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LETTER TO THE EDITOR

Trapping of particles by lasers: the quantum Kapitza pendulum

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Abstract

It is demonstrated that a bound rapidly oscillating potential typically traps particles even if its time average vanishes. In particular, it is shown that in one dimension there is *always* a resonance state and its energy and lifetime are calculated from an effective time-independent potential. This is the quantum analogue of the classical Kapitza pendulum. This work may be relevant for the manipulation of cold atoms and for the suppression of photo-ionization by electromagnetic fields.

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The effect of trapping and cooling of particles, specifically atoms, is of great interest due to the applicability in fields such as atom optics, precision spectroscopy, optical communication, and in the developing field of quantum computing [1].

In this letter we will demonstrate that typically a rapidly oscillating, smooth, bounded one-dimensional potential with vanishing average leads to trapping of particles. This sounds counter intuitive since one may expect that because of the high energy of the photons the particles will rapidly obtain energy that will be sufficient to overcome any potential barrier. It will be demonstrated that this is *not* the case and the situation is similar to that found in classical mechanics, where stabilization by a rapidly oscillating potential with vanishing mean is possible.

Trapping of a classical particle can be achieved by introducing an external rapid time periodic potential $V(q,t) = V_0(q) + V_1(q,t)$ [2, 3]. The classical particle is trapped by an effective time-independent potential which is approximately given by

$$V_{\rm eff}(q) = V_0(q) + \overline{F^2}(q)/(2m\omega^2) \tag{1}$$

where $\overline{F^2}(q)$ is the time average of the square of the force $F = -\partial V_1(q,t)/\partial q$, which is exerted by the oscillating field $V_1(q,t) = V_1(q,t+T)$, where $T = 2\pi/\omega$ and its time average $\bar{V}_1$ vanishes. In this case the trapping is obtained when the frequency of the external oscillatory field, ω, is much larger than the frequency Ω of the bound motion or the inverse of the shortest characteristic time scale of the motion, which for this comparison plays the role of Ω. Note that the motion can be bounded even in the absence of V_0, namely when the time average of the potential vanishes. Such a stabilization was proposed by Kapitza for a pendulum with a vibrating point of suspension [3]. In such a situation the pendulum can perform stable vibrations around the point where it points upwards, which is unstable in the absence of the vibrations of the point of suspension. It was generalized to arbitrary oscillating potentials in [2]. This is also the principle of operation of the Paul trap [4] where $V_1(q, t)$ and the resulting $V_{\mathrm{eff}}(q)$ are harmonic. In this letter it will be argued that for high frequency the action of the potential V_1 on quantum particles can be approximated by the action of the time-independent potential $V_{\mathrm{eff}}(q)$ also beyond the validity of the semiclassical approximation. In particular, if $V_{\mathrm{eff}}(q)$ has a minimum at $q = 0$, and maxima at $\pm\bar{q}_{\max}$ and it vanishes in the limit $|q| \to \infty$, the classical particle will be bounded in a region around $q = 0$ if its energy is lower than $V_{\mathrm{eff}}(\bar{q}_{\max})$, while under these conditions the quantum particle will exhibit some long lived resonances. The potential $V_{\mathrm{eff}}(q)$ that describes the classical dynamics for the rapidly oscillating potential $V_1(q, t)$ will be demonstrated to also describe the quantum dynamics. For simplicity a one-dimensional notation is used in most of the letter, but generalization to higher dimensions is straightforward.

This problem is relevant for the modelling of manipulation of cold atoms by electromagnetic fields. Resonant coupling between a field and an atom results in a potential, proportional to the intensity, on the centre of mass of the atom [5]. This potential may oscillate with a frequency that is much larger than the frequencies related to the dynamics of the centre of mass (but much lower than the frequency of the light of the laser). This is the way the atoms are trapped in an effective light billiard [6, 7].

The model studied here may also be relevant for the analysis of the electronic motion of atoms and molecules in the presence of strong laser fields. In this case the potential experienced by the electrons is a result of the combined effect of the internal interactions in the atom and of the external field. For example, the Kramers–Henneberger (KH) transformation [8] results in a potential of the form $V(q, t) = V_{\mathrm{atom}}(\mathbf{q} - \hat{\mathbf{z}}\alpha_0 \cos\omega t)$, where V_{atom} is the potential in the absence of an external field, and α_0 is a constant.

