# Diffusion in momentum space for systems in a random time-dependent electric field: the 1D hydrogen atom



1992 J. Phys. A: Math. Gen. 25 L727

(http://iopscience.iop.org/0305-4470/25/12/004)

J. Phys. A: Math. Gen. 25 (1992) L727–L732. Printed in the UK

LETTER TO THE EDITOR

# Diffusion in momentum space for systems in a random time-dependent electric field: the 1D hydrogen atom

J C Flores†

Department of Physics, Purdue University, West Lafayette, IN 47907, USA

Received 5 February 1992, in final form 1 April 1992

**Abstract.** It is argued that diffusion in momentum space exists for 1D quantum systems ($H_0 = p^2 + V(x)$) in a random external electric wavefield ($Fb(t)x$). In the high-field regime, a diffusion type equation is found explicitly for the probability density. In this regime, diffusion is a consequence of *randomization* in the quantum system. Particularly, this result is also valid for the 1D hydrogen atom in a random wavefield. So the interference phenomenon, which is a typical property in quantum systems, is disturbed by *randomization*. This could have important inferences in the phenomenon known as quantum suppression of classical chaos where interference gives dynamical localization.

The one-dimensional (1D) hydrogen atom in the presence of microwave frequency radiation is the object of great interest because of the dynamical localization of chaos in quantum systems [1, 2]. So it seems that quantum mechanics has a suppressive effect on classical chaos. In fact, the hydrogen atom in a microwave field is a complex system and it is only at high frequencies that this phenomenon occurs. A more simple system which displays suppression of chaos by quantum effect is the so-called kicked rotator. Classically, the kicked rotator becomes chaotic above a critical threshold in the external force (the amplitude of the kick). So the energy becomes unbounded in time with a diffusive behaviour. On the other hand, it has been conjectured that in the quantum model the energy is bounded in time, outside of the resonance regime, which is the opposite of the classical case [3]. At present, a clear explanation of the divergence between the classical and quantum systems does not exist. So, quantum suppression of classical chaos has important implications in the foundations of quantum mechanics and its relation to classical mechanics. Also, it is interesting to note that quantum mechanics was developed and tested from analogies and observations of systems which are classically integrable.

A qualitative (partial) accord between the classical and quantum descriptions can be found when noise is assumed in the quantum kicked rotator. In different random quantum models [4–6], a diffusive behaviour at the energy could be found in partial accord with the classical system. Nevertheless, this accord is obtained by considering *randomization* in the quantum system while the classical system is itself random. Moreover, no diffusion threshold has yet been found. However from the above results, the following idea can be suggested: *if we assume that the Hamiltonian*

† Supported by the Swiss National Science Foundation.

  

*of the microscopic system (the quantum rotator) cannot be known exactly then a (partial) qualitative accord with the classical system can be found.* A similar idea, to explain irreversibility in the microworld, has been used in [7].

In this work it is argued that diffusion, in momentum space, exists when *randomization* is considered on a quantum system with a time-variating electric field (for example the 1D hydrogen atom in a random microwave field). Explicitly we consider the Hamiltonian

$$H = H_0 - \tfrac{1}{2}b(t)Fx \tag{1}$$

where the Hamiltonian

$$H_0 = p^2 + V(x) \tag{2}$$

has a discrete spectrum. $F$ is the amplitude of the electric field and $b(t)$ is a time-function which can be either periodic or random.

The model where $b(t)$ is a periodic function and $V(x) = -e^2/x, x > 0$ is known as the 1D hydrogen atom which displays quantum suppression of classical chaos in the high-frequency regime. More information can be found in [2].

In our case we consider $b(t)$ related to a series of (square) pulses. We assume that every pulse has random height and it is argued that diffusion, in momentum space, exists because of *randomization*.

The Schrödinger equation related to the Hamiltonian (1) is given by ($\hbar = 1$)

$$\mathrm{i}\frac{\partial}{\partial t}\psi = -\frac{\partial^2}{\partial x^2}\psi + V(x)\psi - \tfrac{1}{2}b(t)Fx\psi. \tag{3}$$

The important point for us is that equation (3) can be transformed to another equation where the time-dependence comes directly in the potential $V(x)$ [8]. To see this, we consider the unitary transformation $T$, given by the expression

$$T = \mathrm{e}^{\mathrm{i}\gamma p}\mathrm{e}^{-\mathrm{i}(\alpha x+\beta)} \qquad p = -\mathrm{i}\frac{\partial}{\partial x} \tag{4}$$

where the quantities $\alpha, \beta$ and $\gamma$ are related to $b(t)$ by

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \frac{1}{2}Fb(t) \qquad \frac{\mathrm{d}\beta}{\mathrm{d}t} = -\alpha^2 \qquad \frac{\mathrm{d}\gamma}{\mathrm{d}t} = 2\alpha. \tag{5}$$

So, using the transformation (4) in equation (3) we have

$$\mathrm{i}\frac{\partial}{\partial t}\psi = -\frac{\partial^2}{\partial x^2}\psi + V(x - \gamma(t))\psi \tag{6}$$

where explicitly

$$\frac{\mathrm{d}^2\gamma}{\mathrm{d}t^2} = Fb(t). \tag{7}$$

Calulations on the 1D hydrogen atom, with a strong deterministic time-dependent external field and using the above method can be found in [8].

