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A quantum particle in a quadrupole radio-frequency trap

by

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ABSTRACT. — The quantum motion of a charged particle in a quadrupole radio-frequency trap is solved exactly in terms of the classical trajectories. Thus the quantum stability regions are exactly given in terms of the stability regions for the associated Mathieu equations, and quantum trapping is demonstrated inside these stability area. These exact results enable us to test a commonly believed « static effective potential approximation » for a particle in a rapidly oscillating time-periodic potential: our results exhibit serious limitations to this approximation. As a subproduct of our approach, we solve the eigenvalue problem for the Floquet operator of our system. This exactly solvable system should be a good starting point for the study of quantum instabilities under small perturbations.

RÉSUMÉ. — Le mouvement quantique d'une particule chargée dans un piège quadrupolaire de radio-fréquence est soluble exactement en termes des solutions du mouvement classique. Il en résulte que les régions de stabilité quantique sont exactement les régions de stabilité pour les équations de Mathieu correspondantes, et on démontre le piégeage quantique à l'intérieur de ces régions. Ces résultats exacts permettent de tester « l'approximation de potentiel effectif statique » communément admise pour une particule dans un potentiel périodique dans le temps rapidement oscillant, et mettent en évidence de sérieuses limitations à cette approximation. Comme sous-produit de cette approche, on résoud l'équation aux

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valeurs propres pour l'opérateur de Floquet de ce système. Ce problème exactement soluble devrait être un bon point de départ pour l'étude de la stabilité quantique sous de petites perturbations.

1. INTRODUCTION

The possibility of confining charged particles by means of alternating and static electric fields has been discovered thirty years ago [13] [15]. It is still intensively used in conjonction with laser cooling techniques, for the purpose of confining a few or even single ions at rest: thus Doppler shifts vanish, which is a powerful advantage for the measurement of time [12]. A striking feature, in these experiments, is that classical mechanics predicts the stability regions with a very good accuracy so that one can forget that these particles are actually quantum mechanical! By « stability regions » is meant the values of the parameters, namely strength and frequency of the field, size of the trap and mass of the particle, such that the classical motion will be stably bound. In fact it is known for the quadrupole trap, for which the potential is quadratic in each space coordinate, that the quantum problem is exactly solvable in terms of the classical motion [5] [1]. However the actual traps used in experiments are never exact realizations of this ideal quadrupole trap, but rather perturbed versions of them, due for example, to finite size effects, presence of holes, etc. [4]. It is our purpose in this paper to derive in a rigorous manner several aspects of the exact resolution of the quantum problem in terms of the classical motion for the quadrupole trap. Namely it is desirable to investigate on the qualitative, but also on the quantitative level, how a certain set of perturbations can produce quantum instabilities [2] [3]. This will be done elsewhere, using the exact results provided in this work. As a subproduct of our exact analysis, we give some estimates at large radio-frequencies that invalidate, or at least provide serious limitations to a commonly believed approximation: the so-called « effective potential approximation » [5]. In this approximation, one usually exhibits a *static* confining potential such that the evolution associated with it simulates in an appropriate way the true evolution associated with the time-periodic potential. This approximation is believed to become more and more accurate when the radio-frequency increases. We prove that, if we consider the system at a sequence of times that are very close to each other, namely $\frac{2k\pi}{\Omega}$ where k is integer and Ω the frequency of the field, then the exact quantum states are given, with a good agreement, by the evolution associated to the effective potential: in particular, starting from an eigenstate of the effective hamiltonian, the state at time $\frac{2k\pi}{\Omega}$ looks like a « stationary states ». But inbetween these instants $2k\pi/\Omega$, the particle visits other eigenstates of the effective hamiltonian, so that the average excitation probability during a period is not very small when Ω becomes large, contrarily to what was expected in ref. [5] on the basis of a perturbation argument. We note that this system is not expected to have a naive quantum perturbation theory around this « effective potential approximation » because, as we shall see, it exhibits small divisors problems. We believe that such a solvable quantum trapping problem gives an indication of what can be expected in more general cases where the true evolution is not known exactly.

A charged particle in a three dimensional quadrupole trap is subject to a time-dependent potential of the form

$$V_t = \frac{e}{r_0^2}\left(z^2 - \frac{x^2+y^2}{2}\right)(V_{dc} - V_{ac}\cos\Omega t) \tag{1.1}$$

where e is the charge of the particle, r_0 the size of the trap, (x, y, z) the 3-dimensional coordinates, and V_{dc}(resp. $-V_{ac}$) the constant (resp. alternating) voltages. Thus if m is the mass of the particle, the quantum-mechanical time-dependent hamiltonian is

$$H_t = \frac{-\hbar^2}{2m}\Delta + V_t \tag{1.2}$$

Δ being the 3-dimensional Laplacian. We shall prove that to H_t can be associated a unitary evolution group $U(t, s)$ such that $i\hbar\frac{d}{dt}U(t, s) = H_t U(t, s)$. If the quantum state ψ of the particle is a square integrable function of $(x, y, z) \in \mathbb{R}^3$ at time 0, its state at time t is $U(t, 0)\psi = \psi_t$. Quantum trapping will be expressed by the fact that, for any initial state ψ

$$\operatorname*{Sup}_t \int_{x^2+y^2+z^2>R^2} dxdydz\,|\psi_t(x, y, z)|^2 \to 0 \quad \text{as} \quad R \to \infty \tag{1.3}$$

It is known that a convenient relationship between the quantum evolution and the classical motion can be established, in the limit $\hbar \to 0$ through the coherent states [8]. Furthermore this relationship appears to be exact, for all $\hbar$, when the potential is quadratic in the space coordinates [7] which is the case for the potential V_t given by (1.1). This will allow us to derive the quantum stability region for the quadrupole trap, i. e. the set of values of Ω for which (1.3) holds, given e, r_0, m, V_{dc} and V_{ac} as the parameters: it is given exactly by the classical stability region, i. e. by the stability region for some Mathieu equations. We shall give these results in section 2.

Furthermore a convenient way of studying time-periodic problem is to consider the operator of « quasi-energy »:

$$K = -i\hbar\frac{\partial}{\partial t} + H_t \tag{1.4}$$

as an operator on the space of functions of (t, x, y, z) that are $\frac{2\pi}{\Omega}$ periodic in t, and square integrable in $\mathbb{T}_\Omega \times \mathbb{R}^3$, $\mathbb{T}_\Omega$ being the torus $\mathbb{R}/\frac{2\pi}{\Omega}\mathbb{Z}$. We then use a beautiful property of the group $U(t, s)$ when applied to suitable Hermite functions, inspired by a work by Hagedorn [*6*] [*7*] in the time independent case. This allows us to solve the eigenvalue problem for the operator K, and thus for the Floquet operator $U(2\pi/\Omega, 0)$. It will be given in section 3 of this paper.

The « effective potential approximation » claims that at sufficiently large frequencies Ω, a particle in a time-periodic potential $V(r)\cos\Omega t$ behaves as if it was subject to the static potential $|\nabla V|^2/2m\Omega^2$. If this were exact, any eigenstate of the effective hamiltonian should be stationary with respect to the true evolution. As the true evolution is known exactly, we calculate the probability of such a state to be stationary, or to get excited, at any time t, when Ω becomes large. Of course we do these calculations only in the case $V_{dc} = 0$, because only in this case the stability region contains every sufficiently large frequency. We discuss these estimates as a test of the « effective potential approximation » in the last section of this paper.

