Numerical multi-scale time averaging approach to quantum systems with pseudo random potentials

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Abstract

We consider the problem of numerically solving the Schrödinger equation with a quasi periodic in space time potential, approximating multiplicative noise term. We introduce a numerical scheme based on a newly developed multi-time scale averaging technique. We show that with this new method we can solve efficiently and with rigorous control of the error the above equation for large times. A comparison with the standard split-step method shows order of magnitude improvement in computational times, besides the controlled errors. We apply this method to a free particle perturbed by quasi-periodic potential with many frequencies.

We observe the (anomalous) diffusion in momentum space, over large time intervals, as large as the system is away from the Chirikov resonance strips. In the limit of zero potential, the diffusion rate becomes standard, but with a coefficient that approaches zero.

Keywords: Numerical solution, time dependent ODE

1. Introduction

In the present work a novel numerical method for the exploration of the dynamics for time dependent potentials [1] is implemented for the numerical
solution of the Schrödinger equation with a potential that is random in both space and time. Exploration of the dynamics for such potentials was motivated by experiments in optics [2] where hypertransport, namely transport faster than ballistic was found experimentally and numerically. In theoretical work that followed [2, 3, 4, 5] a classical theory was developed for the potentials relevant for these optics experiments. In particular it was found that for smooth potentials the spreading in momentum as function of time stops. For short times, relevant for the existing experiments it was found that quantum and classical dynamics agree in general features.

For long times it turned out impossible to compute numerically the quantum dynamics using the standard methods [6, 7], while with the method introduced in [1] and implemented here, calculations for such long times are feasible. Such calculations and comparison with the classical results, is of fundamental importance for the issue of quantum classical correspondence. The main objective of the present paper is to demonstrate the power of the method introduced in [1] for a physically relevant example.

Potentials which are random both in space and time can manifest a high degree of complexity and are subject of many studies over the last decade mostly in the framework of classical physics [8, 9, 10, 11, 12, 13, 14, 15]. For time independent potentials a particle can exhibit Anderson localization [16, 17]. Such potentials have been also experimentally realized for many systems. For example Anderson localization was realized using light trapping in disordered wave-guides (see [18, 19] and references therein) that is most relevant for our work. If the potential fluctuates in time as well as in space, the arguments indicating Anderson localization break down. Recently such potentials have also been implemented experimentally [2] and it was shown that in such settings a wave packet can exhibit faster than ballistic transport.

With different experimental realizations of such potentials there is also a need for a numerical approach to investigate them and their asymptotic behavior. The standard way to numerically investigate time dependent potentials is based on either spectral methods [20, 21] or explicit/implicit finite difference schemes.
In this paper we implement numerically a recently developed rigorously controlled multi-time scale averaging technique \[1\]. The above mentioned method has two distinct advantages. The first is that at each step of the averaging hierarchy there is a well defined and completely known bound on the numerical error. The second advantage and one which has far greater impact is the reduction in computational time accompanied with each of the hierarchical averaging steps. This reduction enables to go to long time scales. In this paper we will introduce the methods and perform the first steps in the hierarchy.

1.1. The model

The random potentials which are prepared in optics \[19,2\] and atom optics \[23,24,25\], experiments are described by a series of random Fourier components. Motivated by such experiments we will examine potentials composed out of a large number of random independent Fourier components \(N\).

More specifically we will study the Schrödinger equation for a potential

\[ V(x,t) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} A_n \exp(i(k_n x - \omega_n t)) + C.C \]  

Here the \(A_m\) are independent, identically distributed complex random variables.

The expectation values of these variables satisfy

\[ <A_m> = <A_mA_n> = 0 \quad <A_mA_n^*> = \sigma^2 \delta_{nm} \]  

In particular we will study models where \(A_n = Ae^{i\phi_m}\) with \(\phi_m\) uniformly distributed in the interval \([-\pi, \pi]\) and \(A > 0\).

Our equation of motion is the time dependent Schrödinger equation

\[ i\partial_\tau \psi(x,\tau) = H\psi(x,\tau) \]  

Where

\[ H = \frac{1}{2} \partial^2 + V(x,\tau) \]  

In the following section we will introduce the reduction of the problem into a framework where the multi-scale averaging technique \[1\] is applicable.
1.2. Reduction of the problem

In the classical version of the model the potential $V$ the particle is expected to be accelerated most effectively in the regime of velocities where the Chirikov resonances

$$v_n^{(r)} = \frac{\omega_n}{k_n}$$

(5)

are formed [26, 27]. In this paper we choose $v_n^{(r)}$ and $k_n$ uniformly distributed in the intervals $[v^{(\text{min})}, v^{(\text{max})}]$ and $[k^{(\text{min})}, k^{(\text{max})}]$ respectively.

