Generation of a spin-polarized electron beam by multipole magnetic fields

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The propagation of an electron beam in the presence of transverse magnetic fields possessing integer topological charges is presented. The spin–magnetic interaction introduces a nonuniform spin precession of the electrons that gains a space-variant geometrical phase in the transverse plane proportional to the field’s topological charge, whose handedness depends on the input electron’s spin state. A combination of our proposed device with an electron orbital angular momentum sorter can be utilized as a spin-filter of electron beams in a mid-energy range. We examine these two different configurations of a partial spin-filter generator numerically. The results of this analysis could prove useful in the design of an improved electron microscope.

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1. Introduction

A few years ago, the existence of electron beams carrying orbital angular momentum (OAM) was predicted theoretically [1]. A couple of years later, two different techniques, based on the holography and random phase changes in a graphite sheet, were used to generate electron beams carrying OAM, i.e., electron vortex beams, experimentally [2–4]. Such an intriguing topic is of particular interest to materials scientists, since it can be used to probe the magnetic and spin-dependent properties of materials with atomic resolution [5,6]. The OAM as a “rotational-like” degree of freedom of an electron beam induces a magnetic moment, in addition to the spin magnetic moment, of up to few hundred Bohr magnetons per electron, which gives a possibility to interact with an external magnetic field [3,5]. The interaction of OAM magnetic moments with a uniform longitudinal magnetic field or a flux has been recently examined theoretically and experimentally [7–9]. This interaction enhances or diminishes the kinetic OAM of the beam, and can be used to measure or sort the OAM of electron beams spatially. However, besides its interesting and fascinated applications, this novel degree of freedom of free electrons can be utilized to investigate some fundamental quantum concepts such as the Bohr–Pauli impossibility of generating a spin-polarized free electron beam [10,11].

The spin–orbit coupling in a non-uniform balanced electric–magnetic field, named a “q-filter”, was proposed by some of the authors as a novel tool to generate an electron vortex beam from a pure spin-polarized electron beam. In that configuration, the spin of an electron follows the Larmor precession up and acquires a geometrical phase, which depends on both the spin–magnetic field direction and the time of interaction. A non-uniform magnetic field introduces a non-uniform phase profile whose topological structure is that of the magnetic field. Several different topological charge configurations, proposed in the previous paper, have been achieved in practice [11]. A locally orthogonal electric field was proposed to compensate for the “net” magnetic force. Furthermore, the reverse process was suggested to filter the spin component of an electron beam spatially, where two different longitudinal electron’s spin components suffer opposite precession directions, thus possess opposite OAM values.

In this work, we suggest a scheme based on non-uniform magnetic fields, rather than a balanced space-variant Wien q-filter, to manipulate electron OAM. Analogous to the q-filter, the proposed scheme imprints a topological charge – identical to the topological charge of magnetic field – onto the incoming electron beam with a handedness depending on the longitudinal component of electron spin; positive for spin up (↑) and negative for spin down (↓) with the advantage that no compensating electric field is needed. Unlike in the q-filter, however, the beam structure is now
strongly affected by the magnetic field. A TEM₀₀ Gaussian beam splits out into multi Gaussian-like beams after passing through the nonuniform magnetic field of the device, each beam oscillates in the opposite direction of the gradient of A₀, i.e., along −∇A₀. In particular, the incident Gaussian electron beam splits into two and three semi-Gaussian beams in quadrupole and hexapole magnetic fields, respectively. It is worth noting, however, that a multi-Gaussian-like beam does recover its original Gaussian shape at certain free-space propagation distance, provided its phase distribution does not acquire sudden changes in the transverse plane. In this work, we introduce and numerically simulate two realistic configurations of a spin-filter for electron beams, based on the new proposed device. Our numerical simulations confirm that a portion of the electrons, typically small, remains polarized after passing through the device and can be easily separated form the rest of the beam by suitable apertures.

2. Propagation of electron beams in an orthogonal uniform magnetic field

Let us assume that the electron beam moves along the z-direction perpendicular to a uniform magnetic field \( B = B_0 \cos \theta, \sin \theta, 0 \), which lies in the \( (x,y) \) transverse plane at angle \( \theta \) with respect to the \( x \)-axis. As associated vector potential we may take \( A = A_0(0,0,y \cos \theta - x \sin \theta) \). We assume a paraxial beam with average linear momentum \( p_c \) and average energy \( E_c = p_c^2/2m \), so that \( \psi(x,y,z,t) = \exp\left(-i\mathbf{p}z - E_c t\right)\tilde{u}(x,y,z) \), with \( \tilde{u}(x,y,z) \) a slow-envelope spinor field [1]. Inserting this ansatz into Eq. (1) and neglecting the second derivatives of \( \tilde{u} \) with respect to \( z \), we obtain the paraxial Pauli equation

\[
\left( \partial_z^2 + \mathbf{k} \cdot \mathbf{A} \right) \tilde{u}(x,y,z) = 0,
\]

where \( \mathbf{A} \) stands for the transverse coordinate, and \( k_c = p_c/h \) is the central de Broglie wave-vector.

