Vortices in atomic wave functions

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Abstract. Vortices in atomic wave functions are shown to have observable consequences. It is shown that time-dependent electron wave functions in coordinate space go over to electron emission amplitudes in the limit that time becomes infinite. This relation between wave functions and emission amplitudes is called the imaging theorem. According to this theorem vortices in wave functions at small times when particles interact in a complex way appear as vortices in electron momentum distributions where they produce observable features. Conversely, some observable structures may be interpreted in terms of vortices no matter how they are seen or computed. We verify that previously unexplained features in (e,2e) triply differential cross sections can be interpreted in terms of vortices.

1. Introduction
Structures in triply differential cross sections (TDCS) are often markers for a particular type of motion represented in the quantum theory by time-dependent Schrödinger wave functions [1]. Cusps and some zeros in TDCS have been interpreted in terms of particle-particle interactions and the interference of Schrödinger waves that underlie the momentum distributions of observed electrons. For example, double slit type interferences are predicted and observed for electrons ejected from diatomic molecules. In these instances the interference produces a distribution that vanishes along a nodal surface [1].

Almost all structures can be interpreted in the terminology given above, however, isolated zeros in TDCS have been observed [2] which do not fit into standard dynamical pictures of atomic processes [1]. It has been known since the early days of quantum mechanics that isolated zeros appear in complex single-particle wave functions, and the relation of these zeros to vortices has been explored by earlier workers. The imaging theorem discussed below suggests that isolated zeros in TDCS may be related to vortex structures in atomic wave functions.

2. The imaging theorem
One usually associates electron momentum distributions \( P(k) dk = |A(k)|^2 dk \) with Fourier transforms \( \tilde{\psi}(k) \) of free-particle coordinate-space wave functions \( \psi(k) \) at large times where the bound state components are explicitly subtracted off. As usually happens the free-particle waves have evolved from a bound or otherwise tightly confined wave packet at earlier times. In this case, the wave function incorporates an "explosion factor" equal to \( t^{-3/2} \exp(i m r^2/2\hbar t) \) so that

\[
\psi(r, t) = \left( \frac{m}{\hbar} \right)^{-3/2} \exp \left( i \frac{m r^2}{2\hbar t} \right) f(r, t)
\]

(1)
where \( f \) is a "reduced" wave function. Upon taking the Fourier transform of \( \psi(r, t) \) using the method of stationary phases for large times one sees that

\[
\tilde{\psi}(k, t) = f \left( \frac{\hbar kt}{m}, t \right) \exp \left( -i \frac{k^2 t}{2m} + 3i \frac{\pi}{4} \right) = \left( \frac{\hbar t}{m} \right)^{3/2} \psi \left( \frac{\hbar kt}{m}, t \right) \exp \left( -i \frac{k^2 t}{m} + 3i \frac{\pi}{4} \right)
\]

in the limit of large times. This identity shows that

\[
\lim_{t \to \infty} \left( \frac{m}{\hbar t} \right)^{3/2} \left| \psi(kt, t) \right|^2 d^3r = \left| A(k) \right|^2 d^3k,
\]

which is one version of the imaging theorem. In the remainder of this report atomic units with \( m = \hbar = e = 1 \), where \( m \) is the electron mass, will be used.

The derivation of the imaging theorem applies to a single electron in external time-dependent fields which effectively shut off after some finite time \( t_{\text{off}} \). It is readily extended to processes where more than one electron is ejected in the final state. The theorem also applies to \((e,2e)\) processes where it is understood that the incident electron \( a \) is confined to a wave packet of microscopic dimensions. Only after colliding with an atom and ejecting a second electron \( b \) do we apply the identity of Eq. (3) to both electrons. In this case \( k_a, k_b \) in the amplitudes \( A(k_a, k_b) \) are understood to satisfy energy conservation, so that the \( k_a, k_b \) variable space is actually 5 dimensional.

3. Vortices in TDCS for proton impact

Computations of electron momentum distributions using a modified Lattice-Time-Dependent Schrödinger Equation method (LTDSE) for proton impact on atomic hydrogen found unusual structures in the electron momentum distributions also called the Triply Differential Cross Sections (TDCS) [3,4]. The results for the amplitude \( |A(k_y = 0, k_x, k_z)| \) are shown in in Fig. (1) where isolated holes are present near the continuum capture and direct ionization cusps. The computational method showed that these holes emerged from similar holes in the time-dependent coordinate space wave function. The local probability current \( \text{Im} \nabla \psi \psi \) circulates around these holes and integration of the current around the holes gives a value of \( 2\pi \), indicating that they correspond to isolated first order zeros in \( A(k) \), i.e. to vortices [5]. Because the vortices produce holes in the TDCS, they are observable features. The first indication, to our knowledge, that vortices in atomic wave functions eventually appear as vortices in the TDCS were the "holes" in momentum distributions reported in Ref. [3].