Here we would like to study what is the acceleration of a particle prepared with momentum or velocity $v$ (we assume unit mass), so that all $v_n^{(r)}$ are far from $v$.

For the classical corresponding system we found that the acceleration is negligible. Here we study the corresponding quantum mechanical system. For this purpose it is convenient to work in a frame of reference where the initial velocity of the particle vanishes. For this we perform the Galilean transformation

$$x' = x - vt, \quad t = \tau v$$

(6)

where $v$ is the velocity of the moving frame (in later stages we will relate this quantity to the required small parameter) on the potential $V$

$$V(x' + vt, t) = \frac{A}{\sqrt{N}} \sum_{n=1}^{N} \cos (k_n x' + (k_n - \omega_n) t + \phi_n)$$

(7)

re-scaling time as

$$t = \tau v$$

(8)

the potential takes the form

$$V(x + vt, t) = \frac{A}{\sqrt{N}} \sum_{n=1}^{N} \cos \left( k_n x' - \frac{(\omega_n - k_n v)t}{v} + \phi_n \right)$$

(9)

and defining

$$\omega'_n = \frac{(\omega_n - k_n v)}{v}$$

(10)
The potential in the moving frame takes the form

$$V(x', t) = \frac{A}{\sqrt{N}} \sum_{n=1}^{N} \cos (k_n x' - \omega'_n t + \phi_n) \quad (11)$$

The time dependent Schrödinger equation is

$$i \partial_t \psi (x', t) = \frac{1}{\hbar} H(\hat{p}', \hat{x}', t) \psi (x', t) \quad (12)$$

Introducing the small parameter $\beta = \frac{1}{\sqrt{v}}$

$$i\hbar \partial_t \psi (x', t) = \beta H(\hat{p}', \hat{x}', t) \psi (x', t) \quad (13)$$

From here and on we drop the ′ replacing in the notation $p' \rightarrow p$, $x' \rightarrow x$, $\omega'_m \rightarrow \omega_n$ and the time is $t$. From this point on we will use the small parameter $\beta$ to perform the averaging steps introduced in the next section. In what follows we will also relate the small parameter $\beta$ to time scale on which we average.

2. The averaging schemes

The calculation follows the steps and notation of [1].

2.1. Zero order

The multiscale averaging method is based on replacing the original Hamiltonian by a hierarchical set of averaged Hamiltonians. In each step we perform a "peeloff" transformation and average a part of the Hamiltonian, for a chosen time interval of length $T_0 = \frac{1}{\sqrt{\beta}} = \sqrt{v}$. For the purpose of this article we will only look at the first two orders. We use the fact that Eq (13) is of the form of (2.1) in [1].

the zero order average on the jth interval has the form

$$\bar{V}^{(j)}_0 = \frac{1}{T_0} \int_{jT_0}^{(j+1)T_0} V(t) \, dt \quad (14)$$

In the case of the potential (11), the zero order averaging can be performed analytically

$$\bar{V}^{(j)}_0 = \frac{1}{T_0} \int_{jT_0}^{(j+1)T_0} V(t) \, dt = \frac{A}{\sqrt{NT_0}} \int_{jT_0}^{(j+1)T_0} \sum_{n=1}^{N} \cos (k_n x' - \omega'_n t + \phi_n) = \ldots$$
\[
\begin{align*}
&= \frac{A}{\sqrt{NT_0}} \sum_{n=1}^{N} \frac{1}{\omega_n'} \left[ \sin \left( k_n x' - \omega_n' \left( j + \frac{1}{2} \right) T_0 + \phi_n \right) - \sin \left( k_n x' - \omega_n' j T_0 + \phi_n \right) \right] = \\
&= 2 \frac{A}{\sqrt{NT_0}} \sum_{n=1}^{N} \frac{1}{\omega_n'} \sin \left( \frac{1}{2} \omega_n' T_0 \right) \cos \left( k_n x' - \omega_n' \left( j + \frac{1}{2} \right) T_0 + \phi_n \right) 
\end{align*}
\]

