Time Independent Description of Rapidly Oscillating Potentials

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The classical and quantum dynamics in a high frequency field are found to be described by an effective time independent Hamiltonian. It is calculated in a systematic expansion in the inverse of the frequency (ω) to order ω^{-4}. The work is an extension of the classical result for the Kapitza pendulum, which was calculated in the past to order ω^{-2}. The analysis makes use of an implementation of the method of separation of time scales and of a quantum gauge transformation in the framework of Floquet theory. The effective time independent Hamiltonian enables one to explore the dynamics in the presence of rapidly oscillating fields, in the framework of theories that were developed for systems with time independent Hamiltonians. The results are relevant, in particular, for exploring the dynamics of cold atoms.

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The classical and quantum dynamics of a particle in a field that oscillates rapidly relative to the motion of the particle will be studied. The variation of the field in space is smooth but otherwise arbitrary. Such fields are applied experimentally to cold atoms, where a very high degree of control is possible. The exploration of the dynamics of cold atoms in strong electromagnetic fields resulted in many novel, interesting experimental observations [1–3]. The results of this Letter [4] are expected to enable further discoveries in this field, as well as in related fields.

For atom optics, the effect of the internal degrees of freedom on the center of mass motion is important. The force on the center of mass due to the internal degrees of freedom that couple to the external field is given approximately by a dipole force [2]. The motion of the atoms can be manipulated by fields with amplitudes which vary spatially, resulting in a force on the center of mass of the atoms. In the present work, the effect of the laser on the center of mass motion is modeled by a time dependent potential. For some situations of physical interest, this simpler model still describes the dynamics of the center of mass without the need to specify the dynamics of the internal degrees of freedom or the quantum aspects of the light field. In the situation that is of interest for the Letter, the frequency of this potential is large compared to the inverse of the characteristic time scale of the center of mass dynamics. An example of such systems that was recently realized experimentally and that motivated the present work is of atomic billiards [5,6]. The boundary of the billiards is generated by a laser beam that rapidly traverses a closed curve, which acts as the boundary of the billiard, approximated by the time average of this beam. The force applied by the boundary on the particles is approximately the mean force applied by the beam.

The influence of a high frequency field on a classical particle was derived by Landau and Lifshitz [7] generalizing the work on the Kapitza pendulum [8], which is a classical pendulum with a periodically moving point of suspension. The motion was separated into a slow part and a fast part. The leading order (in the inverse frequency) of the slow motion was calculated. This mechanism is used to trap ions in electromagnetic fields. The most notable example is the Paul trap [9] that can be described approximately by a Hamiltonian of a time dependent harmonic oscillator [10–12]. It is of interest to solve more general problems even if only approximately. The work of Kapitza was first extended to quantum mechanical systems in a pioneering paper by Grozdanov and Raković [13]. They introduced a unitary gauge transformation resulting in an effective Hamiltonian that describes the slow motion. In that paper, the analysis is restricted to a driving potential that has a particularly simple time dependence. Moreover, the final results are restricted to forces that are uniform in space, a situation natural in standard spectroscopy, but too restrictive for the interesting problems in atom optics. These restrictions are avoided in the present work. Many investigations of periodically driven quantum systems were performed [14–21].

In the present work, a coherent theoretical treatment of the dynamics of classical and quantum high frequency driven systems is presented. Classically the motion can be considered approximately as one that consists of a rapid oscillation around a slowly varying trajectory. Therefore for the classical problem the motion is separated into a "slow" part and a "fast" part and a systematic perturbation theory is developed for the motion of the slow part. This slow motion is computed to order ω^{-4} and demonstrated to result from an effective Hamiltonian. It is an extension of the order ω^{-2} (that is presented in Ref. [7]). Floquet theory is used to separate the slow and fast time scales in the corresponding quantum problem. An effective (time independent) Hamiltonian operator is defined following [13]. The eigenvalues of this operator are the quasienergies of the system. This effective Hamiltonian is then computed perturbatively (to order ω^{-4}). It is obtained by a gauge transformation that is simply related to the canonical transformation leading to the corresponding classical effective Hamiltonian.

