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Quantum mechanics in strong time dependent external fields

by

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ABSTRACT. — In quantum mechanics, time dependent Hamiltonians are most often studied by perturbation methods, the amplitude of the unsteady force being assumed to be small. On two examples (two level system with a large time dependent coupling, and atoms in large external unsteady field). I show that the opposite limit (large time dependent field) can be analyzed in some details too. For a particle in a central potential and submitted to a large periodic external field, one is led to make a Kapitza averaging because the intrinsic frequency tends to zero when the external field diverges. In that way one has to introduce a steady effective potential with singular turning points.

RÉSUMÉ. — En mécanique quantique, l'étude des hamiltoniens dépendants du temps se fait le plus souvent à l'aide d'un calcul de perturbation dans l'amplitude de la force instationnaire, qui est donc supposée petite. Nous montrons sur 2 exemples (système à 2 degrés de liberté, particule dans un champ extérieur variant périodiquement) que la limite opposée des grandes perturbations instationnaires peut aussi être analysée assez en détail. Dans le cas d'une particule soumise à un potentiel central et à un champ extérieur intense variant périodiquement avec le temps, on est conduit à faire une moyenne de Kapitza, puisque la fréquence intrinsèque du système devient très petite. On fait ainsi apparaître un potentiel effectif constant avec un point tournant singulier.

INTRODUCTION

In the course of theoretical investigations on quantum chaos, I have been led to consider the effect of strong unsteady external fields on quantum systems. That limit turns out to be tractable, at least in a certain sense. I give below two such examples: first the case of two levels coupled by a strong time dependent field that could be a spin 1/2 in a constant external magnetic field H_0 plus a time dependent field $H_1(t)$ not parallel to H_0 and such that $|H_1| \gg |H_0|$), then a charged particle submitted both to a steady potential and to a large uniform and oscillating electric field. In this last situation, one may get rid of the time dependent external field by introducing a steady effective potential through a Kapitza averaging.

Let us summarize the most relevant results of this work. In two levels systems, I consider perturbations proportional to a large time dependent real function $b(t)$. As long as this function does not take the value zero, the quantum state of the system is an arbitrary linear superposition of two « quasi-eigenstates » with constant amplitudes. These amplitudes are constant, in the same sense as adiabatic invariants are. Whenever $b(t)$ crosses zero, those two « constants » or adiabatic invariants exchange a small amount of norm. If $b(.)$ is a random function of time, this leads to a diffusion-like process on the sphere S_3 where the dynamics of the adiabatic invariants is constrained by unitarity.

The second case studied is an electron in a steady potential and a large oscillating electric field uniform in space. There the Kapitza averaging allows to replace the time dependent hamiltonian by the one of an electron in a stationary effective potential. In one space dimension, this effective potential is attracting whenever the mean value of the initial potential is negative, as we assume it. When the externally imposed electric field varies sinusoidally with time, one may analyze in a rather detailed fashion bound states of the effective potential. The fundamental and first few excited states have (negative) energies of order $\lambda^{-2/3}$, λ being the amplitude of the external field. However, most bound states have energies of order λ^{-1}, as shown by a semiclassical approach. In this semiclassical limit, one turning point at the transition between classically accessible and forbidden regions is singular. This changes the constant phase in the Bohr-Sommerfeld quantization condition. Then I consider an electron in three dimensional central Coulomb field, and a large external oscillating electric field. The first bound state has an energy of order $\lambda^{-2/3}$ and most excited states have energies of order $\lambda^{-1} \ln \lambda$ (again λ is the amplitude of the external field). In this last case, the semiclassical analysis cannot be as complete as in one spatial dimension, because the Schrödinger equation in the effective potential is not separable.

1. TWO LEVELS COUPLED BY A STRONG TIME DEPENDENT FIELD

The simplified equation of motion for this system may be written as:

$$i\dot{\psi}_1 = a_1\psi_1 + b(t)\psi_0 \qquad (1.a)$$

$$i\dot{\psi}_0 = a_0\psi_0 + b(t)\psi_1 \qquad (1.b)$$

where dots represent time derivative, $\psi_{0/1}$ are the (complex) amplitudes of the two states, $a_{0/1}/2\pi$ their bare Planck frequencies (i. e. a_0 and a_1 are two given real quantities) and where the real function of time $b(t)$ represents the coupling between the two levels. Moreover, any physical quantity as the Planck constant, the Bohr magnetron, ... has been incorporated into parameters bearing the dimension of a frequency, that is in a_0, a_1 and b.

Indeed, the equation (1) constitutes the Schrödinger picture of this two levels system, although a Heisenberg picture could be equally used. To obtain the latter, one needs a closed linear system for three real quadratic forms built from ψ_0 and ψ_1. Define

$$Q = |\psi_1|^2 - |\psi_0|^2,\ Q' = i(\psi_0^*\psi_1 - \psi_1^*\psi_0),\ Q'' = \psi_1\psi_0^* + \psi_1^*\psi_0,$$

then elementary manipulations show from (1) that

$$\dot{Q} = 2bQ' \qquad (2.a)$$

$$\dot{Q}' = -2bQ - (a_0 - a_1)Q'' \qquad (2.b)$$

and

$$\dot{Q}'' = Q'(a_0 - a_1) \qquad (2.c)$$

The constant of the motion $Q^2 + Q'^2 + Q''^2$ is the square of the total probability ($|\psi_1|^2 + |\psi_0|^2$). All the forthcoming analysis could be done by starting from (2) instead of (1), but I have chosen to deal with (1) instead of (2).

