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QUANTUM DYNAMICS OF A PARTICLE IN A PLANE WAVE

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Abstract

We discuss quantum dynamics of a particle in a time and space periodic field. We consider a soluble model of a particle in a plane wave. We reduce the quantum problem to a random Riccati equation. We show that solutions of the Riccati equation experience an abrupt change from a periodic to non-periodic behaviour under a variation of classical parameters with respect to the Planck constant. As a consequence the classical results on the particle trapping by an electromagnetic wave need a quantum correction.

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I. Introduction.

It is a basic question in the theory of periodic quantum systems (see e.g. ref.[1]) whether the solutions are quasiperiodic or not. The problem is closely related to the stability of these systems. We cannot answer this question through a perturbation expansion, because of the small denominators, which are an obstacle to a proof of the quasiperiodicity of the sum. We discuss in this paper a soluble model of stochastic dynamics equivalent to the quantum mechanics. The model allows a classical description of the phenomena which lead to quantum instability. Our model is a particular example of a particle in an electromagnetic field discussed in refs.[2]-[5]. It is known that the particle is either trapped by the wave (if the wave amplitude is large with respect to its frequency) or moves in a complicated oscillatory way (if the frequency of the wave is sufficiently large).

We consider in our model the following scalar potential

$$V = \frac{m}{4}(\alpha^2 - \beta^2) \cos(2x + 2\omega t) - \frac{m\alpha\beta}{2} \sin(2x + 2\omega t) + m\alpha\omega \sin(x + \omega t) + m\beta\omega \cos(x + \omega t) \quad (1)$$

We can find a particular solution of the classical Hamilton-Jacobi equation

$$\partial_t S_t + \frac{1}{2m}(\nabla S_t)^2 + V = 0 \quad (2)$$

The solution is

$$S_t(x) = m\alpha \cos(x + \omega t) - m\beta \sin(x + \omega t) + \frac{m}{4}(\alpha^2 + \beta^2)t \quad (3)$$

$S_0(x)$ could be considered as the Hamilton-Jacobi description of the separatrix. The classical equation of motion resulting from the solution (3) has the form (it becomes the conventional pendulum's separatrix equation when $\omega = \beta = 0$)

$$\frac{dx}{dt} = \alpha \sin(x + \omega t) + \beta \cos(x + \omega t) \quad (4)$$

Eq.(4) is explicitly integrable. Let

$$\xi = x + \omega t \quad \text{and} \quad u = \text{tg}(\frac{1}{2}\xi) \quad (5)$$

Then,

$$\frac{du}{dt} = \frac{1}{2}(\omega - \beta)u^2 + \alpha u + \frac{1}{2}(\omega + \beta) \quad (6)$$

It is clear from eq.(6) that properties of its solution depend in a crucial way on whether

$$\alpha^2 + \beta^2 \leq \omega^2 \quad (\text{a particle is trapped}) \quad \text{or} \quad \alpha^2 + \beta^2 > \omega^2 \quad (\text{lack of trapping})$$

In the first case the particle moves with the wave and for large time the only effect of the non-linear dynamics is a phase shift (the phase shift tends to a constant with an exponential speed). In the second case the particle oscillates with its own frequency

$$\mu = \sqrt{\omega^2 - \alpha^2 - \beta^2} \quad (7)$$

II. Stochastic description.

In order to investigate the quantum dynamics we apply a probabilistic formulation of the Feynman integral . So, we write the solution of the Schroedinger equation in the form

$$\psi_t(x) \equiv (U_t \psi)(x) = E[\exp\left(\frac{i}{\hbar} \int_0^t V(x + \sigma b_s) ds\right) \psi(x + \sigma b_t)] \quad (8)$$

Here, $t \geq 0$

$$\sigma = (1+i) \sqrt{\frac{\hbar}{2m}}$$

and the expectation value is with respect to the Brownian motion defined as the Gaussian process with the covariance

$$E[b(t) b(s)] = \min(t, s) \quad (9)$$

The generator of U_t is

$$\frac{1}{i\hbar} H = \frac{i\hbar}{2m} \Delta + \frac{1}{i\hbar} V \quad (10)$$

Assume we know a particular (complex) solution S_t of the Hamilton-Jacobi equation (2) with the initial condition S_0 . Let us write the initial state ψ in the form

$$\psi = \exp\left(\frac{i}{\hbar} S_0\right) \phi \quad (11)$$

Then, the formula (8) can be expressed as

$$\psi_t(x) = \exp\left(\frac{i}{\hbar} S_t(x)\right) E\left[\exp\left\{-\frac{1}{2m} \int_0^t \Delta S_\tau(q_\tau(x)) d\tau\right\} \phi(q_0(x))\right] \quad (12)$$

where q_τ is the solution of the stochastic equation

$$dq_\tau = -\frac{1}{m} \nabla S_\tau d\tau + \sigma db \quad (13)$$

with the boundary condition $q_\tau(x)|_{\tau=t} = x$.

