quasi-modes

These are the simplest quasi-modes to construct: it suffices to exploit the properties of robust states. Recall that $n \in \Lambda$ is a robust state if it is possible to construct a ball $B_{\tilde{R}}$ of radius $\tilde{R}(n)$ and centre n which does not intersect any resonant gap. Define

$$\delta_1 = \min_{a \in B_{\bar{k}}} \tilde{\delta}_1(a). \tag{24}$$

If $a, b \in B_{\tilde{R}}$, then $|a - b| < 2\tilde{R}(n) < 4\tilde{R}(a)$ so that $|E_a - E_b| > 2\delta_1$. In particular, there is a gap $2\delta_1$ between E_n and any other level of H_0 in $B_{\tilde{R}}$. If $\tilde{V}_0 \ll \delta_1$, one can therefore conclude from perturbation theory that the eigenstates of $H_{\tilde{R}}$ (restriction of H to the ball $B_{\tilde{R}}$) are exponentially localized around some lattice point; if this lattice point lies in the centre of $B_{\tilde{R}}$, then the eigenstate is a quasi-mode.

The following theorem is a direct corollary of lemma 7 (where $C_4(\alpha)$ has been replaced by 1) and lemma 8 in the appendix.

[†] Strictly speaking, levels do not generically cross (unless they are completely decoupled) but a new set of eigenstates temporarily forms, which removes the degeneracy.

Theorem 1. Consider a ball B_R in the lattice Λ of radius R and centre n, and define

$$\alpha = \min(\log 4, \min_{s \in B_R} \tilde{\alpha}(s)) \tag{25}$$

$$V_0 = \max_{s \in B_p} \tilde{V}_0(s). \tag{26}$$

Assume that for all $s, s' \in B_R$, $|E_s - E_{s'}| \ge 2\delta \ge 8C_1(\alpha)V_0$. Then to each $s \in B_R$ corresponds an eigenstate $|x\rangle$ of H_R (restriction of H to B_R) exponentially localized around s: for all $t \in B_R$

$$|\langle x|t\rangle| \leqslant \frac{13V_0}{\delta} e^{-\alpha/2\sqrt{|t-s|}}.$$
(27)

Moreover,

$$E_s - C_1 V_0 \leqslant E_x \leqslant E_s + C_1 V_0. \tag{28}$$

In particular, the eigenstate $|q\rangle$ localized around n is a quasi-mode: for all $m \notin B_R$

$$|\langle q|V|\boldsymbol{m}\rangle| \leqslant V_0 C_5 \left(1 + \frac{4}{C_1}\right) \mathrm{e}^{-\alpha(d_m + 1/8\sqrt{R})}$$
⁽²⁹⁾

where $d_m = \operatorname{dist}(m, B_R)$.

We call $|q\rangle$ a *KAM quasi-mode*. It is worthy of note that the above estimates are obtained with perturbative methods only[†]. If most lattice points are robust and $\tilde{\alpha}\sqrt{\tilde{R}}$ grows as some power of the energy, then this result is in a sense equivalent to KAM theorem: according to the foregoing discussion, most quasi-modes can be seen as accurate approximations of the exact modes, so that a large fraction of the perturbed eigenstates can be obtained with perturbative methods. Moreover, the corresponding quantum numbers keep their significance, quite like invariant tori in the classical system. We refer to section 4 for a more complete discussion of KAM quasi-modes through concrete examples.

We stress here that the name KAM quasi-mode is not meant to imply any sophisticated perturbative technique (only standard Rayleigh–Schrodinger theory is used in the present work). In quantum mechanics indeed, the positiveness of the convergence radius of the perturbation series has nothing to do with integrability; discreteness of the spectrum and smallness of the perturbation are the important ingredients. Genuine quantum small divisors come from *global* resonances, whereas the small divisors of KAM theory are related to *local* tangency of the energy surface with the lattice of quantum numbers; this problem disappears as soon as robust points are considered, whence the name of the corresponding quasi-modes.

3.3. Quasi-modes in single resonant gaps

Suppose that the functions $\tilde{R}(n)$, $\tilde{\delta}_1(n)$ defined in 2.2 are such that, above a certain energy, resonant gaps fill only a small fraction of the space of quantum numbers. Then the intersections of two or more gaps (with linearly independant resonant vectors) are included in the neighbourhood of sets of codimension 2 and it is natural to consider a region intersected by one maximal gap only. The aim of this section is to demonstrate how quasi-modes can be constructed in such a region; unlike their KAM analogues, however, these quasi-modes cannot be computed by treating V as a perturbation.

Let B_r be a ball of radius r in the lattice Λ , intersected by one maximal gap \overline{G}_m only. As explained in 2.2, in such a ball the lattice can be described as a family of resonant chains whose

[†] There is a non-perturbative step in the application of lemma 7, namely the diagonalization of the Hamiltonian H_1 ; however, this step is trivial in our case.

spectra do not overlap. The exact spectrum of a chain depends of course on the integrable system under consideration; however, the curvature assumptions of section 2.2 imply that the distance between levels generally increases with the distance to the centre of the chain. These characteristics of the spectrum are the key to the construction of quasi-modes. The smooth perturbation V leads to the appearance of eigenstates delocalized in the centre of the chain; however, this delocalization is limited by the increasing distance between levels in the chain: when two neighbouring points become separated by an energy gap of the order of \tilde{V}_0 , states become localized.

We consider an integer $j_0 > J$ and a ball $B_r = \{v \in \Lambda : |v - n_0| < r\}$ where the point n_0 is the centre of a resonant chain C_{n_0} and $E_{n_0} > E_0$. We define

$$\delta_1 = \min_{v \in B_r} \tilde{\delta}_1(v) \tag{30}$$

and we assume that B_r intersects only one maximal resonant gap \overline{G}_m , with $2j_0m < r < \widetilde{R}(n_0)$; consequently, inside of B_r , $|E_{n,j} - E_{n',j'}| \ge 2\delta_1$ if $n \ne n'$. In the following we set $E_{n_0} = 0$ and

$$\delta_2 = \frac{5}{21} \kappa_{n_0} ((j_0 - 2)m). \tag{31}$$

Typically $\delta_2 \ll \delta_1$; here we shall simply assume $\delta_2 < \delta_1/2$.

Proposition 2. There exist

$$j_0 - 2 \le j_+ \le j_0 + 2$$
 $-j_0 - 2 \le j_- \le -j_0 + 2$

and $\Delta > 0$ such that:

(1) If $j \in [j_-, j_+]$ then $E_{n_0, j} \in [0, \Delta]$. (2) If $j \notin [j_-, j_+]$ then $E_{n_0, j} \ge \Delta + 21\delta_2/10$.

Moreover, if $E_{n_0,j} \leq E_{n_0,k} \leq E_{n_0,l}$ are three consecutive levels of C_{n_0} and $E_{n_0,j} \notin [0, \Delta]$, then $\max(E_{n_0,k} - E_{n_0,j}, E_{n_0,l} - E_{n_0,k}) \geq 21\delta_2/10$.

Proof. Consider E_{n_0,j_0} . According to the curvature assumptions of 2.2, the closest level E_{n_0,j_j} to E_{n_0,j_0} , j < 0, is $E_{n_0,-j_0+\epsilon}$ and $\epsilon \in \{0, 1, -1\}$. Suppose that $E_{n_0,-j_0+\epsilon} \leqslant E_{n_0,j_0}$; then $E_{n_0,-j_0+\epsilon-1} > E_{n_0,j_0} + 21\delta_2/10$, so that we can choose $j_+ = j_0$, $j_- = -j_0 + \epsilon$, $\Delta = E_{n_0,j_+}$. Similarly if $E_{n_0,-j_0+\epsilon} \geqslant E_{n_0,j_0}$, then $j_- = -j_0 + \epsilon + 1$, $j_+ = j_0 - 1$, $\Delta = E_{n_0,j_-}$.

Suppose now that $\max(E_{n_0,k} - E_{n_0,j}, E_{n_0,l} - E_{n_0,k}) \leq 21\delta_2/10$. Then by definition of δ_2 , jk < 0 and kl < 0. Therefore j and l have the same sign; but $E_{n_0,l} - E_{n_0,j} < 21\delta_2/5$, which is a contradiction. This completes the proof.

We give now localization conditions insuring that the eigenfunctions of the Hamiltonian H, restricted to a ball B_r in the lattice, are exponentially localized in B_r . The subsequent propositions are devoted to the proof of this fact; as we have explained, this proof rests entirely on the existence of large gaps in the spectrum of H_0 restricted to B_r . Let us define

$$V_0 = \max_{s \in B_r} \tilde{V}_0(s) \tag{32}$$

$$\alpha = \min(\log 4, \min_{s \in B_r} \tilde{\alpha}(s)). \tag{33}$$

In what remains of this section, the argument of the functions C_1, \ldots, C_5 always takes the above value of α .

Localization conditions:

$$\frac{o_2}{V_0} > \max(20C_1, 10C_3, 60C_2) \tag{34}$$

$$\frac{\delta_1}{V_0} > 10C_1(2r+2)^{\nu/2} \tag{35}$$

$$\frac{r}{2m} > (2j_0 + 5)\left(2 + \frac{1}{\alpha m} + \frac{1}{\alpha^2 m^2}\right).$$
(36)

We shall now demonstrate that the above conditions imply the existence of quasi-modes. We want to diagonalize the Hamiltonian H_r (restriction of H to B_r); observe that, by the Gerschgorin theorem, the levels of H_0 are shifted by an amount less than $C_1V_0 < \delta_2/20$, so that many characteristics of the spectrum remain almost unchanged. In particular, there remains a gap $2\delta_2$ around the enlarged interval

$$b = [-\delta_2/20, \Delta + \delta_2/20] \tag{37}$$

and there are exactly $j_+ - j_- + 1$ levels of H_r in b. Moreover, there remain gaps of width $3\delta_1/2$ between the spectra of different chains, so that it is still meaningful to say that an eigenstate of H_r belongs to a chain C_n .

Proposition 3. Let H_r be the restriction of the Hamiltonian H to the ball B_r , and assume that the first localization condition is satisfied (condition (34)). Let $|x\rangle$ be an eigenstate of H_r belonging to C_{n_0} , but not to the energy interval b. Then $|x\rangle$ is exponentially localized around one or two lattice points $s, s' \in C_{n_0}$. More precisely, $s = n_0 + jm$, $s' = n_0 + j'm$, $j, j' \notin [j_-, j_+], |j + j'| \leq 1$ and

$$|\langle x|t\rangle|^2 \leqslant \frac{7}{C_1^2} \exp(-\alpha\sqrt{r_t})$$
(38)

where t is any lattice point in B_r and $r_t = \text{dist}(\{s, s'\}, t)$.