In the case of a periodic wavefield $b(t) = \cos t/\tau$, the variations of $\gamma$ are bounded in time namely

$$-F\tau^2 < \gamma(t) < F\tau^2 \qquad \text{when} \qquad b = \cos t/\tau. \tag{8}$$

This relation suggests that we could consider a simplified model where the parameter $\gamma$ is related to square-pulses. *Randomization* is provided by the variation in height of each pulse. Explicitly we assume

$$\gamma(t) = F\tau^2 \sum_j \xi_j \{\theta(t - j\tau) - \theta(t - (j+1)\tau)\} \\ - \mu_j \{\theta(t - (j+1)\tau) - \theta(t - (j+2)\tau)\} \qquad j = 0, 2, 4, \ldots \tag{9}$$

where $\theta(t)$ is the step-function and $\xi_j, \mu_j$ are random independent quantities for any $j$ with dispersion $\sigma$ and average equal to one

$$\sigma^2 = [\xi_j^2] = [\mu_j^2] \qquad [\xi_j] = [\mu_j] = 1. \tag{10}$$

So $\gamma$ takes consecutively the values $+F\tau^2\xi_j$ and $-F\tau^2\mu_j$, or

$$\gamma(t) = \begin{cases} +F\tau^2\xi_j & j\tau < t < (j+1)\tau \\ -F\tau^2\mu_j & (j+1)\tau < t < (j+2)\tau. \end{cases} \tag{11}$$

We note that the deterministic case $\xi_j = \mu_j = 1$ is related to the periodic square-pulse with period $2\tau$.

Because $\gamma$ is a constant between $j\tau < t < (j+1) < \tau$ and $(j+1)\tau < t < (j+2)\tau$, the evolution operator $U_j$ (between two consecutives pulses) is

$$U_j = e^{i(p^2 + V(x - F\tau^2\xi_j))\tau} e^{i(p^2 + V(x + F\tau^2\mu_j))\tau} \tag{12}$$

which is a random operator and can be written as

$$U_j = e^{iF\tau^2\xi_j p} e^{iH_0\tau} e^{-iF\tau^2(\xi_j + \mu_j)p} e^{iH_0\tau} e^{iF\tau^2\mu_j p}. \tag{13}$$

At this point is interesting to note the similarity between this operator and another related to the kicked rotator. In fact in the periodic case, the above evolution operator gives a (formal) tight-binding type equation for the wavefunction because of the analogy of this operator with another of the periodic kicked rotator.

We now consider the case where $\xi_j, \mu_j$ are random quantities in the model defined above. We found that in the limit where $F\tau^2$ is sufficiently large, diffusion in the momentum space exists because of *randomization*.

The time-evolution, at the density operator $\rho$, from $t = j\tau$ to $t = (j+2)\tau$ is given by

$$\rho^{j+2} = U_j \rho^j U_j^{-1} \tag{14}$$

where the random unitary operator $U_j$ was defined above.

The idea is to show that the evolution of the average-density operator, is given by a diffusion type equation in the limit where $F\tau^2$ is sufficiently large. To see this we use the fact that in the momentum space representation (14) becomes

$$\rho_{pq}^{j+2} = \sum_{k_1 k_2 k_3 k_4} \mathrm{e}^{\mathrm{i}F\tau^2 \xi_j (p-k_1+k_4-q)} \mathrm{e}^{\mathrm{i}F\tau^2 \mu_j (k_2+k_4-k_1-k_3)} J_{pk_1} J_{k_1 k_2} J^*_{k_4 k_3} J^*_{qk_4} \rho^j_{k_2 k_3} \tag{15}$$

where

$$J_{pq} = \langle p | \mathrm{e}^{\mathrm{i}H_0 \tau} | q \rangle \tag{16}$$

and we have a sumation over $k_1, \ldots, k_4$ because we assume that the system is in a great-box of length $L$ namely ($\hbar = 1$)

$$p = \frac{n}{L} \qquad \Delta p = \frac{1}{L} \qquad n \in Z. \tag{17}$$

In the approximation $F\tau^2\sigma \gg L$, the sample-averaging at the random phase becomes proportional to $\delta_{p,0}$ or

$$[\mathrm{e}^{\mathrm{i}F\tau^2 p \xi_j}] \sim \delta_{p,0} \qquad \text{when} \qquad F\tau^2 \Delta p \sigma \gg 1 \tag{18}$$

where the symbol [. . .] denotes sample-average on the random quantities. From (15) and (18), the diagonal elements of $\rho$ are related at different times by

$$[\rho_{pp}^{j+2}] = \sum_q |\, G_{pq} \,|^2 \, [\rho^j_{qq}] \tag{19}$$

where

$$|\, G_{pq} \,|^2 = \sum_k |\, J_{pk} \,|^2 |\, J_{kq} \,|^2 \tag{20}$$

and

$$\sum_q |\, G_{pq} \,|^2 = 1 . \tag{21}$$

Condition (21) gives the normalization condition $\sum_p [\rho^j_{pp}] = 1$ for any time.