A model Hamiltonian for the motion in a periodic field is

$$H = p^2/2m + V_0(x) + V_1(x, \omega t), \tag{1}$$

leading to Newton's equation,

$$m\ddot{x} = -V_0'(x) - V_1'(x, \omega t), \tag{2}$$

where V_1 is a 2π periodic function of ωt and its average over a period vanishes. (We denote $\dot{X} = dX/dt$, $V_0' = dV_0/dx$, etc.) An instructive example of such a system is

$$V_0 = 0, \qquad V_1 = \gamma e^{-\beta x^2} \cos(\omega t). \tag{3}$$

The system is of particular interest since (i) the time average of the potential vanishes, consequently any interesting effect is due to the rapidly oscillating potential; (ii) when $x \to \infty$ the potential vanishes and therefore one expects to find scattering quasienergy states.

We look for a solution of (2) that has the form

$$x(t) = X(t) + \xi(X, \dot{X}, \omega t), \tag{4}$$

where X is the slow part, $\dot{X} = \frac{dX}{dt}$ while ξ is the fast part which is periodic (in the variable ωt) with *vanishing average*. This determines uniquely the functions X and ξ. One could use a different functional dependence of ξ on X and its time derivatives, but such a change cannot affect the dependence of the solution for ξ on time. Our method of solution is to choose ξ so that (2) leads to an equation for X which is explicitly time independent. An exact solution using (4) is too complicated to obtain in general. However, at high frequencies, one can determine ξ order by order in $1/\omega$, using

$$\xi = \sum_{i=1}^{\infty} \frac{1}{\omega^i} \xi_i. \tag{5}$$

The ξ_i are chosen so that the equation for X does not depend on $\tau \equiv \omega t$. One may also expand X in powers of $1/\omega$ as $X = \sum_{i=0}^{\infty} X_i/\omega^i$. When one does so, the equation of motion for X is replaced by a series of equations for X_i. In this series of equations, each X_i can be determined from the lower order terms X_j, where $j < i$. This is the standard method of separation of time scales [22]. These equations are equivalent, in any order, to the equation of motion of the (unexpanded) X which will be used in what follows. At a given order ω^{-n} of the present calculation, *all* contributions that are found by the method of separation of time scales are included, but *some* of the higher order terms are included as well.

The slow motion is found to be controlled by the Hamiltonian [4]

$$H_{\rm eff} = \frac{P^2}{2m} + V_{\rm eff}(X) + \frac{1}{\omega^4} g(X) P^2 + O(\omega^{-5}), \tag{6}$$

where $g(X) = [3/(2m^3)]\overline{(\int^{(2)\tau}[V_1''])^2}$ and P is the momentum conjugate to X. We define the integrals

$$\int^{(j)\tau}[f] = \underbrace{\int^{\tau}\Big[\cdots\int^{\tau}[f]\cdots\Big]}_{\text{j times}},$$

where $f(x,\tau) = \sum_{n\neq 0} f_n(x) e^{in\tau}$ and $\int^{\tau}[f] \equiv \sum_{n\neq 0}\frac{1}{in}\times f_n e^{in\tau}$. The effective potential is found to be