Perturbation theory [*1*] shows that, if $b(.)$ is small and periodic with a period nearby $((a_1 - a_0)/2\pi)^{-1}$, the dynamics described by (1) are made of slow regular oscillations between the two quantum states. Near $|b| \sim 0$, the frequency of these oscillations is proportional to the amplitude of b. This has many important applications, both in magnetic resonance and molecular and atomic spectroscopy. More generally, the Floquet theorem [*2*] states that for any periodic $b(.)$ of period T, the general solution of (1) has the form:

$$\psi_0(t) = f_\mu(t)e^{i\mu t} + f_\nu(t)e^{i\nu t}$$

$$\psi_1(t) = -f_\mu(t)e^{i\mu t} + f_\nu(t)e^{i\nu t}$$

where μ and ν are real and $f_{\mu,\nu}$ are T-periodic functions. As said before,

perturbation theory gives access to μ, ν and $f_{\mu,\nu}$ for small b's. I want to show here – among other things – that these quantities can be also computed in the other limit, i. e. for b large.

I shall assume $a_0 \neq a_1$, since otherwise the problem is trivial. Moreover, it will appear that the large b-limit means that $| a_0 - a_1 |$ is much smaller than $| b |$. Actually, this limit will be understood as if b were of the form $\lambda \hat{b}(t)$, $\hat{b}$ being some fixed function of time and λ tending to infinity, although this formal device won't be used explicitely. The analysis will run as follows: a few elementary transformations lead from (1) to the second order equation (3). And this equation can be solved for large b by a WKB-like approximation. This one fails near turning points defined by $b = 0$. The inner solution near these (eventual) turning points is expressed by Fresnel integrals at the dominant order, and one can get from that the monodromy transformation (M. T.) solving the problem, at least locally in time. Roughly speaking the time dependence of the WKB solution has the form

$$\sum_{j=\pm 1} C_j(t) e^{ji \int^t b(t')dt'}$$

where the two functions $C_\pm(t)$ are such that $| C_+ |^2 + | C_- |^2$ stays constant in the course of time. Moreover, in the WKB limit these two functions are just constants, they change only near the turning points (i. e. near the zeroes of $b(.)$ if there are any). If β is the (large) time derivative of b at one of its zeroes, $C_\pm$ change by a relative amount of order $| \beta |^{-1/2}$ near this turning point, so that the time scale for the dynamics of $C_\pm(.)$ is much larger than the time scale for the phase dynamics, the latter being of order b^{-1}. For a random $b(.)$, this yields a diffusion process for C_+ and C_- on the unit $3d$ sphere, although for a periodic $b(.)$, this allows one to compute explicitly the quantities μ, ν and $f_{\mu/\nu}$ that appear in the Floquet theory.

So, let us derive first the announced second order differential equation (3) from (1). For that purpose, we define two phase factors

$$\chi_\pm(t) = \exp\left[\pm i \int^t b(t')dt' \right],$$

and use as new unknown functions $\hat{\varphi}_+$ such that

$$\psi_1 = \hat{\varphi}_+ \chi_+ + \hat{\varphi}_- \chi_-$$
$$\psi_0 = - \hat{\varphi}_+ \chi_+ + \hat{\varphi}_- \chi_-$$

The equation of motion for $\hat{\varphi}_\pm$, as deduced from (1), reads:

$$2i\dot{\hat{\varphi}}_- = (a_1 - a_0) \frac{\chi_+}{\chi_-} \hat{\varphi}_+ + (a_1 + a_0)\hat{\varphi}_-$$
$$2i\dot{\hat{\varphi}}_+ = (a_1 - a_0) \frac{\chi_-}{\chi_+} \hat{\varphi}_- + (a_1 + a_0)\hat{\varphi}_+$$

Taking now $((a_1 - a_0)/2)^{-1}$ as time unit, and introducing the new functions $\varphi_\pm = e^{\frac{i}{2}(a_1 + a_0)t}\hat{\varphi}_\pm$, one has:

$$i\dot{\varphi}_- = \frac{\chi_+}{\chi_-}\varphi_+$$

$$i\dot{\varphi}_+ = \frac{\chi_-}{\chi_+}\varphi_-$$

a pair of equations having the total probability $|\varphi_+|^2 + |\varphi_-|^2$ as a constant of the motion. Putting now ϕ for φ_+, one gets readily the sought second order equation:

$$\ddot{\phi} + \phi - 2ib\dot{\phi} = 0 \tag{3}$$

This equation has $|\phi|^2 + |\dot{\phi}|^2$ as a constant of motion. Furthermore, its Wronskian can be exactly calculated. Let ϕ_α and ϕ_β be two solutions of (3), and let their Wronskian be $W_{\alpha\beta} = \dot{\phi}_\alpha\phi_\beta - \phi_\alpha\dot{\phi}_\beta$. From (3): $\dot{W}_{\alpha\beta} = 2ibW_{\alpha\beta}$, and thus

$$W_{\alpha\beta}(t) = C_{\alpha\beta}\exp\left[2i\int_0^t b(t')dt'\right]$$

where the constant $C_{\alpha\beta}$ depends on the initial values of $\phi_{\alpha\beta}$.

If $b(.)$ is large, and so can be considered as almost constant over time intervals of order $|b^{-1}|$, it is natural to seek a solution of (3) by a WKB-type of analysis. Putting $\phi \sim e^{i\sigma t}$ into (3), and taking b a constant, one finds

$$\sigma = b \pm (b^2 + 1)^{1/2},$$

so that, for $b \gg 1$, the WKB solution of (3) reads:

$$\phi = \hat{A} + \hat{B}\exp\left[-2i\int^t dt'b(t')\right] \tag{4.a}$$

where $\hat{A}$ and $\hat{B}$ are – for the moment – arbitrary complex numbers. Pursuing the expansion at next order, one finds:

$$\hat{A} = A\left(1 + \int^t \frac{dt'}{2ib(t')} + \ldots\right) \tag{4.b}$$

and

$$\hat{B} = \frac{B}{2b(t)}(1 + \ldots) \tag{4.c}$$

where now A and B are constant on the time scale of the variations of $b(.)$, i. e. 1. Moreover, one may verify that – thanks to the $1/2b(t)$ factor in (4.c) – the previous constant of the motion is simply equal (at dominant order) to $|A|^2 + |B|^2$, if one admits that $|A|$ and $|B|$ have the same order of magnitude, a point proved later.