For the sake of clarity we briefly sketch below the *quantum* derivation that will lead to an effective time-independent potential. It employs a unitary transformation of the time-dependent Schrödinger equation which provides an alternative transformed time periodic potential, $V^{\mathrm{alt}}(q, t)$ [9]. For a Hamiltonian of the form

$$\mathcal{H}(q, t) = \mathcal{H}_0 + V_1(q, t) \tag{2}$$

with

$$\mathcal{H}_0 = \frac{\hat{p}_q^2}{2m} + V_0(q) \tag{3}$$

where the average over a period of V_1 vanishes, the unitary transformation

$$\hat{U} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int^t V_1(q,t')\,\mathrm{d}t'} \tag{4}$$

will result in a Schrödinger equation with a Hamiltonian where the potential is given by $V_0 + V^{\mathrm{alt}}$ with

$$V^{\mathrm{alt}}(q, t) = \frac{(\hat{p}_q - A(q, t))^2}{2m} - \frac{\hat{p}_q^2}{2m} \tag{5}$$

where

$$A(q, t) = \int^t \frac{\partial V_1(q, t')}{\partial q}\,\mathrm{d}t'. \tag{6}$$

Averaging over a period results in an effective potential

$$V_{\text{eff}}(q) = V_0(q) + \frac{1}{T}\int_0^T V^{\text{alt}}(q,t)\,\mathrm{d}t = V_0(q) + \frac{1}{2m\omega^2}\sum_{n\neq 0}\frac{f_n(q)f_{-n}(q)}{n^2} \tag{7}$$

where $f_n(q)$ is the nth Fourier component of the force:

$$f_n(q) = \frac{1}{T}\int_0^T \mathrm{e}^{-\mathrm{i}n\omega t}\frac{\partial V_1(q,t)}{\partial q}\,\mathrm{d}t. \tag{8}$$

In our calculations we use

$$\mathcal{H}_{\text{eff}} = \frac{\hat{p}_q^2}{2m} + V_{\text{eff}}(q) \tag{9}$$

rather than $\mathcal{H}_0$ as the unperturbed Hamiltonian where the perturbation is $V^{\text{alt}}(q,t) - V_{\text{eff}}(q)$. This perturbation will be ignored in the calculations presented here. In the studies of the photo-induced dynamics of atoms in strong laser fields the time average over the time-dependent Hamiltonian in the KH representation [8], $\mathcal{H}_0$, has been used as the unperturbed Hamiltonian (see, for example, [10] and references therein). Our modified time-independent zero-order Hamiltonian depends explicitly on the maximum field amplitude and the frequency. The Hamiltonian $\mathcal{H}_{\text{eff}}$ turns out to be the leading part in a systematic expansion of the Floquet operator in powers of ω^{-1}. The corrections are of order ω^{-4}. This expansion is rather involved and will be given elsewhere [11]. Usually when the interaction of the system with the laser field is described within the framework of the acceleration representation (known as the KH representation), $V_0(q)$ is taken as the unperturbed part. The additional term included here compared to previous work is $V_{\text{eff}}(q) - V_0(q)$. This correction potential term describes the average kinetic energy of the rapid oscillations of the particle in the oscillatory field. It acts as an effective potential energy when the motion of the 'slow' coordinate of the particle is studied. This term is just the second term of (1) which is presented in the framework of classical mechanics in [2]. The effective potential (7) was obtained in the quantum framework and its classical limit is (1).