This defines the potential on one interval, accordingly we can write the Hamiltonian of one interval as

\[
\tilde{H}_0^{(j)} (x) = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \tilde{V}_0^{(j)}
\]

The global Hamiltonian corresponding to (2.1) of [1] is

\[
\tilde{H}_0^{g} = \tilde{H}_0^{(j)} (t) \quad \text{for} \quad j T_0 \leq t < (j + 1) T_0
\]

Using this notation a general time evolution can be written as the product of the interval propagators:

\[
U_0(t) = e^{-i\beta \tilde{H}_0^{g} (t-j T_0)} \ldots e^{-i\beta \tilde{H}_0^{g} (0)}
\]

for \( j T_0 \leq t < (j + 1) T_0 \) and evolution in this order is

\[
\psi (x', t) = U_0 (t) \psi (x', 0)
\]

The propagator satisfies

\[
i \frac{\partial}{\partial t} U_0(t) = \beta \tilde{H}_0^{g} U_0(t)
\]

corresponding to (2.10) of [1]. This propagator was numerically implemented and used to solve the time dependent equation of motion.

2.2. First order

The first order averaging is based upon a "peeloff" transformation of the zero order. In such a transformation the next order Hamiltonian is constructed from the zero order in the following way

\[
H_1 (t) = U_0^{-1} (t) \left[ H_0 (t) - \tilde{H}_0^{g} (t) \right] U_0 (t)
\]
and its average in the $j$-th interval is

$$\bar{H}_1^{(j)} = \frac{1}{T_0} \int_{jT_0}^{(j+1)T_0} H_1(t) \, dt$$  \hspace{1cm} (22)$$

The propagator is

$$U_1(t) = e^{-i\beta \bar{H}_1^{(j)}(jT_0)} \ldots e^{-i\beta \bar{H}_1^{(0)}T_0}$$  \hspace{1cm} (23)$$

Before diagonalizing this operator to calculate the time evolution, there are several steps needed to be taken. First we write explicitly the operator using integration by parts

$$\bar{H}_1^{(j)}(t) = \frac{1}{T_0} \int_{jT_0}^{(j+1)T_0} U_0^{-1}(t) \left[ H_0(t) - \bar{H}_0^g(t) \right] U_0(t) dt = \bar{H}_1^{(j,1)} + \bar{H}_1^{(j,II)} + \bar{H}_1^{(j,III)}$$  \hspace{1cm} (24)$$

Where

$$\bar{H}_1^{(j,1)}(t) = \frac{1}{T_0} \int_{jT_0}^{(j+1)T_0} U_0^{-1}(t) \left( \int_0^t [H_0(t') - \bar{H}_0^g(t')] \, dt' \right) U_0(t) \right]_{t=jT_0}^{(j+1)T_0}$$  \hspace{1cm} (25)$$

$$\bar{H}_1^{(j,II)}(t) = -\frac{1}{T_0} \int_{jT_0}^{(n+1)T_0} dt' \left( \frac{\partial}{\partial t'} U_0^{-1}(t') \right) \left[ \int_0^{t'} \left[ H_0(s) - \bar{H}_0^g(s) \right] ds \right] U_0(t')$$  \hspace{1cm} (26)$$

and

$$\bar{H}_1^{(j,III)}(t) = \frac{1}{T_0} \int_{jT_0}^{(j+1)T_0} U_0^{-1}(t') \left[ \int_0^{t'} \left[ H_0(s) - \bar{H}_0^g(s) \right] ds \right] \left( \frac{\partial}{\partial t} U_0 \right)(t') dt'.$$  \hspace{1cm} (27)$$

we note that for any integer $j$

$$\int_{jT_0}^{(j+1)T_0} \left[ H(t') - \bar{H}_0^g(t') \right] dt' = 0$$  \hspace{1cm} (28)$$

by construction. Therefore $\bar{H}_1^{(j,1)}(t) = 0$ and $\bar{H}_1^{(j,II)}(t)$ can be simplified. Moreover the expression in $\bar{H}_1^{(j,III)}$ is just the hermitian conjugate of $\bar{H}_1^{(j,II)}$ so we only need to analyze the second term