From (3-4), it is clear that this WKB solution has to be changed when b

approaches zero, a situation that I shall analyse now. For simplification, I will assume that b crosses 0 in a generic fashion, and that it does that at $t = 0$. Thus, this « generic » $b(t)$ has near $t = 0$ the following Taylor expansion:

$$b(t) = \beta t + \beta' t^2 + \ldots \tag{5}$$

where β, β' are large, as well as the higher order coefficients. Delightful mathematics could be made if $b(.)$ were to behave in a more complicated way near its zeroes. One could think, for instance, to a « general » algebraic behavior of $b(.)$ as $b \simeq \beta \mid t \mid^{\alpha}, \alpha > 0$ or $b \simeq \beta \operatorname{sgn} t \mid t \mid^{\alpha}$ [$\operatorname{sgn}(.) = \text{sign of}(.)$], or even more complicated things. Such power laws could be handled more or less as the generic case of eq. (5), although a transcendental behavior as $b(t) \sim \beta t \exp - (t_0^2/t^2)$ for instance would pose a more difficult and specific problem.

The general strategy for dealing with turning points is to formulate an inner problem with « stretched variables » and then, by asymptotic matching, to get the M.T. relating the values of the WKB parameters (here A and B) on both sides of the turning point. We shall do this now.

Near this turning point, one replaces in (3) the function $b(.)$ by the first term in its Taylor expansion (5), to get the « inner equation »:

$$\tilde{\phi} + \tilde{\phi} - 2i\beta t \dot{\tilde{\phi}} = 0,$$

where $\tilde{\phi}$ is for the value of ϕ in the inner domain. Assuming first $\beta > 0$, one makes the stretching transformation $t \to \theta = \beta^{1/2} t$ that yields:

$$\tilde{\phi}_{\theta\theta} + \beta^{-1}\tilde{\phi} - 2i\theta\tilde{\phi}_{\theta} = 0. \tag{6.a}$$

where the subscript θ means derivative with respect to θ, to avoid confusion with the dots meaning derivative with respect to the original time variable t. At large β, one can solve this equation by power expansion in β^{-1}. The formally dominant term as well as the first correction read:

$$\phi = u + v \int_0^{\theta} d\theta' e^{i\theta'^2} - \beta^{-1}\left[\int_0^{\theta} d\theta' e^{i\theta'^2} \int_0^{\theta'} d\theta'' e^{-i\theta''^2} \times \left(u + v\int_0^{\theta''} d\theta''' e^{i\theta'''^2}\right)\right] + \mathcal{O}(\beta^{-2}) \tag{6.b}$$

where u and v are arbitrary complex numbers.

Before to go on, we have to give the order of magnitude of u and v with respect to β. From the following asymptotics of the Fresnel integral:

$$\int_0^{\theta} d\theta' e^{i\theta'^2} \underset{\theta\to\infty}{\simeq} \frac{\sqrt{2\pi}}{4}(1+i)\operatorname{sgn}\theta + \frac{ie^{i\theta^2}}{2\theta} + \ldots,$$

the first two terms on the right hand side of eq. (6.*b*) give:

$$u+v\int_0^{\theta} d\theta' e^{i\theta'^2} \underset{\theta\to\infty}{\simeq} \left(u+v\frac{\sqrt{2\pi}}{4}(1+i)\,\mathrm{sgn}\,\theta\right)+\frac{ive^{i\theta^2}}{2\theta}+\ldots, \tag{7}$$

or with the unstretched time:

$$u+v\int_0^{\theta} d\theta' e^{i\theta'^2} \underset{t\sim\beta^{-1/2}}{\simeq} \left(u+v\frac{\sqrt{2\pi}}{4}(1+i)\,\mathrm{sgn}\,t\right)+\frac{ive^{i\beta t^2}}{2\beta^{1/2}t}+\ldots \tag{8}$$

By comparison with the small t-behavior of the WKB solution given in (3, 4), one has – again at dominant order in β:

$$u \simeq A \tag{9.a}$$

and

$$v \simeq -iB\beta^{-1/2} \tag{9.b}$$

If one assumes (as it will be proved later on) that both A and B have the order of magnitude 1, thus $u \sim 1$ and $v \sim \beta^{-1/2}$. On the other hand, one deduces from (9) that, at the dominant order, the M. T. is trivial because A and B keep the same value on both sides of the turning point. However, this does not imply that these crossings have a negligible effect. For many successive crossing may become effective by accumulating small perturbations. And it will turn out that this is what happens.

The M.T. for A is easy to find from (8) and (9): the $(\mathrm{sgn}\,t)$ term leads to a change of order $\beta^{-1/2}$ [that is the order of magnitude of v, from (9.*b*)] for A. Let A_+ (resp. A_-) be the value of A after (resp. before) the turning point. Thus:

$$A_{\pm} = u \pm \frac{v\sqrt{2\pi}}{4}(1+i)$$

or, from (9.*b*), at the dominant order in $\beta^{-1/2}$:

$$A_+ = A_- + \frac{B_-\sqrt{2\pi}}{2}(1-i)\beta^{-1/2} \tag{10.a}$$

The equivalent transformation for B follows from the consideration of terms behaving asymptotically as $(e^{i\theta^2}/\theta)$ on the right hand side of (6.*b*). One of those terms is already written explicitly on the right hand side of eq. (7), and yields the relation between v and B given in (9.*b*), and valid at the dominant order only. The first correction to this (trivial) M.T. requires the knowledge of the large θ behavior of

$$I(\theta) \equiv \int_0^{\theta} d\theta' e^{i\theta'^2} \int_0^{\theta'} d\theta'' e^{i\theta''^2}.$$

By integration in polar coordinates:

$$I(\theta) = \frac{i}{2}\int_{\pi/4}^{\pi} d\gamma (e^{-i\theta^2/\sin^2\gamma} - 1)$$

and after a few elementary transformations:

$$I(\theta) = \frac{i \mid \theta \mid e^{-i\theta^2}}{4} \int_0^{\theta^2} \frac{d\eta}{\eta^{1/2}(\eta + \theta^2)} (e^{-i\eta} - e^{i\theta^2}),$$

from which one deduces:

$$I(\theta) \simeq -\frac{i\pi e^{i\theta^2}}{4} + e^{-i\theta^2} \frac{\sqrt{2\pi}}{8} (1 - i) \operatorname{sgn} \theta + \ldots$$

