Directed transport and Floquet analysis for a periodically kicked wavepacket at a quantum resonance

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The dynamics of a kicked quantum mechanical wavepacket at a quantum resonance is studied in the framework of Floquet analysis. It is seen how a directed current can be created out of a homogeneous initial state at certain resonances in an asymmetric potential. The almost periodic parameter dependence of the current is found to be connected with level crossings in the Floquet spectrum.

I. INTRODUCTION

The kicked rotor is, due to its relative simplicity, one of the most studied and best understood models of chaotic mechanics. In essence, it models a particle that is exposed to a sinusoidal potential during periodically repeated, delta-function shaped kicks. The quantum mechanical version of the kicked rotor has attracted special attention lately, due to the realization of the model in optical lattices [1, 2, 3]. It turns out that there exist two peculiar quantum mechanical effects that distinguish the quantum kicked rotor from its classical counterpart. These two, mutually exclusive, effects are Anderson localization in momentum space, which occurs for generic (almost all) values of the kicking period [4], and quantum resonances, which occur when the kicking period matches a resonance criterion [2, 3, 5, 6, 7, 8, 9]. The latter phenomenon, quantum resonances, is the subject of this paper.

Classically, the energy growth of the kicked rotor is diffusive, i.e., linear. In the quantum case and off resonance, the energy growth will also be diffusive but eventually saturate due to Anderson localization in momentum space. In contrast, a quantum resonance will result in an energy growth that is quadratic in time. Such resonances occur when the period of the potential kicks on the particle matches a rational value times the so-called Talbot time of the system. In the context of optical lattices, the corresponding frequency is identical to the recoil frequency [10]. It is common to state the resonance criterion in terms of an effective Planck constant which is defined as a combination of the physical parameters.

We have recently found that a slight generalization of the kicked rotor to an asymmetric, sawtooth-shaped potential will, combined with quantum resonances, result in a ratchet effect of sorts – a directed current which increases linearly with time [10]. In general, a classical or quantum particle in a flashing periodic potential will not pick up a finite velocity even if the potential is asymmetric, i.e., there is no ratchet effect. However, quantum resonances may change the situation and allow for a directed current. The effect hinges on the fact that a specific momentum eigenstate is chosen as the initial state, since a proper averaging over all of phase space would necessarily cancel out any directed current. Nevertheless, it was seen in Ref. [10] that the proposed setup could give a constant acceleration to an initially zero-momentum plane wave.

The spectral properties of the quantum kicked rotor were first studied by Izrailev and Shepelyanskii [2, 3]. It was found that the quasienergy spectrum is in general discrete, but in the case of a quantum resonance it forms a band structure with a continuum of quasienergies. This was found to explain the quadratic energy growth. In the present paper, the same type of analysis is exploited in order to understand how a directed current is created out of a motionless initial state with the help of an asymmetric potential. In Sec. II we describe the problem and set up the definitions. In Sec. III we show how the general solution of the problem at hand is constructed and cover the cases of two simple resonances. In Sec. IV a resonance of special interest is analyzed by perturbative and numerical means. Finally, in Sec. V we summarize and conclude.
II. PRELIMINARIES

We wish to study the Schrödinger equation

\[ i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2} \frac{d^2\psi}{dx^2} + U(x)\psi \sum_{n=1}^{\infty} \delta(t-n). \]  

(1)

This equation describes a particle subject to a periodic potential \( U(x) \) that is flashed on for short, periodically repeated pulses. It can be realized with atoms in an optical lattice [1, 2, 3]; the kicked rotor problem corresponds to the case \( U(x) \propto \sin x \), while the superposition of two sines has been predicted to result in a directed current [10].

The parameter \( \hbar \) is a dimensionless, effective Planck constant. Units are chosen so that the spatial periodicity of the potential is \( 2\pi \) and the temporal period of the flashing is unity.