Eq. (2) is solved with initial Cauchy data at \( z = 0 \),

\[
\tilde{u}(r, \phi, 0) = \tilde{u}(r, \phi, z) = \exp(-r^2/w_0^2) \tilde{u}(r, \phi, z) \quad \text{corresponding to a Gaussian beam of width} \ w_0 \ \text{in the cylindrical coordinates of} \ (r, \phi, z). \]

The constant spinor \( \tilde{u}(r, \phi, z) = (\tilde{u}_1, \tilde{u}_2) \) describes the polarization state \( |\psi\rangle = |\tilde{u}_1\rangle \pm i |\tilde{u}_2\rangle \). The input beam in the \( |\uparrow\rangle, |\downarrow\rangle \) basis where the spin is aligned parallel or antiparallel to the beam propagation direction, respectively. We assume the normalization \( |\tilde{u}_1|^2 + |\tilde{u}_2|^2 = 1 \). A straightforward calculation shows that the required solution of the paraxial Pauli equation is given by

\[
\tilde{u}(r, \phi, z) = G(r, \phi, z) M(z) \tilde{u},
\]

where \( M(z) \) is a matrix given by

\[
M(z) = \begin{pmatrix}
\cos \frac{\Lambda_1}{2} & i e^{i\theta} \sin \frac{\Lambda_1}{2} \\
-e^{i\theta} \sin \frac{\Lambda_1}{2} & \cos \frac{\Lambda_1}{2}
\end{pmatrix},
\]

with \( \Lambda_1 = 4\pi h^2 k_c/\mu g B_0 \). The matrix \( M(z) \) accounts for the action of the magnetic field on the particle spin. The action on the electron motion is described in Eq. (3) by the Gaussian-coherent factor \( G(r, \phi, z) \) given by

\[
G(r, \phi, z) = \sqrt{\frac{-k_c z_0}{\pi q_f (z_0^2 + z^2)}} e^{ik_c f_z(r, \phi, z) z_0^2/2 + i f_x(r, \phi, z) z_0/2}.
\]

with

\[
f_x(r, \phi, z) = r^2 \cos^2(\theta - \phi),
\]

\[
f_z(r, \phi, z) = i \left( \frac{\Lambda}{\pi} + r \sin(\theta - \phi) \right) \left( \frac{\Lambda}{\pi} + r \sin(\theta - \phi) \right) + \cos \left( \frac{\pi z}{\Lambda} \right) \left( \frac{\Lambda}{\pi} - r \sin(\theta - \phi) \right) \left( \frac{\Lambda}{\pi} + r \sin(\theta - \phi) \right).
\]

The complex curvature radii of the Gaussian-coherent factor \( G(r, \phi, z) \) are given by

\[
q_+ = z - iz_0
\]

\[
q_- = \frac{\Lambda}{\pi} \left( \frac{\pi z}{\Lambda} \right) - iz_0 \cos \left( \frac{\pi z}{\Lambda} \right),
\]

where \( z_0 = \frac{4k_c w_0^2}{2\pi} = \pi \hbar k_c/eB_0 \). From Eq. (4) we see that the beam spin state oscillates during propagation with spatial period \( \Lambda_1 \).

Moreover, unlike the case with the Wien-filter, in which the mean direction of the beam is not affected, now the beam oscillates perpendicularly to the magnetic field \( \mathbf{B} \) towards \( -\mathbf{A}_0 \), with spatial period \( 2\Lambda_1 = (g/\mu g) \Lambda_1 = \Lambda_1/2 \propto B_0^{-1} \). Fig. 1(a) shows the beam intensity profiles at two different \( z \)-planes; at the entrance plane \( z = 0 \) (central spot) and at \( z = \alpha \Lambda \) with \( \alpha = 0.44\% \) (upper spot). The electron trajectory in the \( yz \)-plane, orthogonal to the magnetic field, is shown in Fig. 1(b): the electron beam follows a sinusoidal oscillation with spatial period \( 2\Lambda_1/\pi \).