Comparing now the coefficient in front of the $(\beta t)^{-1}$ contribution resulting from (4.*b*), (6.*b*) and from the above computation, one obtains:

$$B_+ \simeq B_- - \beta^{-1/2}(1 + i)\sqrt{\frac{\pi}{2}} A_- . \qquad (10.b)$$

Again, this relation, as (10.*a*) is only valid up to the order $\beta^{-1/2}$ included. Let us also remark that the terms of order $\beta^{-1/2}$ in (10.*a*-*b*) are such that $|A_+|^2 + |B_+|^2 = |A_-|^2 + |B_-|^2$, up to the order $\beta^{-1/2}$ included.

It is thinkable that, although time dependent, $b(.)$ never reaches zero, and one could ask whether A_0 and B_0 become exact invariants in that case. Indeed these invariants should be equal to A_0 and B_0 at lowest order only, but it can be shown that these quantities are the dominant terms in infinite expansions involving formally two constants of motion. However this is only an algebraic property of these expansions, and it is not true in general [*3*] that such adiabatic invariants are exact invariants. In particular, unless special circumstances, the radius of convergence of these expansions is zero. As it is well known, these adiabatic expansions (unless they are turning points) never couples the two rapid phase factors, that is – in the present case – one may assume (for instance) that A is zero, and get all terms in this expansion that are proportional to the phase χ_-^2. However, if the complex extension of $b(.)$ has a finite strip of analyticity near the real time axis, the Fourier component of $b(.)$ at the large frequency b is of order $\exp -(1/|b|t_0)$, where t_0 is the distance of the nearest singularity of this complex extension of $b(.)$ to the real axis. Thus, if $b(.)$ never crosses zero, and if $t_0 \neq 0$, the speed of variation of the adiabatic invariants is transcendentally small for b large, as well as the Floquet eigenvalues μ and ν defined before for a periodic large b.

In what follows, I shall be only concerned with situations where $b(.)$ crosses zero at a more or less constant rate, so that the evolution of A and B is mainly due to the M.T. described by eq. (10).

To understand the secular effect of the M.T. given by eq. (10), let us consider first the case of a periodic $b(.)$ taking the zero value twice per period. At the price of some more formalism, situations with more than two zeroes per period could be handled too. Let T be this period of $b(.)$, i. e. the smallest T such that $b(t+T)=b(t)$ for any t. Let furthermore $\beta_\pm$

be the values of b at these zeroes. From (10), it is natural to introduce the linear operator

$$\tilde{H}=(|\beta_+|^{-1/2}+|\beta_-|^{-1/2})\sqrt{\frac{\pi}{2}}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}+(|\beta_+|^{1/2}-|\beta_-|^{-1/2})\sqrt{\frac{\pi}{2}}\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}.$$

The action of many periods of $b(.)$ on $\psi \equiv \begin{pmatrix}A\\ B\end{pmatrix}$ (that may be seen as a 1/2 spinor) can thus be described by saying that $\psi(t) \equiv \begin{pmatrix}A(t)\\ B(t)\end{pmatrix}$ is the solution of a « Schrödinger like » equation with constant coefficients:

$$i\frac{d}{dt}\psi = \mathscr{H}\psi$$

where $\mathscr{H}$ is the Hermitian operator $(-i\hat{\mathscr{H}}/T)$. With this definition of $\mathscr{H}$, the eigenvalue of $\mathscr{H}$ are the two Floquet exponents μ and ν introduced at the beginning.

If the behavior of $b(.)$ is less regular than the one of a simple periodic function, the above method, as it stands cannot be applied to estimate the long term behavior of ψ. Thus, it becomes convenient to measure the time by the number n of crossing of $b(.)$ through zero, and thus to consider n as continuous, because each crossing yields a small variation of ψ only. If $b(.)$ is a random function with a finite correlation time, i. e. if $b(.)$ is of the form $\lambda\hat{b}(t)$, $\lambda \to \infty$, $\hat{b}(.)$ random and λ-independent the analysis can be pursued because, again, the variation of ψ at each crossing of $b(.)$ with zero is small. The state of the system is a vector in C^2, bound to lie on the unit Hermitian sphere S^2_C (or $S^4_{\mathbb{R}}$), by the conservation of probability, and each crossing induces a small shift of ψ on this sphere. For a random $b(.)$ this shift has a mean value plus some fluctuating part. As each step is small, this is typically the kind of assumption needed to have Brownian diffusion on S^2_C. The corresponding diffusion equation can be derived by applying standard methods in the theory of stochastic processes. To simplify the writing, let us introduce the (small) random variable ε_j, where j is the index of the j^{th} crossing, the M.T. at this crossing being represented as

$$\psi_{j+1} = \begin{pmatrix}1 & \varepsilon_j\\ -\varepsilon_j^* & 1\end{pmatrix}\psi_j \tag{11}$$

and from our previous discussion:

$$\varepsilon_j = \left|\frac{\pi}{2\beta_j}\right|^{1/2}.(1 + i\,\mathrm{sgn}\,\beta_j)$$

β_j being the value of $\dot{b}$ at the j^{th} value of the time such that $b(t) = 0$. The

spinor $\psi = \begin{pmatrix} A \\ B \end{pmatrix}$ can be represented by three angles φ, η_A and η_B such that $A = \cos\varphi e^{i\eta_A}$, $B = \sin\varphi e^{i\eta_B}$. If $|\varepsilon_j| \ll 1$, the M.T. given by eq. (11) induces small changes of φ, $\eta_{A/B}$ that can be found easily from the above equation in the small ε-limit :

$$\Delta_j\eta = \frac{1}{2}\cot 2\varphi \operatorname{Im}(\varepsilon_j e^{i\eta}) \tag{12.a}$$

$$\Delta_j\varphi = -\operatorname{Re}(\varepsilon_j e^{i\eta}) \tag{12.b}$$

where $\eta \equiv \eta_A - \eta_B$, $\Delta_j(.)$ is for the small difference $(.)_{j+1} - (.)_j$ and where Re( ) and Im( ) are for real and imaginary part of their argument.