The time development of the wave packet is given by

\[ \psi(x, t+1) \equiv U[\psi(x, t)] = e^{-iV(x)} \int_0^{2\pi} dx' \sum_{k=-\infty}^{\infty} e^{-ik(x-x')} e^{i k^2 \hbar \frac{t}{2}} \psi(x', t), \]  

(2)

where the operator \( U \) was implicitly defined. We assume that the wave function has the same spatial periodicity as the potential, and hence the momentum variable \( k \) is restricted to integers. The extension to non-integer momenta is straightforward but not important to the objectives of this paper. For notational convenience we have defined \( V(x) = U(x)/\hbar \).

The time development can be written in terms of the Floquet states \( w_j(x) \), which are eigenstates with associated quasi-energies \( \omega_j \) of the evolution operator for one temporal period:

\[ e^{-i\omega_j} w_j(x) = U[w_j(x)]. \]  

(3)

Since \( U \) is unitary, the quasi-energies \( \omega_j \) are real. The time evolution of an initial state \( \psi(x, 0) \) is constructed as follows:

\[ \psi(x, t) = \sum_j c_j e^{-i\omega_j t} w_j(x), \]  

(4)

with

\[ c_j = \int dx w_j(x)^* \psi(x, 0). \]  

(5)

Note that since the evolution operator \( U \) propagates the system for one unit of time \( \Delta t = 1 \), Eq. (4) is valid for integer \( t \) only.

This type of analysis was first performed for the kicked rotor in Refs. [5, 6]. It was found that quantum resonances are associated with a banded quasienergy spectrum. In the present paper, the same type of analysis will be employed with a specific goal in mind: It was found numerically in Ref. [10] that when the effective Planck constant \( \hbar \) takes on values that are integer or half-integer multiples of \( \pi \), the ensuing resonant behavior may result in a directed current.

We shall now investigate how this is reflected in the quasienergy spectrum.

III. FLOQUET STATES AT RESONANCES

This section contains mainly a brief repetition and slight generalization of the findings of Ref. [3], so that the formalism can be applied to the case of an asymmetric flashing potential. In order to get acquainted with the system and define the terminology, we start with the simplest case, where the Planck constant is an integer multiple of \( 4\pi \).

It is well known that in this case, the density stays unchanged at all times, the mean momentum increase is zero and the energy increases quadratically with time for any potential \( V(x) \) [2, 5, 6, 7].

When \( \hbar = 4\pi \), then \( \exp(-i k^2 \pi / 2) = 1 \) for all \( k \), and the unitary operator \( U \) in Eq. (2) simplifies to

\[ U[\psi(x)] = e^{-iV(x)} \int_0^{2\pi} dx' \sum_{k=-\infty}^{\infty} e^{-ik(x-x')} \psi(x', t) = e^{-iV(x)} \psi(x, t). \]  

(6)
Already from here we can see the solution to the full problem, but in order to prepare ourselves for more complicated cases we solve for the time evolution using Floquet analysis. The eigenvalue equation reads

$$e^{-iV(x)}w_j(x) = e^{-i\omega_j}w_j(x).$$

(7)

The phase factor on the left-hand side is space dependent, but that on the right-hand side is not. This has a solution if $w_j(x)$ is nonzero only for a discrete number of spatial points $x$. The discrete index $j$ has to be changed into a continuous one, $x_0$, and the solution for the continuous set of eigenstates, $\{w_{x_0}\}_{0 \leq x_0 < 2\pi}$, is found to be

$$w_{x_0}(x) = \delta(x - x_0), \quad \omega_{x_0} = V(x_0).$$

(8)

The expansion coefficients for the initial state are

$$c_{x_0} = \int dx w_{x_0}(x)^* \psi(x,0) = \psi(x_0,0),$$

(9)

and the wave function at integer time instances $t$ is

$$\psi(x,t) = \int dx_0 c_{x_0} e^{-i\omega_{x_0}} w_{x_0}(x) = \psi(x_0,0) e^{-iV(x)} e^{-itV(x)}.$$  

(10)

We conclude that the system remains unchanged at all times except for a multiplicative phase factor; there is no transport.