$$\bar{H}_1^{(j,II)} = \frac{1}{T_0} \int_{jT_0}^{(j+1)T_0} dt' \left( \frac{\partial}{\partial t'} U_0^{-1}(t') \right) \left[ \int_0^{t'} \left[ H(s) - \bar{H}_0^{(j)}(s) \right] ds \right] U_0(t')$$  \hspace{1cm} (29)$$

$$= \frac{1}{T_0} \int_{jT_0}^{(j+1)T_0} dt' \left( \frac{\partial}{\partial t'} U_0^{-1}(t') \right) \left[ \int_{jT_0}^{t'} H(s) \, ds - (t' - jT_0) \bar{H}_0^{(j)} U_0(t') \right]$$
To evaluate this operator we can use a recursive construction of states based on the zero order averaging, it is important to remember that this is actually a matrix. For convenience of notation we will define

\[ U_0(t) = e^{-i\beta \hat{\mathcal{H}}_0^{(j)} (t-jT_0)} e^{-i\beta \hat{\mathcal{H}}_0^{(1)} T_0} e^{-i\beta \hat{\mathcal{H}}_0^{(0)} T_0} = \prod_{j'=0}^{j} W_j e^{-i\beta \hat{\mathcal{H}}_0^{(j)} T_0}, \quad (30) \]

where

\[ W_j = e^{-i\beta \hat{\mathcal{H}}_0^{(j)} T_0}. \quad (31) \]

The eigenvalues and eigenfunctions of \( \hat{\mathcal{H}}_0^{(j)} \) are

\[ \hat{\mathcal{H}}_0^{(j)} |\psi_j^k\rangle = E_j^k |\psi_j^k\rangle \quad (32) \]

For a base of size \( M \) we will have \( M \) eigenvalues and eigenvectors. Between each pair of propagators \( W_j, W_{j+1} \) we can insert the identity resolution in the corresponding basis

\[ \hat{I}_j = \sum_{k=1}^{M} |\psi_j^k\rangle \langle \psi_j^k| \quad (33) \]

resulting in

\[ U_0 = W_j \cdots W_1 W_0 = W_j I_j \cdots W_1 I_1 W_0 I_0 \quad (34) \]

As an example lets take just the first two terms

\[ W_1 I_1 W_0 I_0 = \sum_{k_1=1}^{M} W_1 |\varphi_1^{k_1}\rangle \langle \varphi_1^{k_1}| \sum_{k_0=1}^{M} W_0 |\varphi_0^{k_0}\rangle \langle \varphi_0^{k_0}| \quad (35) \]

the brakets expressions are just scalars, and since our potential is diagonal this reduces to the sum of eigenvalues \( E_j^k \)

\[ W_1 I_1 W_0 I_0 = \sum_{k_1=1}^{M} W_1 |\varphi_1^{k_1}\rangle \langle \varphi_1^{k_1}| W_0 \sum_{k_0=1}^{M} |\varphi_0^{k_0}\rangle \langle \varphi_0^{k_0}| \quad (36) \]

\[ = \sum_{k_1=1}^{M} e^{-i\beta T_0 E_1^{k_1}} |\varphi_1^{k_1}\rangle \langle \varphi_1^{k_1}| \sum_{k_0=1}^{M} e^{-i\beta T_0 E_0^{k_0}} |\varphi_0^{k_0}\rangle \langle \varphi_0^{k_0}| \]

using the notation

\[ \alpha_{k_1 k_0} = \langle \varphi_1^{k_1} | \varphi_0^{k_0} \rangle \quad (37) \]
this becomes
\[ W_1 I_1 W_0 I_0 = \sum_{k_0=1}^{M} \sum_{k_1=1}^{M} \alpha_{k_0 k_1} e^{-i\beta T_0 E^{k_1}_0} e^{-i\beta T_0 E^{k_0}_0} |\varphi_{k_1}^{}> \langle \varphi_{k_0}^{}| \] \hspace{1cm} (38)

