Nonparaxial Accelerating Electron Beams

Yongfeng Kang, Yiqi Zhang, Changbiao Li, Hua Zhong, Yanpeng Zhang, and Milivoj R. Belić

***Abstract*— We investigate nonparaxial accelerating electron beams theoretically in two and three dimensions. Starting from the Klein–Gordon equation, we obtain the Helmholtz equation for electron beams. We demonstrate that the electron beams can accelerate along semi-circular, parabolic, and semi-elliptic trajectories. The shape of the trajectory is determined by the input beam, which can be constructed by using phase masks that reflect the shape of the relevant special functions: half-Bessel, Weber, or half-Mathieu. The corresponding self-healing and ballistic-like effects of the nonparaxial accelerating beams are also demonstrated. The depth of the focus of the electron beam can be adjusted by the order of the function that is included in the input. Our investigation enriches the accelerating electron beam family, and provides new choices for improving the resolution of transmission electron microscope images.**

***Index Terms*— Electron accelerating beams, Klein-Gordon equation, Bessel beams, Mathieu beams, Weber beams.**

I. Introduction

In 1979, it was demonstrated in quantum mechanics that the Airy function is an eigenmode of the Schrödinger equation [1]; it was also demonstrated that this wave function exhibits the self-accelerating and nondiffracting properties. However, to be a physical quantity, Airy wave function must be truncated, and this was first accomplished in optics by Siviloglou *et al.* [2,3], in 2007. From then on, Airy and other accelerating nondiffracting beams have become one of the hottest fields in optics and have experienced rapid development. Until now, studies of Airy beams have been reported in nonlinear media [4]–[7], optical fibers [8], [9], systems with linear potentials [10]–[12], and elsewhere.

It should be recalled that the Airy beam is a paraxial accelerating beam, being based on the paraxial wave equation, which is equivalent to the Schrödinger equation. If one treats the beams using Maxwell's equations directly, one will arrive at the nonparaxial optical beams, based on the Helmholtz equation [13], [14]. It is known that the solutions of the two-dimensional (2D) Helmholtz equation are plane waves in Cartesian coordinates, Bessel beams in polar coordinates [15]–[19], Mathieu beams in elliptic coordinates [20], [21], and Weber beams in parabolic coordinates [20], [22]. One can also solve the 3D Helmholtz equation for the 3D accelerating beams, by e.g. utilizing the Whittaker integral [15], [23], [24]. For a comprehensive look into this field, one may consult the review articles [25], [26]. A question naturally pops up: What about the matter waves such as electron beams?

Besides in electron optics, electron beams as accelerating waves were reported in [27] and [28]; they also possess self-healing and nondiffracting properties. The investigation of accelerating electron beams has opened a new chapter in the field, adding matter waves to the list. Indeed, research in this field has broadened to cover acoustics [29], surface plasmons [30], Bose-Einstein condensates [31], water waves [32], and other areas. However, one should note that the investigations were mostly focused on the paraxial cases; therefore, we wonder if the nonparaxial accelerating concept can be extended to the electron beams. This is the motivation and the goal of this paper.

In addition, we believe that such a research is meaningful and sorely needed. Since one has to take into account relativistic properties of a single electron, the Helmholtz equation for an electron will be obtained directly from the Klein-Gordon equation [33]. It should be mentioned that the nondiffracting nonparaxial electron Bessel beam was recently demonstrated experimentally [34]; therefore, we believe that theoretically predicted self-accelerating nonparaxial matter beams in this paper can also be experimentally observed, even though there are challenges on that path.

It should also be noted that the traditional electron optics has been researched thoroughly in the last decades, owing to its great applicative potential. In order to calculate higher-order aberrations [35], differential algebra method was applied to the electron optical systems, including electron lens and combined focus and deflection systems [36], [37]. Nevertheless, introducing a novel accelerating concept into electron optics may inspire new designs and supply additional avenues to the management of electron beams.