We are now prepared to discuss the more general case $\bar{k} = \pi/m$, where $m$ is an integer. (The case $\bar{k} = 2\pi$ is more easily solved by simpler means.) We have for the sum over momenta

$$\sum_{k=-\infty}^{\infty} e^{-i\pi \frac{k^2}{2m}} e^{-ikx} = \sum_{j=0}^{2m-1} A_j \delta(x - j \frac{\pi}{m}),$$

(11)

where

$$A_j = \frac{1}{2m} \sum_{n=0}^{2m-1} e^{-i\pi \frac{(n^2 - 2nj)}{m}}.$$  

(12)

The Floquet equation becomes

$$e^{-i\omega_{x_0}} w_{x_0}(x) = e^{-iV(x)} \sum_{j=0}^{2m-1} A_j w_{x_0}(x - j \frac{\pi}{m}).$$

(13)

By the same argument as above in the $\bar{k} = 4\pi$ case, the solution must be of the form

$$w_{x_0}(x) = \sum_{l=0}^{2m-1} \alpha_{x_0,l} \delta(x - x_0 - \frac{\pi}{m}).$$

(14)

We have come to the important conclusion that at a quantum resonance, each Floquet eigenstate is nonzero only at a discrete set of points. As a result, the Floquet spectrum is divided into a number of discrete bands, within each of which the quasienergy depends on the continuous parameter $x_0$. Now, inserting this ansatz and equating the coefficients yields the equations for the factors $\alpha_{x_0,l}$

$$e^{-i\omega_{x_0}} \alpha_{x_0,n} = \sum_{l=0}^{2m-1} M_{nl} \alpha_{x_0,l},$$

(15)

where

$$M_{nl} = e^{-iV(x_0 + n\pi/m)} A_{n-1}.$$  

(16)

The indices $l$ and $n$ are modulo $2m$. There are $2m$ solutions to this eigenvalue equation, which will be labeled $\alpha_{x_0,l}^\mu$, with $\mu = 0..2m$. But there is a degeneracy, since we can choose phases such that $w_{x_0}^{\mu}(x) = w_{x_0}(x)$, or
\( \alpha_{x_0 + r \pi / m, l} = \alpha_{x_0, l + r} \). This degeneracy needs to be taken care of by restricting \( 0 \leq x_0 < \pi / m \), in order to avoid overcounting.

Let us now use these eigenstates to construct the long-time development of the wavepacket. We specialize to the case of homogeneous initial conditions, \( \psi(x, 0) = 1 / \sqrt{2\pi} \), whereby the coefficients \( c \) become

\[
c_{x_0}^{\mu} = \frac{1}{\sqrt{2\pi}} \sum_{l=0}^{2m-1} \alpha_{x_0, l}^{\mu}, \tag{17}
\]

and

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi}} \sum_{\mu} \sum_{l} \alpha_{x_l}^{\mu*} e^{-i\omega_{\mu}^t - i\pi \mu / m} \alpha_{x_l}^{\mu} e^{-i\omega_{\mu}^t} \alpha_{x_l}^{\mu}, \tag{18}
\]

where \( l_x \) is the integer that fulfills \( \pi l_x / m \leq x < \pi (l_x + 1) / m \). After the completeness of the basis \( \psi_{x_0}^{\mu} \) has been exploited, we are free to extend the definition of the amplitudes \( \alpha \) to the whole range \( 0 \leq x < 2\pi \), and there results

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi}} \sum_{\mu} \sum_{l} \alpha_{x_l}^{\mu*} \alpha_{x_0, l}^{\mu} e^{-i\omega_{\mu}^t} \alpha_{x_l}^{\mu}. \tag{19}
\]

