Influence of laser pulse shape and spectral composition on strong-field Kapitza-Dirac scattering

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Abstract. Diffractive scattering of an electron beam from an intense standing wave of light (Kapitza-Dirac effect) is analyzed theoretically. The corresponding Schrödinger equation is solved in the Bragg regime by combined analytical and numerical means. Our goals are twofold: On the one hand, we examine the influence of the nature of the field’s turning-on phase and demonstrate that a smooth, adiabatic envelope restricts the transitions to those satisfying the Bragg condition. On the other hand, we study signatures of quantum mechanical interference when the standing light wave comprises two commensurate frequencies. Characteristic modifications of the Rabi oscillation dynamics and a dependence on the relative phase between the frequency modes are revealed.

1. Introduction

Based on the newly established rules of quantum mechanics, Kapitza and Dirac predicted in 1933 that an electron beam can diffractively scatter from a standing wave of light, formed by two counterpropagating waves of equal frequency and intensity [1, 2]. The effect, which henceforth has been named after them, relies on the quantum wave nature of the electron. It represents an analogue of the classical diffraction of light on a periodic grating, but with the roles of light and matter interchanged. In its original version, the Kapitza-Dirac effect can be understood as a combined absorption and emission process involving two photons: the electron absorbs a photon of momentum \( \vec{k} \) from one of the laser beams and emits a photon of momentum \( -\vec{k} \) into the counterpropagating laser beam (stimulated Compton scattering). The incoming electron momentum thus changes by \( 2\vec{k} \), provided that it is incident under the Bragg angle which follows from the requirements of energy and momentum conservation.

The scattering probability predicted by Kapitza and Dirac was very small, though, because of the low intensities of light sources available at that time. Consequently, the interest in the Kapitza-Dirac effect was newly inspired in the 1960s when much higher light intensities were delivered by the first laser devices. This has led to several experimental attempts to observe the effect [3, 4, 5] and to seminal theoretical work on Kapitza-Dirac scattering in strong laser fields [6].

Nevertheless, a convincing experimental confirmation of the Kapitza-Dirac effect as originally proposed has been achieved only recently [7]. This successful observation has once again revived the interest of theoreticians in the effect. In recent years, various novel aspects of Kapitza-Dirac scattering have been examined. For example, a theory based on electronic wave packets was developed [8] and diffractive scattering in the case of counterpropagating laser beams of non-
equal frequencies was studied [9]. Besides, a relativistic formulation of the Kapitza-Dirac effect based on the Dirac equation was presented [10, 11], which generalizes earlier treatments within Klein-Gordon theory [12, 13] and provides the proper framework to analyze the electron’s spin dynamics in the process.

In this contribution, we study Kapitza-Dirac scattering in the nonrelativistic domain, focussing on the impact of the applied laser pulse shape and its frequency composition. After having established the theoretical framework in Section 2, we analyze the role played by the field’s turning-on phase in Section 3. Using the leading order of perturbation theory we show that, in general, characteristic temporal oscillations are imprinted on the scattering amplitude. However, in the case when the switching duration is very long, the scattering amplitude for resonant electron momenta shows a linear growth in time, whereas off-resonant transitions are strongly suppressed. A tight interplay between the switching duration and the detuning from the resonance is revealed.

Afterwards, in Section 4 we consider Kapitza-Dirac scattering from a bichromatic standing wave which comprises, apart from the fundamental frequency \( \omega \), also its third harmonic \( 3\omega \). Due to quantum mechanical interference effects, the Rabi oscillations are modified in a characteristic manner which is revealed via comparison with the corresponding monochromatic scattering dynamics. Also the influence of the relative phase between the frequency modes is illustrated. We finish with some concluding remarks in Section 5.

2. Theoretical framework

The nonrelativistic evolution of the quantum mechanical wave-function \( \psi \) of an electron in the presence of an external electromagnetic field is described by the time-dependent Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} \psi = \frac{1}{2m} \left( \hbar \frac{i}{\hbar} \nabla + \frac{e}{c} \vec{A} \right)^2 \psi.
\]  