The theory of Ref. [4] also relates these vortices to angular momentum transfer from the relative motion of target and projectile to angular momentum of continuum electrons in the final state. By angular momentum transfer we imply that the vector \( \mathbf{L} \) becomes non-zero. Bound
states with non-zero $L$ are said to be oriented \[6\]. Vortices in continuum functions indicates that continuum states may also be oriented, thus the imaging theorem shows that exact zeros in momentum distributions correspond to oriented electron. Because exact zeros may be seen experimentally, the observation of vortices is also an observation of continuum state orientation. Unusual minima may be present in some observations of TDCS in ion-atom collisions, however, such minima have never been identified with vortices in time-dependent wave functions, thus observations of such features is necessary in order to confirm that vortices are present in electron momentum distributions.

4. Vortices in electron (e,2e) impact

The imaging theorem applies to ionization by electron impact. In the case of ionization by fast electron impact, one can consider that the fast electron $a$ ejects electron $b$ with a velocity that is comparable to the mean velocity in the initial state, which is much less than the velocity of the fast electron. Then electrons initially in s-wave bound states are ejected by predominantly dipole interactions as outgoing p-waves with small admixtures of other partial waves. In the first Born approximation, where no net angular momentum $L$ is transfered from $b$ to $a$, the angular distribution exhibits minima in directions perpendicular to the momentum transfer. Because other partial waves are out of phase with the p-wave amplitude, the TDCS does not vanish exactly at any point.

The situation differs dramatically when angular momentum transfer is included, as in the Coulomb Born approximation. In that case the dipole transitions eject p-wave electrons with $m \neq 0$ so that the states are oriented. Then there is a vortex line, i.e. a line of zeros, along an axis perpendicular to the incident $k_i$ and final $k_b$ momentum of the scattered electron. The coordinate system is chosen so that this axis, parallel to $k_b \times k_i$, is the $y$–axis. The presence of other partial waves shifts the zero away from the $y$–axis to a non-zero value of $k_b$ called the vortex location $k_{b0}$.

In the Coulomb Born calculations of Botero and Macek \[7\] for K-shell ionization of hydrogen by fast electrons, zeros in the electron distribution were found but not recognized as vortices. A partial wave analysis shows that these zeros are due to orientation of the continuum electrons since the ionization amplitude had $p$–wave components with $L_y \neq 0$. Interference with $s$ and $d$–waves shifts the zero away from the $y$–axis where it appears as a zero in the angular distribution of the ejected electron $b$.

Murray and Read \[2\] observed a similar minima in the angular distribution of electrons ejected from He by relatively slow electron impact in a geometry where $k_a = k_b$ and the momentum vectors were symmetrically placed relative to $k_i$. This geometry is shown in Fig. 2, where the angle between the outgoing momentum vectors is $2\Theta$. Calculations by Berackdar and Briggs \[8\]

![Figure 2](image-url)  
**Figure 2.** Symmetric (e,2e) geometry showing incident electron momentum inclined at an angle $\chi$ to an axis perpendicular to the plane of the final scattered and ejected electrons. The angle $2\Theta$ is the angle between the outgoing electrons $a$ and $b$ in the final state.
using highly correlated final state wave functions, and essentially exactly by Colgan et. al [9] showed that the minima was related to an exact zero in the electron momentum distribution. We have repeated the calculations of Ref. [8] as the solid red curve in Fig. 3 and find a similar minima. Also shown are some experimental data points from Ref. [2] which show a minima in the vicinity of the theoretical minima.

To analyze the minima for vortex structure we transform to a coordinate system with $\mathbf{k}_i$ and $\mathbf{b}_a$ fixed in plane and examine the direct ionization amplitude for vortex structure in the neighborhood of the computed minima. A contour plot of the TDCS for values of $\mathbf{k}_b$ near the minima seen in Fig. 3 is shown in Fig. 4.

**Figure 3.** TDCS vs $\Theta$ for 67.4 eV electrons incident on helium at $\chi = 22.5^\circ$ ejecting 20 eV electrons. The solid (red) curve is the calculated cross section and the squares are experimental data from Ref. [2]. The dashed curve is a spline fit to the data.

**Figure 4.** Contour plot of the direct ionization amplitude in a plane parallel to the x-z plane. An arrow (red) points to the computed vortex position in a slice of the TDCS. The contour plot shows a vortex zero and the small black arrows point in the direction of the velocity current. An expanded version of the logarithmic contour plot is shown on the right.

Also shown on the contour plot in Fig. 4 are small black arrows pointing in the direction of the velocity current. It is apparent that there is a vortex near the position of the TDCS minimum, corresponding to probability circulation in a counterclockwise direction. The direction is
consistent with the transfer of angular momentum from the scattered to the ejected electron. Integration of the current around vortex gives a value of $2\pi$ consistent with a first order zero.

This analysis finds a vortex in the direct amplitude for fixed $k_i$ and $k_a$. Experiment does not observe this amplitude rather an incoherent mixture of singlet and triplet amplitudes are observed. An exact zero is unlikely for incoherent mixtures, however the zero was actually observed in the symmetric geometry where only the triplet amplitude contributes. The observed state is therefore a pure state and could exhibit an exact zero. Further analysis, not given here, shows that there is indeed a vortex in the triplet state momentum distribution, and that this zero gives rise to the cross section minimum seen in Fig. 3. It is apparent the role of vortices in atomic dynamics must be understood to form a complete picture of (e,2e) TDCS.

5. acknowledgements
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