$$V_{\rm eff}(X) \equiv V_0(X) + V_2(X) + V_4(X). \tag{7}$$

where $V_2(X) = [1/(2m\omega^2)]\overline{(\int^{\tau}[V_1'])^2}$ and $V_4(X) = [1/(2m^2\omega^4)]\overline{\{V_1''(\int^{(2)\tau}[V_1'])^2 + V_0''(\int^{(2)\tau}[V_1'])^2\}}$. For example, for the system with the potential (3), at the order ω^0, where only the average of the potential over time is taken into account, $V_{\rm eff} = 0$. The effective potential $V_{\rm eff}$ of (7) is plotted in the inset of Fig. 1. The leading order (ω^{-2}) is $V_2(x) = [(\beta^2\gamma^2x^2)/(m\omega^2)]e^{-2\beta x^2}$, which is clearly a double barrier. It is obvious that it traps the particle. This potential is always positive since it is the mean kinetic energy of the rapid oscillation around the slow motion, an energy which is coordinate dependent. For this it is instructive to note that $V_2 = m\overline{\dot{\xi}^2}/2$ in the leading order. In the order ω^{-4}, on the other hand, the Hamiltonian cannot be expressed anymore in terms of an effective potential and terms that mix coordinates and momentum, such as $g(X)P^2$, appear. Such terms result in corrections increasing with energy. It is also more complicated to understand terms of this order intuitively.

Consider a quantum system with a Hamiltonian that is periodic in time, $\hat{H}(t + T) = \hat{H}(t)$. Such a system can be treated using Floquet theory [23–25]. The symmetry with respect to discrete time translations implies that

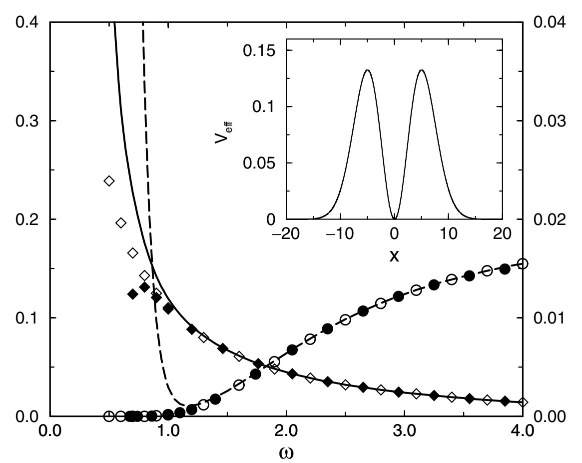

FIG. 1. The lowest quasienergy resonance of the oscillating Gaussian (3), E_0 (solid line) and Γ_0 (dashed line), as a function of the driving frequency, compared to the lowest resonance of the effective Hamiltonian (16), E_0 (diamonds) and Γ_0 (circles), for $\gamma = 9$ and $\beta = 0.02$ (in "atomic units" $\hbar = m = e = 1$). Full symbols correspond to the effective Hamiltonian truncated at order ω^{-4} while empty symbols to order ω^{-2}. The effective potential (7) is depicted in the inset, for $\omega = 1.5$.

the solutions of the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi, \quad (8)$$

are linear combinations of functions of the form

$$\psi_\lambda = e^{-i(\lambda t/\hbar)}u_\lambda(x, \omega t), \quad (9)$$

where λ are the quasienergies and the corresponding quasienergy (or Floquet) states are $u_\lambda(x, \omega(t+T)) = u_\lambda(x, \omega t)$ with $\omega = 2\pi/T$. This is the content of the Bloch-Floquet theorem in time. The states u_λ are the eigenstates of the Floquet Hamiltonian,

$$\hat{\mathcal{H}}_F = -i\hbar\frac{\partial}{\partial t} + \hat{H}. \quad (10)$$

These states have a natural separation into a slow part $e^{-i(\lambda t/\hbar)}$ (with the natural choice $0 \leq \lambda/\hbar \leq \omega$), which includes the information about the quasienergies, and a fast part $u_\lambda(x, \omega t)$ that depends only on the fast time $\tau \equiv \omega t$. In the following, an equation of motion for the slow part of the dynamics is found as was done for classical systems. It establishes a natural link between the separation into fast and slow motion in classical mechanics, that can be formalized by the theory of separation of time scales, and Bloch-Floquet theory in quantum mechanics. For this purpose, following [13], we will look for a unitary gauge transformation $e^{i\hat{F}(t)}$, where $\hat{F}(t)$ is a Hermitian operator (function of $\hat{x}$ and $\hat{p}$) defined at a certain time t, which is a *periodic function* of time with the *same* period as $\hat{H}$, such that in the new gauge the Hamiltonian in the Schrödinger equation is *time independent.* In terms of the functions in the new gauge $\phi = e^{i\hat{F}}\psi$, the Schrödinger Eq. (8) is

