Spin dynamics in the Kapitza-Dirac effect

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Electron spin dynamics in Kapitza-Dirac scattering from a standing laser wave of high frequency and high intensity is studied. We develop a fully relativistic quantum theory of the electron motion based on the time-dependent Dirac equation. Distinct spin dynamics, with Rabi oscillations and complete spin-flip transitions, is demonstrated for Kapitza-Dirac scattering involving three photons in a parameter regime accessible to future high-power X-ray laser sources. The Rabi frequency and, thus, the diffraction pattern is shown to depend crucially on the spin degree of freedom.

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Introduction The diffraction of an electron beam from a standing wave of light is referred to as the Kapitza-Dirac effect [1, 2]. This process points out the quantum wave nature of the electron and may be considered as an analogue of the optical diffraction of light on a grating, but with the roles of light and matter interchanged. Predicted already in 1933, a clear experimental confirmation of the Kapitza-Dirac effect as originally proposed has been achieved only recently [3]. It has stimulated renewed theoretical interest in the process [4], advancing earlier treatments [5, 6]. A related successful experiment observed the (classical) scattering of electrons in a standing laser wave [7]. Both experiments operated at moderate light intensities between 10^9 W/cm^2 and 10^{14} W/cm^2 and near optical wavelengths. The existing theoretical studies, accordingly, have treated the electron quantum dynamics nonrelativistically. The nonrelativistic Kapitza-Dirac effect has been observed experimentally also using atomic beams [8].

The current development of novel light sources, envisaged to provide field intensities in excess of 10^{20} W/cm^2 and field frequencies in the hard X-ray domain [9, 10], raises the question as to how the Kapitza-Dirac effect is modified in this hitherto unexplored parameter regime. This calls for a fully relativistic treatment of the process within the Dirac theory, valid at high electron energies and, in particular, accounting for the electron spin. Relativistic considerations of quantum mechanical electron scattering in two counterpropagating light waves were provided, but assuming nonequal laser frequencies and disregarding the electron spin degree of freedom [11]. Spin signatures in the Kapitza-Dirac effect have so far been examined within the nonrelativistic framework of the Pauli equation [12] and by solving the classical equations of motion [13]. Both studies found negligibly small spin effects. We note that the influence of the electron spin has also been investigated with respect to free-electron motion [14], bound-electron dynamics [15], atomic photoionization [16], and Compton and Mott [17] scattering in strong plane-wave laser fields.

In this Letter, we present a fully relativistic consideration of the Kapitza-Dirac effect within the framework of Dirac theory. We focus on the relevance of spin-flip transitions when the process occurs in X-ray laser fields of high intensity. We demonstrate that under suitable conditions, the diffraction probability depends considerably on the electron spin. Thus, the spin degree of freedom significantly influences the quantum mechanical scattering dynamics.

Relativistic theory We consider a quantum electron wave packet in a standing linearly polarized light wave (see Fig. 1) with maximal electric field strength $\boldsymbol{E}$, wave vector $\boldsymbol{k}$, and wavelength $\lambda = 2\pi/|\boldsymbol{k}| = 2\pi/k$, respectively. The laser is modeled by the vector potential

$$\boldsymbol{A}(\boldsymbol{x}, t) = -\frac{\boldsymbol{E}}{k}\cos(\boldsymbol{k}\cdot\boldsymbol{x})\sin(ckt)w(t) \tag{1}$$

introducing the speed of light c and the temporal envelope function $w(t)$. The relativistic quantum dynamics of an electron with mass m and charge $-e$ is governed by the Dirac equation [18]

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\boldsymbol{x}, t) = \left[c\left(-\mathrm{i}\nabla + \frac{e}{c}\boldsymbol{A}(\boldsymbol{x}, t)\right)\cdot\boldsymbol{\alpha} + \beta mc^2\right]\psi(\boldsymbol{x}, t)\,. \tag{2}$$

In (2), we have introduced the vector $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$, where α_i and β are the Dirac matrices in standard representation [19].