The nature of quantum dynamics depends on the shape of the effective potential (7). If its general form is similar to that of figure 2, a classical particle will be trapped, if its energy is smaller than the maxima, while the quantum particle is expected to tunnel out. Its temporary trapping is associated with a metastable solution of the time-dependent Schrödinger equation with the Hamiltonian (2). For time-independent Hamiltonians (such as $\mathcal{H}_{\text{eff}}(q)$) these metastable states are the complex poles of the scattering matrix or of $(E - \mathcal{H}_{\text{eff}})^{-1}$ and are known as resonance states [12]. For periodically time-dependent Hamiltonians the resonances are associated with the complex poles of $(E - \mathcal{H}_f)^{-1}$, where the Floquet operator is $\mathcal{H}_f(q,t) = -\mathrm{i}\hbar\frac{\partial}{\partial t} + \mathcal{H}(q,t)$ [13, 14]. For time periodic potentials, as in our case, the resonances are the quasi-energy (QE) solutions of the Floquet eigenvalue problem, which are obtained when outgoing boundary conditions are imposed. These resonance solutions are not in the Hilbert space. By carrying out a similarity transformation which is known as the complex scaling transformation the resonance solutions become part of the generalized Hilbert space and become square integrable (see, for example, [15]). We can summarize this discussion by stating that the driven quantum particle is temporarily trapped in a $\Psi(q\mathrm{e}^{-\mathrm{i}\theta},t) = \exp(-\mathrm{i}\mathcal{E}^{\text{QE}}t/\hbar)\Phi_\theta^{\text{QE}}(q,t)$ state, where $\mathcal{E}^{\text{QE}} = E - \frac{\mathrm{i}}{2}\Gamma$ and Γ is the rate of decay of the quantum particle, while $\mathrm{e}^{\mathrm{i}\theta}$ parametrizes the complex rotation. The lifetime of the trapped quantum particle is defined as usual as $\tau_l = \hbar/\Gamma$. The complex eigenfunction and eigenvalue of the complex scaled Floquet operator $\mathcal{H}_f$ are $\Phi_\theta^{\text{QE}}(q,t)$ and $\mathcal{E}^{\text{QE}} = E - \frac{\mathrm{i}}{2}\Gamma$, respectively. We expect that for high frequency these will be approximated by $\hat{U}\phi_{\mathcal{E}}$ and $\mathcal{E}$,

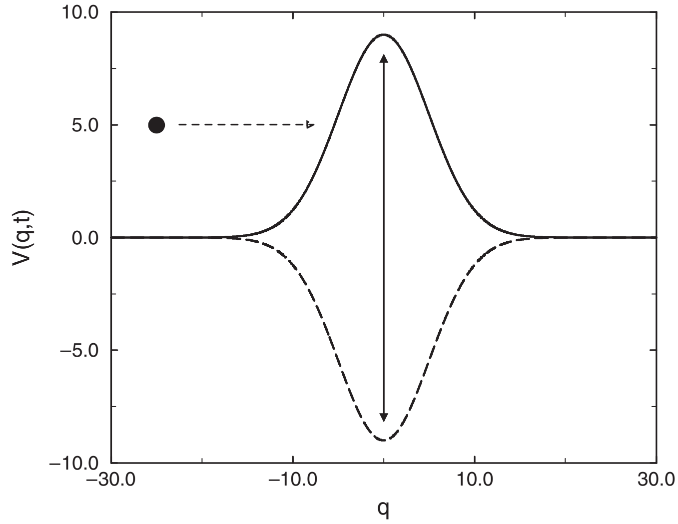

Figure 1. An illustration of a particle scattered by an oscillating Gaussian of (10) with $V_0 = 9$ and $\beta = 0.02$ (in 'atomic units' $\hbar = m = e = 1$).

where $\mathcal{E}$ and $\phi_{\mathcal{E}}$ are the resonance state and the corresponding complex scaled energy state of $\mathcal{H}_{\rm eff}$ (9), and $\hat{U}$ is given by (4).

The model Hamiltonian we have chosen for the demonstration of the application of the theory developed here to the quantum trapping phenomenon is

$$\mathcal{H}(q,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + V_0\,\mathrm{e}^{-\beta q^2}\cos(\omega t). \tag{10}$$