$$i\hbar\frac{\partial}{\partial t}\phi = \hat{G}\phi, \quad (11)$$

where the Hamiltonian is

$$\hat{G} = e^{i\hat{F}}\hat{H}e^{-i\hat{F}} + i\hbar\left(\frac{\partial e^{i\hat{F}}}{\partial t}\right)e^{-i\hat{F}}. \quad (12)$$

Assume that such an operator $\hat{F}$ exists, so that $\hat{G}$ is time independent. Its eigenfunctions $v_\lambda(x)$ evolve as

$$\phi_\lambda(t, x) = e^{-i(\lambda t/\hbar)}v_\lambda(x). \quad (13)$$

These states, in the original gauge, correspond to

$$\psi_\lambda(t, x) = e^{-i\hat{F}}\phi_\lambda = e^{-i(\lambda t/\hbar)}e^{-i\hat{F}}v_\lambda(x). \quad (14)$$

The function $e^{-i\hat{F}}v_\lambda$ is periodic in time with the period of $\hat{H}$, and therefore ψ_λ of (9) is a Floquet state with quasienergy λ (mod $\hbar\omega$), where $u_\lambda = e^{-i\hat{F}}v_\lambda$.

At high frequencies, $\hat{F}$ is found to be small, of the order of $1/\omega$. We expand $\hat{G}$ and $\hat{F}$ in powers of $1/\omega$ and choose $\hat{F}$ so that $\hat{G}$ is time independent in any given order. The expansions are $\hat{G} = \sum_{n=0}^{\infty}\hat{G}_n/\omega^n$ and $\hat{F} = \sum_{n=1}^{\infty}\hat{F}_n/\omega^n$. The calculation is performed by computing $\hat{G}_l$ in terms of $\hat{F}_1, \ldots, \hat{F}_{l+1}$ and then choosing $\hat{F}_{l+1}$ so that $\hat{G}_l$ is time independent. The terms in (12) are calculated with the help of the operator expansion,

$$e^{i\hat{F}}\hat{B}e^{-i\hat{F}} = \hat{B} + i[\hat{F}, \hat{B}] - \frac{1}{2!}[\hat{F}, [\hat{F}, \hat{B}]]\cdots, \quad (15)$$

where for the first term in (12) one takes $\hat{B} = \hat{H}$, while for the second $\hat{B} = \frac{\partial}{\partial\tau}$.

The resulting time independent effective Hamiltonian is [4]

$$\hat{G} = \frac{\hat{p}^2}{2m} + \hat{V}_{\mathrm{eff}}(x) + \frac{1}{4\omega^4}[\hat{p}^2 g(x) + 2\hat{p}g(x)\hat{p} + g(x)\hat{p}^2] + \frac{\hbar^2}{\omega^4}\hat{V}_q + O(\omega^{-5}), \quad (16)$$

where $V_{\mathrm{eff}}(x)$ and $g(x)$ are the classical terms [see (6) and (7)], while $\hat{V}_q = \frac{1}{8m^3}\overline{(\int^{(2)\tau}[V_1^{(3)}])^2}$ is a quantum correction to the classical Hamiltonian that appears first in this order. The Hamiltonian (16) is presented in a form which is manifestly Hermitian.

The effective Hamiltonian (16) is the main result of this work. Its classical limit is the classical effective Hamiltonian (6) that can be obtained from (1) by the canonical transformation that is the classical limit of $-\hbar F$. It should be emphasized that in the derivation of (16) *no* semiclassical approximation was made.