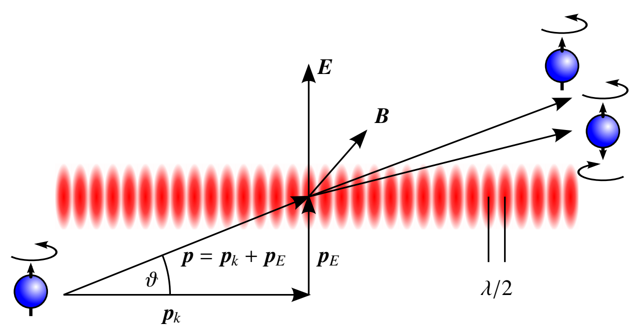

FIG. 1: (Color online.) Schematic setup. An electron with momentum $\boldsymbol{p}$ is incident at an angle ϑ on a linearly polarized standing laser wave with electric and magnetic components $\boldsymbol{E}$ and $\boldsymbol{B}$. The momentum $\boldsymbol{p}$ has components $\boldsymbol{p}_E$ and $\boldsymbol{p}_k$ along the laser's electric field $\boldsymbol{E}$ and wave vector $\boldsymbol{k}$, respectively. The electron is initially spin-polarized along the electric field component. After Kapitza-Dirac scattering, parts of the electron wave packet may have flipped their spin orientation.

The monochromatic light wave (1) allows us to decompose the wave function $\psi(\boldsymbol{x}, t)$ into a discrete set of plane waves, viz.,

$$\psi(\boldsymbol{x}, t) = \sum_{n,\zeta} c_n^\zeta(t)\psi_{n,\boldsymbol{p}}^\zeta(\boldsymbol{x}), \quad \psi_{n,\boldsymbol{p}}^\zeta(\boldsymbol{x}) = u_{n,\boldsymbol{p}}^\zeta \mathrm{e}^{\mathrm{i}(\boldsymbol{p}+n\boldsymbol{k})\cdot\boldsymbol{x}}. \tag{3}$$

The function $\psi_{n,\boldsymbol{p}}^\zeta(\boldsymbol{x})$ denotes a free particle Dirac eigenfunction of momentum $\boldsymbol{p} + n\boldsymbol{k}$ ($n = 0, \pm1, \pm2, \dots$). The index $\zeta \in \{+\uparrow, +\downarrow, -\uparrow, -\downarrow\}$ labels the sign of the energy and the spin projection along the laser electric field vector. Taking advantage of the basis functions' orthonormality the ansatz (3) yields

$$\begin{aligned} \mathrm{i}\dot{c}_n^\gamma(t) = \mathrm{i}\,\langle\psi_{n,\boldsymbol{p}}^\gamma|\dot{\psi}\rangle = \epsilon^\gamma\mathcal{E}(\boldsymbol{p}+n\boldsymbol{k})c_n^\gamma(t) \\ - \frac{w(t)e\sin(ckt)}{2k}\sum_\zeta \langle u_{n,\boldsymbol{p}}^\gamma|\boldsymbol{E}\cdot\boldsymbol{\alpha}|u_{n-1,\boldsymbol{p}}^\zeta\rangle\, c_{n-1}^\zeta(t) \\ - \frac{w(t)e\sin(ckt)}{2k}\sum_\zeta \langle u_{n,\boldsymbol{p}}^\gamma|\boldsymbol{E}\cdot\boldsymbol{\alpha}|u_{n+1,\boldsymbol{p}}^\zeta\rangle\, c_{n+1}^\zeta(t), \end{aligned} \tag{4}$$

where we have introduced the relativistic energy momentum dispersion relation $\mathcal{E}(\boldsymbol{p}) = \sqrt{m^2c^4 + c^2\boldsymbol{p}^2}$ and the signum ϵ^γ, which is 1 for $\gamma \in \{+\uparrow, +\downarrow\}$ and -1 for $\gamma \in \{-\uparrow, -\downarrow\}$.