Proof. It suffices to apply the localization lemma given in the appendix. By proposition 2 and the Gerschgorin theorem the state $|x\rangle$ can be associated with one or two lattice points $s, s' \in C_{n_0}$ such that $|E_s - E_{s'}| \leq 21\delta_2/10$. We identify the subspaces *A* and *B* of lemma 7 with $\{s, s'\}$ and B_r respectively (we refer to the appendix for subsequent notations in this proof). The energy levels of H_1 corresponding to the subspace *A* lie in an interval *a* of width $w_1 \leq 22\delta_2/10$, separated by a gap $2w_2 = 2\delta_2$ from all other levels of H_1 (proposition 2). It is straightforward to verify that all conditions of the lemma are satisfied and that the contour γ surrounds E_x . Moreover, we can replace C_4 by 2. This completes the proof.

Proposition 4. Let $|z\rangle$ be an eigenstate of H_r belonging to the energy interval b, and assume that the localization conditions are satisfied. Then $|z\rangle$ is exponentially localized in the ball $B_{r/2}$. More precisely, for any lattice point $t \in B_r \setminus B_{r/2}$

$$|\langle z|t\rangle|^2 \leqslant \left(\frac{4C_4+1}{C_1}\right)^2 j_0^3 \exp(-\alpha\sqrt{r_t})$$
(39)

where $r_t = \operatorname{dist}(t, B_{r/2})$.

Proof. We want to apply lemma 7 again (we refer to the appendix for subsequent notations). We set $A = B_{r/2}$, $B = B_r$. The diagonalization of H_1 yields normalized eigenstates a_1, a_2, \ldots belonging to A. We identify the interval a of lemma 7 with b, so that there are N eigenstates

 a_1, \ldots, a_N in a and $N = j_+ - j_- + 1$ according to the Gerschgorin theorem. We also have $w_1 = \Delta + \delta_2/10, w_2 = \delta_2$.

Let us first estimate the delocalization of a_1, \ldots, a_N in $B_{r/2}$. We have

$$|\langle s|a_i\rangle| = \left|\frac{\langle s|V|a_i\rangle}{E_s - E_{a_i}}\right| \leqslant \frac{V_0 C_1}{|E_s - E_{a_i}|} \tag{40}$$

so that if $s \notin C_{n_0}$

$$\sum_{1 \leqslant i \leqslant N} |\langle a_i | s \rangle| \leqslant \frac{N V_0 C_1}{\delta_1}$$
(41)

whereas if $|s\rangle = |n_0 + jm\rangle$ and $j \notin [j_-, j_+]$

$$\sum_{1 \leq i \leq N} |\langle a_i | s \rangle| \leq \frac{N V_0 C_1}{E_{n_0, j} - \Delta - \delta_2 / 20}.$$
(42)

We can now estimate the sum

$$I = \sum_{y} \left| \frac{\langle x | W | y \rangle}{E - E_{y}} \right|$$
(43)

where x, y are eigenstates of H_1 and $E \in \gamma$. Suppose first that $x \in B_{r/2}$; in this case the sum runs over lattice points $v \in B_r \setminus B_{r/2}$. Defining $C'_{n_0} = C_{n_0} \cap B_r \setminus B_{r/2}$ we obtain

$$I \leq \sum_{v \in B_r \setminus B_{r/2}} \sum_{s \in B_{r/2}} \left| \frac{\langle v | W | s \rangle \langle s | x \rangle}{E - E_v} \right|$$

$$\leq \frac{V_0}{\delta_1} \sum_s |\langle s | x \rangle| \sum_{v \notin C'_{n_0}} e^{-\alpha |s-v|} + \frac{V_0}{\delta_2} \sum_{v \in C'_{n_0}} \sum_s e^{-\alpha |s-v|}$$

$$\leq \frac{V_0}{\delta_1} C_1 (r+2)^{\nu/2} + 2\frac{V_0}{\delta_2} C_3 < \frac{1}{10} + \frac{1}{5}$$
(44)

where we have used the inequality

$$\sum_{s \in B_{r/2}} |\langle s | x \rangle| \leqslant \left(\sum_{s \in B_{r/2}} 1\right)^{1/2} \leqslant (r+2)^{\nu/2}.$$
(45)

Suppose now that $x = v \in B_r \setminus B_{r/2}$; in this case the sum runs over a_1, a_2, \ldots and $u \in B_r \setminus B_{r/2}$

$$I = \sum_{u \in B_r \setminus B_{r/2}} \left| \frac{\langle v | W | u \rangle}{E - E_u} \right| + \sum_{a_i \in C_{n_0}, i > N} + \sum_{a_i \notin C_{n_0}} + \sum_{i \leqslant N} \left| \frac{\langle v | W | a_i \rangle}{E - E_{a_i}} \right|$$

= $I_0 + I_1 + I_2 + I_3.$ (46)

Clearly $I_0 < \frac{1}{20}$. By proposition 3, for any $s \in B_{r/2}$

$$\sum_{a_i \in C_{n_0}, i > N} |\langle s | a_i \rangle| \leqslant \frac{6C_2}{C_1} \tag{47}$$

so that

$$I_1 \leqslant 6C_2 \frac{V_0}{\delta_2} < \frac{1}{10}.$$
(48)

On the other hand

$$I_2 \leqslant C_1 \frac{V_0}{\delta_1} (r+2)^{\nu/2} < \frac{1}{10}$$
(49)

using an inequality similar to (45). It remains to estimate I_3 . Using (41), (42), we obtain

$$I_{3} \leqslant \frac{V_{0}}{\delta_{2}} \sum_{s \in B_{r/2}} e^{-\alpha |s-v|} \sum_{1 \leqslant i \leqslant N} |\langle a_{i} | s \rangle|$$

$$\leqslant \frac{V_{0}}{\delta_{2}} \left(C_{1} \frac{N V_{0} C_{1}}{\delta_{1}} + N^{3/2} e^{-\alpha (r/2 - (j_{0} + 2)m)} \right)$$

$$V_{0} \left(\sum_{i=1}^{N} \sum_{j \in V_{0}} \frac{N V_{0} C_{1}}{\delta_{1}} + N^{3/2} e^{-\alpha (r/2 - (j_{0} + 2)m)} \right)$$
(50)

$$+\frac{V_0}{\delta_2} \left(\sum_{-h \leqslant j < j_-} + \sum_{j_+ < j \leqslant h} \frac{N V_0 C_1}{E_{n_0, j} - \Delta - \delta_2 / 20} e^{-\alpha (r/2 - |j|m)} \right)$$
(51)

where *h* is the integer part of r/2m. The term (50) is smaller than $\frac{1}{20}$; to estimate term (51), consider for instance

$$NV_{0}C_{1}\sum_{j_{+}< j \leqslant h} \frac{e^{-\alpha(r/2-jm)}}{E_{n_{0},j} - \Delta - \delta_{2}/20} \leqslant NV_{0}C_{1}\sum_{1\leqslant k\leqslant h-j_{+}} \frac{e^{-\alpha m(h-k-j_{+})}}{k\delta_{2}}$$
$$= \frac{NV_{0}C_{1}}{\delta_{2}}\sum_{0\leqslant t\leqslant h-j_{+}-1} \frac{e^{-\alpha mt}}{h-j_{+}-t}$$
$$\leqslant \frac{N}{20} \left(\frac{2}{h-j_{+}} + \exp\left(-\alpha m \frac{h-j_{+}}{2}\right)\right) \left(1 + \frac{1}{\alpha m}\right).$$
(52)

It can be verified, using (36), that this last expression is smaller than $\frac{1}{2}$, so that $I_3 < \frac{1}{20} + \frac{1}{20} = \frac{1}{10}$. We have thus proved that $I < \frac{1}{2}$; lemma 7 can therefore be applied. To complete the proof, it remains to observe that $\Delta < 10j_0\delta_2$.

The results of this section can be restated as follows.

Theorem 5. Assume that the localization conditions are satisfied. Let $|q\rangle$ be an eigenstate of H_r belonging to $C_{n_0} \cap B_{r/2}$; by this we mean

$$-\frac{\delta_2}{20} \leqslant E_q \leqslant \frac{\delta_2}{20} + \max(E_{n_0,h-1}, E_{n_0,-h+1})$$

where h is the integer part of r/2m. Then $|q\rangle$ is a quasi-mode: for any lattice point $n \notin B_r$

$$|\langle q|V|\boldsymbol{n}\rangle| \leqslant V_0 \frac{4C_4 + C_1 + 1}{C_1} C_5 \exp\left(-\alpha \left(\frac{\sqrt{r}}{8} + d_n\right)\right)$$

where $d_n = \operatorname{dist}(n, B_r)$.

Proof. By proposition 3 or 4, $|q\rangle$ is exponentially localized in $B_{r/2}$. We can therefore apply lemma 8 of the appendix.

3.4. A complete determination of the perturbed spectrum

A particularly interesting situation arises when quasi-modes can be constructed around any lattice point in a given energy interval e. In this case one might hope to obtain, with exponential accuracy, the complete spectrum in the interval e; moreover, projectors over either single levels or clusters of exponentially close levels might be expressed, with exponential accuracy, as sums of projectors over quasi-modes. Since we have been able to construct quasi-modes in single resonant gaps only, one has to assume that the energy interval e avoids all multiple resonant gaps (intersection of two or more gaps with linearly independent resonant vectors); as we shall see in a specific example (section 4.1), this is possible only if v = 2 or 3.

Consider an energy interval $e = [e_1, e_2] (e_1 > E_0)$ and define

$$X = \{ s \in \Lambda : E_s \in e \}.$$
⁽⁵³⁾

Assume that one can construct disjoint balls B_{r_1}, \ldots, B_{r_n} of radius r_1, \ldots, r_n so that

$$X \subset B_{r_1} \cup \dots \cup B_{r_n}.$$
 (54)

We write V_{r_i} the restriction of V to B_{r_i} . We would like to obtain an accurate estimate of the eigenstates and eigenvalues of $H = H_0 + V$ in a subinterval $e' = [e_1 + w, e_2 - w]$ by computing a limited number of quasi-modes only, i.e. by diagonalizing $H_{r_1,...,r_n} = H_0 + V_{r_1} + \cdots + V_{r_n}$. To do so we need to demonstrate:

- (1) that no eigenvalue of $H_{r_1,...,r_n}$ outside of e can be shifted inside of e' by $W = V (V_{r_1} + \cdots + V_{r_n})$
- (2) that each eigenstate of $H_{r_1,...,r_n}$ belonging to *e* is a quasi-mode.