2. CLASSICAL AND QUANTUM TRAPPING IN A RADIO-FREQUENCY FIELD

In $\mathbb{R}^3$ with $x = (x_1, x_2, x_3)$, the time-dependent potential of a particle of charge e in a quadrupole trap with a A.C plus D.C electric field can be taken as:

$$V(t, x) = \frac{e}{r_0^2}\left(x_1^2 - \frac{x_2^2 + x_3^2}{2}\right)(V_{dc} - V_{ac}\cos\Omega t) \tag{2.1}$$

r_0 being a characteristic size of the trap, and V_{dc}, (resp. V_{ac}) the constant (resp. alternating) voltages. Therefore the time-dependent quantum hamiltonian

$$H_t = -\frac{\hbar^2}{2m}\Delta + V(t, x) \tag{2.2}$$

of the particle decouples along the three directions of x_1, x_2, x_3 as

$$h_1(t) \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes h_2(t) \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes h_3(t)$$

where

$$h_1(t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} + \frac{e}{r_0^2}x_1^2(\mathrm{V}_{dc} - \mathrm{V}_{ac}\cos\Omega t) \tag{2.3}$$

and similarly for $h_2(t)$ and $h_3(t)$. Therefore it is enough to study the one dimensional Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{x^2}{2}(\alpha - \beta\cos\Omega t)\right]\psi \equiv h_t\psi \tag{2.4}$$

where $\psi \in \mathrm{L}^2(\mathbb{R}) \otimes \mathrm{L}^2(\mathbb{T}_C)$

$$\mathbb{T}_\Omega = \mathbb{R}\Big/\frac{2\pi}{\Omega}\mathbb{Z} \tag{2.5}$$

so that the derivatives in (2.5) are taken in the distributional sense. The aim of this section is to show that the quantum particle whose wave function at time t is $\psi(t, x)$ solution of (2.5) remains « trapped » for all time t provided the frequency Ω lies in a suitable stability interval. We follow an idea of [5] where the quantum probability density $|\psi(t, x)|^2$ is related to the classical trajectories for the hamiltonian h_t. Before we give the precise « quantum trapping » result, we want to draw the reader's attention to the *linear* character of the classical equation of motion associated to h_t. It implies that the classical position and velocity are linear combinations of the initial data which is an essential tool in the determination of the « classically allowed regions » in phase space in the stability regime.

THEOREM 2.1. — Let $u(t, s)$ be the unitary evolution group associated to the time-dependent hamiltonian h_t. Then there exist Ω_0 and $\Omega_1 > 0$ depending on α and β such that for any $\Omega \in (\Omega_0, \Omega_1)$ we have:

$$\forall\psi \in \mathrm{L}^2(\mathbb{R}) \quad \text{and} \quad \forall\varepsilon, \quad \exists\mathrm{R} \text{ such that} \quad \sup_t \| \mathrm{F}(|x| > \mathrm{R})u(t, 0)\psi \| < \varepsilon \tag{2.6}$$

$\mathrm{F}(|x| > \mathrm{R})$ being the operator in $\mathrm{L}^2(\mathbb{R})$ that corresponds to the multiplication by the characteristic function of the exterior of the interval $|x| \leq \mathrm{R}$, and $\|\,.\,\|$ the usual L^2-norm. Moreover Ω_1 is infinite when $\alpha = 0$.

Proof. — The first step of the proof, namely the existence and differentiability of $u(t, s)\psi$ for suitable ψ's is a known fact, that we recall in the following lemma:

LEMMA 2.2. — Let $\mathscr{D} = \mathscr{D}\left(\frac{-d^2}{dx^2} + x^2\right)$. Then the time-dependent hamiltonian h_t defined by (2.5) is essentially self-adjoint on $\mathscr{D}$ for any t, and admits a unitary evolution group $u(t, s)$ satisfying

i) $u(t, s)\mathscr{D} \subset \mathscr{D}$ (any t and s)

ii) $\forall\psi \in \mathscr{D}$, the derivative $\frac{d}{dt}u(t, 0)\psi$ exists for every t and satisfies:

$$i\hbar\frac{d}{dt}u(t, 0)\psi = h_t u(t, 0)\psi$$

Proof. — We apply a general result of Kato [*10*] which is related to the essential self-adjointness of $\frac{-d^2}{dx^2} + x^2$ on $\mathscr{D}$. We can take

$$\mathrm{S} = 1 - \frac{d^2}{dx^2} + x^2$$

as an isomorphism of $\mathscr{D}$ onto $\mathrm{L}^2(\mathbb{R})$. Then

$$\mathrm{S}h_t\mathrm{S}^{-1} - h_t = [\mathrm{S}, h_t]\mathrm{S}^{-1} = 2i\left(x\frac{d}{dx} + \frac{d}{dx}x\right)\left(\alpha\cos\Omega t + \beta - \frac{\hbar^2}{m}\right)\mathrm{S}^{-1}$$

is strongly continuous in t and uniformly bounded in $\mathrm{L}^2(\mathbb{R})$ because

$$\| x^2\varphi \|^2 \leqslant \left\| \left(- \frac{d^2}{dx^2} + x^2 \right)\varphi \right\|^2 + 2 \| \varphi \|^2 \qquad \forall\varphi \in \mathscr{D}$$

and similarly for $\frac{d^2}{dx^2}$ instead of x^2. This completes the proof of lemma 2.2.

An immediate connection between the classical and quantum dynamics is that the time-dependent position and momentum quantum observables obey the classical equation of motion, due to the quadratic character of the interaction:

LEMMA 2.3. — Let x denote the operator of multiplication by x and p denote the operator $-i\hbar\frac{d}{dx}$. Let $x(t) = u(t, 0)^* x u(t, 0)$ and $p(t) = u(t, 0)^* p u(t, 0)$. Then we have as operators on $\mathscr{D}$:

$$\frac{d}{dt}x(t) = p(t)/m$$

$$\frac{d}{dt}p(t) = - x(t)(\alpha - \beta\cos\Omega t)$$

which are the Hamilton equations associated to the hamiltonian h_t.

The proof is immediate and is left to the reader. This implies that the Heisenberg observable $x(t)$ obeys the Mathieu equation:

$$\ddot{x}(t) + x(t)(\alpha/m - \beta\cos\Omega t/m) = 0 \tag{2.7}$$

whose stability regions are well known (see fig. 1 below).

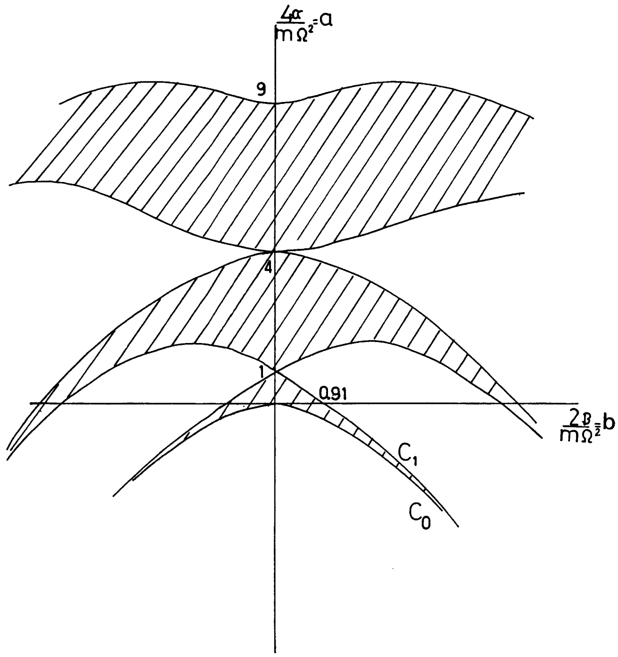

FIG. 1. — Shaded area = stability regions for Mathieu equation (2.7).