Considering now the right hand side of (12.*a-b*) as quantities with a mean value plus some random part of zero average, one get from this an equation for the evolution of the probability distribution $P(\eta, \varphi; n)$ where n is considered as a continuous (time) parameter:

$$\frac{\partial}{\partial n}P + \frac{\partial}{\partial\eta}\left(\frac{1}{2}\cot\varphi \operatorname{Im}(\bar{\varepsilon}e^{i\eta})P\right) - \frac{\partial}{\partial\varphi}(\operatorname{Re}(\bar{\varepsilon}e^{i\eta})P)$$
$$= (D^{\varphi\varphi}P_\varphi)_\varphi + (D^{\eta\eta}P_\eta)_\eta + (D^{\varphi\eta}P_\eta)_\varphi + (D^{\eta\varphi}P_\varphi)_\eta \tag{13}$$

In this equation ε is the mean value of ε (over the discrete time index), although the diffusion coefficients $D^{\varphi\varphi}$, $D^{\eta\eta}$, ... are related to autocorrelation functions of the fluctuating part of ε, i. e. to $\tilde{\varepsilon}_j = \varepsilon_j - \bar{\varepsilon}$, by the Einstein-like expressions:

$$D^{ab} = \sum_{j=1}^{\infty} \langle J^a(j_0)J^b(j + j_0)\rangle \tag{14}$$

where the fluctuating « currents » J^a ($a = \varphi$ or η) have the form

$$J^\varphi(j) = \operatorname{Re}(\tilde{\varepsilon}_j e^{i\eta}) \tag{15.a}$$

and

$$J^\eta(j) = -\cot 2\varphi \operatorname{Im}(\tilde{\varepsilon}_j e^{i\eta}). \tag{15.b}$$

The values of the quantities φ and η that appear on the right hand side of (15.*a-b*) must be considered as j-independent, since the correlation of $\tilde{\varepsilon}$ decays much faster than φ and η varies. Notice also that, except for the case $\bar{\varepsilon} = 0$, where P constant is an obviously steady (= η independent) solution of (13), it does not seem possible to have in general this steady solution in a simple closed from.

2. A PARTICLE IN A CONSTANT POTENTIAL AND A STRONG EXTERNAL FIELD

Below, I consider the following class of problems: a particle is submitted both to a constant potential $v(x)$ that could be, for instance, the Coulomb

potential generated by an ion, plus a large time dependent external field. The Schrödinger equation for this case reads in dimensionless notations:

$$i\dot{\psi} = -\frac{1}{2}\psi_{xx} + v(x)\psi + xb(t)\psi\,. \tag{16}$$

To make the various expressions simpler, this has been written with one space dimension (x) only, although thereafter the results will be extended to the physically more meaningful situation in $3d$. The last term on the right hand side of (16) represents the effect of the large external field. This one is supposed to be homogeneous at the space scales considered, whence the simple x-dependence of this term.

One could try to use methods similar to the ones of the previous section for the present case. However, the situation is quite different here. As we shall see it, the turning point phenomena near the zeroes of $b(.)$ have no specific effect. This is because the operator in front of the large external force, i. e. x, has a continuous spectrum going up to zero. So, at least for small values of x, the fact that $b(.)$ is zero or not is not as important as when this spectrum has a gap, as in the case considered before. I will show first that thanks to a few simple transformations, a large $b(.)$ can be handled by the general method of Kapitza [*4*], developed for mechanical systems having parameters varying with a very small period. Afterwards, I shall discuss, as an example of application of the general theory, the case of a $3d$ Coulomb potential $v(.)$.

To show the possibility of applying the method of Kapitza to the present problem [that is $b(.)$ large in (16)], one has to make first a few simple transformations on (16). As these transformations rely upon elementary manipulations, I shall list them only. First multiply ψ by the phase factor $\exp -i\left[x\int_0^t b(t')dt' + \int_0^t\left[\int_0^{t'} b(t'')dt''\right]^2 dt'\right]$. Then define $\Lambda(t) \equiv \int_0^t dt' \int_0^{t'} dt'' b(t'')$ and take $X = x + \Lambda(t)$, $T = t$ as new pair of variables. The modified wavefunctions obeys the equation

$$i\phi_T = -\frac{1}{2}\phi_{xx} + v(x - \Lambda(T))\phi\,. \tag{17}$$

Indeed, $\Lambda(T)$ is the displacement of a classical particle (of unit mass) submitted to the field $b(t)$ between time 0 and T, so that (17) results from the application to (16) of the canonical mapping describing this displacement. Now we will show that a large b (and thus a large Λ) implies that $v(X - \Lambda(T))$ is a rapidly varying function of time. As this is not completely obvious, I shall show this in some details for a periodic $\Lambda(T)$. Let x_0 be the range of $v(x)$, *a priori* much smaller than the typical value of the displacement Λ, say λ. Thus, if T_0 is the period of $\Lambda(.)$, the amount of time

during which $v(X - \Lambda(T))$ differs from 0 at a fixed X will be of order $(x_0/\lambda)T$ if $|X| < \lambda$, and zero otherwise. This amount of time is thus very short and, for a given X, $v(X - \Lambda(T))$ will be felt as a rapidly varying potential. But this is not enough: to apply the Kapitza averaging, one has to have a potential $v(.)$ varying much more rapidly than any quantity relevant for the particle motion. This implies certainly $|x_0| \ll \lambda$, but also that the frequency of variation of the potential is much larger (for instance) than the typical Planck frequency of the bound states in the effective potential resulting from this Kapitza averaging. This avoids (*) the following paradox: λ diverges in the low frequency limit, and for a fixed field strength, although it is well known that, in the limit of a steady external field, whether small or large, there is certainly no bound state. The answer to this paradox is that the introduction of a constant effective potential is no longer justified if the frequency of the external field is of the same order or less than the typical Planck frequency in the effective potential.