Generalized Bragg condition The elastic scattering of an electron on a standing light wave may be characterized by a Bragg condition [1] provided that the ponderomotive energy of the electron is small (so-called Bragg regime) [5, 20]. This Bragg condition may be generalized to an inelastic process of absorbing and emitting an arbitrary number of photons by utilizing momentum conservation $\boldsymbol{p}' = \boldsymbol{p} + (n_r - n_l)\boldsymbol{k}$ and energy conservation $\mathcal{E}(\boldsymbol{p}') = \mathcal{E}(\boldsymbol{p}) + (n_r + n_l)ck$, where $\boldsymbol{p}$ and $\boldsymbol{p}'$ are the initial and final electron momenta. The integers n_r and n_l denote the net numbers of photons exchanged with the right- and left-traveling laser waves, respectively, with positive (negative) values indicating photon absorption (emission). The momentum and energy conservation laws yield the relativistic generalized Bragg condition

$$\frac{\cos\vartheta}{\lambda_p} = -\frac{n_r - n_l}{2\lambda} + \frac{n_r - n_l}{|n_r - n_l|}\frac{n_r + n_l}{2}\sqrt{\frac{1}{\lambda^2} - \frac{1}{n_r n_l}\left(\frac{\sin^2\vartheta}{\lambda_p^2} + \frac{1}{\lambda_C^2}\right)} \tag{5}$$

by introducing the angle ϑ (see Fig. 1), the de Broglie wavelength $\lambda_p = 2\pi/|\boldsymbol{p}|$, and the Compton wavelength $\lambda_C = 2\pi/(mc)$. To be consistent with the nonrelativistic limit n_r and n_l must have opposite signs. Equation (5) reduces to the Bragg condition of the two-photon Kapitza-Dirac effect [1, 20] by setting $n_r = -n_l = 1$.

From Eq. (5), it follows that for inelastic processes ($n_r + n_l \neq 0$) either the initial electron momentum $\boldsymbol{p}$ or the laser photon momentum k must be of the order of mc, i. e., relativistic, except we allow for a very large number of interacting photons. Thus, an analysis of inelastic Kapitza-Dirac scattering demands a relativistic treatment by the Dirac equation.

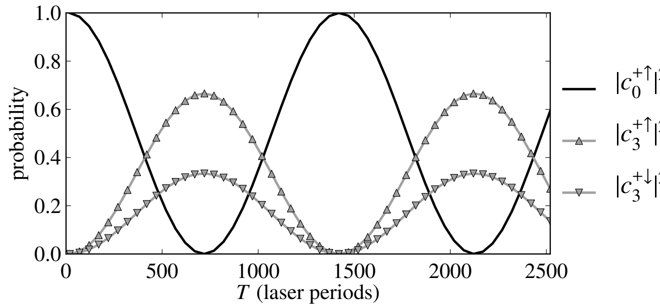

FIG. 2: Rabi oscillations of the spin resolved diffraction probabilities as a function of the interaction time T for a three-photon Kapitza-Dirac effect. Starting from a pure spin-up state the electron is either diffracted with probability $|c_3^{+\uparrow}(T)|^2 + |c_3^{+\downarrow}(T)|^2$ or passes the laser beam without momentum transfer with probability $|c_0^{+\uparrow}(T)|^2$. Laser parameters of this simulation correspond to two counterpropagating X-ray laser beams with a peak intensity of $2.0 \times 10^{23}\,\mathrm{W/cm^2}$ each and a photon energy of 3.1 keV. The electron impinges at an angle of inclination of $\vartheta = 0.4°$ and a momentum of 176 keV/c, in order to fulfill the Bragg condition (5).

A setup for spin-sensitive Kapitza-Dirac scattering Equation (4) couples momentum components having momenta that differ by $\pm\boldsymbol{k}$ and equal or opposite spin orientation. An explicit calculation of $\langle u_{n,\boldsymbol{p}}^\gamma|\boldsymbol{E}\cdot\boldsymbol{\alpha}|u_{n\pm1,\boldsymbol{p}}^\zeta\rangle$ reveals that if $\boldsymbol{p}$ and $\boldsymbol{E}$ are orthogonal then $c_n^\gamma(t)$ couples only to components $c_{n\pm1}^\zeta(t)$ having opposite spin orientation. Therefore, a distinct spin dynamics may be expected for Kapitza-Dirac scattering with an odd number of photons provided that the initial electron momentum $\boldsymbol{p}$ is almost orthogonal to the electric field $\boldsymbol{E}$. Thus, we focus on a three-photon Kapitza-Dirac effect, i. e., $n_r = 2$, $n_l = -1$, in the subsequent sections.