3. Propagation of electron beams in an orthogonal uniform nonuniform magnetic field possessing a specific topological charge

Eq. (3) represents an exact solution of the beam paraxial equation, with explicit boundary conditions, for a uniform constant magnetic field at angle \( \theta \) with respect to the \( x \)-axis. If the angle \( \theta = \theta(x,y) \) changes slowly in the transverse plane, we may assume that the solution (3) is still approximately valid. This Geometric Optics Approximation (GOA) is quite accurate in the present case, since the electron beam wavelength in a typical Transmission Electron Microscope (TEM) is in the range of tens of picometers, while \( \theta \) changes over length of several microns. Within this slowly varying approximation, the effect of a nonuniform magnetic field is obtained simply by replacing \( \theta \) with \( \theta(x,y) \) in Eqs. (4)-(6). We assume a singular space distribution of the magnetic field where \( \theta(x,y) = \theta(r, \phi) \) is given by

\[
\theta(\phi) = \phi \phi + \beta,
\]

where \( \phi = \arctan(y/x) \) is the azimuthal angle in the beam transverse plane and \( \beta \) is a constant angle, which defines the inclination on the \( x \)-axis. Finally \( q \) is an integer which fixes the topological charge of the singular magnetic field distribution. Such magnetic structures can be generated in practice by multipolar lenses (for negative charges \( q \)) or by a set of appropriate longitudinal currents at origin (for positive
charge $q$. Inserting Eq. (9) into Eqs. (4) and (6) yields

$$\dot{M}(z) = \left( \begin{array}{c} \cos \frac{2z}{\Lambda} \\
\hfill \end{array} \right)$$

(10)

and

$$f_\phi(r, \phi, z) = r^2 \cos^2((q - 1)\phi + \beta),$$

$$f_z(r, \phi, z) = i\left( \frac{\pi}{\Lambda} \right) \left( \frac{\Lambda}{\pi} r \sin((q - 1)\phi + \beta) \right) \times \left( \begin{array}{c} 2i\left( \frac{\Lambda}{\pi} \right)^2 + \left( \frac{\pi}{\Lambda} \right)^2 z_r \left( q_z z + iz_r \cos \left( \frac{\pi z}{\Lambda} \right) \right) \\
\hfill \end{array} \right) \times \left( \frac{\Lambda}{\pi} r \sin((q - 1)\phi + \beta) \right) + \cos \left( \frac{\pi z}{\Lambda} \right) \times \left( \frac{\Lambda}{\pi} r \sin((q - 1)\phi + \beta) \right) \times \left( 2 \left( \frac{\Lambda}{\pi} \right)^2 + r \sin((q - 1)\phi + \beta) \right).$$

(11)

Eq. (10) shows that in passing through a multipole magnetic field of length $L$, a fraction $|\eta|^2 = |\sin(2\pi L/\Lambda)|^2$ of the electrons in the beam flip their spin and acquire a phase factor $\exp(\pm i\eta\phi)$ according to whether the initial spin was up $|\uparrow\rangle$ or down $|\downarrow\rangle$. The rest of the electrons, i.e., $1 - |\eta|^2$, pass through without changing their initial spin state. When $L = \Lambda/2$ (mod 2\pi), all electrons emerge with their spins reversed and acquire the abovementioned phase factor, which means that an amount of $\pm h\eta$ is added to their initial OAM value. In this case the Spin-To-OAM Conversion (STOC) process is complete and we say that the device is “tuned” [11]. Tuning can be achieved by altering the strength of the magnetic field or changing the device length. The STOC process is governed by the $\exp(\pm i\eta\phi)$ factors in Eq. (10), which is of geometrical origin [12]. As a consequence, the STOC process even if the field amplitude $B_0$ is (slowly) dependent on the radial coordinate $r$ in the beam transverse plane. The capability of changing the electron OAM and of creating a correlation between OAM and spin are the main features of the non-uniform magnetic multipoles. Eq. (11) shows that the device significantly alters the transverse profile of the beam which acquires multi quasi-Gaussian shapes as shown in Figs. 2(b) and 3(b) for quadrupole and hexapole magnetic field, respectively. The initial Gaussian beam breaks up upon propagation through the magnetic field into two and three astigmatic quasi-Gaussian beams for quadrupole and hexapole, respectively. The cleft number depends on the number of local vector potential minima. Both the STOC and non-STOC parts of the beam possess the same intensity profile; but the STOC part only acquires a helical phase structure according
to the magnetic field topological charge. For a small beam distortion, it can be shown that in the far-field the multi-Gaussian-like beam with the helical structure assumes a doughnut shape, while the vortex free non-STOC beam assumes a Gaussian shape.