More precisely, for any eigenstate $|x\rangle$ of H_{r_1,\ldots,r_n} , we define

$$\Gamma_x(W) = \sum_{y} |\langle x | W | y \rangle|$$
(55)

where the sum runs over the eigenstates of $H_{r_1,...,r_n}$. By the Gerschgorin theorem, to demonstrate 1 it is enough to prove that

$$\Gamma_x \leqslant w + \operatorname{dist}(E_x, e) \tag{56}$$

for any eigenstate x such that $E_x \notin e$. Observe that this method opens the way for a perturbative computation of the *exact* levels in the energy interval e' (by treating W as a perturbation).

Before we carry out this program, we make the following assumption about H_0 : let n_0 $(E_{n_0} > E_0)$ be the centre of a resonant chain with resonant vector m. Consider a ball B_r of centre n_0 and radius r > 10m and define $s_{\pm} = n_0 \pm lm$ where l is the smallest integer exceeding r/m. For any chain C_n of resonant vector m intersecting B_r , we assume that

$$|n - s_{\pm}| \geqslant \frac{4r}{5}.\tag{57}$$

Roughly speaking, this assumption has the following geometrical meaning: the minimum angle between m and the hypersurface $m \cdot \partial_n E = 0$ is greater than some constant. Notice that it implies $|n - n_0| < 2r$.

In the following theorem it is proved that, under appropriate circumstances, quasi-modes yield a complete picture of the spectrum in the subinterval $e' = [e_1 + w_1 + w_2, e_2 - w_1 - w_2]$. Some preliminary definitions are necessary:

$$R = \min_{s \in X} \tilde{R}(s) \tag{58}$$

$$\delta_1 = \min_{s: \operatorname{dist}(s, X) < R} \tilde{\delta}_1(s) \tag{59}$$

$$V_0 = \max_{s:\operatorname{dist}(s,X) < R} \tilde{V}_0(s) \tag{60}$$

$$\alpha = \min(\log 4, \min_{\substack{s: \text{dist}(s, X) < R}} \tilde{\alpha}(s)).$$
(61)

In what remains of this section, the argument of C_1, \ldots, C_5 always takes the above value of α . We also assume that $e_2 - e_1 < \delta_1$. See section 4 for an application of this theorem in two and three dimensions.

Theorem 6. Assume that there exists an integer $j_0 > J$ and a number r < R/4 such that the following conditions are satisfied:

(1) For any resonant chain C_n intersecting X.

$$e_2 - e_1 < \frac{\kappa_n(2r/5)}{4}.$$
 (62)

- (2) For any $s \in X$ we can construct a ball of centre s and radius 6r intersecting at most one maximal resonant gap.
- (3) For any resonant chain C_n such that $dist(C_n, X) < r/10$

$$\kappa_n(r/10) > 8C_1 V_0. \tag{63}$$

(4) Define

$$r' = \frac{r}{2(2j_0 + 5)(2 + \alpha^{-1} + \alpha^{-2})}.$$
(64)

For any centre n of a chain $C_n \subset G_m$ such that dist(n, X) < 3r and m < r', we can define $\delta_2(n) = 5/21\kappa_n((j_0 - 2)m) < \delta_1/2$ so that $j_0, \delta_2(n), \delta_1, r$ satisfy the localization conditions (34), (35) ((36) is automatically satisfied).

Then it is possible to construct disjoint balls B_{r_1}, \ldots, B_{r_n} $(r_i \ge r'/4)$ with the property dist $(B_{r_i}, B_{r_j}) > r_i + r_j$, so that each eigenstate of H_{r_1,\ldots,r_n} belonging to the energy interval e is a quasi-mode. Moreover, for any eigenstate $|x\rangle$ not belonging to e

$$\Gamma_x(W) \leqslant w_1 + w_2 + \operatorname{dist}(E_x, e) \tag{65}$$

where

$$w_1 = V_0(C_1 + C_5(5C_4 + 1) + 12C_2)$$
(66)

and w_2 decreases exponentially with r:

$$w_{2} = C_{4}V_{0}\sum_{i} (2r_{i}+2)^{\nu/2} e^{-\alpha r_{i}/4} + \max_{i} (2r_{i}+2)^{\nu/2} C_{4}V_{0} \sum_{j \neq i} (2r_{j}+2)^{\nu/2} \exp\left(-\frac{\alpha}{2}\left(d(i,j)-\frac{r_{i}}{2}\right)\right)$$
(67)

 $(d(i, j) = \operatorname{dist}(B_{r_i}, B_{r_i})).$

Proof. Let us first describe the construction of the Hamiltonian $H_{r_1,...,r_n}$. If $s \in X$ and s is robust, then the distance between s and any other point in X is greater than R; we therefore construct a ball $B_{R/4}$ of centre s and radius R/4 around any such point. If s is not robust, then s belongs to some resonant chain C_n with resonant vector m (condition 2 insures that the primitive vector m is unambiguously defined). Suppose first that m < r' and |s - n| > 2r/5; by condition 1, the distance between s and radius r/10. If |s - n| < 2r/5 then we construct a ball $B_{r/10}$ of centre s and radius r/10. If |s - n| < 2r/5 then we construct a ball B_r of centre n and radius r. Finally, if $m \ge r'$, then we construct a ball $B_{r'/4}$ of centre s and radius r'/4. It is not difficult to convince oneself that the distance between any two balls is greater than the sum of their radii.

Let us verify that any eigenstate of $H_{r_1,...,r_n}$ belonging to *e* is a quasi-mode. Consider first a ball $B_{r/10}$ of centre $s \in C_n$; for any chain $C_{n'}$ intersecting $B_{r/10}$, we have $|n'-(n\pm(r/m)m)| > 4r/5$ so that dist $(n', B_{r/10}) > r/10$. Now by condition 3, $\kappa_{n'}(r/10) > 8C_1V_0$ so that the minimum distance between levels in $B_{r/10} > 8C_1V_0$. Therefore theorem 1 can be applied and the only eigenstate in the ball belonging to *e* is a quasi-mode. The same is true, of course, in balls $B_{R/4}$ and $B_{r'/4}$. Consider then a ball B_r constructed around the centre of a resonant chain; using condition 4 and theorem 5, we see again that eigenstates in *e* are quasi-modes.

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Consider now an eigenstate $|x\rangle$ of $H_{r_1,...,r_n}$ such that $E_x \notin e$. If $|x\rangle = |v\rangle$ and if the distance between v and any ball is greater than half the radius of the ball, then

$$\Gamma_{x}(W) = \sum_{y} |\langle v|W|y \rangle|$$

$$\leq C_{1}V_{0} + \sum_{i=1}^{n} \sum_{y \in B_{r_{i}}} \sum_{t} V_{0}e^{-\alpha|v-t|}|\langle t|y \rangle|$$

$$\leq C_{1}V_{0} + C_{4}V_{0} \sum_{i=1}^{n} (2r_{i}+2)^{\nu/2}e^{-\alpha r_{i}/4}$$

$$\leq w_{1} + w_{2}.$$
(68)

Suppose now that $|x\rangle$ either belongs to a ball B_{r_i} or $|x\rangle = |v\rangle$ and dist $(v, B_{r_i}) < r_i/2$. For each ball B_{r_i} , we define

$$W_{r_i} = V_{2r_i} - V_{r_i} (69)$$

where V_{2r_i} is the restriction of V to a ball B_{2r_i} of radius $2r_i$ concentric with B_{r_i} . We have

$$\Gamma_x(W) \leqslant \Gamma_x(W - W_{r_i}) + \Gamma_x(W_{r_i}) \tag{70}$$

and

$$\Gamma_{x}(W - W_{r_{i}}) = \sum_{y} |\langle x|V - V_{2r_{i}}|y\rangle|
\leq \sum_{j \neq i} \sum_{y \in B_{r_{j}}} \sum_{v,t} V_{0} e^{-\alpha|v-t|} |\langle x|v\rangle \langle t|y\rangle| + \sum_{t \notin B_{2r_{i}}} \sum_{v} V_{0} e^{-\alpha|v-t|} |\langle x|v\rangle|
\leq (2r_{i}+2)^{\nu/2} C_{4} V_{0} \sum_{j \neq i} (2r_{j}+2)^{\nu/2} \exp\left(-\frac{\alpha}{2} \left(d(i,j) - \frac{r_{i}}{2}\right)\right)
+ C_{4} V_{0} (2r_{i}+2)^{\nu/2} e^{-\alpha r_{i}/4}
\leq w_{2}.$$
(71)

It remains to prove that

$$\Gamma_x(W_{r_i}) < w_1 + \operatorname{dist}(E_x, e). \tag{72}$$

To obtain accurate estimates, it is necessary to examine the localization properties of all the eigenstates in a ball.

Consider first a ball B_r constructed around the centre n_0 of a resonant chain and denote H_r as the restriction of H to B_r . Recall that, for each chain C_n intersecting B_r , $|n - n_0| < 2r$; using condition 4 and proposition 2, we can therefore define an energy interval b_n for each chain with the following properties: there are two gaps $2\delta_2(n)$ around b_n in the spectrum of H_r and b_n contains at most $2j_0 + 5$ eigenvalues. Consider now an eigenstate $|z\rangle$ of H_r belonging to an interval b_n . We can use proposition 4 to demonstrate that $|z\rangle$ is exponentially localized in a ball $B_{r/2}(n)$ of centre n and radius r/2. More precisely, for any $t \notin B_{r/2}(n)$

$$|\langle z|t\rangle| \leqslant \frac{4C_4 + 1}{C_1} r^2 \exp\left(-\frac{\alpha\sqrt{r_t}}{2}\right)$$
(73)

where $r_t = \text{dist}(t, B_{r/2}(n))$. Actually, we apply proposition 4 to the Hamiltonian $\tilde{H} = \tilde{H}_0 + V_r$, where \tilde{H}_0 is the restriction of H_0 to the ball $B_{3r}(n)$ and V_r is the restriction of V to $B_r(n_0) \subset B_{3r}(n)$ (proposition 4 remains valid if we replace B_r by B_{3r} , as long as B_{3r} intersects no other resonant gap than \bar{G}_m ; in our case this is true because, by hypothesis, $B_{3r}(n) \subset B_{5r}(n_0)$). If $|z\rangle$ belongs to C_n but not to b_n then again, applying proposition 3 to the Hamiltonian \tilde{H}

$$|\langle z|t\rangle| \leqslant \frac{\sqrt{7}}{C_1} \left(\exp\left(-\frac{\alpha}{2}\sqrt{|t-s|}\right) + \exp\left(-\frac{\alpha}{2}\sqrt{|t-s'|}\right) \right)$$
(74)

where $s, s' \in C_n \cap B_r(n_0)$. A similar inequality holds when $|z\rangle$ is localized around one lattice point only. Moreover, there is a bijection between such states (or pair of states) $|z\rangle$ and lattice points (or pairs of points) s.