So, under the conditions of applicability of the Kapitza approximation, one may replace $v(x - \Lambda(T))$ by its mean value over time. To be more specific, I shall assume a simple sinusoidal dependence of $\Lambda(T)$ in the form $\Lambda(T) = \lambda \sin\left(\frac{2\pi T}{T_0}\right)(\lambda > 0)$, so that the effective potential $V_\lambda(x)$ will be given by

$$V_\lambda(x) = \frac{1}{T_0}\int_0^{T_0} dT\, v\left(x - \lambda \sin\left(\frac{2\pi T}{T_0}\right)\right). \tag{18.a}$$

This effective potential is an Abel transform of $v(x)$:

$$V_\lambda(x) = \frac{3}{\pi}\int_{-1}^{+1} \frac{du}{\sqrt{1-u^2}}\, v(x - \lambda u). \tag{18.b}$$

If λ much larger than the range of v that is the limit in which we are interested, one has:

$$V_\lambda(x) \simeq \frac{w}{(\lambda^2 - x^2)^{1/2}} \tag{18.c}$$

for $|x| < \lambda$ and $V_\lambda(x) = 0$ otherwise. In this last expression, $w = \frac{1}{2}\int_{-\infty}^{+\infty} dy\, v(y)$ is assumed to be non zero and finite.

The energy E of the bound states in the potential $V_\lambda(x)$ appears as the negative eigenvalue defined by:

$$\left[\frac{1}{2}\frac{\partial^2}{\partial X^2} + (E - V_\lambda(X))\right]\psi(X) = 0 \tag{19}$$

(*) As pointed out to me by C. Itzykson.

where $V_\lambda(x) = \dfrac{w}{(\lambda^2 - x^2)^{1/2}}$ for $|x| < \lambda$ and zero otherwise, $\psi(x)$ being C^1 at $x = \pm\lambda$ and tending to zero at $x \to \pm\infty$. Indeed such bound states exist if $w < 0$ only. The case $w = 0$ would require to go to next order, in a way rather similar to the one followed by Cook at al. [5]. As the limit $\lambda \to \infty$, w fixed > 0 poses by itself an interesting problem, we shall sketch now its solution. In this limit, the potential $V_\lambda(x)$ cannot be replaced by an uniform approximation, because of the two inverse square root singularities at $x = \pm |\lambda|_{\mp}$. For the « highly excited » bound states, these square root singularities lead to a special kind of turning point in the WKB solution of (19). Otherwise, the low bound states split by tunnelling between the two potential walls near $x = \pm\lambda$.

Let us consider these « deep » bound states. Putting $x = -\lambda + z$, one may replace $V_\lambda(x)$ near $z \sim 0$ by:

$$V_\lambda(z + \lambda) \underset{z \to 0_+}{\simeq} \frac{w}{(2\lambda z)^{1/2}} \tag{20}$$

and $V_\lambda = 0$ for $z < 0$. But for this kind of dependence of V_λ, it is possible to get rid of the λ-parameter. This is done by scaling energies as $\lambda^{-2/3} |w|^{4/3}$ and lengths as $\lambda^{1/3} |w|^{2/3}$ and yields the following dimensionless form for the « Schrödinger equation » for the first bound states:

$$\left(\frac{1}{2}\frac{d^2}{d\bar{z}^2} + (\bar{E} - \bar{V}(\bar{z}))\right)\psi(\bar{z}) = 0\,, \tag{21}$$

where the bars indicate that the quantities have been scaled as explained before, so that $\bar{V}(\bar{z}) = -(\bar{z})^{-1/2}$ for $\bar{z} > 0$ and $\bar{V} = 0$ otherwise. Note that the length scaling with $\lambda^{1/3}$ is in agreement with the fact that one has taken an approximate form of $V_\lambda(x)$ near $x = \lambda$, since $V_\lambda(x)$ varies over a length of order λ. By tunnelling between the two potential wells near $x = +\lambda$ and $x = -\lambda$, the bound states given by the solution of (21) split into two levels, one symmetric (the one with the lowest energy) and one antisymmetric with respect to $x = 0$.

The highly excited state are outside of the range of applicability of the scaling leading to (21), as their wavefunctions extend significantly over the full range of potential $V_\lambda(x)$, and not only nearby its singularities. These excited states are amenable to a WKB-analysis, but this one is more complicated than usually, because the turning points ($x = \pm\lambda$) represent also singularities of the potential, so that the wave function near the turning point is not given by the solution of the usual Airy equation, but merely by the solution of (21) for $\bar{E}$ very close to zero.

Actually they are two possible sorts of turning point. If the energy is between the ground state energy and w/λ, the equation $E = V_\lambda(x)$ has four

solutions: $x = \pm \lambda$ and $\pm\left(\lambda - \frac{w^2}{E^2}\right)^{1/2}$, the « regular » turning points although if $\frac{w}{\lambda} < E < 0$, the only turning point are at $x = \pm \lambda$.

Let us consider first this last situation. Outside the vicinity of the (irregular) turning point, the WKB solution reads:

$$x > \lambda \qquad \psi = a_+ e^{-2|E|^{1/2}x} \tag{22.a}$$

$$x < -\lambda \qquad \psi = a_- e^{+2|E|^{1/2}x} \tag{22.b}$$

$$-\lambda < x < +\lambda \; \psi = \sum_{j=\pm} \alpha_j \exp \pm i \int_0^x [2(E - V_\lambda(x'))]^{1/2} dx'. \tag{22.c}$$

To match the different forms of this WKB solution on both sides of each turning point, one needs to have the solution of the « inner problem » near the inverse square root singularity. As seen before, the energy scale near this singularity is of order $\lambda^{-2/3}$, although we are interested here by energies of order λ^{-1}, so that in (19) one may neglect near this singularity the energy E with respect to the other terms and the wave equation near the turning point reads:

$$\left(\frac{1}{2}\frac{d^2}{dz^2} - \tilde{V}_\lambda(z)\right)\psi(z) = 0 \tag{23}$$

where $z = \lambda - x$, $\tilde{V}_\lambda(z) = \frac{w}{(-2\lambda z)^{1/2}}$ for $z < 0$ and zero otherwise.