The perturbation theory that was developed here enables one to calculate not only the quasienergies that are the eigenvalues of $\hat{G}$ but also the corresponding quasienergy states. If the eigenfunctions of $\hat{G}$ are known, then the quasienergy (or Floquet) states can be computed up to order ω^{-4} using Eq. (14) with

$$\hat{F} = \frac{1}{\hbar\omega}\int^{\tau}[V_1] + \frac{i}{m\omega^2}\int^{(2)\tau}\left(\frac{1}{2}[V_1''] + [V_1']\frac{\partial}{\partial x}\right) + \cdots, \quad (17)$$

where the explicit expressions of terms of order ω^{-3} and ω^{-4} will be given elsewhere [4].

The theory is demonstrated for the oscillating Gaussian (3). The system demonstrates trapping by an oscillating field, a phenomenon that is of physical interest. For this problem, the effective potential (7), depicted in the inset of Fig. 1, is a double barrier, therefore it exhibits resonances. Each resonance is characterized by a complex energy $E - i\Gamma/2$. (For a relevant review, see [26].) For any resonance of (16), it is natural to look for the corresponding resonance of the original time dependent Hamiltonian (3). More precisely, one looks for the resonances of the Floquet Hamiltonian (10) with $\hat{H}$ of (3). This is done numerically using a combination of the (t, t') method and complex scaling [26].

The energy E_0 and the width Γ_0 of the lowest (smallest real part E_0) quasienergy resonance of (3) are compared with the lowest resonance of the corresponding effective Hamiltonian (16) in Fig. 1. It is clear that for large frequencies there is excellent agreement. The results for the effective Hamiltonian truncated at orders ω^{-4} and ω^{-2} are comparable at large frequencies. At low frequencies, the results of order ω^{-2} turn out to be more accurate, indicating that the series do not converge at those frequencies. For comparison, the characteristic frequency for the slow motion of the particle is in the range 0.1–0.3.

It was found that the perturbation theory leads to a time independent effective Hamiltonian. This effective Hamiltonian may give physical insight, based on experience with time independent systems, which is absent when examining the corresponding time dependent problem. For example, consider a system where the time averaged potential consists of two barriers in addition to some high frequency time dependent perturbation (with vanishing average). If the perturbation is mainly in the region of the barriers, one expects that the perturbation slightly raises the barriers in the effective Hamiltonian. In contrast, if the perturbation is in the region between the barriers, it tends to raise the energy of the resonance. Therefore one expects that applying a time dependent perturbation in the region of the barriers will tend to increase the lifetime of the resonance ($\hbar/\Gamma$), while applying it in between the barriers will tend to decrease it. All the well-developed techniques for time independent quantum systems can be used to compute the eigenvalues of $\hat{G}$, in particular, in the case where the eigenvalues and eigenstates of $\hat{G}_0 = \hat{p}^2/(2m) + V_0(x)$ are known. The effective Hamiltonian can also be used to predict trapping by oscillating potentials that were thus far investigated mainly numerically [27].

We have investigated the dynamics of high frequency driven general classical and quantum systems. High frequency perturbation theory, which exploits the idea of separation of time scales, was used to obtain an effective time independent Hamiltonian for the slow part of the classical and quantum motion. The spectrum of the effective quantum Hamiltonian is the quasienergy spectrum of the time dependent system. This effective Hamiltonian is computed to order ω^{-4} in a perturbation theory. While in the order ω^{-2} the effect of the rapid oscillations around the slow motion could be expressed in terms of a classical scalar potential, the order ω^{-4} involves both coordinates and momentum. Quantum corrections to the Hamiltonian also appear at this order.

Some properties of the perturbation theory for $\hat{F}$ and $\hat{G}$, such as its convergence and validity, are not well understood and should be further studied. For instance, in one dimension the classical slow motion is integrable while the exact time dependent dynamics may have chaotic regions in phase space. This may hint that the perturbation theory may describe correctly only part of the phase space (whose fraction grows with ω).

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