The condition (5) allows us to determine the initial electron momentum $\boldsymbol{p}$ and the laser wave number k for a resonant three-photon Kapitza-Dirac effect. The impinging electron is modeled by a plane wave; thus, the initial condition $c_0^{+\uparrow}(0) = 1$ and $c_n^\zeta(0) = 0$ else will be applied for the remainder of the Letter. We solve the Dirac equation (4) until time T to compute the transition amplitudes $c_n^\zeta(T)$.

Spin-flip probability and Rabi frequency Figure 2 shows the final occupation probabilities $|c_n^\zeta(T)|^2$ after laser-electron interaction, which have been calculated by numerical propagation of the Dirac equation (4) by a combination of the explicit and the implicit Euler method [21]. The laser profile was modeled by an envelope function $w(t)$ that starts with a $\sin^2$-shaped turn-on ramp of 10 laser cycles and finishes with a $\sin^2$-shaped turn-off ramp of 10 laser cycles having a flat plateau in between. The experimental setup was chosen to meet the Bragg condition (5) for a three-photon process. As illustrated in Fig. 2, only zeroth-order and third-order modes are nonzero after interaction. The occupation probabilities oscillate in Rabi cycles of frequency Ω_R

$$|c_0^{+\uparrow}(T)|^2 = \cos^2(\Omega_R T/2), \tag{6a}$$

$$|c_3^{+\uparrow}(T)|^2 + |c_3^{+\downarrow}(T)|^2 = \sin^2(\Omega_R T/2), \tag{6b}$$

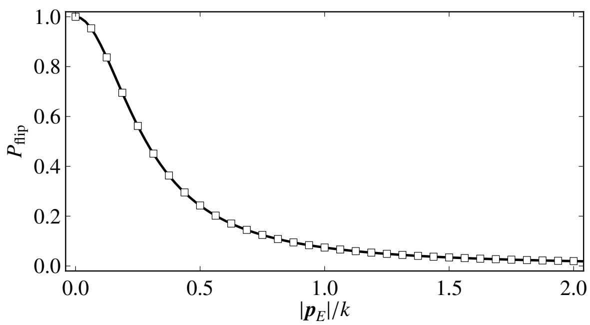

FIG. 3: The spin-flip probability P_{flip} as a function of the electron momentum $|\boldsymbol{p}_E|$ in electric field direction. The solid black line is given by (8). White squares result from simulations with the Dirac equation (4). All simulation parameters except $\boldsymbol{p}_E$ are the same as those for Fig. 2.

similarly to the two-photon Kapitza-Dirac effect [2] and the Kapitza-Dirac effect in atomic beams [8]. In the present case, however, the scattered portion of the electron wave packet consists of two parts which are distinguished by opposite spin orientations. The period of the Rabi oscillations is $2\pi/\Omega_R = 1.9$ fs for parameters of Fig. 2.

For short times with $\Omega_R T \ll 1$, the Dirac equation (4) can also be solved analytically via time-dependent perturbation theory. This yields for parameters compatible with the three-photon Bragg condition (5) the probabilities

$$|c_3^{+\uparrow}(T)|^2 = \left(\frac{1}{2}\Omega_0 T\right)^2 \left(\frac{5}{\sqrt{2}}\frac{|\boldsymbol{p}_E|}{k}\right)^2 , \tag{7a}$$

$$|c_3^{+\downarrow}(T)|^2 = \left(\frac{1}{2}\Omega_0 T\right)^2 , \tag{7b}$$

with $\Omega_0 = e^3|\boldsymbol{E}|^3/(24m^3c^5k^2)$. The $|\boldsymbol{E}|^3$ dependence clearly indicates the three-photon nature of the transition. From Eq. (7), we can derive the spin-flip probability P_{flip} within the scattered portion of the electron wave packet

$$P_{\text{flip}} \equiv \frac{|c_3^{+\downarrow}(T)|^2}{|c_3^{+\uparrow}(T)|^2 + |c_3^{+\downarrow}(T)|^2} = \frac{1}{\frac{25}{2}\left(\frac{|\boldsymbol{p}_E|}{k}\right)^2 + 1} . \tag{8}$$