We have thus obtained bounds on the delocalization of eigenstates of H_r . We can now compute $\Gamma_x(W_r)$ for a ball B_r constructed around the centre n_0 of a resonant chain. Suppose first that $|x\rangle \in B_r$ $(E_x \notin e)$; if $|x\rangle \notin C_{n_0}$, then

$$\Gamma_x(W_r) \leqslant C_1 V_0 (2r+2)^{\nu/2} \leqslant \frac{\delta_1}{10} < \operatorname{dist}(E_x, e).$$
 (75)

If $|x\rangle \in C_{n_0}$ and $E_x \notin b_{n_0}$ we obtain, using (74)

$$\Gamma_x(W_r) \leqslant 2\sqrt{7C_2V_0} \leqslant w_1 \tag{76}$$

whereas if $E_x \in b_{n_0}$, $|x\rangle$ is a quasi-mode and (73) yields the rough estimate

$$\Gamma_x(W_r) \leqslant V_0(5C_4 + 1)C_5 < w_1. \tag{77}$$

Suppose now that $|x\rangle = |s\rangle$, where $r < |s - n_0| \leq 3r/2$. In this case

$$\Gamma_x(W_r) \leqslant C_1 V_0 + \sum_{y \in B_r} \sum_{t \in B_r} |\langle t|y \rangle| V_0 e^{-\alpha |s-t|}.$$
(78)

If $s \notin C_{n_0}$ then

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$$\begin{aligned} V_x(W_r) &\leq C_1 V_0 + C_1 V_0 (2r+2)^{\nu/2} \\ &\leq \frac{\delta_2(n_0)}{20} + \frac{\delta_1}{10} < \operatorname{dist} (E_x, e) \end{aligned}$$
(79)

while if $s \in C_{n_0}$ (and for instance $(s - n_0) \cdot m > 0$)

$$\Gamma_x(W_r) \leqslant C_1 V_0 + \sum_{y,t} |\langle t|y \rangle| V_0 \mathrm{e}^{-\alpha |s_* - t|}.$$

$$\tag{80}$$

Consider first $y \in b_n$; since $|s_+ - n| > 4r/5$ we obtain, using (73)

$$\sum_{|s_{+}-t| < r/5} + \sum_{r/5 \leqslant |s_{+}-t| \leqslant 2r} |\langle t|y \rangle| V_{0} e^{-\alpha |s_{+}-t|} \\ \leqslant V_{0}(4C_{4}+1)r^{2} \exp\left(-\frac{\alpha}{2}\sqrt{\frac{r}{10}}\right) + V_{0}C_{4} \exp\left(-\frac{\alpha r}{10}\right).$$
(81)

On the other hand, each state (or pair of states) y which does not belong to an interval b_n is exponentially localized around one or two lattice points in B_r , according to (74). Summing over y and taking the maximal value with respect to r, we finally obtain

$$\Gamma_x(W_r) \leqslant C_1 V_0 + V_0 C_5 (5C_4 + 1) + 12 V_0 C_2$$

$$\leqslant w_1.$$
 (82)

It remains to estimate $\Gamma_x(W_{r_i})$ for a ball $B_{R/4}$, $B_{r/10}$ or $B_{r'/4}$. In every case, the minimum distance between levels in the ball is larger than $8C_1V_0$, so that eigenstates of $H_{r_1,...,r_n}$ are exponentially localized around some lattice point in the ball (theorem 1). From this it is readily deduced that

$$\Gamma_x(W_{r_i}) \leqslant V_0 C_1 + 4V_0 C_2 < w_1 \tag{83}$$

where either $|x\rangle \in B_{r_i}$ or $|x\rangle = |s\rangle$ and $0 < \text{dist}(s, B_{r_i}) < r_i/2$. This completes the proof of the theorem.

4. Examples

4.1. Free particle on a Euclidean torus

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The configuration space of this system is a ν -dimensional torus with Euclidean coordinates $0 \le x_i < L_i, i = 1, ..., \nu$. The integrable Hamiltonian H_0 is simply the kinetic energy

$$H_0 = \frac{p^2}{2m} = -\frac{\hbar}{2m} \sum_{i=1}^{\nu} \frac{\partial^2}{\partial x_i^2}.$$
 (84)

This system is especially simple for several reasons. First of all, the semi-classical quantization rules are exact and the actions

$$I_k = \frac{p_k L_k}{2\pi} \qquad k = 1, \dots, \nu \tag{85}$$

simply take integer values multiplied by \hbar . If we define the *k*th quantum number as

$$n_k = \frac{L_1 p_k}{2\pi\hbar} = \frac{L_1}{L_k} \times \text{integer}$$
(86)

and

$$e_0 = \left(\frac{2\pi\hbar}{L_1\sqrt{2m}}\right)^2\tag{87}$$

then $E_n = e_0 n^2$ and the energy surface is simply a sphere in the lattice Λ . Moreover, if $L_1 \ge L_k, k = 1, ..., \nu$, then the norm of the shortest vector in the lattice and the volume of the unit cell are >1.

In the following, we shall consider a perturbation V depending analytically on the coordinates x_i ; its matrix elements are then simply Fourier coefficients and the functions \tilde{V}_0 , $\tilde{\alpha}$ take constant values V_0 , α .

There are several possible definitions of resonant gaps; here we shall define δ_1 , \tilde{R} so as to avoid intersections of ν resonant gaps whose resonant vectors are linearly independent. We set

$$\tilde{R}(n) = \frac{1}{4} \left(\frac{2Cn}{\nu}\right)^{1/(1+\nu)}$$
(88)

$$\tilde{\delta}_1(n) = e_0 \tilde{R}(n) \tag{89}$$

where $C \ll 1$. Now the resonant gap G_m is included in the set

$$g_m = \{ n \in \Lambda : 4\tilde{R}(n) > m \text{ and } |\hat{m} \cdot n| < 2\tilde{R}(n) + 1 \}$$

$$\tag{90}$$

(where $\hat{m} = m/m$). To see this, suppose that $n \notin g_m$ and $4\tilde{R}(n) > m$; then $|E_{n\pm m} - E_n|/e_0 \ge |2|n \cdot m| - m^2| \ge 2\tilde{R}(n)$, so that $n \notin G_m$. We can therefore estimate the fraction x of the energy surface occupied by resonant gaps: each set g_m fills a volume $\sim \tilde{R}n^{\nu-2}$ on the energy surface, so that

$$x \leq \text{constant} \times \frac{\tilde{R}^{\nu} \tilde{R} n^{\nu-2}}{n^{\nu-1}} \sim C \ll 1$$
(91)

where the constant depends only on ν . Moreover, the intersection of ν gaps $g_{m_1}, \ldots, g_{m_\nu}$, whose resonant vectors are linearly independant is always empty. For if $n \in g_{m_1} \cap \cdots \cap g_{m_\nu}$, we can choose \hat{n} as an unit axis in the coordinate system and estimate the volume

$$|m_1 \times \dots \times m_{\nu}| \leq (m_1, \dots, m_{\nu}) \sum_{1 \leq j \leq \nu} \frac{|m_j \cdot \hat{n}|}{m_j}$$
$$\leq \nu (4\tilde{R})^{\nu} \frac{2\tilde{R} + 1}{n} \simeq C \ll 1.$$
(92)

This is impossible, since the volume of the unit cell is >1. This result has a simple corollary: if v = 2, it is possible to choose *C* so that any ball of centre *n* and radius $2\tilde{R}(n)$ intersects at most one resonant gap (cf condition 2 of theorem 6).

The function $\kappa_n(x)$ defined in 2.2 is readily estimated, seeing that $|n \cdot m| < m^2/2$ for any centre *n* of a chain with resonant vector *m* (because the set $\{u \in \mathbb{R}^{\nu} : |u \cdot m| < m^2/2\}$ is a strip of width *m*)

$$2mxe_0 \geqslant \kappa_n(x) \geqslant mxe_0. \tag{93}$$

Moreover, the curvature assumptions stated in 2.2 are verified. It is also easy to check that condition (57) of 3.4 is satisfied.

We have seen that most lattice points are robust. By theorem 1, a KAM quasi-mode can be constructed around any robust point of energy

$$E > \text{constant} \times e_0 \left(\frac{C_1 V_0}{e_0}\right)^{2(1+\nu)}.$$
(94)

Moreover, the ratio

$$\epsilon(V_0, \alpha, \hat{R}(n))$$
/average distance between levels (95)

decreases exponentially with some power of the energy; thus most KAM quasi-modes represent true eigenstates.

Quasi-modes can also be constructed in a single resonant gap \bar{G}_m if we define, for a given amplitude V_0

$$j_0 \ge 2 + \frac{21}{5} \frac{V_0}{e_0} \max(20C_1, 10C_3, 60C_2)$$
(96)

$$r = \frac{R^{2/\nu}}{3(1+10C_1V_0/e_0)^{2/\nu}}$$
(97)

and if m < r', where

$$r' = \frac{7}{2(2j_0 + 5)(2 + \alpha^{-1} + \alpha^{-2})}.$$
(98)

Localization conditions (34)–(36) are then satisfied; it remains to choose an energy sufficiently large so that r' > m.

In two dimensions, theorem 6 can be applied at all sufficiently large energies: we choose an interval e of width $|e_2 - e_1| = e_0 r/10$ and e_1 large enough so that $r > 80C_1V_0/e_0$ and $|w_1 + w_2| < (e_2 - e_1)/4$. Quasi-modes thus provide a complete picture of the perturbed spectrum beyond some energy threshold.