There is another (equivalent) formula which expresses ψ_t by a solution of the stochastic equation (13)

with the initial condition

$$q(x)|_{\tau=0} = x \quad (14)$$

In such a case $\phi(q_0(x))$ in eq (6) is replaced by $\phi(q_t(x))$.

We assume that all functions discussed here are boundary values of analytic functions. Then, the formulas (12)-(13) make sense. We discussed a slightly modified version of eqs.(12)-(13) in our earlier papers [6]-[7]. There, we applied a particular solution of the Schroedinger equation instead of the Hamilton-Jacobi equation. In such a case the exponential factor in the square brackets of eq.(12) is absent.

Note that $\hbar$ enters eq.(12) only through q . The formal classical limit ($\hbar \rightarrow 0$) of eqs.(12)-(13) is

$$\psi_t(x) = \exp\left(\frac{i}{\hbar} S_t(x)\right) \exp\left(-\frac{1}{2m} \int_0^t \Delta S_\tau(x_\tau(x)) d\tau\right) \phi(x_0(x)) \quad (15)$$

$$\frac{dx_\tau}{d\tau} = -\frac{1}{m} \nabla S_\tau(x) \quad (16)$$

where $x_\tau|_{\tau=t} = x$.

We discuss in this paper the model (3)

$$dq = \alpha \sin(q + \omega t) dt + \beta \cos(q + \omega t) dt + \sigma db \quad (17)$$

Using the exponential representation of the trigonometric functions we can transform eq.(17) into the Riccati equation

$$\frac{dz}{dt} = f_0(t) + f_1(t) z + f_2(t) z^2 \quad (18)$$

The Riccati equation can subsequently be linearized by the substitution

$$W(t) = \exp\left(-\int_0^t f_2(s) z(s) ds\right) \quad (19)$$

Then, W fulfills a linear equation

$$\frac{d^2 W}{dt^2} - \left(f_1(t) + \frac{d}{dt} \ln f_2(t)\right) \frac{dW}{dt} + f_0(t) f_2(t) W = 0 \quad (20)$$

In the model (17) we may choose

$$W = \exp\left(-\frac{1}{2}(\alpha - i\beta) \int_0^t \exp(-i\omega s - iq(s)) ds\right) \quad (21)$$

or

$$W_* = \exp\left(-\frac{1}{2}(\alpha + i\beta) \int_0^t \exp(i\omega s + iq(s)) ds\right) \quad (22)$$

Both fulfil linear equations

$$\frac{d^2 W}{dt^2} + i(\omega + \sigma \frac{db}{dt}) \circ \frac{dW}{dt} - \frac{1}{4} (\alpha^2 + \beta^2) W = 0 \quad (23)$$

whereas W_*

$$\frac{d^2 W_*}{dt^2} - i(\omega + \sigma \frac{db}{dt}) \circ \frac{dW_*}{dt} - \frac{1}{4} (\alpha^2 + \beta^2) W_* = 0 \quad (24)$$

where $\circ$ means the Stratonovitch differential [8] (the Stratonovitch form in eq.(24) follows from eq.(17)).

Eqs.(23) -(24) can be rewritten as a well-defined system of two linear stochastic differential equations.

For this purpose let us introduce the notation

$$V^T = (W, \frac{dW}{dt}) \quad (25)$$

then we can write eq.(23) in the form

$$\frac{dV}{dt} = \mathcal{A} \circ V \quad (26)$$

where (the multiplication is understood in the Stratonovitch sense)

$$\mathcal{A} = \begin{bmatrix} 0 & 1 \\ \gamma^2 & \nu_b \end{bmatrix} \quad (27)$$