The goal is to calculate the time dependence of the momentum. It is given by

\[
\langle \psi(t) \frac{dV}{dx} \psi(t) \rangle = \frac{1}{2\pi} \sum_{\mu, \mu'} \sum_{l'l} \int_0^{2\pi} dx \frac{dV(x)}{dx} e^{-i(\omega_{\mu}^t - \omega_{\mu'}^t) t} \alpha_{x_l}^{\mu*} \alpha_{x_{l'}}^{\mu'} \alpha_{x_0}^{\mu} \alpha_{x_0}^{\mu}. \tag{20}
\]

The sum can divided into a part that oscillates in time and a constant part. The constant part will be responsible for a linear increase of the momentum, if there is one. This term is denoted by \( F \) and is given by

\[
F = \frac{1}{2\pi} \sum_{\mu} \sum_{l, l'} \int_0^{2\pi} dx V'(x) \alpha_{x_l}^{\mu*} \alpha_{x_{l'}}^{\mu'} |\alpha_{x_0}^{\mu}|^2. \tag{21}
\]

This is the final expression for the rate of momentum increase for an initially homogeneous wavepacket.

The solution method outlined above will now be applied to the case \( k = \pi \), i.e. \( m = 1 \). We have \( \exp(-i\pi k^2 / 2) = 1 \) for even \( k \) and \(-i\) for odd \( k \), and the kernel is

\[
\sum_{k} e^{-ikx} e^{-i\pi k^2} = \frac{1-i}{2} \delta(x) + \frac{1+i}{2} \delta(x - \pi). \tag{22}
\]

The solutions to the Floquet equation consist of two bands, whose discrete indices \( \mu \) will be labeled + and -. The eigenvectors are

\[
\alpha_{x_0, 0}^{\pm} = \left[ \frac{e^{-i\Delta V}}{2} \left( 1 \pm \frac{\sin \Delta V}{\sqrt{1 + \sin^2 \Delta V}} \right) \right]^{1/2},
\]

\[
\alpha_{x_0, 1}^{\pm} = \pm \left[ \frac{e^{i\Delta V}}{2} \left( 1 \pm \frac{\sin \Delta V}{\sqrt{1 + \sin^2 \Delta V}} \right) \right]^{1/2}, \tag{23}
\]

with the eigenvalues

\[
e^{-i\omega_{x_0}^{\pm}} = \frac{1-i}{2} e^{-V} \left[ \cos \Delta V \pm i \sqrt{1 + \sin^2 \Delta V} \right], \tag{24}
\]

where \( \Delta V = (V(x_0) - V(x_0 + \pi))/2 \), and \( V = (V(x_0) + V(x_0 + \pi))/2 \). Thus,

\[
\omega_{x_0}^{\pm} = \frac{\pi}{4} + V(x_0) \mp \arctan \sqrt{1 + \sin^2 \Delta V(x_0) / \cos \Delta V(x_0)}. \tag{25}
\]
Now insert this into the general expression, Eq. (21), for the time development. There results for the time-independent part of the force

\[
F = \sum_{+, -} \int_{0}^{2\pi} dx \frac{dV(x)}{dx} \left[ \frac{e^{-i\Delta V}}{2} \left( 1 \pm \frac{s}{\sqrt{1+s^2}} \right) \right] + \frac{1}{2} \int_{0}^{2\pi} dx \int_{0}^{2\pi} dx' \Delta V(x, x') \frac{s}{1+s^2}
\]

where \( s \) and \( c \) are short for \( \sin \Delta V(x) \) and \( \cos \Delta V(x) \), respectively. The presence of a term odd in \( \Delta V(x) \) is crucial. Now use the periodicity of \( V \) to transform

\[
F = \int_{0}^{2\pi} dx V'(x) + \frac{1}{2} \int_{0}^{2\pi} dx dx' V'(x) \frac{s}{1+s^2} + \frac{1}{2} \int_{0}^{2\pi} dx dx' \Delta V(x, x') \frac{s}{1+s^2}
\]

by the periodicity of the potential. This could be done because the integrand of the second term depends on the coordinate solely through the potential difference \( \Delta V \). This concludes the demonstration that the drift is zero in an initially homogeneous system for any potential \( V \) at the resonance \( \bar{k} = \pi \).