Here the free particle interacts with an external time-dependent field which is a Gaussian oscillating up and down periodically as shown in figure 1. The effective time-independent potential (7)

$$V_{\rm eff}(q) = \frac{V_0^2\beta^2}{m\omega^2}q^2\,\mathrm{e}^{-2\beta q^2} \tag{11}$$

is plotted in figure 2. For this specific model Hamiltonian the periodic time-dependent potential $V(q,t)$ is described as a simple product of two functions where one is a coordinate-dependent function whereas the second is time dependent. However, this form is not essential for the conclusions of the paper. As one can see from figure 2 the time-averaged effective potential supports two potential barriers separated by a potential well. The quantum particle is temporarily trapped inside this potential well in definite resonance states. The resonance energy, E, and width, Γ (i.e. inverse lifetime), of the ground state were calculated by solving the eigenvalue problem $\mathcal{H}_f(q_c,t)\Phi^{\rm QE}(q_c,t) = \left(E - \frac{\mathrm{i}}{2}\Gamma\right)\Phi(q_c,t)$ where $q_c = q\exp(\mathrm{i}\theta)$, by combining the (t,t') and the complex scaling methods [13, 15, 16].

For a potential of the form (11), namely a one-dimensional potential that is positive and vanishes in the limit $|q| \to \infty$, there is always at least one resonance below the maximum of the potential. The reason is that in one dimension for a negative potential that vanishes at infinity there is always a bound state [17–19]. With the help of analytic continuation one can show that the existence of a bound state for a static potential V implies existence of a low energy resonance for $-V$. The sufficient condition for such a continuation is that $V(q)$ falls off exponentially (or faster) with q (for the precise statement see [18]). A general argument

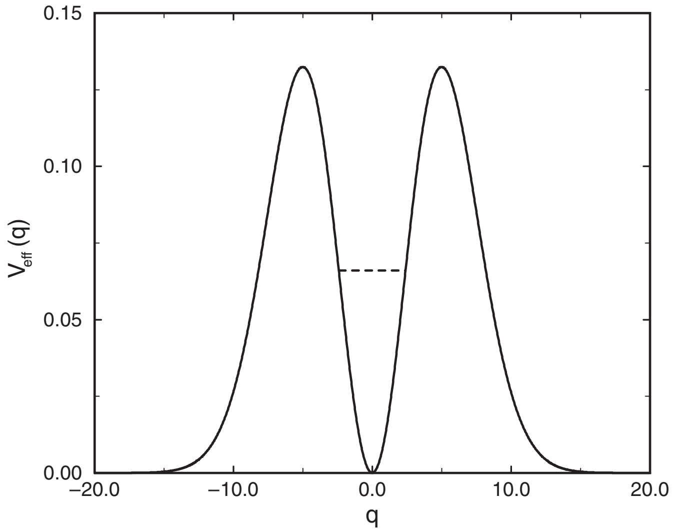

Figure 2. Effective time-independent potential of equation (11) for the parameters of figure 1 and with $\omega = 1.5$.

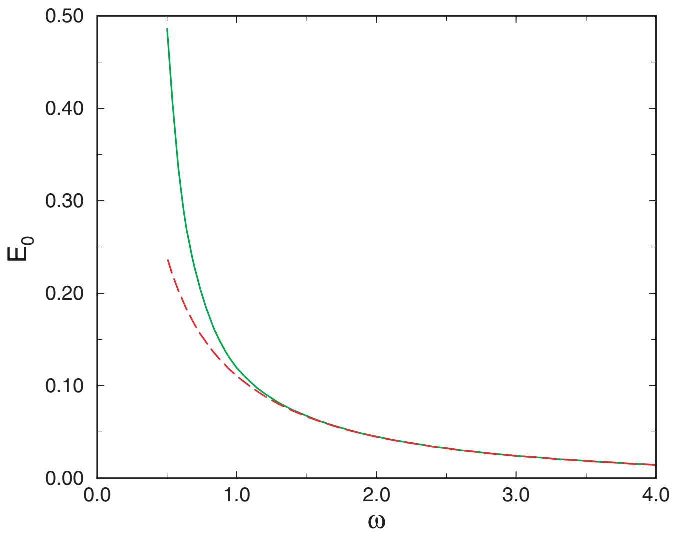

Figure 3. The energy position of the lowest resonance for the potentials of figures 1 and 2 versus the driving frequency ω. The solid line is a result of the exact calculation for (10) and the dashed line for the effective potential of equation (11).

