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IT-16-P-3287 Electron vortex beam diffraction via multislice solutions of the Pauli equation

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Electron magnetic circular dichroism (EMCD) has gained plenty of attention as a possible route to high resolution measurements of, for example, magnetic properties of matter via electron microscopy. However, certain issues, such as low signal-to-noise ratio, have been problematic to the applicability. In recent years, electron vortex beams\cite{Uchida2010,Verbeeck2010}, i.e. electron beams which carry orbital angular momentum and are described by wavefunctions with a phase winding, have attracted interest as potential alternative way of measuring EMCD signals. Recent work has shown that vortex beams can be produced with a large orbital moment in the order of l = 100 [6, 7]. Huge orbital moments might introduce new effects from magnetic interactions such as spin-orbit coupling.

The multislice method[2] provides a powerful computational tool for theoretical studies of electron microscopy. However, the method traditionally relies on the conventional Schrödinger equation which neglects relativistic effects such as spin-orbit coupling. Traditional multislice methods could therefore be inadequate in studying the diffraction of vortex beams with large orbital angular momentum. Relativistic multislice simulations have previously been done with a negligible difference to non-relativistic simulations[4], but vortex beams have not been considered in such work.

In this work, we derive a new multislice approach based on the Pauli equation, Eq. 1, where $q = -e$ is the electron charge, $m = \gamma m_0$ is the relativistically corrected mass, $\boldsymbol{p} = -\mathrm{i}\,\nabla$ is the momentum operator, $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ is the magnetic flux density while $\boldsymbol{A}$ is the vector potential and $\boldsymbol{\sigma} = (\sigma x\ ,\ \sigma y\ ,\ \sigma z\ )$ contains the Pauli matrices. $\psi_{\pm}(\mathbf{r})$ represent wavefunctions for spin up (+) and down (-) electrons. A two component fast electron equation of the form given in Eq. 2 is found. The solutions of this equation are studied computationally via a real-space multislice[1] approach. Results are presented for large orbital angular momentum vortex beams passing through model systems, such as bcc Fe, and are compared to results from the traditional Schrödinger equation based calculations.

$$\left\{\frac{1}{2m}\left[\left[\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right]^2+\frac{e\hbar}{c}\boldsymbol{\sigma}\cdot\boldsymbol{B}(\boldsymbol{r})\right]-eV(\boldsymbol{r})\right\}\begin{pmatrix}\psi_+(\boldsymbol{r})\\ \psi_-(\boldsymbol{r})\end{pmatrix}=E\begin{pmatrix}\psi_+(\boldsymbol{r})\\ \psi_-(\boldsymbol{r})\end{pmatrix}, \tag{1}$$

$$\frac{\partial}{\partial z}\psi_\pm(\boldsymbol{r})=f(\boldsymbol{r})\left\{\frac{\hbar^2}{2m}\nabla_{xy}^2+\frac{ie\hbar}{mc}\boldsymbol{A}_{xy}\cdot\nabla_{xy}-\frac{4\pi e\hbar A_z}{\lambda c}-\frac{e^2A^2}{2mc^2}\mp\frac{e\hbar}{2mc}B_z+eV\right\}\psi_\pm(\boldsymbol{r})-b_\pm(\boldsymbol{r})\psi_\mp(\boldsymbol{r}), \tag{2}$$

$$b_\pm(\boldsymbol{r})=\frac{e\hbar}{2mc}f(\boldsymbol{r})(B_x\mp iB_y),\quad f(\boldsymbol{r})=\frac{i}{2\hbar}\left(\frac{\pi\hbar}{m\lambda}+\frac{e}{c}A_z(\boldsymbol{r})\right)^{-1} \tag{3}$$

Fig. 1: Equations referred to in the text.

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Fig. 2: References referred to in the text.