In the same way for the complete sequence of propagators
\[ U_0 = \prod_{j'=0}^{j} W_{j'-j'} = \prod_{j'=0}^{j} [W_{j'-j'} I_{j-j'}] = \sum_{k_0=1}^{M} \sum_{k_1=1}^{M} \cdots \sum_{k_j=1}^{M} \alpha_{k_j k_{j-1}} \alpha_{k_{j-1} k_{j-2}} \cdots \alpha_{k_1 k_0} e^{-i\beta (t-jT_0) E^{k_j}_j} \cdots e^{-i\beta T_0 E^{k_0}_0} |\varphi_{k_j}^{}> \langle \varphi_{k_0}^{}| \] \hspace{1cm} (39)

and
\[ i \frac{\partial}{\partial t} U_0 (t) = \beta \bar{H}_0^{(g)} (t) U_0 (t) \] \hspace{1cm} (40)

The inverse takes the form
\[ U_0^{-1} (t) = e^{i\beta \bar{H}_0^{(0)} t_0} e^{i\beta \bar{H}_0^{(1)} T_0} \cdots e^{i\beta \bar{H}_0^{(j-1)} T_0} = \prod_{j=0}^{j} W_{j}^\dagger \] \hspace{1cm} (41)

\[ = \sum_{k_0=1}^{M} \sum_{k_1=1}^{M} \cdots \sum_{k_j=1}^{M} \alpha_{k_0 k_1}^* \alpha_{k_1 k_2}^* \cdots e^{i\beta (t-jT_0) E^{k_0}_0} e^{i\beta (j-1) E_0} |\varphi_{k_0}^{}> \langle \varphi_{k_j}^{}| \] \hspace{1cm} (42)

and
\[ \frac{\partial}{\partial t} U_0 (t) = -\sum_{k_0=1}^{M} \sum_{k_1=1}^{M} \cdots \sum_{k_j=1}^{M} i\beta E^{k_j}_j \alpha_{k_j k_{j-1}} \alpha_{k_{j-1} k_{j-2}} \cdots \alpha_{k_1 k_0} e^{-i\beta (t-jT_0) E^{k_j}_j} \cdots e^{-i\beta T_0 E^{k_0}_0} |\varphi_{k_j}^{}> \langle \varphi_{k_0}^{}| \] \hspace{1cm} (43)

The full form of \( \bar{H}_1^{(j,\Pi)} \) is
\[ \bar{H}_1^{(j,\Pi)} (t) = -\frac{1}{T_0} \sum_{k_0=1}^{M} \sum_{k_1=1}^{M} \cdots \sum_{k_j=1}^{M} \beta E^{k_j}_j \alpha_{k_0 k_1}^* \cdots \alpha_{k_j k_{j-1}}^* \alpha_{k_{j-1} k_{j-2}} \cdots \alpha_{k_1 k_0} \] \[ \int_{jT_0}^{(j+1)T_0} dt' e^{i\beta T_0 E^{k_0}_0} e^{-i\beta T_0 E^{k_0}_0} \cdots e^{i\beta (t-jT_0) E^{k_j}_j} e^{-i\beta (t'-jT_0) E^{k_j}_j} \] \[ \beta E^{(j)}_j |\varphi_{k_0}^{}> \langle \varphi_{k_j}^{}| \int_{jT_0}^{t'} H (s) ds - (t' - jT_0) \bar{H}_0^{(j)} \] \hspace{1cm} (44)
\[
\begin{align*}
&= -\frac{1}{T_0} \sum_{k_0=1}^{M} \sum_{k_j=1}^{M} \ldots \sum_{k_{j-1}=1}^{M} \sum_{k_{j-1}=1}^{M} \beta E_j^{k_j} \alpha_{k_0}^{*} \alpha_{k_1}^{*k_1} \ldots \alpha_{k_{j-2}}^{*} \alpha_{k_{j-1}}^{*k_{j-1}} \alpha_{k_{j-1}} \ldots \alpha_{k_1} \alpha_{k_0} \\
&\quad \int_{0}^{T_0} \int_{jT_0}^{(j+1)T_0} e^{-i\beta t_0 E_{k_0}^{j} \ldots e^{i\beta (t-jT_0) E_{j}^{j}} e^{-i\beta (t-jT_0) E_{j}^{j}}} \\
&\quad \left\langle \varphi_{k_0} \right| \int_{jT_0}^{t'} H(s) ds - (t-jT_0) \bar{H}_0^{(j)} \left| \varphi_{k_0} \right| \right\rangle \left\langle \varphi_{k_0} \right| \left( \varphi_{k_0} \right| \right. \\
&\quad \left(44\right)
\end{align*}
\]