Since we are mainly interested in the « high frequency regime », we concentrate our attention to the stability area which is closest to the origin, namely that is contained between the curves (C_0) and (C_1). Of course the other stability areas have their interest, but they do not seem to have been so much exploited in experiments [*15*]. The diagram above exhibits the main characteristic features of the classical motion:

1) For fixed α and β (D.C and A.C voltages respectively), the values of a and b where Ω varies belong to a half line going through the origine with slope $\frac{2\alpha}{\beta}$ therefore the high frequencies Ω that give rise to a « stable » classical motion correspond to the portion of the above half line which is contained between curves C_0 and C_1.

2) The sign of α, namely of the D.C voltage is important: since it is known [*11*] that C_0 is tangent to the axis $a = 0$ at the origin, the radio-frequencies Ω leading to a stable classical motion are

$$\Omega \geq \Omega_1 \quad \text{if} \quad \alpha \geq 0$$
$$\Omega_1 \leq \Omega \leq \Omega_2 < \infty \quad \text{if} \quad \alpha < 0$$

where Ω_1 and Ω_2 can be determined numerically [11]. For example, when $\alpha = 0$, we get

$$\Omega \gtrsim \left(\frac{2eV_{ac}}{0.91\, mr_0^2}\right)^{1/2}$$

Therefore the values of Ω for which the quantum particle remains trapped is exactly given by the classical « stability regions ». A proof of theorem 2.1 is easily obtained by considering coherent states along the classical trajectories, as was done by Hepp [8] for more general purposes: they allow to « linearize » the quantum motion around the classical trajectories, the quantum fluctuation being given by the second order terms.

Here, due to the quadratic character of the interaction, the hamiltonian for the quantum fluctuations is exactly the original hamiltonian h_t!

Given any complex number α, we define

$$C(\alpha) = \exp(\alpha a^+ - \bar{\alpha} a) \tag{2.8}$$

where a is the operator in $L^2(\mathbb{R})$ given by

$$a = \frac{1}{\sqrt{2}}(x - ip/\hbar) \tag{2.9}$$

and a^+ is the adjoint of a. Thus if

$$\alpha = \frac{1}{\sqrt{2}}(-u + iv/\hbar) \qquad u, v \in \mathbb{R} \tag{2.10}$$

we get

$$C(\alpha) = e^{(ixv - ipu)/\hbar} = e^{-iuv/2\hbar} e^{ixv/\hbar} e^{-ipu/\hbar} \tag{2.11}$$

Thus if $u(t)$ is a solution of equation (2.7), and if

$$\alpha_t = \frac{1}{\sqrt{2}}(-u(t) + im\dot{u}(t)/\hbar) \tag{2.12}$$

we say that $C(\alpha_t)$ is the « coherent state along a classical trajectory ». Let $S(t, s)$ be classical action along the trajectory $u(t)$ between time s and time t:

$$S(t, s) = \int_s^t d\tau \left\{ \frac{m}{2}\dot{u}(\tau)^2 - \frac{1}{2}u(\tau)^2(\alpha - \beta \cos \Omega\tau) \right\} \tag{2.13}$$

We shall prove:

LEMMA 2.4. — For any s and t, we have

$$S(t, s) = \frac{m}{2} u(\tau)\dot{u}(\tau) \Big|_s^t$$

$$u(t, s)^* C(\alpha_t) u(t, s) = C(\alpha_s)$$

Proof. — It is enough to check that the operator

$$T(t) \equiv u(t, s)^* C(\alpha_t) u(t, s) \tag{2.14}$$

is independent of t. But, when applied to any vector in $\mathscr{D}$, we have, using (2.7) and (2.13):

$$\frac{d}{dt} T(t) = u(t, s)^* \left\{ \frac{i}{\hbar} [h_t, C(\alpha_t)] + \frac{d}{dt} C(\alpha_t) \right\} u(t, s) \tag{2.15}$$

But

$$[h_t, C(\alpha_t)] = \frac{\dot{u}}{2}(pC(\alpha_t) + C(\alpha_t)p) - \frac{m\ddot{u}}{2}(xC(\alpha_t) + C(\alpha_t)x)$$

and

$$\frac{d}{dt} C(\alpha_t) = -\frac{im}{2\hbar}(\dot{u}^2 + u\ddot{u})C(\alpha_t) + \frac{im\ddot{u}}{\hbar} xC(\alpha_t) - \frac{i\dot{u}}{\hbar} C(\alpha_t)p$$

so that

$$\frac{i}{\hbar}[h_t, C(\alpha_t)] + \frac{d}{dt} C(\alpha_t) = \frac{i\dot{u}}{2\hbar}[p, C(\alpha_t)] + \frac{im\ddot{u}}{2\hbar}[x, C(\alpha_t)] - \frac{im}{2\hbar}(\dot{u}^2 + u\ddot{u})C(\alpha_t) \tag{2.16}$$

Now

$$[p, C(\alpha_t)] = m\dot{u}(t)C(\alpha_t)$$
$$[x, C(\alpha_t)] = u(t)C(\alpha_t)$$

Therefore (2.15) is zero, which yields the result.

Let now Π be the operator of space symmetry, i. e.:

$$(\Pi\psi)(x) = \psi(-x) \tag{2.17}$$

We define, for any $\psi \in L^2(\mathbb{R})$:

$$F(u, v, t) = \langle \psi, \Pi u(t, 0)^* e^{ivx - iup} u(t, 0)\psi \rangle \tag{2.18}$$

Assume u and v are the initial position and momenta at time 0 for the classical motion governed by equation (2.7) and let $x(t, u, v)$ be the corresponding solution at time t. Then as an immediate consequence of lemma 2.4 and of the invariance of (2.7) under time reversal, we get

COROLLARY 2.5. — Let F be defined by (2.18). Then for any t, we have:

$$F(u, v, t) = F(x(t, u, v), \dot{x}(t, u, v), 0)$$

REMARK 2.1. — $F(u, v, t)$ is up to a phase factor very similar to the Wigner function for the state $\psi_t = u(t, 0)\psi$. Therefore the idea developped here is very similar to that of ref. [*5*], where it is argued that the Wigner function associated to suitable states ψ satisfies the classical Liouville equation for an ensemble of points in phase space that move in accordance with Hamilton's equations for hamiltonian h_t, which implies a result similar to Corollary 2.5.

We now assume that we are in a « stability region » for the Mathieu equation (2.7), namely that the classical trajectories stay bounded. Then it is known [*11*] that there exists ρ *real* $\left(\text{depending on } a = \frac{4\alpha}{m\Omega^2} \text{ and } b = \frac{2\beta}{m\Omega^2}\right)$ such that the solution of (2.7) with initial data $x(0)=u$, $\dot{x}(0)=v/m$ is of the form

$$x(t, u, v) = \frac{u}{C}\sum_{-\infty}^{+\infty} c_n \cos(2n+\rho)\frac{\Omega t}{2} + \frac{2v}{m\Omega D}\sum_{-\infty}^{+\infty} c_n \sin(2n+\rho)\frac{\Omega t}{2} \tag{2.19}$$

where c_n is a real sequence, and

$$C \equiv \sum_{-\infty}^{+\infty} c_n \tag{2.20}$$

$$D \equiv \sum_{-\infty}^{+\infty} (2n+\rho)c_n \tag{2.21}$$

We recall that the « stability regions » are delimited by curves (C_j) for which (2.7) has periodic solutions, i. e. for which $\rho = j \in \mathbb{N}$. We immediatly deduce from (2.19) that, uniformly in t:

$$|x(t)| \leqslant C'\left(\frac{|u|}{|C|} + \frac{2|v|}{m\Omega|D|}\right), \qquad \left(C' = \sum_{-\infty}^{+\infty} |c_n|\right) \tag{2.22}$$

so that if our initial data satisfy for some $R > 0$

$$\left\{\begin{array}{l} |u| < R|C|/C' \\ |v| < \dfrac{m\Omega R|D|}{2C'} \end{array}\right. \quad \textit{then} \quad |x(t)| < 2R \,(\text{any } t) \tag{2.23}$$

This property, which relies heavily on the *linearity* of Mathieu equation will be used below.