The general solution of the differential equation

$$\left(\frac{d^2}{dz^2} + uz^{-1/2}\right) f(z) = 0 \tag{24}$$

$$u > 0, \; z < 0 \quad \text{is} \quad f(z) = z^{1/2} Z_{2/3}\left(\frac{4\,|u|^{1/2}}{3} z^{3/4}\right),$$

where Z is any linear combination of the Bessel functions J and N. These two functions differ by their Laurent expansion near $z = 0_+$. They are $f \simeq C_0\left(1 - \frac{4u}{3} z^{3/2} + \ldots\right)$ or $f \simeq C_0'\left(z - \frac{4u}{15} z^{5/2} + \ldots\right)$, as can be seen by direct substitution into (24). In the domain $z < 0$, the wavefunction is a slowly decreasing exponential. At dominant order, this exponential can be matched only with the first Laurent expansion above, that corresponds to the N-solution of (24). Furthermore, the inner-outer matching fixes — as usual — the undetermined phase of the outer oscillating solution and finally specifies the constant part of the phase shift in the Bohr-Sommerfeld quantization condition.

The asymptotic behavior of the inner solution is:

$$z^{1/2}N_{2/3}\left(\frac{4\,|\,u\,|^{1/2}}{3}\,z^{3/4}\right)\underset{z\to\infty}{\simeq}\left(\frac{3}{2\pi\,|\,u\,|}\right)^{1/2}z^{1/8}\sin\left(\frac{4\,|\,u\,|^{1/2}}{3}\,z^{3/4}+\frac{\pi}{12}\right)\quad(25)$$

although the phase of the W.K.B. solution, as given by (22.*c*), is of the form $\int_0^x (2(E - V(x'))^{1/2}dx' + \varphi_0$, where φ_0 is —for the moment arbitrary. Near $x = 0$, one may neglect in this expression the energy E and replace $V_\lambda(x')$ by $(w/2\lambda z)^{1/2}$, with $z = \lambda - x$, as done before. Whence the W.K.B. phase factor takes the form $\varphi_0 + \frac{4}{3}\left(-\frac{w}{3}\right)^{1/2} z^{3/4}$. Assuming now that the W.K.B. phase occurs in a sine function and comparing the argument of this function with eq. (25), one obtains $\varphi_0 = \frac{\pi}{12}$. In case of wavefunctions with two singular turning points $\left(0 < -E < -\frac{w}{\lambda}\right)$, the phase shift has to be added twice in the Bohr-Sommerfeld quantization rule that reads:

$$\int_{-\lambda}^{+\lambda} dx'(2(E - V_\lambda(x'))^{1/2} = \left(n + \frac{1}{6}\right)\pi \qquad (26.a)$$

n being some (large) index level. This equation, relating E to n, was derived under the assumption that they are two singular turning points at $x = \pm\lambda$. If the (negative) energy E is such that

$$\lambda^{-1/3} \gg -E > -\frac{w}{\lambda}$$

the wavefunction has both a regular turning point at one of the two roots $x(E)$ of $V_\lambda(x) = E$, and a singular one at $x = +$ or $-\lambda$. If one neglects tunnelling through the middle part of the potential $V_\lambda(x)$, one finds as a quantization condition

$$\int_{-\lambda}^{x(E)} dx'\,[2(E - V_\lambda(x')]^{1/2} = \left(n' + \frac{1}{3}\right)\pi$$

where $x(E)$ is the negative root of $E = V_\lambda(x)$, i.e. $(E^2\lambda^2 - w^2)^{1/2}/E$ [recall that $V_\lambda(x) = \frac{w}{(\lambda^2 - x^2)^{1/2}}$].

Indeed they are two levels with the same energy on both sides of the central potential barrier. They are actually split in two by tunnelling. However, this tunnelling contribution to splitting may be dominated by an assymmetry of $V_\lambda(x)$ near its two minima arising from an assymmetry in $w(x)$. This effect is absent only at dominant order in λ^{-1}. It would be

proportionnal to $\lambda^{-2} \int_{-\infty}^{+\infty} dx . xw(x)$ (if this integral converges to a non zero value).

Let us extend now the previous considerations to electrons in a central attracting Coulomb field. A simple remark has to be made first. Particles with the same e/m ratio have the same $\Lambda(.)$, so that the Coulomb repulsion between identical electrons remains unchanged by the presence of the strong external electric field. But, as we shall see it, the attraction by a central ion is considerably lowered. Accordingly, it is reasonable to believe that bound states in a strong external field will exist for single electron atoms or ions only, that is what we shall consider now.

Let a linearly polarized electric field act on an electron bound to an ion in the dipolar approximation, i. e. I shall assume that the wavelength of the incident e. m. wave is much larger than any other typical length, in particular $|\Lambda|$. In dimensionless variables (energies are measured in Rydberg, length in Bohr radius and electric fields in Volts/Bohr radius), the Schrödinger equation of this system reads:

$$i\dot{\psi} = -\frac{1}{2}\Delta\psi - \frac{1}{r}\psi + xb(t)\psi \tag{27}$$

x being the direction of polarization of the electric field, of intensity $b(.)$, Δ is the $3d$-Laplacian and $r = (x^2 + y^2 + z^2)^{1/2}$ is the distance of the electron to the central ion, supposed to be fixed. Transformations similar to the one leading from (16) to (17) allow to transform (27) into

$$i\phi_T = -\frac{1}{2}(\partial_{x^2}^2 + \partial_{y^2}^2 + \partial_{z^2}^2)\phi - ((x - \Lambda(t))^2 + y^2 + z^2)^{-1/2}\phi \tag{28}$$