Finally the full expression for the first order averaged Hamiltonian is

\[
\bar{H}_1^{(j)}(t) = \bar{H}_1^{(j,II)}(t) + \left( \bar{H}_1^{(j,II)}(t) \right)^\dagger \\
\left(45\right)
\]

\[
\bar{H}_1^{(j)}(t) = 2 \Re \left\{ -\frac{1}{T_0} \sum_{k_0=1}^{M} \sum_{k_j=1}^{M} \ldots \sum_{k_{j-1}=1}^{M} \sum_{k_{j-1}=1}^{M} \beta E_j^{k_j} \alpha_{k_0}^{*} \alpha_{k_1}^{*k_1} \ldots \alpha_{k_{j-2}}^{*} \alpha_{k_{j-1}}^{*k_{j-1}} \alpha_{k_{j-1}} \ldots \alpha_{k_1} \alpha_{k_0} \\
&\quad \int_{0}^{T_0} \int_{jT_0}^{(j+1)T_0} e^{-i\beta t_0 E_{k_0}^{j} \ldots e^{i\beta (t-jT_0) E_{j}^{j}} e^{-i\beta (t-jT_0) E_{j}^{j}}} \\
&\quad \left\langle \varphi_{k_0} \right| \int_{jT_0}^{t'} H(s) ds - (t-jT_0) \bar{H}_0^{(j)} \left| \varphi_{k_0} \right| \right\rangle \left\langle \varphi_{k_0} \right| \left(46\right)
\]

At first sight this expression might seem very complicated but can be understood quite easily, in fact what we have here is a matrix constructed from the sum of matrix products and the terms of the matrix involve only the products of the zero order eigenvalue and eigenvector. The benefit of calculating the propagator in this manner is that one only needs to diagonalize the Hamiltonian only once in the beginning of the simulation.

2.3. Normal form transformation

To implement the normal form transformation, we will use the form given in Eq. 3.10 of \[1\]. In our notation this becomes

\[
\dot{U}(t) = 1 + i\beta U_1^{-1}(t) \left( \int_{0}^{t} \left[ H_1(t') - \bar{H}_1(t') \right] dt' \right) U_1(t) . \\
\left(47\right)
\]

The manner in which we will simplify the above expression will be similar to the method used to calculate \(U_1\) and \(H_1\) given in Eq (23) and (20) splitting into
intervals of length $T_0$ and using (28) replacing $H$ by $H_1$

$$
\hat{U}(t) = 1 + i\beta U^{-1}_1 \left( \sum_{j=0}^{\bar{j}} \int_{jT_0}^{(j+1)T_0} dt' \left[ H_1(t') - \bar{H}_1^{(j)}(t') \right] \right) + \int_{jT_0}^{t} \left[ H_1(t') + \bar{H}_1^{(j)}(t') \right] dt' U_1(t).
$$

(48)

Therefore

$$
\hat{U}(t) = 1 + i\beta U^{-1}_1 \int_{jT_0}^{t} \left[ H_1(t') - \bar{H}_1^{(j)}(t') \right] dt' U_1(t) = 1 + i\beta U^{-1}_1 \left( \int_{jT_0}^{t} H_1(t') dt' \right) - (t - jT_0) \bar{H}_1^{(j)} U_1(t)
$$

(49)

and explicitly

$$
\hat{U}(t) = 1 + e^{i\beta \bar{H}_1^{(0)}(t - jT_0)} \ldots e^{i\beta \bar{H}_1^{(j)}(t - jT_0)} \left( \int_{jT_0}^{t} H_1(t') dt' \right) - (t - jT_0) \bar{H}_1^{(j)} e^{-i\beta \bar{H}_1^{(0)}(t - jT_0)} \ldots e^{-i\beta \bar{H}_1^{(j)}(t - jT_0)}.
$$

(50)

For numerical convince we introduce

$$
W_j^0 = e^{i\beta \bar{H}_1^{(j)}(t - jT_0)} \left( \int_{jT_0}^{t} H_1(t') dt' \right) - (t - jT_0) \bar{H}_1^{(j)}
$$

(51)

and then performing $j - 1$ times the transformation

$$
\hat{U}(t) = W_0^* \ldots W_{j-1}^* W_j^0 W_j W_{j-1} \ldots W_0,
$$

(52)

where $W_j$ is given by (31). This relation can be computed recursively.