In this third and last step of the proof of theorem 2.1, we shall establish that for a dense set of states, namely $\mathscr{C}_0^\infty(\mathbb{R})$, $F(.,.,0) \in L^1(\mathbb{R}^2)$, and we shall deduce (2.6) from property (2.23) and Corollary 2.5. From now on in this section, the presence of $\hbar$ is irrelevant, so that we can assume $\hbar = 1$. It is easy to see that $F(u, v, 0)$, as given by (2.18), can be written as the absolutely convergent integral

$$F(u, v, 0) = (2\pi)^{-1}\int dy e^{iyv}\overline{\psi}\left(-y-\frac{u}{2}\right)\psi\left(y-\frac{u}{2}\right)$$

As $\psi \in \mathscr{C}_0^\infty(\mathbb{R})$, there exists some $r > 0$ such that supp ψ is contained in $[-r, +r]$; therefore supp F is contained in $\{u : |u| \leq 2r\}$, and

$$F(u, v, 0) = (2\pi)^{-1} \int_{-2r}^{2r} dy e^{iyv} \overline{\psi}\left(-y - \frac{u}{2}\right) \psi\left(y - \frac{u}{2}\right)$$

which implies, by integration by parts:

$$|F(u, v, 0)| \leqslant (2\pi)^{-1} \operatorname{Min}(1, v^{-2}) \|\psi\|^2_{\mathscr{H}_0^2}$$

($\mathscr{H}_0^2$: Sobolev space), so that $F(.,.,0) \in L^1(\mathbb{R}^2)$ with

$$\|F(.,.,0)\|_{L^1} \leqslant Cr \|\psi\|^2_{\mathscr{H}_0^2}$$

Furthermore it follows from lemma 2.2 that $\psi(t, .) \equiv u(t, 0)\psi \in \mathscr{D}$, so that

$$F(u, v, t) = -(2\pi v^2)^{-1} \int_{-\infty}^{+\infty} dx e^{ixv} \frac{d^2}{dx^2}\left(\overline{\psi}\left(t, -x - \frac{u}{2}\right) \psi\left(t, x - \frac{u}{2}\right)\right)$$

where, again, the integral is absolutely convergent. This implies that $F(u, ., t) \in L^1(\mathbb{R})$ for any u, t, and that

$$\overline{\psi}\left(t, -x - \frac{u}{2}\right) \psi\left(t, x - \frac{u}{2}\right) = \int_{-\infty}^{+\infty} dv e^{-ixv} F(u, v, t)$$

where both sides are continuous functions of x. Therefore

$$\left|\psi\left(t, -\frac{u}{2}\right)\right|^2 = \int dv F(u, v, t)$$

so that

$$\|F(|x| > R) u(t, 0)\psi\|^2 = \int_{|u| > 2R} du dv F(u, v, t)$$

$$= \int_{|u| > 2R} du dv F(x(t, u, v), \dot{x}(t, u, v) 0)$$

(using Corollary 2.5),

$$= \int_{\substack{|u| > 2R \\ |\dot{x}(t,u,v)| \leqslant \lambda(\Omega) R}} F(x(t, u, v), \dot{x}(t, u, v), 0) + \int_{\substack{|u| > 2R \\ |\dot{x}(t,u,v)| > \lambda(\Omega) R}} du dv \ldots$$

$$\leqslant \int_{|x(t,u,v)| > R|C|/C'} du dv |F(x(t, u, v), \dot{x}(t, u, v), 0)| + \int_{|\dot{x}(t,u,v)| > \lambda(\Omega) R} du dv \ldots \quad (2.24)$$

where we have used (2.23). But the Jacobian of the change of variable $(u, v) \rightarrow (x, \dot{x})$ is

$$\det \begin{vmatrix} \frac{1}{C} \Sigma c_n \cos(2n + \rho) \frac{\Omega t}{2} & \frac{2}{m\Omega D} \Sigma c_n \sin(2n + \rho) \frac{\Omega t}{2} \\ \frac{-m\Omega}{2C} \Sigma c_n (2n + \rho) \sin(2n + \rho) \frac{\Omega t}{2} & \frac{1}{D} \Sigma c_n (2n + \rho) \cos(2n + \rho) \frac{\Omega t}{2} \end{vmatrix}$$

$$\leq \frac{2E}{D} \quad \text{uniformly in } t \quad (2.25)$$

where

$$\mathrm{E} = \sum_{-\infty}^{+\infty} | c_n | | 2n + \rho | \tag{2.26}$$

Therefore (2.24-25) imply

$$\| \mathrm{F}(|x| > \mathrm{R}) u(t,0)\psi \|^2 \leqslant \frac{2\mathrm{E}}{\mathrm{D}} \left(\int_{|x| > \mathrm{R}|\mathrm{C}|/\mathrm{C}'} dxd\xi \mathrm{F}(x,\xi,0) + \int_{|\xi| > \lambda(\Omega)\mathrm{R}} dxd\xi \mathrm{F}(x,\xi,0) \right)$$

where $\lambda(\Omega)$, E, C, C′ and D are independent of t. Thus as $\mathrm{F}(.,.,0) \in \mathrm{L}^1(\mathbb{R}^2)$, (2.6) follows.

We have thus established the following three-dimensional trapping result (which might be n-dimensional as well, n being arbitrary !).

THEOREM 2.6. — Let $\mathrm{H}_t = -\Delta + \mathrm{V}(x, t)$, with V being the time-dependent potential given in (2.1). Then there exists a unitary evolution group $\mathrm{U}(t, s)$ associated with H_t such that

$$i\hbar \frac{d}{dt} \mathrm{U}(t,s)\psi = \mathrm{H}_t \mathrm{U}(t,s)\psi \qquad \forall \psi \in \mathscr{D}(-\Delta + x^2)$$

Furthermore there exist positive constants θ_1, θ_2 such that if

$$-\theta_1 < \mathrm{V}_{dc}/\mathrm{V}_{ac} < \theta_2$$

there exists a non-empty interval $(\Omega_0, \Omega_1) \subset [0, \infty)$ depending upon V_{ac}, V_{dc}, e, m, r, such that

$$\forall \Omega \in (\Omega_0, \Omega_1), \quad \forall \psi \in \mathrm{L}^2(\mathbb{R}^3) \quad \text{and} \quad \forall \varepsilon, \quad \exists \mathrm{R} \quad \text{s. t.}$$

$$\operatorname*{Sup}_t \| \mathrm{F}(|x| > \mathrm{R})\mathrm{U}(t,0)\psi \| < \varepsilon$$

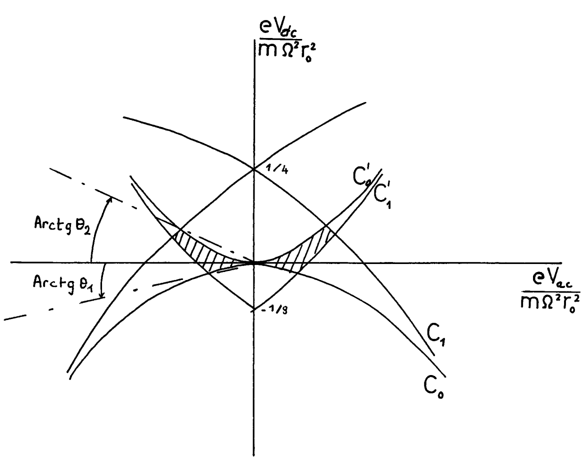

FIG. 2. — The 3 dimensional radio-frequency stability area.