with $\nu_b = -i(\sigma \frac{db}{dt} + \omega)$ and

$$\gamma^2 = \frac{\alpha^2 + \beta^2}{4} \quad (28)$$

The solution of eq.(27) can be expressed in the form

$$V_t = \mathcal{R}_t V_o \quad (29)$$

where we write $\mathcal{R}$ as a product

$$\mathcal{R}_t = \mathcal{M}_t \mathcal{D}_t \quad (30)$$

where

$$\mathcal{M} = \begin{bmatrix} 1 & 0 \\ 0 & \rho \end{bmatrix}$$

$$\rho_t = \exp \int_0^t \nu_b = \exp(-i\omega t - i\sigma b_t) \quad (31)$$

and $\mathcal{D}_t$ is the solution of the equation (with the initial condition $\mathcal{D}_0 = 1$)

$$\frac{d\mathcal{D}_t}{dt} = \mathcal{B}_t \mathcal{D}_t \quad (32)$$

where

$$\mathcal{B} = \mathcal{M}^{-1} \begin{bmatrix} 0 & 1 \\ \gamma^2 & 0 \end{bmatrix} \mathcal{M} \equiv \begin{bmatrix} 0 & \rho \\ \delta & 0 \end{bmatrix} \quad (33)$$

where

$$\delta(t) = \gamma^2 \rho_t^{-1} = \gamma^2 \exp(i\omega t + i\sigma b_t) \quad (34)$$

We can solve eq.(32) by iteration (the series is convergent).

III. The effect of quantum noise.

At $\sigma = 0$ we would get the classical solution (6). We are interested in the effect of a complex noise on the behaviour of the deterministic solution.

Let us denote $\frac{dW}{dt} = W'$, then eq.(26) can be expressed as a system of two Ito equations

$$\begin{aligned} dW &= W' dt \\ dW' &= -i \left(\omega - \frac{\hbar}{2m} \right) W' dt + \gamma^2 W dt - i\sigma W db \end{aligned} \quad (35)$$

where the relation $f \circ db = f db + \frac{1}{2} df db$ (see ref.[8]), between Stratonovitch and Ito differentials has been used. Let $w = E[W]$, then w is the solution of a deterministic equation

$$\frac{d^2 w}{dt^2} + i \left(\omega - \frac{\hbar}{2m} \right) \frac{dw}{dt} - \gamma^2 w = 0 \quad (36)$$

In order to derive eq.(36) we write eqs.(35) in the Ito integral form, then we take the expectation value and use the property of the Ito integral

$$E[\int f db_s] = 0$$

Rewriting the resulting integral equation for the expectation value $E[W]$ again in a differential form we get eq.(36). We can see from eq.(36) that the only effect of noise on the expectation value is a change of the frequency

$$\omega \rightarrow \omega - \frac{\hbar}{2m}$$

Hence, from eq.(7) we can see (γ is defined in eq.(28)) that if

$$|\omega^2 - 4\gamma^2| > \left| \frac{\omega\hbar}{m} - \frac{\hbar^2}{4m^2} \right| \quad (37)$$

then the quantum noise has no effect on stability changing only the frequency (or the Lyapunov exponent). However, if the condition (37) is not fulfilled ,then the noise can change the exponential increase of $w(t)$ into an oscillatory behaviour or vice versa . So, if

$$|\omega| > 2\gamma > \left| |\omega| - \frac{\hbar}{2m} \right| \quad (38)$$

then the classical variable $W(t)$ (eq.(23) at $\sigma=0$) is periodic whereas the quantum expectation value $E[W]$ grows exponentially. If

$$\left| \left| \omega| + \frac{\hbar}{2m} \right| \right| > 2\gamma > |\omega| \quad (39)$$

then classical variable grows exponentially whereas the quantum expectation value is periodic. We can conclude that quantum effects are important for the particle trapping near the critical value of the wave frequency $|\omega|=2\gamma$.

The explicit form of the solution of eq.(36) is

$$w(t) = A(t)w(0) + C(t)\frac{dw}{dt}(0) \quad (40)$$

where

$$A = \frac{1}{\nu} [\nu_+ \exp(i\nu_- t) - \nu_- \exp(i\nu_+ t)] \quad (41)$$

and

$$C = -\frac{1}{\nu} [\exp(i\nu_+ t) - \exp(i\nu_- t)] \quad (42)$$

with

$$\nu_{\pm} = \frac{1}{2} (\nu_0 \pm \nu) \quad (43)$$

where

$$\nu_0 = \omega - \frac{\hbar}{2m} \quad \text{and} \quad \nu = \sqrt{\nu_0^2 - 4\gamma^2} \quad (44)$$

The formulas (40)-(44) are interesting from the point of view of an expansion in γ in eqs.(32)-(33) and in the Feynman formula (8) (the Dyson expansion). We can see by the comparison of the expansion in γ of $w(t)$ (eq.(40)) with eqs.(32)-(33) that ν_0 will be the small denominator in the expansion. The appearance of the small denominator indicates a qualitative change of the dynamics when $\nu_0 \rightarrow 0$. It is clear that this structural change is the trapped-untrapped transition discussed above.