The mass of the electron being \( m \), its charge \( -e \). Besides, \( c \) is the speed of light and \( h \) the reduced Planck constant. A standing light wave of frequency \( \omega = ck \) is described by the vector potential \( \vec{A} \) in Coulomb gauge as

\[
\vec{A} = f(t) A_0 \vec{\varepsilon} \cos(\omega t) \cos(kz)
\]  

where the linearly polarized laser beams (counter-) propagate along the \( z \)-axis and \( \vec{\varepsilon} \) is a polarisation vector of unit length perpendicular to \( \hat{z} \). The constant amplitude \( A_0 \) is multiplied by an envelope function \( f(t) \) to model entering and leaving of the electron in the interaction region, thereby giving it compact support in time. The intensity of the standing wave amounts to \( I = \frac{ck^2 A_0^2}{16\pi} \). From the spatial \( \frac{2\pi}{k} \)-periodicity of the potential in \( z \)-direction and its transverse invariance it follows, that only the subset of momentum eigenstates which differ by an integral multiple of the photon momentum \( \hbar k \) can interact. Assuming that the incident electron momentum is perpendicular to the polarization vector \( \vec{\varepsilon} \), the transverse dynamics can be separated, leaving an effectively one-dimensional situation. Therefore we use an ansatz in the form

\[
\psi(t,z) = \sum_n b_n(t) e^{inkz + ip_z z/h} =: \sum_n b_n(t) \left| n \right\rangle
\]  

with time-dependent expansion coefficients \( b_n(t) \). Note, that \( p_z \) is not necessarily the \( z \)-component of the initial electron momentum, but merely an offset from the integral multiples of \( \hbar k \). We arrive at the equation of motion for \( b_n \) as the coupled system of differential equations:

\[
i\hbar \dot{b}_n(t) = -\frac{(p_z + nh\hbar)^2}{2m} b_n(t) + \frac{e^2 A_0^2}{8mc^2} f(t)^2 \cos^2(\omega t) (b_{n-2}(t) + 2b_{n}(t) + b_{n+2}(t))
\]

This will be the foundation of the following considerations.
3. Adiabatic switching and frequency detuning

In this section we study to which extent the scattering dynamics of the electron is influenced by the switching-on phase of the interaction [14]. For algebraic simplicity, to simulate the adiabatic switching-on procedure, we use \( f \) as an envelope function such that

\[
f(t) = \begin{cases} 
\frac{t}{\tau} & \text{if } 0 < t \leq \tau \\
1 & \text{if } \tau < t \leq T \\
\frac{T-t}{\tau} & \text{if } T < t \leq T + \tau \\
0 & \text{elsewhere}
\end{cases}
\]  

(5)

This way we have established, that \( f(t)^2 \) is continuous with compact support and gives an effective interaction duration of

\[
\int dt f(t)^2 = T
\]

(6)

Its derivative being bound by the inverse switching time \( 1/\tau \).

The time evolution operator \( U \), which solves (4) as a Green’s function, can be expressed by the recurrent integral equation

\[
U(t) = U_0(t) + \frac{1}{i\hbar} \int_0^t dt' U_0(t-t') \frac{e^{2iA(t')^2}}{2mc^2} A(t')^2 U(t')
\]

(7)

where the unperturbed version is given by

\[
U_0(t) = \sum_n \exp \left( \frac{1}{i\hbar} \frac{\hbar k + p_z}{2m} t \right) |n\rangle \langle n|
\]

(8)

The square of the vector potential can be written, with the help of the electron momentum eigenstates \( |n\rangle \), as

\[
A(t)^2 = \left[ \frac{1}{2} f(t) A_0 \cos(\omega t) \sum_n \left( |n+1\rangle \langle n| + |n-1\rangle \langle n| \right) \right]^2
\]

\[
= \frac{1}{4} f(t)^2 A_0^2 \cos^2(\omega t) \sum_n \left( |n+1\rangle \langle n-1| + 2 |n\rangle \langle n| + |n-1\rangle \langle n+1| \right)
\]

(9)

Equation (7) can be expanded in the time-dependent perturbation series for small values of \( A_0 \) as

\[
U(t) = U_0(t) + U_1(t) + U_2(t) + \ldots
\]

(10)

where the first-order term reads

\[
U_1(t) = \frac{1}{i\hbar} \int_0^t dt' U_0(t-t') \frac{e^{2iA(t')^2}}{2mc^2} A(t')^2 U_0(t')
\]

(11)

The transition amplitude from the state \( |-1\rangle \) with momentum \( p_z = \hbar k \) to the state \( |1\rangle \) with momentum \( p_z + \hbar k \) to the lowest order in \( A_0^2 \) is

\[
\langle 1| U_1(T + \tau) |-1 \rangle = \frac{e^2 A_0^2}{2ihmc^2} \int dt \exp \left( -i \frac{(\hbar k + p_z)^2}{2hm} (T + \tau - t) \right) f(t)^2 \cos^2(\omega t) \exp \left( -i \frac{(-\hbar k + p_z)^2}{2hm} t \right)
\]

\[
= \frac{e^2 A_0^2}{2ihmc^2} \exp \left( -i \frac{(\hbar k + p_z)^2}{2hm} (T + \tau) \right) \int dt \exp \left( i \frac{2kp_z t}{m} \right) f(t)^2 \cos^2(\omega t)
\]