$F(|x|>R)$ being the operator in $L^2(\mathbb{R}^3)$ corresponding to the multiplication by the characteristic function of the exterior of ball $x_1{}^2+x_2{}^2+x_3{}^2 \equiv x^2 \leq R^2$. Moreover if $V_{dc}=0$, Ω_1 is infinite, thus trapping holds for every high frequency in this case.

We only draw a picture exhibiting the usual stability region for this problem [*11*].

3. THE EIGENVALUE PROBLEM FOR THE FLOQUET OPERATOR

We now return to the one-dimensional Schrödinger hamiltonian h_t where we assume $m = 1$ for simplicity. It is very convenient, in time-periodic problems to introduce and study the following operator:

$$K = -i\hbar\partial/\partial t + h_t \tag{3.1}$$

in the space $\mathcal{K} = L^2(\mathbb{R}) \otimes L^2(\mathbb{T}_\Omega)$ of functions depending both on x and t. This was first recognized for spectral and scattering quantum problems by Howland [*9*] and Yajima [*16*]. Namely this operator is closely related to the time evolution group $u(t, s)$:

THEOREM 3.1. — *i*) Assume $\Psi \in \mathcal{K}$ is an eigenstate of K of eigenvalue λ. Then for any $t \in \mathbb{T}_\Omega$ (the one-dimensional torus, cf. (2.5)), $\Psi(t) \in L^2(\mathbb{R})$ and Ψ satisfies:

$$u\left(t + \frac{2\pi}{\Omega}, t\right)\Psi(t) = e^{-i\lambda 2\pi/\hbar\Omega}\Psi(t) \tag{3.2}$$

ii) Conversely let $\psi \in L^2(\mathbb{R})$ satisfy

$$u(2\pi/\Omega, 0)\psi = e^{-2i\pi\lambda/\hbar\Omega}\psi \tag{3.3}$$

Then $\Psi = e^{i\lambda t/\hbar}u(t, 0)\psi \in \mathcal{K}$ and satisfies

$$K\Psi = \lambda\Psi \tag{3.4}$$

The proof is standard [*16*].

As h_t is quadratic in $\frac{d}{dx}$ and x, it is natural to introduce states in $\mathcal{K}$ that are « time-scaled » versions of Hermite functions. They have already been introduced by Hagedorn [*6*] [*7*] for the purpose of semi-classical estimates for the time evolution of time-independent hamiltonian. But for quadratic potentials, these estimates are expected to yield actually exact results! Again, the classical motion plays an essential role: let A_t and B_t be complex functions satisfying:

$$\frac{d}{dt}A_t = iB_t \tag{3.5}$$

$$\frac{d}{dt}B_t = iA_t f(t) \tag{3.6}$$

where

$$f(t) \equiv (\alpha - \beta \cos \Omega t) \tag{3.7}$$

and assume they satisfy the initial condition

$$A_0 B_0^* + A_0^* B_0 = 2 \tag{3.8}$$

Let $H_n(.)$ be the usual Hermite polynomials, $n = 0, 1, \ldots$ We define:

$$\Phi_n(A_t, B_t, x) \equiv \frac{2^{-n/2}(n!)^{-1/2}}{(\pi\hbar)^{1/4}} \frac{1}{\sqrt{A_t}} \left(\frac{A_t^*}{A_t}\right)^{n/2} H_n(x/\sqrt{\hbar}\,|\,A_t\,|).\exp\left(-\frac{x^2}{2\hbar}\frac{B_t}{A_t}\right) \tag{3.9}$$

where the determination of the square root is followed by continuity from $t = 0$. We shall make the convenient choice:

$$A_0 = (\Omega D/2C)^{-1/2} = B_0^{-1} \tag{3.10}$$

and for this choice we define:

$$\Psi_n(x, t) = e^{i\left(n+\frac{1}{2}\right)\rho\Omega t/2} \Phi_n(A_t, B_t, x) \tag{3.11}$$

Then we have:

THEOREM 3.2. — Assume Ω lies in a stability region for the Mathieu equation (2.7). Then:

i) $$u(t, 0)\Phi_n(A_0, B_0, .) = \Phi_n(A_t, B_t, .) \quad (\text{any } t) \tag{3.12}$$

ii) Let ρ be the Floquet characteristic exponent for the classical Mathieu equation (2.7) (see 2.19). Then assuming (3.10), we get

$$K\Psi_n = \left(n + \frac{1}{2}\right)\hbar\rho\Omega/2\Psi_n \tag{3.13}$$

Proof. — *i)* Will hold without assumption (3.10). Assuming *i)* for the moment, we show that (3.10) implies (3.13). It immediatly follows from equations (3.5-7) and (2.19) that A_t and B_t are given by

$$A_t = \frac{A_0}{C} e^{i\rho\Omega t/2} \sum_{-\infty}^{+\infty} c_n e^{in\Omega t} \tag{3.14}$$

$$B_t = \frac{B_0}{D} e^{i\rho\Omega t/2} \sum_{-\infty}^{+\infty} c_n(2n + \rho) e^{in\Omega t} \tag{3.15}$$

so that $|\,A_t\,|$ and $\frac{B_t}{A_t}$ are T-periodic. Furthermore $e^{i\left(n+\frac{1}{2}\right)\frac{\rho\Omega t}{2}} \frac{1}{\sqrt{A_t}} \left(\frac{A_t^*}{A_t}\right)^{n/2}$

is also T-periodic, so that $\Psi_n(x, .)$ is T-periodic. Moreover, using (3.12) we get

$$u(\mathrm{T}, 0)\Phi_n(\mathrm{A}_0, \mathrm{B}_0, .) = e^{-i\rho\pi\left(n+\frac{1}{2}\right)}\Phi_n(\mathrm{A}_0, \mathrm{B}_0, .) \tag{3.16}$$

which implies precisely (3.13), using theorem 3.1 *ii*).

We now prove *i*). Coming back to the proof of the existence and differentiability of $u(t, s)$ [*10*] and [*14*, p. 285] we know that $\forall n$, and t

$$u(t, 0)\Phi_n(\mathrm{A}_0, \mathrm{B}_0, .) = \lim_{\mathrm{N}\to\infty} u^{(\mathrm{N})}(t, 0)\Phi_n(\mathrm{A}_0, \mathrm{B}_0, .) \tag{3.17}$$

where

$$u^{(\mathrm{N})}(t, 0) = e^{-i(t-[\mathrm{N}t]/\mathrm{N})h_{[\mathrm{N}t]/\mathrm{N}}}e^{-\frac{i}{\mathrm{N}}h_{([\mathrm{N}t]-1)/\mathrm{N}}} \dots e^{-i\mathrm{N}^{-1}h_0} \tag{3.18}$$

But, if $\mathrm{A}_t^{(\mathrm{N})}$ and $\mathrm{B}_t^{(\mathrm{N})}$ are solutions of:

$$\begin{cases} \dfrac{d}{dt}\mathrm{A}_t^{(\mathrm{N})} = i\mathrm{B}_t^{(\mathrm{N})} \\ \dfrac{d}{dt}\mathrm{B}_t^{(\mathrm{N})} = i\mathrm{A}_t^{(\mathrm{N})}f_{\mathrm{N}}(t) \end{cases} \tag{3.19}$$

with

$$f_{\mathrm{N}}(t) = f(j/\mathrm{N}) \qquad \text{when} \quad j/\mathrm{N} \leqslant t < (j+1)/\mathrm{N} \tag{3.20}$$

and

$$\mathrm{A}_0^{(\mathrm{N})} = \mathrm{A}_0, \qquad \mathrm{B}_0^{(\mathrm{N})} = \mathrm{B}_0$$

we know that for any $k \in \mathbb{N}$

$$e^{-i\mathrm{N}^{-1}h_{k/\mathrm{N}}}e^{-i\mathrm{N}^{-1}h_{k-1/\mathrm{N}}} \dots e^{-i\mathrm{N}^{-1}h_0}.\Phi_n(\mathrm{A}_0, \mathrm{B}_0, .) = \Phi_n(\mathrm{A}_{k/\mathrm{N}}^{(\mathrm{N})}, \mathrm{B}_{k/\mathrm{N}}^{(\mathrm{N})}, .) \tag{3.21}$$