The organization of the paper is as follows. In Sec. II, we obtain the Helmholtz equation for electrons from the Klein-Gordon equation. In Sec. III, we display the nonparaxial electron beams based on the 2D Helmholtz equation. The discussion is divided into three cases based on the accelerating trajectories: the half-Bessel beams in Subsec. III-A, the Weber

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beams in Subsec. III-B, and the half-Mathieu beams in Subsec. III-C. In Sec. IV, we briefly investigate the nonparaxial electron beams in 3D. We conclude the paper in Sec. V and also give a brief outlook on the future investigations.

II. Mathematical Modeling

The Klein-Gordon equation is used to calculate the wave function of a relativistic electron when the spin effects are neglected. In free space, it is expressed as

$$-\hbar^2 \frac{\partial^2}{\partial t^2}\Phi = \left(m_e c^2\right)^2 \Phi - c^2\hbar^2\nabla^2\Phi, \tag{1}$$

where $\hbar$ is the reduced Planck constant, m_e is the mass of electron, c is the light speed in vacuum, and ∇^2 is the Laplacian. For our purposes, it is sufficient to consider the time-independent solutions, so we seek here a solution with an ansatz

$$\Phi(r,t) = \psi(r)\exp\left(-i\frac{E}{\hbar}t\right), \tag{2}$$

where E is the energy of the electron. For a relativistic electron, it can be written as $E = \sqrt{c^2p^2 + (m_ec^2)^2}$, with p being the corresponding momentum. Plugging Eq. (2) into Eq. (1) and after some algebra, one obtains

$$\nabla^2\psi(r) + k_B^2\psi(r) = 0, \tag{3}$$

where $k_B = p/\hbar$ is the de-Broglie wavenumber of the electron. Equation (3) is the Helmholtz equation that is frequently considered in the literature [16], [20], [21].

First, we consider the Laplacian in two dimensions that in Cartesian coordinates can be written as

$$\left(\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial x^2}\right)\psi(r) + k_B^2\psi(r) = 0 \tag{4}$$

in which x and z are the transverse and longitudinal coordinates, and $r = \sqrt{x^2+z^2}$. Equation (4) is also the governing equation for the nonparaxial accelerating electron beams that will be discussed below. For the forward propagation-invariant beams, the solution of the 2D Helmholtz equation can be written as [15], [38]–[40]

$$\psi(x,z) = \int_{-\pi/2}^{\pi/2} A_m(\phi)\exp[ik_B(x\sin\phi + z\cos\phi)]d\phi, \tag{5}$$

where $A_m(\phi)$ is the angular spectral function, which determines the pattern of ψ, and ϕ is the wave propagation angle measured from the z axis.

Classically, one has $E = \gamma m_e c^2$ and $p = \gamma m_e \upsilon$ when the relativistic effects are considered, where $\gamma = 1/\sqrt{1-\beta^2}$ and $\beta = \upsilon/c$, with υ being the speed of the electron. In electron optics, the cathode surface in the electron gun is usually chosen to be the equipotential surface. Then, the potential at the point of observation is identical with the voltage φ applied between this point and the cathode. The relativistic modified electric potential can be written as

$$\varphi^* = \varphi\left(1 + \frac{e\varphi}{2m_ec^2}\right), \tag{6}$$

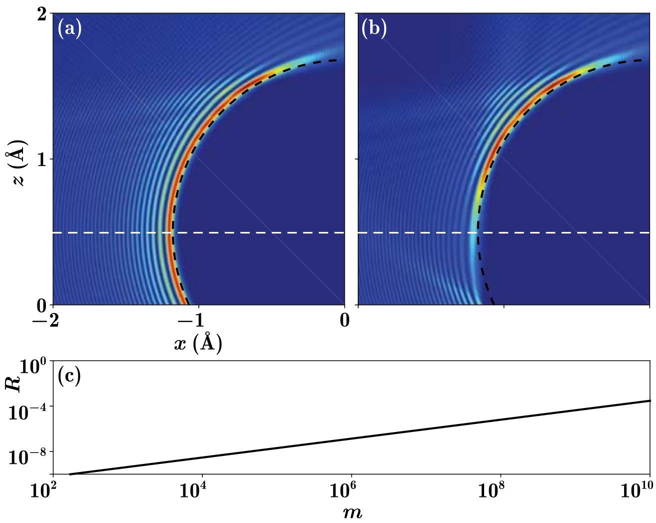

Fig. 1. (a) Propagation of a half-Bessel beam that accelerates along a circular trajectory. The black dashed curve indicates the theoretical accelerating trajectory, and the white dashed line the axis of symmetry of the trajectory. (b) Self-healing of the beam when the main lobe is removed. (c) Dependence of R on the order m of the half-Bessel beam.