**IV. RESONANCE AT \( k = \pi/2 \)**

The half-integer resonances are especially interesting since they are known to result in directed transport even if the initial state is homogeneous \[10\]. We therefore study the case \( \bar{k} = \pi/2 \) with special care. The momentum sum is now

\[
\sum_{k} e^{-ikx} e^{-i\pi k^2/4} = \frac{1}{2} \left[ e^{-i\pi/4} \delta(x) + \delta(x - \pi/2) - e^{-i\pi/4} \delta(x - \pi) + \delta(x - 3\pi/2) \right], \tag{28}
\]

and correspondingly the matrix \( M \) for the Floquet eigenvectors reads

\[
M = V \frac{1}{2} \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & e^{-i\pi/4} & e^{-i\pi/4} & -e^{-i\pi/4} \\
e^{-i\pi/4} & 1 & e^{-i\pi/4} & -e^{-i\pi/4} \\
e^{-i\pi/4} & e^{-i\pi/4} & 1 & e^{-i\pi/4}
\end{pmatrix}, \tag{29}
\]

where

\[
V = \text{diag} \left( e^{-iV(x)}, e^{-iV(x-\pi/2)}, e^{-iV(x-\pi)}, e^{-iV(x-3\pi/2)} \right). \tag{30}
\]

We first solve this system by perturbative means. The quasienergies and eigenvectors to zeroth order in the potential \( V(x) \) are

\[
\omega_{(0)}^{0} = \pi, \quad \alpha_{(0)}^{0} = (-1, 1, -1, 1)^T, \\
\omega_{(0)}^{1} = 0, \quad \alpha_{(0)}^{1} = (1, 1, 1, 1)^T, \\
\omega_{(0)}^{2} = -\pi/4, \quad \alpha_{(0)}^{2} = (0, -1, 0, 1)^T, \\
\omega_{(0)}^{3} = -\pi/4, \quad \alpha_{(0)}^{3} = (-1, 0, 1, 0)^T, \tag{31}
\]

so the correction to first order is

\[
\alpha_{(1)}^{0} = \frac{1}{2} i (-V_0 + V_1 - V_2 + V_3) (1, 1, 1, 1)^T + \frac{e^{-i3\pi/8}}{\sqrt{2} + \sqrt{2}} (\Delta_0, -\Delta_1, -\Delta_0, \Delta_1)^T,
\]
FIG. 1: rate of momentum increase on an initially homogeneous wavefunction for $a = 0.3$, as a function of potential strength $U$, assuming the form of Eq. (33) for the potential.

$$\alpha^1_{(1)} = \frac{1}{2}i(-V_0 + V_1 - V_2 + V_3)(1, -1, 1, -1)^T + \frac{e^{i\pi/8}}{\sqrt{2 - \sqrt{2}}}(-\Delta_0, -\Delta_1, \Delta_0, \Delta_1)^T,$$

$$\alpha^2_{(1)} = -\sqrt{2}\Delta_1(e^{i\pi/4}, 1, e^{i\pi/4}, 1)^T,$$

$$\alpha^3_{(1)} = -\sqrt{2}\Delta_0(1, e^{i\pi/4}, 1, e^{i\pi/4})^T,$$

(32)

where we defined $V_j = V(x + j\pi/2)$ for $j = 0, 1, 2, 3$; $\Delta_0 = V_0 - V_2$; and $\Delta_1 = V_1 - V_3$. These eigenvectors can now be inserted into the expression for the force, Eq. (21). In order to obtain a closed expression, one has to make an assumption about the potential. We make the physically motivated choice

$$V(x) = U(\sin x + a \sin 2x),$$

(33)

which models an atom subject to standing laser waves \[10\]. There results for small $U$

$$F = (3 + 2\sqrt{2})aU^3 - (1 + \sqrt{2})a^3U^5.$$

(34)