In higher dimensions it is impossible to approximate all eigenstates by quasi-modes, because intersections of several resonant gaps become unavoidable. If v = 3 however, it is possible to confine double resonant gaps to a small fraction of the energy spectrum; in the remaining parts of the spectrum theorem 6 can be applied. Let us explain this point in more detail. Define

$$g'_{m} = \{ n \in \Lambda : 4R'(n) > m \text{ and } |\hat{m} \cdot n| < 2R'_{1}(n) + 1 \}$$
(99)

where $R' \ll \tilde{R}^{1/8}$. As before, g'_m contains the gap G'_m defined by the function $\delta'_1 = e_0 R'$. If $s \in g'_{m_1} \cap g'_{m_2}$, then there is a decomposition (not necessarily unique)

$$s = n + z_1 m_1 + z_2 m_2 \quad (z_1, z_2 \in \mathbb{Z})$$
(100)

with $|n \cdot m_i| < m_i^2/2$, i = 1, 2. We call n a *double centre* and we select an unique double centre for each sublattice generated by m_1, m_2 . Moreover, if $s' \in g'_{m_1} \cap g'_{m_2}$ and s - s' is not a linear combination of m_1, m_2 , then

$$\left|s \cdot \frac{s-s'}{|s-s'|}\right| > 2\tilde{R}(s) + 1. \tag{101}$$

To prove this, consider the set

$$K = \{ u \in \mathbf{R}^3 : |u \cdot m_i| < m_i^2/2, i = 1, 2 \}.$$
(102)

When projected on the plane (m_1, m_2) , K is a parallepiped of area greater than m_1m_2 . Consequently, there always exists a pair of integers z_1, z_2 , such that $s - z_1m_1 - z_2m_2 = n \in K$. On the other hand, if $|s \cdot (s - s')|/|s - s'| < 2\tilde{R} + 1$, then $s \in g_{s-s'} \cap g'_{m_1} \cap g'_{m_2}$ so that s - s' must be a linear combination of m_1, m_2 .

Let $s = n + z_1 m_1 + z_2 m_2 \in g'_{m_1} \cap g'_{m_2}$ where *n* is a double centre; it is not difficult to see that $|s - n| \leq \text{constant} \times R'/\theta$, where θ is the angle between m_1 and m_2 . Now $\theta \geq 1/R'^2$ (consider the cell defined by the lattice vectors m_1, m_2 and v, where $|v| \sim 1$; the volume of this cell is smaller than $vm_1m_2\theta < R'^2\theta$ and is >1) so that

$$|s^{2} - n^{2}| = |(s - n)^{2} + 2(s - n)n| \leq \text{constant} \times \frac{R^{\prime 2}}{\theta^{2}} \leq \text{constant} \times R^{\prime 6}.$$
 (103)

We can now describe the contribution of a double resonant gap to the spectrum: to each double centre *n* is associated a two-dimensional lattice generated by m_1 , m_2 and included in $g'_{m_1} \cap g'_{m_2}$. The corresponding energy levels belong to an interval of width $\sim e_0 R'^6$ and there is a gap $2\tilde{\delta}_1$ between intervals corresponding to different double centres. Therefore, since there are $\sim R'^2$ double resonant gaps at a given energy, the fraction of the energy spectrum occupied by them can be estimated as

$$\frac{e_0 R'^8}{\tilde{\delta}_1} \ll 1. \tag{104}$$

By choosing an energy interval e included in the complementary part of the spectrum, we obtain a set $X = \{s : E_s \in e\}$ which is sufficiently separated from double resonant gaps. It becomes therefore possible to satisfy condition 2 of theorem 6.

4.2. A particle in a class of two-dimensional separable potentials

The discussion of the next example will be of a more qualitative nature. Consider the separable Hamiltonian (in appropriate units)

$$H = \sum_{i=1}^{\nu} H_i = \sum_{i=1}^{\nu} -\frac{\partial^2}{\partial x_i^2} + x_i^K$$
(105)

where *K* is a positive, even integer. If we number $n_i = 0, 1, 2, ...$ the energy levels E_{n_i} of H_i , then to each eigenstate of *H* corresponds a vector $n = (n_1, ..., n_v) \subset N^v = \Lambda$. In the limit of large energies, the eigenfunctions of H_i can be approximated by WKB wavefunctions

$$\Psi_n(x) \simeq \frac{C_n}{\sqrt{p(x)}} \sin\left(\int_x^{x_+} p \, \mathrm{d}x + \frac{\pi}{4}\right) \tag{106}$$

where $x_{\pm} = \pm E_n^{1/K}$ are the turning points and $p(x) = \sqrt{E_n - x^K}$. The semi-classical energy E_n is implicitely defined by the Bohr–Sommerfeld quantization rule

$$\int_{x_{-}}^{x_{+}} p \, \mathrm{d}x = \frac{\pi}{2} (2n+1). \tag{107}$$

The above expression of Ψ_n is only valid if p is real and $p^3 \gg Kx^{K-1}$; it can be replaced by an Airy function when x is close to one of the turning points (the domains of validity of these two approximations overlap at sufficiently large energies). Ψ_n decreases exponentially outside of the classically accessible region. The semi-classical energy E_n can be given a more explicit form

$$\int_{x_{-}}^{x_{+}} p \, \mathrm{d}x = 2 \int_{0}^{E_{n}^{1/K}} \sqrt{E_{n} - x^{K}} \, \mathrm{d}x$$
$$= \frac{2E_{n}^{1/2 + 1/K}}{K} \int_{0}^{1} t^{1/K - 1} \sqrt{1 - t} \, \mathrm{d}t$$
(108)

so that

$$E_n = A_K (2n+1)^{2X} (109)$$

where A_K depends only on K and X = K/(K+2). The normalization constant C_n can be estimated as follows: in the interval $|x| < 10^{-1/K}x_+$ we have $p/\sqrt{E_n} = 1 \pm 0.1$; in this interval the semi-classical approximation is of course valid, namely the wavelength p^{-1} is almost constant over distances equal to the wavelength itself, so that

$$1 = \int |\Psi_n|^2 \ge 10^{-1/K} x_+ \frac{C_n^2}{\sqrt{E_n}}.$$
(110)

Consider now a smooth perturbation

$$V(\boldsymbol{x}) = \int \mathrm{d}\boldsymbol{k} \, V_k \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}} \tag{111}$$

where $x = (x_1, \ldots, x_{\nu})$ and assume that $V_k \leq V_0 \exp(-\beta k^{1/X})$. This requirement is somewhat stronger than analycity; as we shall see however, it yields an exponential decrease of the matrix elements of V. For the sake of simplicity, we shall also assume that V(x) is exponentially localized in a finite region around the origin (for instance, $V = \exp(-x^2)$). The matrix elements of V are then readily estimated: if $n_i, m_i, i = 1, \ldots, \nu$ are large enough, then

$$\begin{split} |\langle \boldsymbol{n} | \boldsymbol{V} | \boldsymbol{m} \rangle| &= \left| \int \prod_{1 \leq i \leq \nu} \mathrm{d}x_{i} \, \Psi_{n_{i}}(x_{i}) \Psi_{m_{i}}^{\star}(x_{i}) \boldsymbol{V}(\boldsymbol{x}) \right| \\ &\simeq \left| \int \prod_{1 \leq i \leq \nu} \mathrm{d}x_{i} \, \mathrm{d}k_{i} \, \frac{C_{n_{i}} C_{m_{i}}^{\star}}{E_{n_{i}}^{1/4} E_{m_{i}}^{1/4}} \right. \\ &\qquad \times \sin(\sqrt{E_{n_{i}}} x_{i} + \phi_{n_{i}}) \sin(\sqrt{E_{m_{i}}} x_{i} + \phi_{m_{i}}) \boldsymbol{V}_{k} \mathrm{e}^{\mathrm{i}k_{i}x_{i}} \right| \\ &\leq \mathrm{constant} \times \left(\prod_{i} E_{n_{i}} E_{m_{i}} \right)^{-1/2K} \int \mathrm{d}\boldsymbol{k} | \boldsymbol{V}_{k} | \prod_{i} \sum_{\epsilon_{i}, \epsilon' = \pm 1} \\ &\qquad \times \delta(k_{i} + \epsilon \sqrt{E_{n_{i}}} + \epsilon' \sqrt{E_{m_{i}}}) \\ &\leqslant \mathrm{constant} \times \left(\prod_{i} E_{n_{i}} E_{m_{i}} \right)^{-1/2K} \boldsymbol{V}_{0} \exp\left(-\beta \left| \sum_{i} \left(\sqrt{E_{n_{i}}} - \sqrt{E_{m_{i}}} \right)^{2} \right|^{1/2X} \right). \end{split}$$

We would like to write

$$\beta \left| \sum_{i} \left(\sqrt{E_{n_i}} - \sqrt{E_{m_i}} \right)^2 \right|^{1/2X} \simeq \beta' \left| \sum_{i} (n_i^X - m_i^X)^2 \right|^{1/2X} \\ \geqslant \tilde{\alpha}(n) |n - m|.$$
(112)

Suppose that the index *i* is such that for $k = 1, ..., \nu$

$$|n_i^X - m_i^X| \ge |n_k^X - m_k^X| \tag{113}$$

and similarly, j is such that

$$|n_j - m_j| \ge |n_k - m_k|. \tag{114}$$

Clearly, it is enough to find a function $\tilde{\alpha}(n)$ satisfying

$$|n_i^X - m_i^X|^{1/X} \ge \tilde{\alpha}(n)|n_j - m_j|\sqrt{\nu}.$$
(115)

The following notation will be convenient: we write $f \sim g$ if f, g are two functions such that ag < f < bg, where a, b are two constants. Suppose now that 2n > m. In this case

$$|n^{X} - m^{X}| = n^{X-1} \left| \frac{1 - (m/n)^{X}}{1 - m/n} \right| |n - m| \sim n^{X-1} |n - m|.$$
(116)

On the other hand, if 2n < m

$$|n^{X} - m^{X}| = m^{X}|1 - (n/m)^{X}| \sim m^{X} \sim m^{X-1}|n - m|$$
(117)

and similarly

$$|n^{X} - m^{X}|^{1/X} \sim m \sim |n - m|.$$
(118)

Thus if i = j we have proved that

$$n_i^X - m_i^X|^{1/X} \ge \text{constant} \times n_j^{(X-1)/X}|n_j - m_j|.$$
(119)

Using similar arguments for $i \neq j$, we finally obtain

$$\tilde{\alpha}(n) = \text{constant} \times (\max_{1 \le k \le \nu} n_k)^{-2/K}.$$
(120)

We can also define

$$\tilde{V}_0(n) = \text{constant} \times V_0 \left(\prod_k n_k\right)^{-1/(2+K)}$$
(121)

so that

$$|\langle \boldsymbol{n}|\boldsymbol{V}|\boldsymbol{m}\rangle| \leqslant \tilde{V}_0(\boldsymbol{n}) \mathrm{e}^{-\tilde{\alpha}(\boldsymbol{n})|\boldsymbol{n}-\boldsymbol{m}|} \tag{122}$$

in accordance with our general definition of smooth perturbations.