4. Fringe fields and their effect on spin-filtering

In practice, it is impossible to generate a completely transverse magnetic field. Further non-transverse components, known as fringe fields, cannot be avoided. In this section, we examine the effect of the fringe fields on the spatial distribution of an electron beam when our proposed device is not tuned. A non-tuned device, based on its length and magnetic field strength, converts only a portion of the incoming beam – the remaining part of the beam left unchanged. When the non-tuned device is applied to an unpolarized electron beam, the beam exits in a mixture state of spin up and down with opposite OAM values, given by

$$\psi_{\text{STOC}} = \eta \begin{cases} |\uparrow, -\ell\rangle & \text{for spin } |\uparrow\rangle \text{ input,} \\ |\downarrow, +\ell\rangle & \text{for spin } |\downarrow\rangle \text{ input,} \end{cases}$$ (12)

where $|\ell\rangle$ stands for the OAM state given by topological charge of device, i.e., $\ell = q$, and $|\eta\rangle = |\sin(2\pi Lr/L_0)|^{1/2}$ is the device STOC’s efficiency. The main fringe fields appear at the entrance and the exit face of the device as nonuniform longitudinal magnetic fields. The interaction of longitudinal magnetic field with both spin and orbital angular momentum of electron beams has been recently theoretically investigated [8]. The longitudinal magnetic field introduces a phase rotation $\Phi(\ell, s) \propto B_2(\ell \cdot g)z$ on the beam, where $s = \pm 1$ is the spin eigenvalues in units of $\hbar/2$ corresponding to spin up and down, respectively, and $B_2$ is in general a function of transverse radial coordinate $r$ [8]. This phase rotation comes out from the Zeeman interaction. The longitudinal fringe field introduces a different phase change in each term of Eq. (12) which is therefore changed into

$$\psi_{\text{STOC}} = \eta \begin{cases} e^{i\Phi(-\ell,1)}|\uparrow, -\ell\rangle & \text{for spin } |\uparrow\rangle \text{ input,} \\ e^{i\Phi(-\ell,-1)}|\downarrow, +\ell\rangle & \text{for spin } |\downarrow\rangle \text{ input.} \end{cases}$$ (13)

Since the fringe fields are nonuniform, in general, the phases in Eq. (13) are coordinate dependent and produce dual converging and diverging astigmatic effects. However, even in the presence of fringe fields, the two spin states of the emerging beam are still labeled by the two values $\pm \ell$ of OAM so that an OAM sorter can be used to separate the electrons according to their spin value. In the next section, we determine numerically the efficiency of this method of obtaining polarized electron beams by using a pitchfork hologram with topological charge $\ell$ as an OAM sorter. The final state after an OAM sorter, then, is

$$|\psi\rangle_{\text{final}} = \eta \begin{cases} e^{i\Phi(-\ell,1)}|\uparrow, 0\rangle & \text{for spin } |\uparrow\rangle \text{ input,} \\ e^{i\Phi(-\ell,-1)}|\downarrow, 2\ell\rangle & \text{for spin } |\downarrow\rangle \text{ input.} \end{cases}$$ (14)

The first term tends to recover the Gaussian shape, while the second term will have a doughnut shape in the far-field. Both of the non-STOC terms possess OAM = $\ell$ since the hologram, i.e., OAM sorter, is spin independent. A spatial selector, e.g. a pinhole, can be used to select the central part, which has a uniform coherent spin up state. The efficiency and purity of the spin filter depends on the pinhole radius, which for an optical field has been discussed in [13]. Thus, a combination of this device with an OAM sorter yields an electron spin-filter that is practical, since the multipoles of magnetic magnets are available commercially as aberration correctors for TEM as well as OAM sorters.

5. Numerical simulation and technical discussions

The GOA analytical solution presented in Section 2 may be used to obtain preliminary information on the STOC efficiency and beam intensity profile in the device. However, more details on the interaction of a space-variant magnetic field with an electron beam can be examined by implementing both a ray tracing technique and the spin–orbit interaction simultaneously. In order to overcome this issue, we developed a research software based on the multi-slice method used in electron microscopy, where Eq. (2) has been considered as a free particle motion under the force of a “local potential” of A, $\Delta^2$ and Pauli terms. Therefore, one can evolve both temporal and $z$-dependence of the wave-function based on a well-known Dyson-like decomposition, since both operators of the scalar wave equation and local potential do not commute [14,15]. The potential was divided and projected onto multi-slices where the beam wave-function was constructed by free-space propagation between each slice. After each iteration the wave-function turns into