In order to go beyond perturbation theory, the $k = \pi/2$ problem has to be solved numerically. Again we assume the form Eq. 33 for the potential. Figure 1 depicts the numerically calculated force $F$ as a function of potential strength $U$, for the choice $a = 0.3$. The force rises initially as the third power of $U$ as the perturbative calculation indicated, but for longer times the time dependence displays an approximate periodicity of $F$ as a function of $U$. We shall now see that it can be related to the structure of the Floquet spectrum. In Fig. 2 we display the numerically obtained eigenvalues $\omega_{\mu x}$ for a range of values of $U$. It is seen that a level crossing as a function of the continuous parameter $x_0$ appears when $U = 3.3$ and then separates when $U$ is increased. At this point, two energy bands momentarily merge into one. This crossing is reflected in Fig. 1 as a pointed feature in the force curve $F(U)$. Closer inspection reveals that there is a discontinuity in the first derivative at the turning point, but there does not appear to be a cusp.

Level crossings in Floquet spectra have been seen in various contexts to be associated with resonance phenomena \[11,12\]. However, in Refs. \[11,12\], the situation is different: the eigenvalue spectra are discrete and the level crossings occur as a control parameter is varied. In the present system, the eigenvalues form a continuous set and the level crossings take place in the two-dimensional space formed by the continuous index $x_0$ and the parameter $U$; in other words, the crossing is a merging of two quasienergy bands. The crossings are not easily interpreted as a resonance phenomenon, but they are connected with the sharp turning points of the force $F$ as a function of $U$ that can be seen in Fig. 1. In fact, every such sharp turning point coincides with a level crossing, i.e., a merging of bands, in the continuous spectrum. In Fig. 3, we see how a number of level crossings appear around $U = 19$. Here, the minimum in the curve $F(U)$ is smoother, and accordingly it is associated with a sequence of level crossings instead of just one.

A straight level crossing originates from two eigenvectors $\bar{\alpha}^\mu$ that have different symmetry in the sense that the
overlap with respect to a small change $\delta U$ of the control parameter $U$ vanishes;

$$\left(\tilde{\alpha}^{\mu_1}\right)^T dA \frac{dU}{dU} \delta U \tilde{\alpha}^{\mu_2} = 0.$$ (35)

(Alternatively, a small variation in the index $x_0$ can be considered, since the level crossing takes place in the two-dimensional space of $U, x_0$.) The generic situation is that the overlap is nonzero, which results in an avoided crossing and a mixing of the eigenvectors; when the overlap vanishes the energies cross and the eigenvectors do not mix. Indeed, this decoupling of eigenvectors is clearly seen in the plots of the components $\alpha$ of the eigenvectors, a selection of which is displayed in Fig. 4. The avoided level crossing is accompanied by the crossing at $x \approx 0.9$ of the components of the corresponding eigenvectors. Close to the turning point the slope gets steeper and eventually the two lines do not cross at all, indicating that the overlap between the modes vanishes. This is, in turn, reflected in the force integral (21) and manifests itself in the sharp bending of the curve.
FIG. 4: A selection of eigenvector components $\alpha_{x,l}^\mu$ as functions of $x$, for a few choices of $U$.

V. CONCLUSIONS

We have investigated the Floquet spectrum for a wavepacket subject to periodic forcing, with special attention to quantum resonances, where the effective Planck constant is equal to a rational multiple of $\pi$ and the quasienergies form a band structure. We derived an expression for the force on the wavepacket in terms of Floquet eigenstates and concluded that a nonzero mean velocity is obtained from homogeneous initial conditions only at minor resonances when the Planck constant is equal to a half-integer multiple of $\pi$. The oscillatory dependence of the current on the potential strength was investigated for the special case of a potential composed of two harmonics, and it was seen how turning points in the curve of drift as a function of potential strength arise from level crossings in the Floquet spectrum.

VI. ACKNOWLEDGMENTS

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