The proof is immediate, via the Trotter product formula for each factor $\exp\left(\dfrac{-i}{\mathrm{N}}h_{k/\mathrm{N}}\right)$ as in [*6*]. We omit the details. Therefore, we conclude from (3.18, 22) that

$$u(t, 0)\Phi_n(\mathrm{A}_0, \mathrm{B}_0, .) = \lim_{\mathrm{N}\to\infty} \Phi_n(\mathrm{A}_t^{(\mathrm{N})}, \mathrm{B}_t^{(\mathrm{N})}, .)$$

But $f^{(\mathrm{N})}(t)$ is simply the step function corresponding to the continuous function $f(t)$ given by (3.7) which steps getting more and more narrow. But it is known, from the theory of ordinary differential equations that, as $f^{(\mathrm{N})}(t) - f(t)$ tends to 0 uniformly in t, so do $\mathrm{A}_t^{(\mathrm{N})} - \mathrm{A}_t$ and $\mathrm{B}_t^{(\mathrm{N})} - \mathrm{B}_t$, so that *i*) is proven, using the dominated convergence theorem.

COROLLARY 3.3. — Assume Ω lies in a stability region, and let $\Psi_{n,m}(x, t) = e^{im\Omega t}\Psi_n(x, t)$, $n \in \mathbb{N}$, $m \in \mathbb{Z}$. Then $(\Psi_{n,m})_{\substack{n\in\mathbb{N}\\ m\in\mathbb{Z}}}$ are the eigenstates of the « quasi-energy » operator K, with eigenvalues $\lambda_{n,m}=\left[m+\left(n+\frac{1}{2}\right)\frac{\rho}{2}\right]\hbar\Omega$, ρ being the characteristic Floquet exponent for the Mathieu equation (2.7).

REMARK 3.1. — ρ being a continuous function of Ω, it takes all values between 0 and 1 when Ω lies in the stability region under consideration (delimited by curves C_0 and C_1 of fig. 1). If ρ happen to be rational, then each eigenvalue of K is infinitely degenerate. On the contrary if $\rho \notin \mathbb{Q}$, the $\lambda_{n,m}$ form a dense set in $\mathbb{R}$, because, if $\frac{p_j}{q_j}$ is a suitable sequence of rationals converging to ρ, $(p_j, q_j \in \mathbb{N})$ then the difference between the eigenvalues $\lambda_{n,m}$ and $\lambda_{n+2q_j,m-p_j}$ tends to zero as $j \to \infty$.

REMARK 3.2. — The states $\Phi_n(A_t, B_t, x)$ are quantum fluctuations, in the sense of Hagedorn, around the trivial classical solution $x(t) \equiv 0$. Hagedorn [6] [7] has constructed more general states that are quantum fluctuations around general classical solutions. However they do not yield eigenstates of the Floquet operator, because the general classical trajectories are not T-periodic inside the open stability interval (Ω_0, Ω_1).

REMARK 3.3. — The states $(\Psi_{n,m})_{\substack{m\in\mathbb{N}\\ n\in\mathbb{Z}}}$ obviously form a complete basis in $\mathscr{K}$. Therefore all the eigenstates and eigenvalues of K are obtained in Corollary 3.3. As an alternative formulation of Theorem 3.2, let us mention ref. [1] where $u(t, 0)$ is written explicitely (as long as $\alpha \neq 0$ between 0 and t) as:

$$u(t, 0) = \exp(ix^2\alpha'/2\alpha)\exp(-\,i(xp + px)/2\alpha)\exp\left(-\,ip^2\int_0^t ds\alpha^{-2}(s)/2\right)$$

where α solves the equation $\alpha'' + \alpha f(t) = 0$ with $\alpha(0) = 1$, $\alpha'(0) = 0$. However we feel that our construction of the eigenstates in Theorem 3.2 starting from Hermite functions is more intuitive.

4. A TEST FOR THE EFFECTIVE POTENTIAL APPROXIMATION

In ref. [5], the authors try to perform a perturbative treatment of the quantum motion in a rapidly oscillating field, in order to exhibit the commonly believed « effective potential approximation » and the first corrections to it. However it is clear that perturbation theory is not expected to be dealt with in the usual way because the spectrum of the unperturbed operator $-\,i\hbar\,\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\Delta + \frac{|f(x)|^2}{4mQ^2}$ (where $f(x)$ is the space component of the force $f(x)\cos\Omega t$) exhibits the same characteristics as that of our Floquet operator K: namely either isolated eigenvalues with infinite multiplicities or a dense point spectrum, depending on the value of the parameters. The perturbative treatment of such a system clearly exhibits « small divisors » problems, and therefore requires a refined version of K. A. M. theorem techniques, as in [*2*]. Here we do not want to perform this refined version of perturbation theory because, as we have already seen, the perturbed problem is exactly solvable. However our exact results are a test of what is expected from the « effective potential » belief. We do this comparison in the special case of the one dimensional hamiltonian h_t given by (2.4) with $\alpha = 0$, so that from Theorem 2.1 the stability interval for Ω is of the form (Ω_0, ∞). In the « effective potential approximation », it is believed that if a particle of mass m is subject to a high-frequency force $f(x)\cos\Omega t$ then it moves as if acted upon by a *time-independent* effective potential

$$V_{\text{eff}}(x) = |\,f(x)\,|^2/4m\Omega^2 \tag{4.1}$$

Therefore it happens as if its time evolution were

$$e^{-i(t-s)h_{\text{eff}}} \tag{4.2}$$

where

$$h_{\text{eff}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\beta^2}{4m\Omega^2}x^2 \tag{4.3}$$

which is just a harmonic oscillator hamiltonian. The normalized eigenstates of h_{eff} are $\Phi_n(\tilde{A}_0, \tilde{B}_0, x)$ as given by (3.9) with the special choice

$$\tilde{A}_0 = \tilde{B}_0^{-1} = (\Omega\sqrt{2}/\beta)^{1/2} \tag{4.4}$$

different from (3.10) but close to it when Ω is large, as we shall see below. Therefore if we take $\Phi_n(\tilde{A}_0, \tilde{B}, x)$ as an initial state at time zero for the true evolution $u(t, 0)$, then the state at time t is $\Phi_n(\tilde{A}_t, \tilde{B}_t, x)$, so that we can evaluate the probabilities

1) for the state at time t to be again $\Phi_n(\tilde{A}_0, \tilde{B}_0, x)$ (up to a phase) as it would be the case if the effective potential approximation were exact.

2) For the state at time t to be $\Phi_{n'}(\tilde{A}_0, \tilde{B}_0, x)$ with $n' \neq n$, which precisely measures the failure of the effective potential approximation.

We first give a qualitative description before giving quantitative estimates for these probabilities.