and the de-Broglie wavelength λ_B is

$$\lambda_B = \frac{h}{p} = \frac{h}{\sqrt{2em_e\varphi^*}}. \tag{7}$$

In our calculation, we assume $\beta \approx 0.5479$, so that the de-Broglie wavelength λ_B of the electron is about 3.7 pm, which can be reached in the field emission gun transmission electron microscope that operates at 100 keV. In the following section, we present results obtained in other 2D coordinate systems.

III. Results and Discussion

A. Half-Bessel Beam

In polar coordinates, one of the solutions of Eq. (4) is the Bessel beam [15], i.e.

$$\psi_m(x,z) = u_0 i^m J_m(k_Br)\exp[im\arctan(z,x)], \tag{8}$$

where u_0 is a constant that determines the amplitude of ψ_m, and J_m is the Bessel function of the first kind and order m. However, it was demonstrated before that the forward beam only exhibits half of the Bessel beam structure [16]. Since the analytical solution in Eq. (8) is symmetric about the vertical axis $x = 0$ at certain propagation distance z, one can consider half of it to be the input. Instead of using the integration formula in Eq. (5), we directly use the half-Bessel beam as the input, to observe the corresponding propagation according to the 2D Helmholtz equation (4).

We take the left part of $\psi_m(x, z = -0.5\,\text{Å})$ with $m = 200$ as the input, and the propagation is displayed in Fig. 1(a). One finds that the input beam exhibits accelerating and nondiffracting properties during propagation, and that the trajectory is circular. This is in accordance with the analytical result, as shown by the black dashed curve, which is a part of a circle with radius $R \sim m/k_B$. Since the input is $\psi_m(x, z = -0.5\,\text{Å})$, the symmetry point moves from 0 to 0.5 Å, as depicted by the

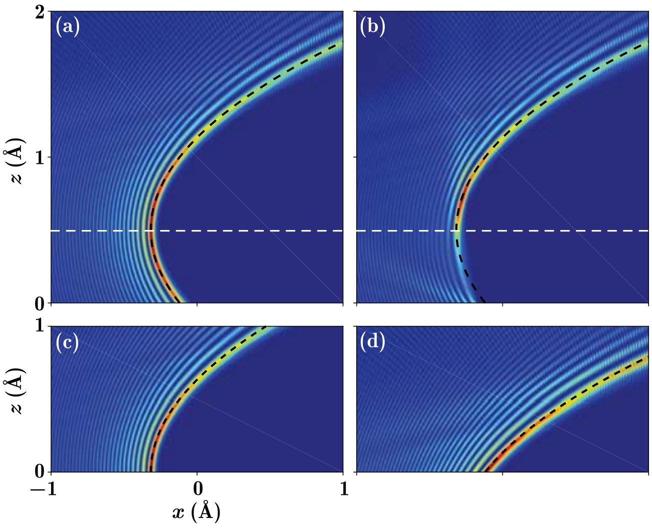

Fig. 2. (a) and (b) Same as Fig. 1, but for the Weber beam. (c) and (d) Propagation of Weber beams with the input at $z = 0$ and at $z = 0.5$ Å.

white dashed line. According to the simulation, one observes that the electron beam can bend nearly 90° and exhibits the ballistic-like effect [41], [42]. To check the self-healing effect, we remove the main lobe of the input beam deliberately, and then follow the propagation in Fig. 1(b). One finds that the main lobe recovers fast during propagation.

We would like to emphasize that the length of the focus can be well adjusted over a long range, because this quantity is controlled by the radius of accelerating trajectory $R \sim m/k_B$. In Fig. 1(c), we display the relation between R and m, from which one finds that the nonparaxial electron beam can have a very large length of focus if one further increases the order m without changing the transverse distribution. In experiment, one has to prepare a proper phase mask, similar to that used in the equivalent optical experiments [17], [20], [27].