It is obvious from these formulae that quasi-modes can easily be constructed when K is large, since in this limit the system is very close to the example discussed in the preceding section. We shall conclude our discussion by showing that KAM quasi-modes yield accurate approximations of the exact eigenstates if K > 12 (in the two-dimensional case).

We shall henceforth consider the region $n_1 < n_2$. KAM quasi-modes are good approximations only if

$$\tilde{\alpha}(n)\tilde{R}^{1/2}(n) \sim n_2^{-2/K}\tilde{R}^{1/2}$$
(123)

grows as some power of the energy. We choose therefore

$$\tilde{R}(n) \sim n_2^{\delta + 4/K} \tag{124}$$

where δ is some positive constant. On the other hand, the function $\tilde{\delta}_1$ must grow with the energy. This is possible only if, for any robust state and any $|m| < 4\tilde{R}$, the linear term $m \cdot \partial_n E$ is dominant in the expansion

$$E_{n+m} - E_n = m \cdot \partial_n E + \frac{1}{2}m^t \cdot \partial_n^2 E \cdot m + \cdots.$$
(125)

Otherwise, the curvature of the energy surface determines the distribution of levels, which can be very close to each other. Of course, $|\partial_n E|$ itself must grow, which implies K > 2. Using Taylor expansion (125) and restricting ourselves to the region $n_1 \ge 8\tilde{R}$, we obtain

$$E_{n+m} - E_n = m \cdot \partial_n E + O(m^2 n_1^{2X-2}).$$
(126)

Therefore we can choose a constant C and define

$$g_m = \{ n \in \Lambda : 4\tilde{R}(n) > m \text{ and } | m \cdot \partial_n E | \leq 2C n_1^{2X-2} \tilde{R}^2(n) \}$$
(127)

and

$$\tilde{\delta}_1(n) = \frac{C}{2} n_1^{2X-2} \tilde{R}^2(n)$$
(128)

so that the resonant gap G_m is included in g_m . Notice that δ_1 grows as some power of the energy, so that KAM quasi-modes can be constructed around robust states. It remains to prove that a large fraction of states in Λ are robust. The intersection of g_m with the energy surface is a curve whose length is approximately given by

$$\frac{2\rho}{m|\partial_n E|} 4\tilde{\delta}_1 \sim \frac{\tilde{R}^2}{m} \tag{129}$$

where ρ is the curvature of the energy surface. Consequently, the fraction of the energy surface intersected by resonant gaps is bounded from above by

$$\frac{1}{n_2} \int_0^R \frac{\tilde{R}^2}{m} m \, \mathrm{d}m \sim n_2^{12/K - 1 + 3\delta}.$$
(130)

This fraction is small if K > 12, and in this case most states are robust. The difficulties encountered for $K \leq 12$ show how the construction of quasi-modes may fail in certain situations.

5. Stochasticity in single resonant gaps

5.1. Weak stochasticity of the classical system

Quasi-modes in a single maximal gap \bar{G}_m are obtained by diagonalizing the restriction H_r of $H = H_0 + V$ to a ball B_r of centre n_0 , where n_0 is the centre of a resonant chain; as noted previously, the eigenstates of H_r cannot be obtained by treating V as a perturbation (unless the amplitude of V is smaller than the minimum distance between levels in the resonant chain). This difficulty is not necessarily related to the appearance of stochastic trajectories around classical resonant tori. If indeed chaotic zones fill only a very small fraction of the energy surface, then the quantum system will not be seriously affected by this fine structure of phase space; in this case the non-perturbative nature of quasi-modes can merely be related to the formation of 'islands' of regular motion around the resonances.

Let us examine this question more closely in the case of a free particle on a two-dimensional torus, submitted to a smooth perturbing potential V(x). We refer to the example discussed in 4.1 for subsequent notations in this section. We choose $L_1 = L_2 = L$ and we focus on a resonance $p_1 = 0$.

Consider a Poincaré surface of section

$$\Sigma = \{ (x, p) : x_2 = 0, H(x, p) = H_0 + V = E \}$$
(131)

 (x_1, p_1) are natural coordinates on Σ and the Hamiltonian flow defines an area-preserving map $T : \Sigma \to \Sigma$. The invariant curves of the unperturbed system are simply $p_1 = \text{constant}$. When $V \neq 0$, robust invariant curves are smoothly transformed into rotational KAM curves, while a finite set of elliptic and hyperbolic fixed points appear instead of the resonant curve $p_1 = 0$. Around each elliptic point new KAM curves form ('islands'); the region enclosed between these islands and the rotational KAM curves closest to the resonance is called the instability zone. This zone itself contains the stochastic layer, whose Lebesgue measure is yet unknown. The stochastic behaviour of the classical system will presumably reflect on quantum eigenstates if the volume Ω filled by the instability zones between p_2 and $p_2 + \delta p_2$ exceeds \hbar^2 ; here $\delta p_2 = 2\pi \hbar/L$ is the minimal uncertainty on p_2 corresponding to a resonant chain $C_{(0,n_2)}$ with resonant vector m = (1, 0).

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Lazutkin [10] has obtained an estimate of the width W_k of the instability zone for the standard map (around the main resonance)

$$W_k \sim \frac{1}{k} \exp(-\pi^2/\sqrt{k}). \tag{132}$$

The standard map is a one-parameter family of area-preserving maps $S_k : (\phi_0, I_0) \to (\phi, I)$ defined by

$$\phi = \phi_0 + I I = I_0 - \frac{k}{2\pi} \sin 2\pi \phi_0.$$
(133)

We can obtain a heuristic estimate of the volume Ω by bringing the Poincaré map T: $(x_1(0), p_1(0)) \rightarrow (x_1(\tau), p_1(\tau))$ into a form qualitatively similar to (133). The time τ is approximately given by $mL/p_2 \simeq L\sqrt{m/2E}$; if we introduce the coordinates

$$\phi = \frac{x_1}{L}$$

$$I = \frac{p_1 \tau}{mL}$$
(134)

then the map T becomes

$$\phi = \phi_0 + I_0 + \cdots$$

$$I = I_0 - \frac{V_0 \tau^2}{mL^2} f(\phi_0, I_0) + \cdots$$
(135)

Identifying $k = V_0 \tau^2 / mL^2 \simeq V_0 / 2E$ and returning to the variables (x, p), we obtain the tentative estimate

$$\Omega \sim W_k \times \frac{Lm}{\tau} \times \delta p_2 \times L^2 = W_k \hbar L \sqrt{mE}.$$
(136)

Introducing the quantum numbers n defined by (86), so that $E = e_0 n^2$, we can write the condition $\Omega > \hbar^2$ as

$$\frac{n^3 e_0}{V_0} \exp\left(-\pi^2 n \sqrt{\frac{e_0}{V_0}}\right) > 1.$$
(137)

The solutions n of this inequality lie approximately in an interval

$$C_1 \sqrt{\frac{V_0}{e_0}} \leqslant n \leqslant C_2 \sqrt{\frac{V_0}{e_0}} \log \sqrt{\frac{V_0}{e_0}}.$$
(138)

In such a region the construction of quasi-modes is clearly impossible, since $V_0 \sim e_0 n^2$ is much larger than the distance between levels in any ball in the lattice. These qualitative arguments suggest therefore that the lattice of quantum numbers is completely obliterated by instability zones filling a volume $\sim \hbar^{\nu}$ in phase space. The above estimate of the width of the instability zone is of course quite debatable; nevertheless, our conclusion is consistent with the fact that a new set of quantum numbers can be defined in single resonant gaps whenever quasi-modes can be constructed (we shall return to this point in the next section). In this sense, quasi-modes in single resonant gaps may be seen as resulting mainly from the quantization of islands of stability.

5.2. Irregularity of the quasi-modes

The considerations of the preceding section indicate that whenever quasi-modes can be constructed in a single resonant gap, the corresponding classical system is only weakly stochastic. It turns out indeed that quasi-modes can be computed perturbatively, starting from a suitably chosen integrable Hamiltonian. However, as we shall see below, this is possible only if the perturbation is not too strong; room is thus left for an interesting situation, in which quasi-modes and quasi-energies still can be constructed, but escape from perturbative methods and depend thereby in an intricate manner on the perturbing potential. This 'irregular' behaviour may be thought of as a precursory mark of chaos.

In order to illustrate these remarks, we adopt an alternate point of view on resonances. We decompose the perturbation V into a sum of two terms

$$V = V_{\rm tan} + V_{\rm res} \tag{139}$$

where V_{tan} has non-zero matrix elements only in the direction tangent to m:

$$\langle \boldsymbol{n}|V_{\text{tan}}|\boldsymbol{n}'\rangle = \begin{cases} \langle \boldsymbol{n}|V|\boldsymbol{n}'\rangle & \text{if } (\boldsymbol{n}-\boldsymbol{n}')//\boldsymbol{m}\\ 0 & \text{otherwise.} \end{cases}$$
(140)

The classical analogue of this decomposition is readily obtained if we interpret n as a vector of quantized actions and $\langle n|V|n' \rangle$ as the Fourier coefficient

$$V_{n'-n}^{\rm cl}(n) \tag{141}$$

in the series

$$V^{\rm cl}(\boldsymbol{I},\boldsymbol{\theta}) = \sum_{\boldsymbol{k}\in\boldsymbol{Z}^{\nu}} V_{\boldsymbol{k}}^{\rm cl}(\boldsymbol{I}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\theta}}.$$
(142)

Here (I, θ) are action-angle variables in the phase space of the classical Hamiltonian $H_0^{cl}(I)$. We see that V_{tan}^{cl} is a periodic function of $m \cdot \theta$. We can introduce new canonical coordinates J, ϕ

$$\boldsymbol{J}^{t} = \boldsymbol{I}^{t} \boldsymbol{M}^{-1} \qquad \boldsymbol{\phi} = \boldsymbol{M} \boldsymbol{\theta} \tag{143}$$

where *M* is a matrix of determinant 1 such that $M_{1i} = m_i$. In these coordinates it is obvious that the Hamiltonian $H_{\text{tan}}^{\text{cl}} = H_0^{\text{cl}} + V_{\text{tan}}^{\text{cl}}$ is integrable, since it does not depend on ϕ_2, \ldots, ϕ_ν . However, all invariant tori of $H_{\text{tan}}^{\text{cl}}$ are not obtainable by a smooth deformation of those of H_0^{cl} , since the implicit solution $J_1(\phi_1)$ of

$$H_{tan}^{cl}(\phi_1, J_1, J_2, \dots, J_{\nu}) = E$$
(144)

 (J_2, \ldots, J_ν) are constants of the motion) has singular points on the resonant torus $m \cdot \partial_I H_0^{cl} = 0$ (for V_{tan}^{cl} infinitesimal). The islands of regular motion are obtained by a smooth deformation of these newly created tori; the residual perturbation V_{res}^{cl} is responsible for the appearance of stochastic trajectories in the instability zones.