The states $\Phi_n(A_t, B_t, .)$ where A_t and B_t evolve by the classical equations (3.5-6) with initial data (3.10) provide the exact quantum evolution starting from the state $\Phi_n(A_0, B_0, .)$. But these states are precisely the eigenstates of a static harmonic oscillator hamiltonian:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{x^2}{2m}\left(\frac{m\Omega D}{2C}\right)^2 \tag{4.5}$$

which is close to h_{eff} when Ω becomes large. But the $\Phi_n(A_t, B_t, x)$ equal a T-periodic function, (where $T = 2\pi/\Omega$ is very small), modulated by a periodic secular wave and therefore so do the probabilities

$$c_n(t) \equiv \langle \Phi_{2n}(A_0, B_0, .), \Phi_0(A_0, B_0, .) \rangle \tag{4.6}$$

which for $n \geq 1$ measure the transition probability to an excited state $\Phi_{2n}(A_0, B_0, .)$ of H, starting from the ground state Φ_0. Therefore if we look at the system at the sequence of times $t = kT$ ($k \in \mathbb{N}$) that are very close from each other, we will observe it again in the initial state Φ_0 with probability one, because $c_0(kT) = 1 \ \forall k \in \mathbb{N}$. However, the system spends enough time inbetween these periods near excited states of H, that its transition probability to, say, the first excited state $\Phi_2(A_0, B_0, .)$ be quite large when integrated over a period interval. More precisely, we shall show that the « time average of the excitation probability to the state $\Phi_2'' : P_1 = T^{-1} \int_0^T dt \, | c_1(t) |^2$ is $O(1)$ and not $O(\Omega^{-4})$ as was claimed in ref. [5] on the basis of first order calculations. Thus it invalidates the « effective potential approximation » even at very high frequencies, because, as we shall see the difference between P_1 and $\tilde{P}_1$ (calculated with $\tilde{A}_0$ and $\tilde{B}_0$ given by (4.4) in place of (3.10)) is of order $O(\Omega^{-2})$. But if we only consider the sequence of times kT ($k \in \mathbb{N}$) which are very close together, the system looks as if it were in the stationary state Φ_0 for the evolution e^{-itH}, and thus the « effective potential approximation » in this sense is very good. Let us now give the quantitative meaning of that:

THEOREM 4.1. — *i*) With the choice (3.10) for A_0 and B_0, we have

$$c_0(t) \equiv \langle \Phi_0(A_0, B_0,.), u(t,0)\Phi_0(A_0, B_0,. \rangle = e^{-i\rho\Omega t/4}F(t) \tag{4.7}$$

where F(*t*) is the T-periodic function

$$F(t) \equiv \left(\sum_{-\infty}^{+\infty} c_n \left(\frac{1}{2C} + \frac{2n + \rho}{2D} \right) e^{in\Omega t} \right)^{-1/2} \tag{4.8}$$

which equals one for $t = kT$ ($k \in \mathbb{Z}$).

ii) Let $c_n(t)$ be given by (4.6), with any choice of A_0, B_0 satisfying (3.8). Then:

$$c_n(t) = \frac{\sqrt{(2n)!}}{n!} 2^{-n} \left(\frac{1}{2}\frac{A_t}{A_0} + \frac{1}{2}\frac{B_t}{B_0} \right)^{-n-\frac{1}{2}} \left(\frac{1}{2}\frac{A_t}{A_0} - \frac{1}{2}\frac{B_t}{B_0} \right)^n \tag{4.9}$$

iii) With the choice (4.4) for A_0 and B_0, we get

$$(1 + O(b)) \left(\frac{3 + \sqrt{2}}{2} \right)^{-1/4} \leqslant | \tilde{c}_0(t) | \leqslant 1$$

and

$$\tilde{P}_1 \equiv T^{-1}\int_0^T dt\,|\tilde{c}_1(t)|^2 \geqslant \frac{1}{8}\left(\frac{3+\sqrt{2}}{2}\right)^{-3/2}(1+0(\Omega^{-2}))$$

Proof. — *i)* and *ii)* easily follow from explicit calculations on Hermite functions, that we leave to the reader. We only note, as a verification that $\sum_0^\infty |c_n(t)|^2 = 1$ (conservation of probabilities) using the relation $(1-x)^{-1/2} = \sum_0^\infty \frac{(2n)!}{(n!)^2 2^{2n}} x^n$. In order to prove *iii)*, we need to investigate the high frequency regime for the Mathieu equation (2.7) with $\alpha = 0$. Restoring the mass $m \neq 1$ in formula (3.10) for A_0 and B_0, we get:

LEMMA 4.2. — Let ρ be the Floquet characteristic exponent for the Mathieu equation (2.7) with $\alpha = 0$. Then as Ω becomes large, we get:

$$\rho = \frac{\beta\sqrt{2}}{m\Omega^2}(1+0(\Omega^{-2})) \tag{4.10}$$

$$0 \leqslant \rho C - D = \frac{2\beta^2\sqrt{2}}{m^2\Omega^4}(1+0(\Omega^{-2})) \tag{4.11}$$

$$\| \Phi_0(A_0, B_0, .) - \Phi_0(\tilde{A}_0, \tilde{B}_0, .) \| \leqslant 0(\Omega^{-2}) \tag{4.12}$$

$$\| \Phi_2(A_0, B_0, .) - \Phi_2(\tilde{A}_0, \tilde{B}_0, .) \| \leqslant 0(\Omega^{-2}) \tag{4.13}$$

Proof. — Let $(c_n)_{n\in\mathbb{Z}}$ be the sequence determining the solutions (2.19) of Mathieu equation (2.7). Then they obey the recurrence relation:

$$c_n + \gamma_n(\rho)(c_{n+1} + c_{n-1}) = 0 \tag{4.14}$$

where

$$\gamma_n(\rho) \equiv \frac{-b}{(2n+\rho)^2 - a} \tag{4.15}$$

Thus if $\Delta(\rho)$ is the (infinite) determinant for the system (4.14), ρ is given by the equation $\Delta(\rho) = 0$. It is easy to prove that [*11*]

$$\sin^2 \pi\rho/2 = \Delta(0)\sin^2 \pi\sqrt{a}/2 \tag{4.16}$$

and that, to the second order in $b = \frac{2\beta}{m\Omega^2}$:

$$\begin{aligned}\Delta(0) &= 1 - 2b^2 \sum_0^\infty [(2n)^2 - a]^{-1}[(2n+2)^2 - a]^{-1} \\ &= 1 + \frac{b^2}{2a} + \frac{b^2}{16(a-1)} \sum_1^\infty \left(\frac{1}{n^2 - a/4} - \frac{1}{n^2 - 1/4}\right)\end{aligned} \tag{4.17}$$

But, using the well known formula

$$\sum_{1}^{\infty} \frac{1}{n^2 - x^2} = \frac{1}{2x^2} - \frac{\pi}{2x} \operatorname{cotg} \pi x \tag{4.18}$$

we get

$$\sum_{1}^{\infty} \frac{1}{n^2 - a/4} - \frac{1}{n^2 - 1/4} = 2\left(\frac{1}{a} - 1\right) - \frac{\pi}{\sqrt{a}} \operatorname{cotg} \frac{\pi\sqrt{a}}{2}$$

$$= -2 + \frac{\pi^2}{6} + 0(\Omega^{-2}) \quad \text{as} \quad \Omega \to \infty \tag{4.19}$$