### 3. Numerical implementation

In this section we will evolve the wave function with the approximate evolution operator and compare the results to the ones found with the help of the standard split step method. In the zeroth order we evolve the wave function with the help of (19), with $U_0$ calculated by (39).

The diagonalization (32) can be performed once and can be done in parallel. In particular the first order (23) requires to diagonalize $\bar{H}_1^{(j)}$ that in turn is given by the diagonalized $\bar{H}_1^{(0)}$ by (46). This enables to compute the $\alpha_{k_1,k_0}$ of (37). To obtain the first order we use the evolution operator

$$
\hat{U}_1 = U_0 U_1,
$$

(53)
where $U_1$ is given by (23) and $\bar{H}_1^{(j)}$ is given by (46). Taking into account the normal form transformation we use

$$U_{(\text{NF})} = \bar{U}_1 \tilde{U}^{-1}. \tag{54}$$

The error on such propagation is rigorously known and stated in Theorem 1 of [1] (see Eq. 2.36 therein) for (53) and Theorem 3 (see Eq. 3.6 therein) for (54). The results are compared to the ones found with the help of the split step method. In this method the wave function is propagated keeping only the kinetic energy or the potential energy in small steps of size $\delta t$. The choice of a time step $\delta t$ is crucial. The way to test the convergence of the scheme is by running the dynamics up to a point $t$ using a time step $\delta t$, running the dynamics up to the same point $t$ only using a new time step $\delta t' = \frac{1}{2}\delta t$. If the wave function is the same within some fixed accuracy then the scheme is said to be converged.

The accuracy is defined as

$$\delta_a = \int_{0}^{t} dx |\psi_1^{(\delta t)}(x,t) - \psi_2^{(\frac{\delta t}{2})}(x,t)|^2. \tag{55}$$

If not converged then one needs to continue adjusting until one converges. Listed in Table 1 are some values of the small parameter and the time scale it dictates. For longer time scale a smaller and a more refined time step is needed in order to converge the split step method. For the values listed in Table 1 an accuracy of $10^{-5}$ was chosen as a convergence criterion, i.e. if the two wave functions obtained at the same time $t$ with different time steps $\delta t$ and $\frac{\delta t}{2}$ differed by less then $\delta_a = 10^{-5}$, the algorithm is considered converged and an appropriate choice of $\delta t$ is obtained. The * marks the fact that the required time was too long for the standard split-step computation to converge.

To evaluate the accuracy of the averaging method we denote by $\psi_a(x,t)$ the wave function computed by the averaging method and by $\psi_s(x,t)$ the one found by the split step method and compute the deviation

$$\Delta(t) = \int_{0}^{t} dx |\psi_s(x,t) - \psi_a(x,t)|^2. \tag{56}$$

The wave function $\psi$ and in particular $\psi_a$ in (56) results of propagation with the help of $U_0$ of (18) for the zeroth order, by $\bar{U}_1$ of (53) for the first order and...
The results are presented for $\Delta(t)$ in Figs 1 for $\beta = 0.01$, Fig. 2 for $\beta = 0.001$. We note that the effects of the normal form transformation is small therefore it was not performed in some cases. To demonstrate the efficiency of the calculation we compare the computer time $T_{\text{comp}}$ required to perform the numerical time propagation (Fig. 3) up to times $T_0^2$ for the zeroth order and time $T_0^3$ for the first order averaging. The calculations were performed on two computational nodes each composed of a 2.4 Ghz Intel Xeon processors.

### 3.1. Spreading in k-space

As a test case for the agreement between the split step and averaging method we can evaluate the spread in momentum space of the wave function calculated. In the presence of a potential the wave function is expected to spread. The spreading in momentum space is defined as

$$\sigma_k = \langle |(p - \bar{p})^2| \psi \rangle$$  \hspace{1cm} (58)

where

$$\bar{p} = \langle |p| \psi \rangle$$  \hspace{1cm} (59)

We can then calculate (58) using the wavefunction obtained by performing the propagation for different values of $\beta$ and compare it to the wave
function obtained by split step propagation. We denote by $\sigma_k^{(0)}$ the initial value of (58). We denote by $\Delta \sigma = \sigma_k - \sigma_k^{(0)}$. Fig. 4 shows $\Delta \sigma$ for one realization of the random potential, where the wave function was propagated by $U_{(NP)}$ (54).