(12)
The last integral in equation (12) can be evaluated for the resonant case \( p_z = 0 \), where \( |−1⟩ \) and \( |1⟩ \) have the same energy, as

\[
\int dt f(t)^2 \cos^2(\omega t) = \frac{T}{2} + \frac{\cos(2\omega \tau) - 1 - \cos[2\omega(T + \tau)] + \cos(2\omega T)}{8\omega^2 \tau}.
\]  

(13)

One can see, that the amplitude grows linearly in time with an oscillating part that is suppressed by \( 1/\tau \). In Fig. 1 the dependence on the duration of the switching is illustrated.

\[\text{Figure 1.} \quad \text{Values of the integral (13) for a range of different switching times } \tau \text{ and interaction times } T.\]

If we allow for the electron momentum to be slightly detuned from the resonant energy-conserving case, described by a non-zero detuning parameter \( \eta := \frac{2kp_z}{\hbar} \neq 0 \), the integral (13) must be replaced by

\[
\int dt f(t)^2 \cos(\omega t)^2 e^{i\eta t} = \frac{1}{2} \frac{(1 - e^{i\eta T})(e^{i\eta \tau} - 1)}{\eta^2 \tau} + \frac{1}{2} \frac{(4\omega^2 + \eta^2)^2}{(4\omega^2 - \eta^2)^2 \tau} \times
\]

\[
\left\{ \left[ (4\omega^2 + \eta^2) \cos(2\omega t) - 4i\omega \eta \sin(2\omega t) \right] e^{i\eta t} \bigg|_{t=0}^{\tau} - \left[ (4\omega^2 + \eta^2) \cos(2\omega t) - 4i\omega \eta \sin(2\omega t) \right] e^{i\eta t} \bigg|_{t=T}^{T+\tau} \right\}. 
\]  

(14)

The second term behaves qualitatively like the corresponding oscillations in (13). The first term shows that, for small interaction time \( T \), the scattering amplitude of the detuned electron has
the same growth as before. But for long interaction time, it is suppressed by a factor of the inverse switching time $1/\tau$ and a factor $1/\eta^2$. This dependence is shown in Fig. 2.

From these observations we infer, that for sufficiently smooth envelope the scattering process complies with the Bragg condition and can therefore be understood in a photon picture, where the electron absorbs and reemits a certain number of photons gaining twice their momentum and no kinetic energy.

4. Interference effects in a bichromatic standing wave

In this section, we study Kapitza-Dirac scattering from a standing light wave which contains two different but commensurate frequency modes. The latter are assumed to be a fundamental frequency $\omega = \frac{ck}{\lambda}$ and its third harmonic $3\omega$. The vector potential of the wave thus reads

$$\vec{A} = f(t)A_0 \left( \alpha \vec{e}_1 \cos(\omega t) \cos(kz) + \sqrt{1 - \alpha^2} \vec{e}_2 \cos \left(3\omega t + \phi \right) \right)$$

where $\alpha \in [0, 1]$ modulates the relative amplitudes of the waves in such a way that the overall laser intensity $I = \frac{e^2 A_0^2}{16\pi}$ does not depend on $\alpha$. The relative phases of the frequency modes in time and space are respectively encoded in $\phi$ and $\delta$. In such a field configuration, quantum mechanical interference effects can occur because it is indistinguishable whether the electron absorbs one big photon of wavelength $3\vec{k}$ or three small photons of wave vector $\vec{k}$ each. Similar two-pathway quantum interferences in strong bichromatic laser fields have also been studied with respect to photoionisation [15, 16], high-harmonic generation [17], electron-atom scattering [18, 19] and electron-positron pair production [20, 21, 22].

Instead of directly using the vector potential (15) in a minimal coupling scheme [see Eq. (1)], we shall apply here the approximation by a ponderomotive potential. The latter results from a suitable time average over the fast oscillations of the interaction Hamiltonian, leading to a space-periodic potential [23]. Then the Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{e^2 A_0^2}{4mc^2} f(t)^2 \left[ \alpha^2 \cos^2(kz) + \frac{1 - \alpha^2}{9} \cos^2 \left(3\omega t + \frac{\delta}{2} \right) \right] \psi$$

which, similarly as before, can be transformed into a coupled system of ordinary differential equations for the momentum amplitudes $b_n(t)$. Compared to the last section, the envelope $f(t)^2$ here is changed to have $\sin^2$-edges. This system of equations has been solved by numerical integration, starting from the initial condition $b_{-3}(0) = 1$ and all other $b_n(0) = 0$. It describes an incident electron with longitudinal momentum $-3\hbar k$ which simultaneously satisfies the Bragg condition for both field frequencies. Consequently, it may be scattered into the mirrored momentum state with $3\hbar k$ (and momentum amplitude $b_3(t)$) by absorbing either one big photon or three small photons with a (total) wave vector of $3\vec{k}$ and, correspondingly, reemitting either one big photon or three small photons with a (total) wave vector of $-3\vec{k}$. A characteristic Rabi oscillation dynamics will occur between the electron momentum states $|\pm 3\rangle$ with momenta $\pm 3\hbar k$ due to the resonant coupling of these two states.