$$u(r, z_{j+1}) = \mathcal{K} \otimes \left( e^{i\phi(r, z_j)} \int_0^{z_{j+1}} V(r, \zeta) d\zeta \right) u(r, z_j),$$ (15)

where $v$ is the electrons velocity, $\otimes$ is the convolution with the wave-function inside parentheses, $z_j$ and $V(r, \zeta)$ stand for position of jth slice and the local potential (third, fourth and fifth term of Eq. (2)), respectively (see Ref. [16] for more details). $\mathcal{K}$ is the Fresnel propagator between each two adjacent slices spaced by
Δz, which is given by
\[ K = \frac{-i k e^{i k / 2 \Delta z^{2} + y^{2}}}{2 \pi \Delta z}. \] (16)

Apart from the simple concept, one may extend such a powerful algorithm to the relativistic case as well [17]. However, since electron microscopes work at mid-range energy, our simulation was carried out in the non-relativistic regime. We considered two possible configurations to generate a spin-polarized electron beam in an electron microscope.

(i) A first scheme can in principle be adopted in various microscopes using a condenser stigmator. In this first scheme, a Gaussian beam is directed to a quadrupolar magnetic field, and then to a pitch-fork hologram as shown in Fig. 4. A lens condenser can be used to form the far-field image of the hologram. However, the intensity required for the magnetic field could make the operation difficult. It also turns out that it is difficult to polarize electrons before the specimen, except in microscopes with two or even three condenser aperture planes. On the other hand, different spin states can be selected by looking at counterpart diffraction orders. Thus, first and minus first orders after being spatially selected possess different spins, i.e., up and down, suitable for examining the spin dependence of materials. Moreover, both beams can be used to perform interference experiments with two spin states to reveal the degree of polarization.

The simulated electron beam shapes after passing through the quadrupole and the pitch-fork hologram for spin up and down input are shown in Fig. 5.

The first and second rows in Fig. 5 show the far-field intensity pattern for input electrons with spin up and down states, respectively. The subrows correspond to expected spin states for the first order of diffraction (left spots). The non-STOC part of both spin up and down, i.e., first and last rows of Fig. 5, forms a Hermite-Gaussian shape of first order, which is affected by the quadrupole’s astigmatism and splits into two parts. Conversely the STOC parts are shaped differently depending on the initial spin state; one as the Hermite-Gaussian of second order while the other one forms a Gaussian beam bearing some astigmatic distortion. It can be seen that an aperture with appropriate size can be used to select the central spot only, which possesses opposite polarizations.

(ii) In the second method, a simplified scheme of a spherical aberration corrector is considered, see Fig. 6. Indeed, normal Cs-correctors contain, as main elements, a set of opposite hexapoles [18]. However, in order to simplify the numerical calculations, we substituted them with quadrupoles. In this sense a set of coupled quadrupoles would probably do the same job but given large diffusion of Cs-corrector it appears interesting to refer also to this device. Therefore, we assume that two quadrupoles with opposite

Fig. 4. First proposed scheme to generate a spin-polarized electron beam based on space-variant magnetic fields.

Fig. 6. Second proposed scheme to generate a spin-polarized electron beam based on coupling with two magnetic quadrupoles (spherical aberration corrector). The second quadrupole corrects the aberration induced by the first one. Nevertheless, the spin-to-orbit coupling efficiency after the second quadrupole can be completely neglected.
electron beam. However, because of the strong astigmatism, the efficiency of the devices proposed here are lower than the ones discussed in Ref. [11]. Finally, it is worth mentioning that the purity of the generated polarized electrons is reasonably higher than other proposed approaches such as the spin-dependent scattering process in diamond loops, and implementing a different photocathode [19,20].

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6. Conclusions

We presented two possible practical devices to generate a spin polarized electron beam via a spin-to-orbit conversion in the presence of a nonuniform transverse magnetic field. The main component of both devices is a multipolar magnet generating a singular transverse magnetic structure with negative integer topological charge. The device action on a pure spin-polarized electron beam is to induce spin-to-orbit conversion, whereby the beam gains a nonuniform phase structure which is defined by the magnetic field topological charge, where the sign is given by the input electron spin value. When the device is combined with an OAM sorter, spiral phase plate, hologram, or even a longitudinal magnetic field, it can be used as a spin-filter to polarize the electron beam. However, because of the strong astigmatism, the efficiency of the devices proposed here are lower than the ones discussed in Ref. [11]. Finally, it is worth mentioning that the purity of the generated polarized electrons is reasonably higher than other proposed approaches such as the spin-dependent scattering process in diamond loops, and implementing a different photocathode [19,20].

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