and specific examples are presented in section 2.2.2 of [15]. Note that this phenomenon might be affected by the presence of an additional time-independent potential. According to the transformations performed in this letter, (2)–(9), which were performed under quite general conditions, it implies existence of a resonance for the time-dependent Hamiltonian (10). Such a resonance was calculated directly for the time-dependent Hamiltonian (10) and for the corresponding time-independent Hamiltonian with the effective potential (11). The comparison is presented in figures 3 and 4. In our calculations we used 'atomic units',

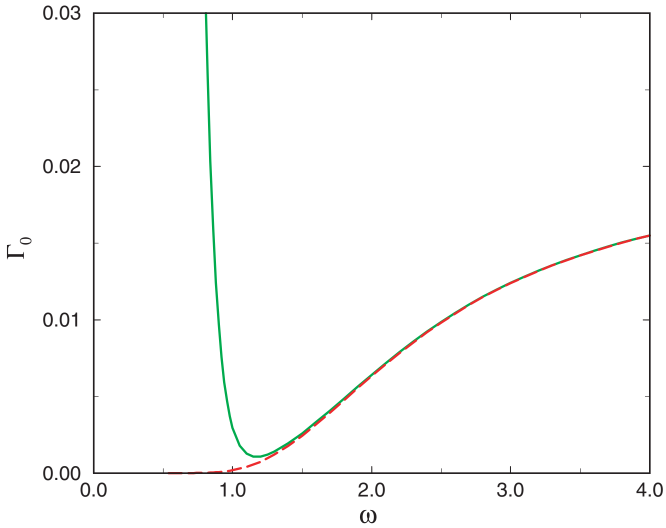

Figure 4. Same as figure 3 for the resonance width.

i.e. $m = \hbar = e = 1$, where m is the mass of the particle considered rather than the mass of the electron. In these units the potential parameters are $\beta = 0.02$ and $V_0 = 9$. The lowest resonance (smallest real part) $\mathcal{E}_0^{\mathrm{QE}} = E_0 - \mathrm{i}\Gamma_0/2$ is presented in these figures. Good agreement between the predictions of (10) and (11) is found for $1 < \omega$. This frequency range should be compared to Ω, the characteristic frequency of the bound motion that satisfies $2\pi/\Omega = \oint \frac{\mathrm{d}q}{\sqrt{2(E_0 - V_{\mathrm{eff}})/m}}$, where the integral is over the closed cycle of the classical motion. The resonance position E_0 and V_{eff} depend on ω. For $\omega = 2$ and $\omega = 1$ one finds $\Omega = 0.10$ and $\Omega = 0.23$, respectively. Note that even for large ω the resonance does not become very wide and the growth of Γ_0 with ω is slower than linear. There is a minimum in the width Γ_0 and the approximation is quite reasonable for frequencies larger than the frequency where the minimum is found.

It is instructive to notice that the agreement between the predictions of (10) and (11) was found here in a regime that is not semiclassical. For this purpose we calculated $\mathcal{R} = L_{\mathrm{ctp}}/\lambda$, where L_{ctp} is the distance between the classical turning points for a trajectory trapped in the well and $\lambda = \hbar/\sqrt{2mE_0}$ is the de-Broglie wavelength. Applicability of the semiclassical approximation requires $\mathcal{R} \gg 1$ while for the results presented here we find $\mathcal{R} < 0.32$. Therefore the behaviour in the regime studied here is *not* semiclassical.

In this work we demonstrated that trapping by a rapidly oscillating potential with a bound amplitude can be approximated by trapping in a static potential that is calculated by averaging the transformed potential $V^{\mathrm{alt}}(q, t)$ over time. It is superior to the averaging of $V(q, t)$ over time, which is traditionally performed in the exploration of the dynamics of atoms in strong laser fields in the context of the KH transformation. The theory presented here is an extension to quantum mechanics of classical stabilization, but its validity is not confined to the semiclassical regime. In particular, the lowest resonance was calculated with the help of an effective static potential. It is argued that a rapidly oscillating smooth potential that decays exponentially or faster at infinity typically exhibits a low energy resonance in one dimension. We emphasize that the effective potential resulting from the rapidly oscillating field is small for high frequencies, resulting in lifetimes that may be short. Nevertheless, as was argued here, even for arbitrarily high frequency, the particle is temporarily trapped in a resonance state.

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