As an example, we consider Kapitza-Dirac scattering of an electron with incident transverse momentum $12\,\text{eV}/c$ from a bichromatic standing wave with $k_1 = 4\,\text{eV}/hc$, $k_2 = 12\,\text{eV}/hc$, $I_1 = 8 \times 10^9 \text{W/cm}^2$ and $I_2 = 5.5 \times 10^9 \text{W/cm}^2$. Two different relative phase values have been considered ($\delta = 0$ and $\delta = \pi$) to demonstrate the dependence of the scattering dynamics on this quantity. Our results are shown by the lower two rows in Fig. 3. Note that our numerical data represent occupation probabilities outside the laser field; that is, after each value of $T$ the interaction between the electron and the field has been faded out in the numerical simulation. For comparison, we have also calculated the corresponding scattering processes when only one
of the two frequency modes is present, which are illustrated by the upper two rows in Fig. 3. We see that the scattering probability in the bichromatic field differs from the sum of the scattering probabilities in the respective monochromatic fields. Besides, the relative phase between the frequency modes can strongly affect the scattering dynamics. Both features indicate the occurrence of quantum interference in the process.

**Figure 3.** Scattering probabilities $|b_3(T)|^2$ after $T = 9.7 \times 10^{-10}$ s interaction time (left) and Rabi oscillation dynamics (right) for Kapitza-Dirac scattering from (a) a monochromatic standing wave with $k_1 = 4$ eV/\(hc\) and $I_1 = 8 \times 10^9$ W/cm$^2$, (b) a monochromatic standing wave with $k_2 = 12$ eV/\(hc\) and $I_2 = 5.3 \times 10^9$ W/cm$^2$, and (c) [(d)] a bichromatic standing wave with the combined parameters and $\delta = 0$ [\(\delta = \pi\)].

To emphasize the influence of the parameters $\alpha^2$ and $\delta$ on the quantum interference, Figs. 4 and 5 show the Rabi frequency $\Omega$ for this resonant transition as a function of them. It can be seen in Fig. 4, that moving between the two phase independent monochromatic cases, while keeping the combined intensity fixed, leads to different minima in $\Omega$ for different phases. Correspondingly, Fig. 5 shows quite different phase dependencies for different colour mixtures.

**Figure 4.** Rabi frequency $\Omega$ of the Kapitza-Dirac scattering from a bichromatic standing wave, as a function of the mixing parameter $\alpha^2$. The wave numbers being $k_1 = 4$ eV/\(hc\) and $k_2 = 12$ eV/\(hc\), the combined intensity $I = 1.3 \times 10^{10}$ W/cm$^2$, and the relative phase is $\delta = 0$ for the blue solid line and $\delta = \pi$ for the red dashed line.

5. Conclusion
Kapitza-Dirac scattering of electrons from a standing light wave was studied in the nonrelativistic regime governed by the Schrödinger equation. We have shown that a finite switching-on duration of the electron-light interaction influences the scattering amplitude in a characteristic way by introducing temporal oscillations. The latter are damped for long switching-on times and lead asymptotically to a linear growth of the scattering amplitude for incident electrons which satisfy the resonant Bragg condition, whereas scattering of electrons with off-resonant momenta is prohibited in this limit. The same conclusion was reached in [14]. From our Eq. (14) one may also deduce a tight interrelation between switching duration and detuning: For short switching
times, also electrons with (slightly) off-resonant momenta can acquire a sizeable scattering probability.

Besides, we have shown that quantum mechanical interference effects may arise in Kapitza-Dirac scattering from a bichromatic standing light wave. Considering the case where the frequency ratio is 1:3, we have demonstrated that the resonant scattering probability in the bichromatic case differs from the sum of the scattering probabilities in the respective monochromatic fields. Accordingly, the dependence of the scattering probability on the interaction time, which exhibits a typical Rabi oscillation dynamics, is modified by the presence of the second mode. The impact of the relative strength of the second mode on the Rabi frequency was examined and a very pronounced sensitivity on the relative phase between the frequency modes found.

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