We can look for an equivalent picture in the quantum system. Instead of the observables A_2, \ldots, A_{ν} commuting with H_0 , we consider operators O_2, \ldots, O_{ν} corresponding to the classical actions I_2, \ldots, I_{ν}

$$O_i = n_i |\mathbf{n}\rangle \langle \mathbf{n}|. \tag{145}$$

Clearly $[O_i, O_j] = 0$, $[O_i, H_0] = 0$. It is then easy to construct operators P_2, \ldots, P_{ν} (corresponding to J_2, \ldots, J_{ν}) which commute with $H_{\text{tan}} = H_0 + V_{\text{tan}}$. We define

$$P_j = \sum_k M_{kj}^{-1} O_k \tag{146}$$

and it is straightforward to verify that

 $\langle r$

$$\boldsymbol{n}|[\boldsymbol{P}_{i}, \boldsymbol{V}_{\text{tan}}]|\boldsymbol{n}'\rangle = 0. \tag{147}$$

Thus H_{tan} is also integrable in the quantum mechanical sense. The corresponding space Λ_{tan} of quantum numbers can be constructed as follows: since V_{tan} can only mix states belonging to the same resonant chain, there are $\nu - 1$ quantum numbers (corresponding to the eigenvalues of P_2, \ldots, P_{ν}) determining the centre of each chain C_{n_0} and one quantum number labelling the energies in a chain. This number differs essentially from $(n - n_0) \cdot m$ (i.e. the coordinate along the chain in Λ) when the states $|n_0 + jm\rangle$, $j \in \mathbb{Z}$, are strongly mixed by V_{tan} ; this occurs only in a region surrounding the centre n_0 , whose width depends on the amplitude of V_{tan} . From an intuitive standpoint, this delocalization of eigenstates in the chain corresponds to the existence of 'bound states' localized in the new tori created by V_{tan} along a resonance; such 'bound states' can exist only if these islands are large enough.

If the amplitude of V_{tan} is large, then the matrix elements of V_{res} do not decrease exponentially in Λ_{tan} , but form instead an intricate function of the quantum numbers (for low-lying states in the chain). One can expect that this irregularity of V_{res} will lead to quasimodes irregularily distributed along each resonant chain; similarly, energy levels will depend on the perturbation in a complicated manner. However, this instability is greatly reduced by the large gaps δ_1 between resonant chains. It is therefore necessary to determine the amplitude \tilde{V}_0 of V for which V_{res} no longer can be treated as a perturbation.

As an example, we consider a particle on the Euclidean torus $0 \le x_i \le L$, i = 1, ..., v, submitted to a Gaussian potential well V(x) of width $\sim L/10$ and depth $\sim V_0$. We refer to section 4.1 for notations and definitions. We select the resonant vector m = (1, 0, ..., 0)and we restrict our attention, for the remainder of this section, to a ball B_r of centre n_0 in the single resonant gap \bar{G}_m , n_0 being the centre of a resonant chain. The potential $V_{tan}(x_1)$ is also a Gaussian well of width $\sim L/10$ and depth $\sim V_0$. To estimate the number N of 'bound states' localized in the x_1 -direction by the well V_{tan} , we use the semi-classical approximation

$$\hbar N \sim \int_{\text{class.traj.}} p_1 \, \mathrm{d}x_1 \sim L \sqrt{mV_0} \tag{148}$$

so that

$$N \sim \sqrt{\frac{V_0}{e_0}}.$$
(149)

We can give a qualitative picture of the eigenstates of H_{tan} . They are labelled by quantum numbers $|n, i\rangle$, where n is the centre of a resonant chain and i = 1, 2, ... numbers the levels in the chain; the first N levels correspond to states 'delocalized' in the unperturbed chain (i.e. $|n, i\rangle$ is a superposition of several states $|n + jm\rangle$, $j \in \mathbb{Z}$, when $i \leq N$). The state $|n, N\rangle$ is delocalized on ~ 10 sites in the lattice Λ , while $|n, 1\rangle$ is delocalized on $\sim Q$ sites, where Q can be estimated by developing $V_{tan}(x_1)$ around its minimum

$$V_{\text{tan}}(x_1) \sim V_0 \left(\frac{x_1}{L}\right)^2.$$
 (150)

The ground state of the corresponding harmonic oscillator has an uncertainty $\Delta p_1 \sim (\sqrt{mV_0}\hbar/L)^{1/2}$ on the momentum so that

$$Q \sim \frac{\Delta p_1}{\hbar L^{-1}} \sim \left(\frac{V_0}{e_0}\right)^{1/4}.$$
(151)

The spectrum of H_{tan} has the following structure (recall that we consider only the subspace spanned by the ball B_r): to each chain corresponds a cluster of levels, separated by a distance $\sim e_0$ from each other (for low-lying levels), and there are gaps $\sim \tilde{\delta}_1$ around each cluster.

The residual potential $V_{\rm res}$ cannot be treated perturbatively if the self-energy

$$S_{|n_0,i\rangle}(E) = \sum_{r,s,\dots} \langle n_0, i | V_{\text{res}} | r \rangle \frac{1}{E - E_r} \langle r | V_{\text{res}} | s \rangle \dots \langle t | V_{\text{res}} | n_0, i \rangle$$
(152)

is divergent. The above sum runs over eigenstates $r, s, \ldots \neq |n_0, i\rangle$ of H_{tan} and the energy E belongs to a contour surrounding the level $E_{|n_0,i\rangle}$. Observe that $\langle x|V_{res}|y\rangle \neq 0$ only if x, y belong to distinct chains.

We seek a situation in which quasi-modes can be constructed but escape from perturbative methods; we shall therefore keep only the most divergent contributions to the sum (152). They come from paths repeatedly visiting the chain C_{n_0} :

$$S_{|n_0,i\rangle} \sim V_0 I_1 + V_0 I_1 I_2 I_1 + \dots + V_0 I_1 (I_2 I_1)^n + \dots$$
(153)

where I_1 , I_2 are abbreviations for two different kinds of sums

$$I_1 = \sum_{n \neq n_0, j} \frac{\langle n_0, k | V_{\text{res}} | n, j \rangle}{E - E_{|n, j\rangle}}$$
(154)

$$I_2 = \sum_{k} \frac{\langle \boldsymbol{n}, j | V_{\text{res}} | \boldsymbol{n}_0, k \rangle}{E - E_{|\boldsymbol{n}_0, k\rangle}}.$$
(155)

Expanding $|n_0, k\rangle$ and $|n, j\rangle$ in the original lattice Λ , we obtain the estimates

$$I_1 \sim \frac{V_0}{\delta_1} \sqrt{NQ} \qquad I_2 \sim \frac{V_0}{e_0} \sqrt{NQ}$$
(156)

whence, using (149) and (151), the criterion for divergence

$$\frac{\delta_1}{V_0} < \left(\frac{V_0}{e_0}\right)^{1+3/4}.$$
(157)

Now the construction of quasi-modes is possible if

$$\frac{\delta_1}{V_0} > r^{\nu/2} \sim j_0^{\nu/2} \sim \left(\frac{\delta_2}{e_0}\right)^{\nu/2} \sim \left(\frac{V_0}{e_0}\right)^{\nu/2} \tag{158}$$

(see localization conditions (34)–(36)). Conditions (157) and (158) are clearly compatible in two and three dimensions, for large values of V_0/e_0 .

6. Conclusion

When a perturbation shifts the energy levels by an amount much larger than the average distance between levels, it is of course impossible to use perturbation theory in its usual form. However, it might happen that eigenstates keep their identity before and after the crossing of levels; in other words, these states are significantly coupled only when their energies are almost degenerate. In an integrable system submitted to a smooth perturbation, most eigenstates have this robustness property, which enables one to use perturbation theory well beyond its usual validity range.

Our main tool in this paper has been the construction of 'block Hamiltonians', restricted to some ball in the lattice of quantum numbers. The eigenstates of such operators, when exponentially localized in a small subset of the ball, are accurate approximations of the true eigenstates. In addition to KAM states, we have thus been able to find quasi-modes in single resonant gaps. In some cases (mainly in two-dimensional systems), it is therefore possible to obtain a precise picture of the perturbed system using quasi-modes only. The results presented here show that such a spectrum is roughly made of two parts, superimposed on each other.

One part is due to KAM quasi-modes and can be obtained by smoothly deforming the energy surface and leaving the lattice of quantum numbers unchanged. The other part is due to resonant quasi-modes and requires a separate study. Level repulsion should be manifest only for exponentially close levels.

It should be emphasized that the above picture most likely concerns this part of the spectrum which corresponds to weakly stochastic regions of phase space. The heuristic considerations of section 5.1 suggest indeed that the lattice of quantum numbers is destroyed by instability zones filling a volume in phase space larger than \hbar^{ν} . Stochasticity may nevertheless be announced by irregular quasi-modes in resonant gaps, as argued in section 5.2.

The possibility of constructing quasi-modes at the intersection of several resonant gaps is more difficult to establish; if one considers for instance resonant discs instead of resonant chains (double resonance), the coupling between resonant discs induces further resonances and the convergence of the perturbation series is hard to control. If such quasi-modes could nevertheless be constructed, they would describe truly chaotic regions of the classical phase space.

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Appendix. A localization lemma

Consider an integrable Hamiltonian H_0 and a smooth perturbation V. Let $A \subset B$ be two subsets of the lattice of quantum numbers Λ , and assume that for all $n \in B$, $n' \in \Lambda$

$$|\langle \boldsymbol{n}|\boldsymbol{V}|\boldsymbol{n}'\rangle| \leqslant V_0 \mathrm{e}^{-\alpha|\boldsymbol{n}-\boldsymbol{n}'|} \tag{159}$$

where $\exp(-\alpha) \ge \frac{1}{4}$. We write V_A the restriction of V to A and $H_1 = (H_0 + V_A)_B$, $H_2 = (H_0 + V)_B$, $W = (V - V_A)_B$ the restrictions of the corresponding operators to B. We shall consider H_1 as the unperturbed Hamiltonian and determine the eigenstates of $H_2 = H_1 + W$ by treating W as a perturbation. Let a_1, a_2, \ldots be the eigenstates of H_1 belonging to the subspace A. Notice that, for all $n \in B \setminus A$

$$|\langle a_i | W | \boldsymbol{n} \rangle| \leqslant C_4 V_0 \exp\left(-\frac{\alpha r_n}{2}\right) \tag{160}$$

where $r_n = \text{dist}(A, n)$ and $C_4 = C_4(\alpha)$ (we shall omit in the following the argument α of the functions C_1, \ldots, C_5).