As expected, one discovers that an electron beam behaves like a light beam, as demanded by the de-Broglie hypothesis. In addition, there exist not only paraxial accelerating electron beams, but also the nonparaxial accelerating electron beams. As investigated previously for the optical beams, we also demonstrate the nonparaxial accelerating electron beams that follow parabolic and elliptic trajectories—the Weber and Mathieu beams.

B. Weber Beam

In parabolic coordinates, one can find another solution of the 2D Helmholtz equation (4)—the Weber wave function. Since the corresponding description is rather technical, to facilitate an easy discussion, we move it to Appendix A.

Similar to the half-Bessel case, we also use $\psi(x, z = -0.5\,\text{Å})$ with $a = 50$ as the input beam (see Appendix A), and the corresponding propagation is shown in Fig. 2(a). As expected, the beam accelerates along a parabolic trajectory with a preserved shape, and the numerical trajectory agrees with the analytical (black dashed curve) [22] very well. If the main lobe of the input beam is removed, the self-healing effect is displayed, as shown in Fig. 2(b).

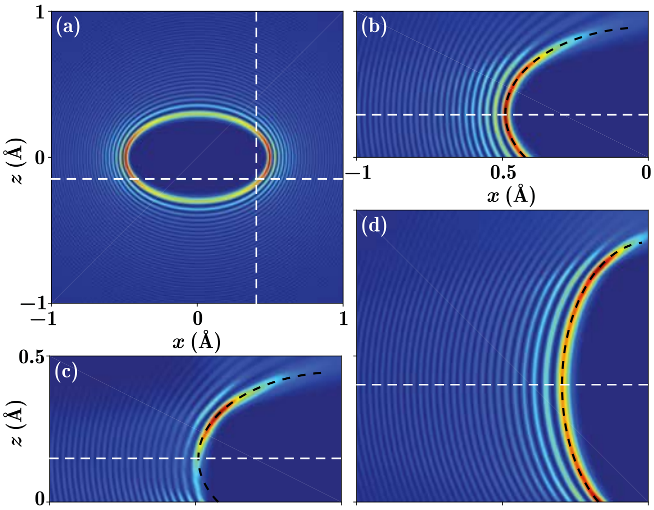

Fig. 3. (a) Intensity of the elliptic mode of the Mathieu electron beam of order $m = 65$ and $q = 1100$. (b) and (c) Setup is as in Fig. 1 (a) and (b), with the half-Mathieu beam along the horizontal dashed line in (a) launched from the major axis. (d) Same as (b), but with the half-Mathieu beam along the direction indicated by the vertical dashed line in (a) launched from the major axis. Panels (b)-(d) share the same scale.

To demonstrate the ballistic effect, we show the propagation of Weber beams with the input at $z = 0$ and at $z = 0.5$ Å, in Figs. 2(c) and 2(d), respectively. One finds that the scenarios in Figs. 2(a), 2(c) and 2(d), which are quite similar to the paraxial cases in [41] and [42], clearly indicate the ballistic effect. As a result, the nonparaxial Weber beam is also feasible for electrons.

C. Half-Mathieu Beam

As shown in Appendix B, the 2D Helmholtz equation in elliptic coordinates supports the accelerating Mathieu beam as a solution, with an elliptic trajectory. In Fig. 3(a), we depict the intensity profile of the elliptic mode from Eq. (14) in Appendix B, with $m = 65$ and $q = 1100$. According to the real parameters provided in Sec. II, one can find that the foci are located at $(\pm h, 0)$, with $h \approx 0.39$ Å.

We first adopt the left part of $\psi(x, z = -0.15\,\text{Å})$ to be the input and display the corresponding propagation in Fig. 3(b). Again, as expected, the acceleration is along an elliptic trajectory $x = -\sqrt{1 - (z - 0.15\,\text{Å})^2/(a^2 - h^2)}a$, with a being the location of the main lobe in Fig. 3(a). If the main lobe is removed, the self-healing effect will recover it soon during propagation, as depicted in Fig. 3(c). One can also use the half-Mathieu beam along the vertical direction shown by the dashed line in Fig. 3(a) to be the input, and such a beam will also accelerate along an elliptic trajectory, as shown in Fig. 3(d). Different from the case in Fig. 3(b) which goes through the apogee point, the case in Fig. 3(d) accelerates by the way of the perigee point.