The evolution equation (19) has an important property: if we assume that the initial state ($j = 0$) is $|\, p\rangle$, with $\langle p \,|\, p \rangle = 1$, then from (19) we have

$$[\rho^j_{pp}] \leqslant |\, G_{pp} \,|^{2j} . \tag{22}$$

Namely, the probability of finding the system in the initial state $|\, p\rangle$ becomes exponentially smaller with time. So we can define, for instance, the 'relaxation-time' of the system $\tau_r$

$$\tau_r \sim \tau \ln \frac{1}{|\, G_{pp} \,|^2} . \tag{23}$$

Expression (23) is general in the sense that we have no restrictions on the matrix elements (16). We recall that in (22), $| G_{pp} | < 1$.

Now, we want to consider systems where the transition matrix, in momentum space, involves only nearest-neighbour elements. Namely we assume that

$$| G_{pq} |^2 = (1 - 2D)\delta_{p,q} + D\delta_{p,q+1} + D\delta_{p,q-1} \tag{24}$$

where $D$ is a positive quantity. Using (24), equation (19) becomes

$$[\rho^{j+2}_{pp}] = [\rho^{j}_{pp}] + 2D\{[\rho^{j}_{pp+1}] + [\rho^{j}_{pp-1}] - 2[\rho^{j}_{pp}]\} \tag{25}$$

which is a discrete diffusion equation. We remark on the similarity of (25) to the continuous diffusion equation $\partial_t \rho = D\partial_{xx}\rho$.

The sample-averaging, for the momentum, is given by

$$\sum_p p^2[\rho^{j}_{pp}] = 2Dj + \sum_p p^2[\rho^{0}_{pp}] \tag{26}$$

namely, a diffusive behaviour exist in momentum space.

So condition (18) gives us the diffusion type equation (25) for the probability density in momentum space. We note that the diffusion equation (25) is obtained in one-step ($j \to j + 2$) namely the diffusive behaviour is rapidly obtained in the system when (18) holds. If (18) is not satisfied, then the behaviour in momentum space is unknown nevertheless, because the similarity of the evolution equation (15) with another of the random kicked rotator [4], it also seems possible that here ($F\tau^2\sigma\Delta p \sim 1$) diffusion exists because of *randomization* but the diffusive behaviour is asymptotic in time.

We have conjectured that for the random model, diffusion exists in momentum space when the condition

$$F\tau^2\sigma\Delta p \gg 1 \tag{27}$$

is assumed. The model is a system with a discrete spectrum (Hamiltonian $H_0$) in a random time-dependent electric field. The amplitude of this field is $F$ and the period $\tau$. In (27), $\sigma$ is the dispersion of the random quantities (10) and $\Delta p = 1/L$ with $L$ the length of the box where the system $H_0$ is operating.

The condition (27) gives us a diffusion type equation, in one-step ($j \to j + 2$), in momentum space (25).

Outside of regime (27) (when $F\tau^2\sigma\Delta \sim 1$), the behaviour is unknow (for me) but because of the similarity between the random time evolution (15), for the density matrix, and another of the random kicked rotator [4] it seems possible that diffusion, related to disorder, also exists here .

Finally, we remark that the hydrogen atom in a wavefield, is a particular case of the general Hamiltonian (1). So it seems possible that dynamical localization, for the hydrogen atom in a wave field, could be broken by *randomization*. So it seems that quantum suppression of classical chaos does not exist when randomization is considered in the quantum model.

## References

[1] Jensen R V, Susskind M S and Sanders M M 1991 *Phys. Rep.* **201** 1

[2] Casati G and Molinari L 1989 *Prog. Theor. Phys. Sup.* **98** 287
[3] Grempel D R, Prange R E and Fishman S 1984 *Phys. Rev.* A **29** 1639
[4] Guarneri I 1984 *Lett. Nuovo. Cimento* **40** 171
[5] Flores J C 1991 *Phys. Rev.* A **44** 3492; *Thesis No 2505* Université de Genève
[6] Cohen D 1991 *Phys. Rev.* A **44** 2292
[7] Peres A 1984 *Phys. Rev.* A **30** 1610
[8] Pomeau Y 1986 *Ann. Inst. H Poincaré* **45** 29