So far, we have computed the expectation value of W and not of q or $\cos q$, which are the

physically meaningful variables. Although q can be expressed by W from eq.(21) , the relation between these variables is non-linear, therefore we need all correlation functions of W in order to compute the correlations of q . For this purpose we need to study the effect of noise on higher order correlation functions. The two-point function is

$$E[W(t) W(s)] = E[W(t,s)] E[W(s)] + E[W(s)^2] \quad (45)$$

where $W(t,s)$ means that the initial condition in eq.(23) is at s instead of 0. We used the additivity of the integral in the derivation of eq.(45) and the independence of increments of the Brownian motion. $E[W(t,s)]$ can be computed from eq.(36). There remains to compute the second term in eq.(45). For this purpose let us compute

$$\begin{aligned} d(W^2) &= 2WdW = 2W W' dt \\ d(W W') &= dW W' + WdW' \\ d(W' W') &= 2W'dW' + dW'dW' \end{aligned} \quad (46)$$

Then, we use the stochastic equations (35) in order to express the differentials of W' in terms of W and W' . We integrate eqs.(46) and subsequently take the expectation value. As a result we get a system of three equations for the expectation values $w_{22}=E[W'W']$, $w_{11}=E[W^2]$ and $w_{12}=E[WW']$. The equations can be expressed in a differential form as an equation for the vector $\mathcal{W}^T=(w_{22}, w_{12}, w_{11})$

$$\frac{d\mathcal{W}}{dt} = \Lambda \mathcal{W} \quad (47)$$

where

$$\Lambda = \begin{bmatrix} M & 2\gamma^2 & 0 \\ 1 & N & \gamma^2 \\ 0 & 2 & 0 \end{bmatrix} \quad (48)$$

with

$$M = -2i(\omega + \frac{\hbar}{4m}) \quad N = -i(\omega - \frac{\hbar}{2m})$$

Eq.(48) is equivalent to a third order equation with constant coefficients. If the inequality (37) is fulfilled , then the quantum corrections do not change the classical behaviour ($w_{11}=w(\hbar=0)^2$); if not

then the quantum corrections can change the periodic behaviour into a non-periodic one. We could continue the method to compute the correlation functions of arbitrary order. The problem is reduced to linear ordinary differential equations of an increasing order.

IV. Change of variables in the Feynman integral.

We wish to rewrite the Feynman formula (12) in terms of the W variables. We can easily check that in the model (3)

$$W(t) W_*(t) = \exp\left(\frac{1}{m} \int_0^t \Delta S_\tau(q(\tau)) d\tau\right) \quad (49)$$

Hence, the Feynman formula can be expressed in the form

$$(U_t \psi)(x) = \exp\left(\frac{i}{\hbar} S_t(x)\right) E\left[\left(\sqrt{W(t)W_*(t)}\right)^{-1} \phi(q_t(W))\right] \quad (50)$$

assuming that we are able to define the square root unambiguously (the right hand side is well-defined for small t , when W is close to 1; the square root can be defined uniquely from 1 by the requirement of the semigroup composition law for U_t).

We are interested now in the variable WW_* in eq.(50). Using eqs.(23)-(24) we can derive an equation for WW_* in the same way as for we got one for W^2 . Denote $\zeta^T = (WW_*, W W_*', W' W_*, W' W_*')$ then ζ fulfills the following Stratonovitch stochastic differential equation

$$\frac{d\zeta}{dt} = \Theta \circ \zeta \quad (51)$$

where

$$\Theta = \begin{bmatrix} 0 & 1 & 1 & 0 \\ \gamma^2 & -\nu_b & 0 & 1 \\ \gamma^2 & 0 & \nu_b & 1 \\ 0 & \gamma^2 & \gamma^2 & 0 \end{bmatrix} \quad (52)$$