As the Coulomb potential has no convergent mean value, one does not have in the present case a simple form for the effective constant potential in the large Λ limit. The form of this effective potential depends on the domain of space where one computes it. Let us consider first the more deeply bound states, for an oscillating $\Lambda(t)$ in the form $\lambda \sin \Omega t$, $\lambda \gg 1$. As in the $1d$ case, the effective potential has two minima near $x = \pm \lambda$. The general expression for this effective potential is:

$$\overline{V}_\lambda(x, \rho) = \frac{1}{2\pi}\int_0^{2\pi} \frac{dt}{(\rho^2 + (x - \lambda \cos t)^2)^{1/2}} \tag{29}$$

where $\rho^2 = x^2 + y^2$. The minimum of V_λ corresponds to the vicinity of $t = 0$, 2π and π in the integration domain. Near these values, one may replace $\cos t$ by its Taylor expansion, and get (for $x \simeq \lambda$ for instance):

$$V_\lambda(x, \rho) \simeq \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\bar{t}}{(\rho^2 + (x - \lambda(1 - \bar{t}^2/2))^2)^{1/2}} .$$

Posing $x - \lambda = \delta$, with $\delta \ll \lambda$, one obtains, after a few elementary transformations:

$$\bar{V}_\lambda(\lambda + \delta, \rho) \simeq \frac{1}{(\lambda \mid \delta \mid)^{1/2}} F(\rho/\delta)$$

where F(.) is defined as

$$F(u) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\theta}{(u^2 + (\operatorname{sgn} u - (\theta^2/2))^2)^{1/2}}$$

and can be expressed by elliptic integrals. Taking now $\lambda^{1/3}$ as unit length and $\lambda^{-2/3}$ as energy unit, one finds that the ground state energy is the lowest (negative) eigenvalue of the parameterless linear operator

$$\frac{1}{2}\left(\partial_{z^2}^2 + \partial_{\rho^2}^2 + \frac{1}{\rho}\partial_\rho\right) + z^{-1/2} F(\rho/z).$$

This possibility of having bound states localized over distances much less than λ depends in an essential manner on the fact that $\Lambda(t)$ reaches a maximum where the attracting potential can be more effective because the electron spends here more time than in other parts of space. For the other polarizations of the external field the situation may be quite different. Consider for instance a circularly polarized external field, that is a perturbation $\omega^2\lambda(x \sin \omega t + y \cos \omega t)$ to the Hamiltonian. The effective potential has the form

$$\bar{V}_\lambda(z, \rho) = \frac{1}{2\pi} \int_0^{2\pi} \frac{d\bar{t}}{(\lambda^2 + z^2 + \rho^2 - 2\lambda\rho \cos \bar{t})^{1/2}} \tag{30}$$

where $\rho = (x^2 + y^2)^{1/2}$ (not to be confused with the quantity called ρ before). This potential has the extremum values λ^{-1} for $z = \rho = 0$. However this corresponds to a local maximum, so that the wavefunction of the ground state is merely concentrated around the minimum of $\bar{V}_\lambda(z, \rho)$. Writing the denominator on the right hand side of (30) as:

$$z^2 + (\lambda - \rho)^2 + 2\lambda\rho(1 - \cos t)$$

one sees that the minimum of $\bar{V}_\lambda(z, \rho)$ is reached for $x = 0$, $\lambda = \rho$, and that $V_\lambda(z, \rho)$ has a logarithmic divergence here.

Putting $R = \rho - \lambda$, one has

$$V_\lambda(z, R) = \frac{2}{(R^2 + z^2 + 4\lambda\rho)^{1/2}} \mathbb{K}\left(\left(\frac{4\lambda\rho}{R^2 + z^2 + 4\lambda\rho}\right)^{1/2}\right) \tag{31}$$

where $\mathbb{K}$ is the elliptic period. We are interested in the limit of λ large $| z | \ll \lambda$ and $\rho \simeq \lambda$. In this limit, the argument of $\mathbb{K}$ is close to 1 and the potential V expands as:

$$V_\lambda(z, R) \simeq \frac{1}{\pi\lambda} \ln\left(\frac{4\lambda\rho + R^2 + z^2}{R^2 + z^2}\right).$$

Scaling now lengths as $\lambda^{1/2}$, one gets the result that, for large λ, the energies of the bound states of the potential $V_\lambda(z, R)$ are of the form $\lambda^{-1}(-\ln\lambda + e_n)$, where e_n is the energy (a dimensionless number) of the n^{th} bound state in the 2^d-potential $2\ln(R^2 + z^2)$, the kinetic energy operator being $-\frac{1}{2}(\partial^2_{R^2} + \partial^2_{z^2})$. However, this approximation fails for very excited states, reaching regions of the (R, z) space such that $R \sim z \sim \lambda$, and that $e_n \sim \ln\lambda$. These states are amenable to a WKB analysis, in the potential $V_\lambda(z, R)$, given by (31) but without any more approximation for V_λ. However, as we are not dealing anymore with a central potential, because R and z (or ρ and z) does not enter only through the combination $(R^2 + z^2)$ (or $(\rho^2 + z^2)$) in (31), the only simple result from this WKB analysis would be contained in a Weyl like formula for the number of levels with an energy less than some fixed quantity.

CONCLUDING REMARKS

As a conclusion, let us recall that — at least for specific examples — it has been possible to treat in a rather detailed fashion the situation of large time independent forces acting on quantum systems. For particles moving in a central potential, this leads quite naturally to the Kapitza averaging method, a point that is not completely obvious when one looks at the formulation of the problem.

Indeed it is natural to ask whether this could have some application to concrete physical systems. Besides atomic physics, that could require prohibitively large electric fields, one might think to much less strongly bounded systems, to decrease the needed external field, as the electrons on the surface of liquid helium or conduction electrons in modulated superlattices. However, if those states are too weakly bound, thermal fluctuations will make it difficult — if not impossible — to observe them, although the coupling with thermal radiation becomes less and less efficient as the frequency decreases, so that this effect of the thermal noise could be more or less suppressed.

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