IV. Three-Dimensional Case

In addition to the 2D nonparaxial accelerating electron beams, there also exist the corresponding

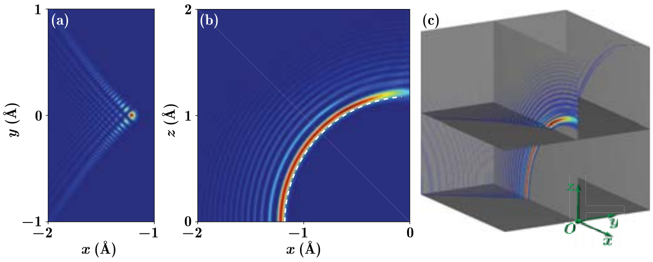

Fig. 4. (a) Intensity of the 3D electron beam in the $x0y$ plane. (b) Same as (a), but in the $x0z$ plane. Dashed curve is the analytical accelerating trajectory of the main lobe. (c) Panels (a) and (b), the beam intensities in the xy plane at $z = 1$ Å and in the yz plane at $x = -2$ Å, and the beam intensity in the xz plane at $y = 1$ Å, put together. The parameters are the same as in Fig. 1.

3D cases [15], [23], [43]. The accelerating solution of the 3D Helmholtz equation in Eq. (3) can be written as [24]

$$\psi(x, y, z) = \int_0^{\pi} d\theta \int_{-\pi/2}^{\pi/2} d\phi A_m(\theta, \phi) \sin\theta \times \exp[ik_B(x \sin\theta \sin\phi + y \cos\theta + z \sin\theta \cos\phi)]. \quad (9)$$

Clearly, if $\theta = \pi/2$, Eq. (9) reduces to Eq. (5), i.e., to the 2D case. Similar to [23], if we consider the beams that accelerate along a semi-circular trajectory, the angular spectral function can be written as $A(\theta, \phi) = g(\theta) \exp(im\phi)$.

In Fig. 4, we present the propagation of a 3D nonparaxial accelerating electron beam with $g(\theta) = 1$. Figure 4(a) is the transverse intensity distribution of the beam in the $x0y$ plane, and Fig. 4(b) is the corresponding intensity distribution in the $x0z$ plane. In order to display the 3D propagation more clearly, Figs. 4(a) and 4(b) are put together in Fig. 4(c), according to the accepted geometric arrangement. In addition, in Fig. 4(c), we also exhibit three intensity distributions that are in the xy plane at $z = 1$ Å, in the yz plane at $x = -2$ Å, and in the xz plane at $y = 1$ Å.

V. Conclusion

In summary, we have demonstrated that electron beams can also exhibit nonparaxial accelerating properties, as well as self-healing and ballistic effects during propagation. We have shown that the accelerating trajectories can be semicircular, parabolic, and semi-elliptic. The bending angle is nearly 90°. These accelerating electron beams can be prepared using the half-Bessel function, the Weber function, and the half-Mathieu function in the phase masks. Our research not only enriches the family of accelerating electron beams, but also exhibits potential applications in improving the resolution of transmission electron microscopes. Owing to the fact that the beam shape can be preserved over a relatively long distance, the depth of the focus can be easily controlled. Since the accelerating trajectories of paraxial accelerating electron beams can be well adjusted, we believe that the trajectories of nonparaxial cases can also be well managed by using magnetic field [27], which will play the role of a linear potential. We also believe that the self-accelerating beams can be potentially used for atmospheric detections [44], which has never been explored before.