Thus, using (4.16-19), we get

$$\rho^2 = a\left(1 + \frac{b^2}{2a} + \left(\frac{\pi^2}{6} - 2\right)\frac{b^2}{16}(1 + 0(\Omega^{-2}))\right)$$

$$= a + b^2/2 + 0(\Omega^{-6}) \quad \text{as} \quad \Omega \to \infty$$

which implies (4.10) in the case $\alpha = 0$. Translating the origin of time by T/2 if necessary, we can assume $b \geq 0$. Therefore, starting from, say, $c_0 = 1$, we see from (4.12) that all c_n are ≥ 0, and that, by induction

$$\frac{b}{(2n+\rho)^2} \leqslant \frac{c_{n+1}}{c_n} \leqslant \frac{b}{(2n-\rho)^2} \leqslant \frac{c_{-n-1}}{c_{-n}} \leqslant \frac{b}{(2n-2+\rho)^2} \quad \forall n \geqslant 2 \tag{4.20}$$

$$0 \leqslant \frac{c_{-n}}{c_{-n+1}} \leqslant \frac{c_n}{c_{n-1}} \leqslant \frac{2b\rho}{n^2} \tag{4.21}$$

$$0 \leqslant c_n \leqslant \frac{(2b)^n}{(n!)^2} \tag{4.22}$$

$$0 \leqslant c_{-n} - c_n \leqslant \frac{(2b)^n}{(n!)^2} 2\rho \tag{4.23}$$

Therefore $\sum_{n \geq 2} n(c_{-n} - c_n) = 0(b^3)$ so that

$$2(c_{-1} - c_1) \leqslant \rho C - D \leqslant 2(c_{-1} - c_1) + 0(b^3)$$

which implies (4.11), using (4.10).
Now $\Phi_0(A, B, .)$ and $\Phi_2(A, B, .)$ being Hermite functions, the LHS of (4.12-13) can easily be calculated:

$$\| \Phi_0(A_0, B_0,.) - \Phi_0(\tilde{A}_0, \tilde{B}_0,.) \|^2 = 2 - 2\left(\frac{A_0}{2\tilde{A}_0} + \frac{\tilde{A}_0}{2A_0}\right)^{-1/2} \tag{4.24}$$

$$\| \Phi_2(A_0, B_0,.) - \Phi_2(\tilde{A}_0, \tilde{B}_0,.) \|^2 = 2 - \frac{1}{\sqrt{A_0 A_0}}\left(\frac{1}{2\tilde{A}_0^2} + \frac{1}{2\tilde{A}_0^2}\right)^{-1/2}$$

$$\cdot \left\{ \frac{3}{A_0^2 \tilde{A}_0^2 (1/2\tilde{A}_0^2 + 1/2A_0^2)} - 1 \right\} \tag{4.25}$$

But using (3.10-11), we see that there exists some constant d such that:

$$\tilde{A}_0/A_0 = 1 - db + 0(b^2)$$

so that, inserting it in (4.24-25), we get (4.12-13).

These results allow us to go on with the proof of Theorem 4.1 *iii*):

$$\left|\frac{1}{2}\frac{A_t}{A_0} + \frac{1}{2}\frac{B_t}{B_0}\right|^2 = \frac{1}{4}\left|\frac{A_t}{A_0}\right|^2 + \frac{1}{4}\left|\frac{B_t}{B_0}\right|^2 + \frac{1}{2} \leqslant \frac{3}{4} + \frac{1}{4}\left(\frac{E}{D}\right)^2$$

where E is defined by (2.26). But an easy calculation yields

$$E = \rho C(1 + \sqrt{2})(1 + 0(b))$$

so that

$$\left|\frac{1}{2}\frac{A_t}{A_0} + \frac{1}{2}\frac{B_t}{B_0}\right|^2 \leqslant \frac{3 + \sqrt{2}}{2} \tag{4.26}$$

(4.9), (4.12-13) and (4.26) together with unitarity of $u(t, 0)$ imply the estimate for $\tilde{c}_0(t)$.

From (4.9) and (4.26) we conclude:

$$|c_1(t)| \geqslant \frac{1}{\sqrt{2}}\left(\frac{3 + \sqrt{2}}{2}\right)^{-3/4}(1 + 0(b)).\left|\sum_{-\infty}^{+\infty} c_n\left(\frac{1}{2C} - \frac{2n + \rho}{2D}\right)e^{in\Omega t}\right| \tag{4.27}$$

Therefore, by Bessel-Parseval relation:

$$P_1 \geqslant \frac{1}{2}\left(\frac{3+\sqrt{2}}{2}\right)^{-3/2}(1+0(b))\sum_{-\infty}^{+\infty} c_n^2\left(\frac{1}{2C} - \frac{2n+\rho}{2D}\right)^2 \tag{4.28}$$

We thus have to evaluate

$$M \equiv \sum_{-\infty}^{+\infty} c_n^2(D - (2n + \rho)C)^2$$

But applying Bessel-Parseval relation to $A_t^*B_t + A_tB_t^* = 2$ we get

$$\sum_{-\infty}^{+\infty} c_n^2(2n + \rho) = CD \tag{4.29}$$

so that

$$M = D^2\sum_{-\infty}^{+\infty} c_n^2 + C^2\sum_{-\infty}^{+\infty} c_n^2(2n + \rho)^2 - 2C^2D^2$$

But using (4.14-15) with $a = 0$, we get

$$\sum_{-\infty}^{+\infty} c_n^2(2n + \rho)^2 = 2b\sum_{-\infty}^{+\infty} c_nc_{n-1} = 2\rho^2C^2(1 + 0(b))$$

and therefore

$$M = \rho^2 C^4 (1 + 0(\Omega^{-2})) \tag{4.30}$$

Inserting (4.30) into (4.28), we get

$$P_1 \geqslant \frac{1}{8}\left(\frac{3 + \sqrt{2}}{2}\right)^{-3/2} (1 + 0(b)) \simeq 0.038(1 + 0(\Omega^{-2})) \tag{4.31}$$

and the same estimate holds for $\tilde{P}_1$ instead of P_1, using estimates (4.12-13) for the comparison of eigenstates of H and those of h_{eff}. This completes the proof of theorem 4.1.

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REFERENCES

[1] A. I. BAZ, Y. B. ZELDOVITCH, A. M. PERELOMOV, *Scattering and break-up reactions in non-relativistic quantum mechanics* (in russian) Moscow, Nauka, 1971.
[2] J. BELLISSARD, *Stability and instability in quantum mechanics*, Marseille-Luminy preprint, 1984.
[3] J. BELLISSARD, private communication.
[4] M. N. BENILAN, C. AUDOIN, *Int. J. Mass Spectrom. Ion. Phys.*, t. **11**, 1973, p. 421-432.
[5] R. J. COOK, D. G. SHAMKLAND, A. L. WELLS, *Phys. Rev.* A, t. **31**, 1985, p. 564-567.
[6] G. HAGEDORN, *Commun. Math. Phys.*, t. **71**, 1980, p. 77-93.
[7] G. HAGEDORN, Semiclassical quantum mechanics IV : large order asymptotics and more general states in more than one dimension, to appear in *Ann. Inst. Henri Poincaré*, t. **42**, 1985, p. 363-374.
[8] K. HEPP, *Commun. Math. Phys.*, t. **35**, 1974, p. 265-277.
[9] J. S. HOWLAND, Two problems with time-dependent Hamiltonians, in Mathematical methods and applications of scattering theory, ed. by J. A. De Santo *et al.* *Lecture Notes in Physics*, t. **130**, 1980, Springei, Berlin-Heidelberg-New-York.
[10] T. KATO, *J. Math. Soc. Japan*, t. **25**, 1973, p. 648-666.
[11] N. W. MCLACHLAN, *Theory and application of Mathieu functions*, Oxford University Press, New York, 1947.
[12] W. NEUHAUSER, M. HOHENSTATT, P. TOSCHEK, H. DEHMELT, *Phys. Rev.* A, t. **122**, 1980, p. 1137-1140.
[13] W. PAUL, M. RAETHER, *Zeitschrift für Physik*, t. **140**, 1955, p. 262-273.
[14] M. REED, B. SIMON, *Methods of Modern Mathematical Physics*, Vol. II, Academic Press, 1975, London, New York.
[15] R. F. WUERKER, H. SHELTON, R. V. LANGMUIR, *J. of Appl. Phys.*, t. **30**, 1959, p. 342-349.
[16] K. YAJIMA, *J. Math. Soc. Japan*, t. **29**, 1977, p. 729-743.

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