The Rabi frequency may be derived by identifying (7) with the Taylor expansion of (6b) for short times T, resulting in

$$\Omega_R = \Omega_0 \sqrt{\frac{25}{2}\left(\frac{|\boldsymbol{p}_E|}{k}\right)^2 + 1} . \tag{9}$$

Figure 3 compares the spin-flip probability as a function of $|\boldsymbol{p}_E|/k$, as obtained from the numerical solution of the Dirac equation (4), with our analytical result (8). The initial electron momentum in laser propagation direction $\boldsymbol{p}_k$ is adjusted according to equation (5) for each value of $\boldsymbol{p}_E$. The analytical formula (8) shows very good agreement with the numerical data.

Considerations on nonrelativistic theory The spin-flip probability (8) can be understood on a qualitative level by analyzing the leading order of the Foldy-Wouthuysen expansion [22] of the Dirac equation (2) which equals the nonrelativistic Pauli equation. This equation features two coupling terms which are linear in the fields, namely $e\boldsymbol{A}\cdot\boldsymbol{p}/(mc)$ and $e\boldsymbol{\sigma}\cdot\boldsymbol{B}/(2mc)$, where $\boldsymbol{\sigma}$ denotes the vector of Pauli matrices. Both terms give rise to couplings between adjacent electron momentum components (differing by $\pm\boldsymbol{k}$), with the first term preserving and the second term flipping the electron spin. Note that such nearest-neighbor couplings are necessarily involved in Kapitza-Dirac scattering with an odd number of photons. The relative strength of the $\boldsymbol{A}\cdot\boldsymbol{p}$ term as compared with the $\boldsymbol{\sigma}\cdot\boldsymbol{B}$ term is just $2|\boldsymbol{p}_E|/k$. This results in the spin-flip probability

$$P_{\text{flip, nonrel.}} = \frac{1}{4\left(\frac{|\boldsymbol{p}_E|}{k}\right)^2 + 1} , \tag{10}$$

which agrees with (8) up to a scale parameter 25/8. The probability (10) can also be derived more rigorously via time-dependent perturbation theory for the Pauli equation, which yields the nonrelativistic Rabi frequency

$$\Omega_{R,\text{ nonrel.}} = \frac{243}{128}\Omega_0 \sqrt{4\left(\frac{|\boldsymbol{p}_E|}{k}\right)^2 + 1} . \tag{11}$$

Note that the relativistic and nonrelativistic spin-flip probabilities (8) and (10) and the relativistic and nonrelativistic Rabi frequencies (9) and (11) agree qualitatively. However, the nonrelativistic expressions cannot be recovered from the relativistic ones by taking a nonrelativistic limit. This is a consequence of the three-photon Bragg condition (5) that enforces a relativistic photon momentum and/or a relativistic electron momentum highlighting the relativistic nature of the three-photon Kapitza-Dirac effect.

The role of the spin Equation (7) indicates that spin-preserving transitions in the three-photon Kapitza-Dirac effect are completely suppressed for setups with $\boldsymbol{p} \perp \boldsymbol{E}$. This means that under such conditions the scattering is rendered possible only because the electron does carry spin, which clearly demonstrates the pivotal role the electron spin can play in Kapitza-Dirac scattering processes.

The above argument suggests that for a spinless particle with $\boldsymbol{p} \perp \boldsymbol{E}$ the three-photon channel of Kapitza-Dirac scattering is not accessible at all. This expectation is confirmed by Fig. 4 (a). It compares numerical results on the Rabi frequency as following from the Dirac equation (4) with corresponding numbers that we obtained by solving the time-dependent Klein-Gordon equation [23]. The predictions significantly differ in the limit $\boldsymbol{p}_E \to 0$. While the Rabi frequency converges to a finite value for spin-half particles [see also (9)], it approaches zero for spinless particles, indicating that the scattering channel closes indeed. In the spinless case, the spin-flipped channel (7b) is missing, which consequently yields the Rabi frequency

$$\Omega_{R,\text{ spinless}} = \Omega_0 \frac{5}{\sqrt{2}}\frac{|\boldsymbol{p}_E|}{k} . \tag{12}$$