Let us denote by $< \Delta \sigma >$ the average of $\Delta \sigma$ over 15 realizations of the random potential, where $\phi_i$ are distributed uniformly in the interval $[-\pi, \pi]$, while $v_n(r)$ and $k_n$ are distributed uniformly in the intervals $[v_{\text{min}} = -15, v_{\text{max}} = 15]$ and $[k_{\text{min}} = -20, k_{\text{max}} = 20]$ respectively. $\omega_n$ is calculated by (5).

Fig. 4 shows $< \Delta \sigma >$ at times $T_0^2 = \frac{1}{\beta}$ and $T_0^3$ accordingly for different values of the small parameter $\beta$, as a function of time. Fig. 6 shows $< \Delta \sigma >$ as a function of $\beta$ for several times. As can be seen both split step and averaging method agree. A small spread for these moderate values of $\beta$ is found. We note that the rapid oscillations found for a single realization (Fig. 4) are rapidly averaged. Therefore on the time scales discussed here the quasiperiodic potential (1) can be considered random.

4. Spreading for very long times

After testing the method of averaging and comparison with the standard split step method for short times we apply it to the study of long times where the standard method is not practical. This enables us to study spreading for extremely small values of $\beta$.

In Fig 7 we plot on a logarithmic scale $< \Delta \sigma >_n = < \Delta \sigma > / \sigma_k$ as a function of time for $\beta = 10^{-2} (v = 100)$ and fit it to

$$< \sigma >_n = C(\beta) \tau^{\alpha(\beta)}$$

(60)

The calculation is repeated for several values of $\beta$ and the functions $C(\beta)$ and $\alpha(\beta)$ are plotted in Fig 8. We note that $C(\beta \rightarrow 0) \approx 0$ and $\alpha(\beta \rightarrow 0) \approx 1$.

5. Conclusions

We have presented a way to implement multi-time scale averaging technique to study the large time behavior of quantum systems. The systems are perturbed by a time dependent quasi-periodic potentials (in space-time), which are
a close approximations of a random space and time potentials.

We use this method which also provides a rigorous explicit bound on the error terms to study the above problem. This method is vastly superior to the standard FFT split step approach, in fact by orders of magnitude as the required accuracy gets higher. In particular, we were able to solve the equations to large times, which are not accessible to the split-step method. It is therefore expected that this method will be useful for other systems where a small parameter can be identified.

By applying this method to a free quantum particle perturbed by a quasi-periodic in space-time potential, we observe the diffusion in momentum space for solutions which are away from all the Chirikov resonances. The observed momentum distribution spreads like

\[
\langle p^2 \rangle \sim C(\beta) t^{\alpha(\beta)}
\]

with \(\alpha(\beta) \to 1\) and \(C(\beta) \to 0\), as \(\beta \to 0\).

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Figure 1: The deviation $\Delta$ of (56) for $\beta = 0.01$ (a) as a function of $t$, (b) a close up of (a), (c) as a function of $t/T_0$ and (d) as a function of $\tau$
Figure 2: Same as Fig 2 but for $\beta = 0.001$
Figure 3: The computation time required for time propagation up to \( t \) where (a) for zero order averaging and \( t = T_0^2 \) (b) for first order (53) averaging method and \( t = T_0^3 \). The lines are a guide to the eye.
Figure 4: $\Delta \sigma$ calculated to first order (53) for one realization of the potential (a) $\beta = 0.01$ and (b) $\beta = 0.001$.
Figure 5: \( \langle \Delta \sigma \rangle \) calculated to first order (53) for (a) \( \beta = 0.01 \) as a function of \( t/T_0 \), (b) \( \beta = 0.01 \) as a function of \( t \), (c) \( \beta = 0.001 \) as a function of \( t/T_0 \), (d) \( \beta = 0.001 \) as a function of \( t \).
Figure 6: $\langle \Delta \sigma \rangle$ as a function of $\beta$ for (a) zero order averaging, at time $t = T_0^2$ (b) zero order averaging and measured at time $t = 200$ for each $\beta$ (c) first order averaging, at time $t = T_0^3$ (d) first order averaging and measured at time $t = 200$
Figure 7: $\langle \Delta \sigma \rangle_n$ calculated to first order (53) as a function of $\tau$ on a logarithmic scale for $\beta = 0.001$
Figure 8: The parameters of the fit (60) as a function of $\beta$