Assume that the states a_1, \ldots, a_N belong to a given energy interval a of width w_1 , separated by gaps $2w_2$ from all other levels of H_1 . The following lemma shows that, under appropriate circumstances, the eigenstates of H_2 belonging to a are exponentially localized in A.

Lemma 7. Assume that

$$\sum_{y} \left| \frac{\langle x | W | y \rangle}{E - E_{y}} \right| < \frac{1}{2}$$
(161)

where x, y are eigenstates of H_1 . Here E belongs to a contour γ that surrounds the interval a so that $|E - E_y| \ge w_2$. Assume further that

$$\frac{V_0C_1}{w_2} \leqslant \frac{1}{4}.\tag{162}$$

Then if $t \in B \setminus A$

$$\frac{1}{2\pi i} \int_{\gamma} dE \langle t | (E - H_2)^{-1} | t \rangle \leqslant c \exp\left(-\alpha \sqrt{r_t}\right)$$
(163)

where

$$c = \left(\frac{w_1}{w_2} + 1\right) \left(\frac{4C_4 + 1}{C_1}\right)^2 \left(\frac{V_0 C_1}{w_2}\right)^2 4N \left(1 + 2V_0 C_1 \frac{N}{w_2}\right).$$
 (164)

Proof. For any given pair r, s of eigenstates of H_1 , we define

$$S_{rs}(E) = \langle r|W|s \rangle + \sum_{x,y,\dots,z \neq t} \frac{\langle r|W|x \rangle}{E - E_x} \frac{\langle x|W|y \rangle}{E - E_y} \cdots \langle z|W|s \rangle$$
(165)

where x, y, ..., z are eigenstates of H_1 and the sum runs over paths of all lengths in B. Let $\Gamma = \{a_1, ..., a_N\}$; we define $S_{rs}^{\Gamma}(E)$ with the additional restriction that no path visits Γ (except at terminal points). Our aim is to compute the self-energy $S_{tt}(E)$. We have

$$S_{tt} = S_{tt}^{\Gamma} + \sum_{1 \leqslant i \leqslant N} S_{ta_i}^{\Gamma} \frac{1}{E - E_{a_i}} S_{a_i t}^{\Gamma} + \sum_{1 \leqslant i, j \leqslant N} S_{ta_i}^{\Gamma} \frac{1}{E - E_{a_i}} S_{a_i a_j} \frac{1}{E - E_{a_j}} S_{a_j t}^{\Gamma}.$$
 (166)

Let us estimate each term in this sum. If $E \in \gamma$ it is straightforward, using (161), to obtain the upper bounds

$$|S_{rs}(E)| \leqslant 2V_0 C_1 \tag{167}$$

$$|S_{rs}^{\Gamma}(E)| \leqslant 2V_0 C_1. \tag{168}$$

This last inequality also holds when *E* lies *inside* of the contour γ , because paths in S_{rs}^{Γ} avoid all states whose energy lies within γ . The following inequality will also be useful:

$$\sum_{s} \left| \delta_{rs} + \frac{S_{rs}}{E - E_s} \right| \leqslant 2 \tag{169}$$

where δ_{rs} is the Kronecker symbol and $E \in \gamma$.

Consider now the decomposition

$$S_{a_it}^{\Gamma} = S_{a_it}^{\Gamma,m-} + S_{a_it}^{\Gamma,m+}$$
(170)

where $S_{a_it}^{\Gamma,m^-}$ contains only paths which terminate with less than (m + 1) consecutive steps in $B \setminus A$. Each path in $S_{a_it}^{\Gamma,m^+}$ terminates therefore with at least (m + 1) consecutive steps in $B \setminus A$. A step in $B \setminus A$ has a natural length, defined as follows: the length of a step $n \to n'$ is |n - n'|, while the length of a step $a_i \to n$ is r_n . Now any path in $S_{a_it}^{\Gamma,m^-}$ contains at least one step in $B \setminus A$ of length greater than r_t/m . In other words, each term of the sum contains a factor

$$|\langle x|W|s\rangle| \leqslant C_4 V_0 \exp\left(-\frac{\alpha r_t}{2m}\right) \tag{171}$$

where $s \in B \setminus A$. We can therefore write, using (169)

$$|S_{a_{i}t}^{\Gamma,m-}| \leq \sum_{x,s} \left| \delta_{a_{i}x} + \frac{S_{a_{i}x}}{E - E_{x}} \right| |\langle x|W|s \rangle| \left| \delta_{st} + \frac{S_{st}}{E - E_{s}} \right|$$

$$\leq 4C_{4}V_{0} \exp\left(-\frac{\alpha r_{t}}{2m}\right).$$
(172)

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Using (169) again, we also obtain

$$|S_{a_{i}t}^{\Gamma,m+}| \leq \sum_{n_{1}} \left| \frac{S_{a_{i}n_{1}}^{\Gamma}}{E - E_{n_{1}}} \right| \sum_{n_{2},...,n_{m}} \left| \frac{\langle n_{1}|W|n_{2} \rangle}{E - E_{n_{2}}} \right| \times \cdots \times \left| \frac{\langle n_{k-1}|W|n_{k} \rangle}{E - E_{n_{k}}} \langle n_{k}|W|t \rangle \right|$$

$$\leq V_{0} \left(\sum_{n}^{\prime} \left| \frac{\langle n|W|n^{\prime} \rangle}{E - E_{n}^{\prime}} \right| \right)^{m-1}$$

$$\leq V_{0} \left(\frac{V_{0}C_{1}}{w_{2}} \right)^{m-1}.$$
(173)

Thus if we choose

$$\sqrt{r_t} \ge m \ge \frac{\sqrt{r_t}}{2} + 1 \tag{174}$$

(assuming $r_t \ge 2$) we finally have

$$|S_{a_{i}t}^{\Gamma}(E)| \leq |S_{a_{i}t}^{\Gamma,m^{-}}(E)| + |S_{a_{i}t}^{\Gamma,m^{+}}(E)| \leq V_{0}(4C_{4}+1)\exp\left(-\frac{\alpha\sqrt{r_{t}}}{2}\right).$$
(175)

The same bound is of course valid for $|S_{ta_i}^{\Gamma}(E)|$.

We can now estimate the projection of $|t\rangle$ on the eigenstates of H_2 surrounded by γ :

$$\int_{\gamma} dE \langle t | (E - H_2)^{-1} | t \rangle = \int_{\gamma} \frac{dE}{E - E_t - S_{tt}(E)}$$
$$= \int_{\gamma} \frac{dE}{E - E_t - S_{tt}^{\Gamma}} + \int_{\gamma} \frac{(S_{tt} - S_{tt}^{\Gamma}) dE}{(E - E_t - S_{tt}^{\Gamma})(E - E_t - S_{tt})}.$$
(176)

Consider the first integral of the sum. Inside the contour $|E - E_t| > w_2$, $|S_{tt}^{\Gamma}| \le 2V_0C_1 < w_2/2$ and S_{tt}^{Γ} is analytic. The integrand is therefore analytic and the integral vanishes. In the second integral we have, according to (166)–(168)

$$|S_{tt} - S_{tt}^{\Gamma}| \leq \frac{N}{w_2} |S_{a_i t}^{\Gamma}|^2 + 2V_0 C_1 \frac{N^2}{w_2^2} |S_{a_i t}^{\Gamma}|^2$$
(177)

$$|(E - E_t - S_{tt}^{\Gamma})(E - E_t - S_{tt})| \ge \frac{w_2^{-2}}{4}$$
(178)

so that finally

$$\frac{1}{2\pi i} \int_{\gamma} dE \langle t | (E - H_2)^{-1} | t \rangle \leqslant c \exp\left(-\alpha \sqrt{r_t}\right)$$
(179)

where

$$c = \frac{w_1 + w_2}{w_2^3} 4N \left(1 + 2V_0 C_1 \frac{N}{w_2} \right) V_0^2 (4C_4 + 1)^2.$$
(180)
proved.

The lemma is proved.

If $A \subset B_{r/2} \subset B_r = B$, where $B_{r/2}$ and B_r are two concentric balls of radii r/2 and r respectively, then the above lemma implies that the eigenstates of H_2 belonging to the interval a are quasi-modes. More generally, we have the following result.

Lemma 8. Consider two concentric balls $B_{r/2} \subset B_r \subset B$, of radii r/2 and r respectively. Let H_r be the restriction of $H = H_0 + V$ to B_r and assume that $|q\rangle$ is an eigenstate of H_r exponentially localized in $B_{r/2}$; in other words, there exists a constant C_0 such that for any $t \in B_r \setminus B_{r/2}$

$$|\langle q|t\rangle|^2 \leqslant C_0 r^4 \exp\left(-\alpha \sqrt{r_t}\right) \tag{181}$$

where $r_t = \text{dist}(t, B_{r/2})$. Then $|q\rangle$ is a quasi-mode: for all $n \notin B_r$

$$\langle q|V|n\rangle| \leq V_0 \left(1 + \sqrt{C_0}\right) C_5 \exp\left(-\alpha \left(d_n + \frac{\sqrt{r}}{8}\right)\right)$$

(182)

where $d_n = \operatorname{dist}(n, B_r)$.

Proof. Let $B_{3r/4}$ be a ball of radius 3r/4 concentric with B_r . We can write

$$\begin{aligned} |\langle q|V|n\rangle| &\leq \sum_{t \in B_{3r/4}} + \sum_{t \in B_r \setminus B_{3r/4}} V_0 |\langle q|t\rangle |e^{-\alpha|t-n|} \\ &\leq V_0 (2r)^{\nu} e^{-\alpha(d_n+r/4)} + V_0 (2r)^{\nu+2} \sqrt{C_0} e^{-\alpha(d_n+1/2\sqrt{r/4})}. \end{aligned}$$
(183)

Using the inequality

$$x^{p} e^{-x} \leqslant \left(\frac{p}{e}\right)^{p} \qquad (x \ge 0)$$
 (184)

we obtain the result.

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