with

$$\nu_b = -i\omega - i\sigma \frac{dh}{dt}$$

For a discussion of solutions of eq.(52) it is useful to decompose the matrix Θ

$$\Theta = \Theta_+ + \mathfrak{B} \quad (53)$$

where

$$\Theta_c = \begin{bmatrix} 0 & 1 & 1 & 0 \\ \gamma^2 & i\omega & 0 & 1 \\ \gamma^2 & 0 & -i\omega & 1 \\ 0 & \gamma^2 & \gamma^2 & 0 \end{bmatrix} \quad (54)$$

and

$$\mathfrak{B} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & B & 0 & 0 \\ 0 & 0 & -B & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (55)$$

where

$$B = i\sigma \frac{db}{dt}$$

Now, the solution of eq.(51) can be expressed in the form

$$\zeta_t = \mathcal{F}_t \zeta_0 \quad (56)$$

where

$$\mathcal{F}_t = \exp(t\Theta_c) \mathcal{G}_t \quad (57)$$

where $\mathcal{G}_t$ is the solution of the equation (with the initial condition $\mathcal{G}_0=1$)

$$\frac{d\mathcal{G}}{dt} = \exp(-t\Theta_c) \mathfrak{B} \exp(t\Theta_c) \mathcal{G} \quad (58)$$

Eq.(58) can be used for a successive expansion in $\hbar$. The exponentiation of Θ_c is equivalent to the problem of solving a system of four linear differential equations with constant coefficients. This can be done in an elementary way. It is sufficient to use the solution (40) of eqs.(23)-24) at $\hbar=0$. Inserting the initial conditions resulting from eq.(17) we get

$$W^c = -\frac{\gamma}{\mu} \exp(-ix - \frac{\omega t}{2}) \sin(\frac{1}{2}\mu t) - \mu^{-1} \exp(-\frac{i\omega t}{2}) \left(\mu_- \exp(-\frac{i\mu t}{2}) - \mu_+ \exp(\frac{i\mu t}{2}) \right) \quad (59)$$

where

$$\mu = \sqrt{\omega^2 - 4\gamma^2} \quad \text{and} \quad \mu_{\pm} = \frac{\omega}{2} \pm \frac{\mu}{2}$$

Then, $W^c_* = \overline{W^c}$ and

$$W(t)W_*(t)|_{\hbar=0} = |W^c|^2 = \mu^{-2} \left[\gamma \sin(\frac{1}{2}\mu t) + \exp(ix) \left(\mu_- \exp(-\frac{i}{2}\mu t) - \mu_+ \exp(\frac{i}{2}\mu t) \right) \right]^2 \quad (60)$$

Eqs. (50) and (59) - (60) give the semiclassical formula (12) for the motion of a quantum particle in a

plane wave.

We can subsequently find the matrix $\exp(t\Theta_c)$ by differentiation of $w(t)$ and $\bar{w}(t)$. Then, we get a convergent expansion in $\hbar$ of $\mathcal{F}$ (eqs.(56)-(58)) ; in particular, an expansion of WW_* .

In order to compute the expectation value of $(\sqrt{WW_*(t)})^{-1}$ we can again use an expansion in $\hbar$. For this purpose we compute $E[(WW_*(t))^n]$. The method is the same as in the computation of $E[W(t)^n]$. For $n=1$ denote

$$X_1=WW_*' - W_*W', \quad X_2=WW_*' - W_*W', \quad X_3=WW_*, \quad X_4=W'W_*'$$

We get for the vector X the equation

$$\frac{dX}{dt} = \Omega \circ X \tag{61}$$

where

$$\Omega = \begin{bmatrix} 0 & -\nu_b & 0 & 0 \\ -\nu_b & 0 & 2\gamma^2 & 2 \\ 0 & 1 & 0 & 0 \\ 0 & \gamma^2 & 0 & 0 \end{bmatrix} \tag{62}$$

From eq.(62) we can compute $E[WW_*]$. The result is that the classical frequencies $\mu_{\pm}$ in eq.(60) are shifted by $\omega \rightarrow \omega \pm \frac{\hbar}{2m}$. We can use the solution of eq.(61) to compute $(WW_*)^2$ and continue the procedure to higher orders.

Summarizing, we have shown that the random variable W linearizing the quantum mechanical model of a particle in a plane wave can undergo an abrupt change of behaviour. This occurs when the wave amplitude is close to the classical critical value corresponding to the particle transition between trapped and untrapped states. The behaviour of variables built from W can be well- approximated by a convergent expansion in $\hbar$. The model can shed some light also on the meaning of small denominators in quantum mechanics.

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