Appendix A
Weber Beam

The transformation between Cartesian coordinates (x, z) and parabolic coordinates (η, ξ) is accomplished by the relation $x + iz = (\eta + i\xi)^2/2$, with $\eta \in (-\infty, \infty)$ and $\xi \in [0, \infty)$. By utilizing variable separation, that is, by writing the solution of the 2D Helmholtz equation as $\psi(\xi, \eta) = R(\xi)\Phi(\eta)$, one obtains two ordinary differential equations:

$$\frac{\partial^2 R(\xi)}{\partial \xi^2} + \left(k_B^2 \xi^2 - 2k_B a\right) R(\xi) = 0, \quad (10a)$$

$$\frac{\partial^2 \Phi(\eta)}{\partial \eta^2} + \left(k_B^2 \eta^2 + 2k_B a\right) \Phi(\eta) = 0, \quad (10b)$$

where $2k_B a$ is the separation constant. The parameter a affects both the scaling and the curvature of parabolic lobes of the Weber beam. The solutions of Eqs. (10a) and (10b) are determined by the same Weber functions, but the corresponding eigenvalues have the opposite signs. If we denote the even and odd solutions of Eq. (10a) as P_e and P_o, the final even and odd transverse stationary solutions of the 2D Helmholtz equation in parabolic coordinates are expressed as

$$W_e(x, z; a) = \frac{1}{\sqrt{2\pi}} |\Gamma_1|^2 P_e\left(\sqrt{2k_B}\xi; a\right) P_e\left(\sqrt{2k_B}\eta; -a\right), \quad (11a)$$

$$W_o(x, z; a) = \frac{2}{\sqrt{2\pi}} |\Gamma_3|^2 P_o\left(\sqrt{2k_B}\xi; a\right) P_o\left(\sqrt{2k_B}\eta; -a\right), \quad (11b)$$

respectively, where $P_{e,o}(t, a) = \sum_{n=0}^{\infty} c_n t^n/n!$, $\Gamma_1 = \Gamma[(1/4) + (1/2)ia]$, $\Gamma_3 = \Gamma[(3/4) + (1/2)ia]$, and the coefficients c_n satisfy the recurrence relation: $c_{n+2} = ac_n - n(n-1)c_{n-2}/4$. For P_e (P_o), the first two c_n coefficients are $c_0 = 1$ and $c_1 = 0$ ($c_0 = 0$ and $c_1 = 1$) [22]. The transverse stationary solution can be written in the form

$$\psi(x, z) = W_e(x, z; a) + iW_o(x, z; a). \quad (12)$$

Appendix B
Mathieu Beam

In the elliptic coordinates $z = h \cosh\xi \cos\eta$ and $x = h \sinh\xi \sin\eta$, with $\xi \in [0, +\infty)$ and $\eta \in [0, 2\pi)$, the solutions of the 2D Helmholtz equation are the Mathieu functions. By utilizing the variable separation, that is, by writing the solution of the 2D Helmholtz equation as $\psi(\xi, \eta) = R(\xi)\Phi(\eta)$, one obtains two ordinary differential equations:

$$\frac{\partial^2 R(\xi)}{\partial \xi^2} - (a - 2q \cosh 2\xi) R(\xi) = 0, \quad (13a)$$

$$\frac{\partial^2 \Phi(\eta)}{\partial \eta^2} + (a - 2q \cos 2\eta) \Phi(\eta) = 0, \quad (13b)$$

where a is the separation constant, $q = k_B^2 h^2/4$ is a parameter related to the ellipticity of the coordinate system, and h is the interfocal separation. The solutions of Eqs. (13a) and (13b) are the radial and angular Mathieu functions. The transverse stationary solution can be written as

$$\psi(x, z) = \mathrm{ce}_m(\eta; q)\mathrm{Je}_m(\xi; q) + i\,\mathrm{se}_m(\eta; q)\mathrm{Jo}_m(\xi; q), \quad (14)$$

where ce_m and se_m are the even and odd angular Mathieu functions of order m, and Je_m and Jo_m represent the corresponding even and odd radial Mathieu functions of the first kind.

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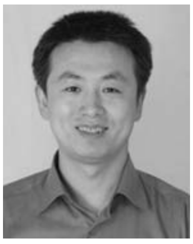

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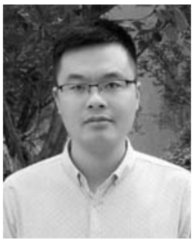

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