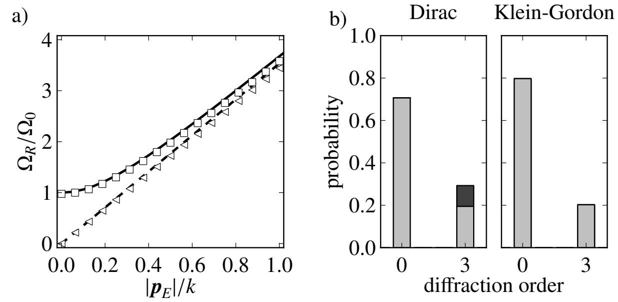

FIG. 4: Panel (a): The Rabi frequency Ω_R as a function of the electron momentum $|\boldsymbol{p}_E|$ in electric field direction for the Dirac equation (squares) and the Klein-Gordon equation (triangles). The solid black line is given by (9) and the dashed black line is given by (12). Panel (b): The diffraction probability after an interaction time of 0.36 fs for particles with and without spin for parameters as in Fig. 2. The light (dark) gray bars represent the spin-up (spin-down) probabilities. In the case of the Klein-Gordon equation there is no spin degree of freedom and, therefore, no dark gray bars appear. Note that the diffraction probability depends on the spin degree of freedom.

For nonzero values of $\boldsymbol{p}_E$, also Klein-Gordon particles may be scattered. But the scattering probability still may be considerably different from the Dirac case, as the example in Fig. 4 (b) shows.

Experimental realization An experimental realization of the three-photon Kapitza-Dirac effect may utilize intense photon beams at near-future X-ray laser facilities to form standing waves. In our numerical simulations, we assumed 3.1 keV photons as envisaged, for example, at the European X-ray free electron laser facility (XFEL) [9], which is currently under construction. The design value of the peak power at this photon energy is 80 GW. Assuming a focus diameter of 7 nm [25], a field intensity of about $2 \times 10^{23}\,\mathrm{W/cm^2}$ results. Laser pulses with duration of about half a Rabi period [which is about 1 fs for the parameters in Fig. 2)] are required for experimental realization [26]. Since the Rabi frequency is much lower than the laser frequency, the photon energy and the electron momentum must be fine-tuned to achieve a resonant transition. Numerical simulations indicate that only electrons whose momentum varies by $0.1\,\mathrm{keV}/c$ around the mean value of $176\,\mathrm{keV}/c$ are diffracted. The photon pulse of the European XFEL with a seeded beam of a primary undulator is expected to be coherent, featuring a photon energy uncertainty far below 0.1 keV [27]. We note that the electron may lose energy due to spontaneous photoemission with resulting quantitative modification of the presented results. Spontaneous emission (scaling with $|\boldsymbol{E}|^2$), however, is substantially suppressed as compared with the very fast momentum transfer through the three-photon Kapitza-Dirac effect which takes place on a femtosecond time scale during a Rabi period ($1/\Omega_R \sim 1/|\boldsymbol{E}|^3$). A numerical solution of the Landau-Lifshitz equation [28] indicates that the momentum transfer into laser propagation direction caused by spontaneous emission is sufficiently small in order not to violate the resonance condition (5) for the current parameters. Finally, the electron beam is diffracted almost in the electron propagation direction by $3 \times 3.1\,\mathrm{keV}/c$. Therefore, a spectrometer with a resolution below $10\,\mathrm{keV}/c$ should be able to separate the diffracted electron beam from the not diffracted one. In the diffracted beam, about one out of three electrons are spin flipped in the case of the scenario in Fig. 2. This spin-flip fraction is independent of the interaction time T of the electron with the laser, in accordance with (8).

Conclusions Pronounced spin effects in Kapitza-Dirac scattering involving three X-ray laser photons interacting with a weakly relativistic electron beam have been revealed. To this end, we deduced a generalized Bragg condition and developed a theoretical description of the quantum dynamics based on the Dirac equation. The process features characteristic Rabi oscillations and a competition between spin-preserving and spin-flipping nearest-neighbor couplings. The spin-flipping transition becomes dominant in the limit of small angles of inclination, where three-photon Kapitza-Dirac scattering crucially relies on the nonzero electron spin. Our predictions may be tested with the aid of near-future high-intensity XFEL sources.

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