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IT-16-P-2085 Calculations of elastic and inelastic scattering processes of relativistic electrons in oriented crystals

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Many modern electron microscopes operate at acceleration voltages of several hundred kV. The accelerated electrons thus reach velocities approaching the speed of light. Therefore the scattering processes have to be treated relativistically. We focus on inelastic scattering in crystals.

In a non-relativistic treatment the movement of the electrons inside the crystal is described using Bloch waves. Before the electrons enter into the crystal they are described by simple plane waves. This view is used in non-relativistic calculations in many cases. The periodic potential of a crystal provides Bloch waves as solutions of the Schrödinger equation. To ensure the boundary conditions at the interface of crystal and vacuum, the transmitted electrons are described using a superposition of plane waves. To obtain a reliable result for the scattering process, many excited Bloch waves have to be considered. The scattering process is mathematically described using matrix elements [1]. The computational complexity depends strongly on the number of Bloch waves considered. The general solution for the wave function of the incident electrons in the crystal is a superposition of many Bloch waves, which are excited at the same time. The excitation of every single Bloch wave is weighted with a excitation coefficient. The number of excited Bloch waves which have to be taken into account depends on the geometry of the crystal.

In this work we focus on an extension of this treatment for relativistic electrons. In contrast to the non-relativistic case the wave functions of the fast incident electrons and the atomic electrons have to be calculated using the Dirac equation. Therefore the incident electrons are described by relativistic four-component Bloch waves (Fig. 1). In our approach we use the relativistic propagator theory where the atomic electrons are seen under influence of a scalar and a vector potential generated by the fast incident electrons via their charge and current (Fig. 2). Furthermore retardation is considered in this relativistic treatment. This approach has previously been used for relativistic plane waves [2]. To consider crystalline materials the incident electrons are described by the relativistic Bloch waves. Consequently the matrix elements contain different sums over reciprocal space and the different single relativistic Bloch waves. The fourier coefficients of these Bloch waves depend on the crystal structure and can be calculated analoguously to the non-relatvistic treatment.

[1] A. Weickenmeier and H. Kohl, Phil. Mag. B60 (1989) 467.

[2] R. Knippelmeyer et al.,Ultramicroscopy 68 (1997) 25-41.

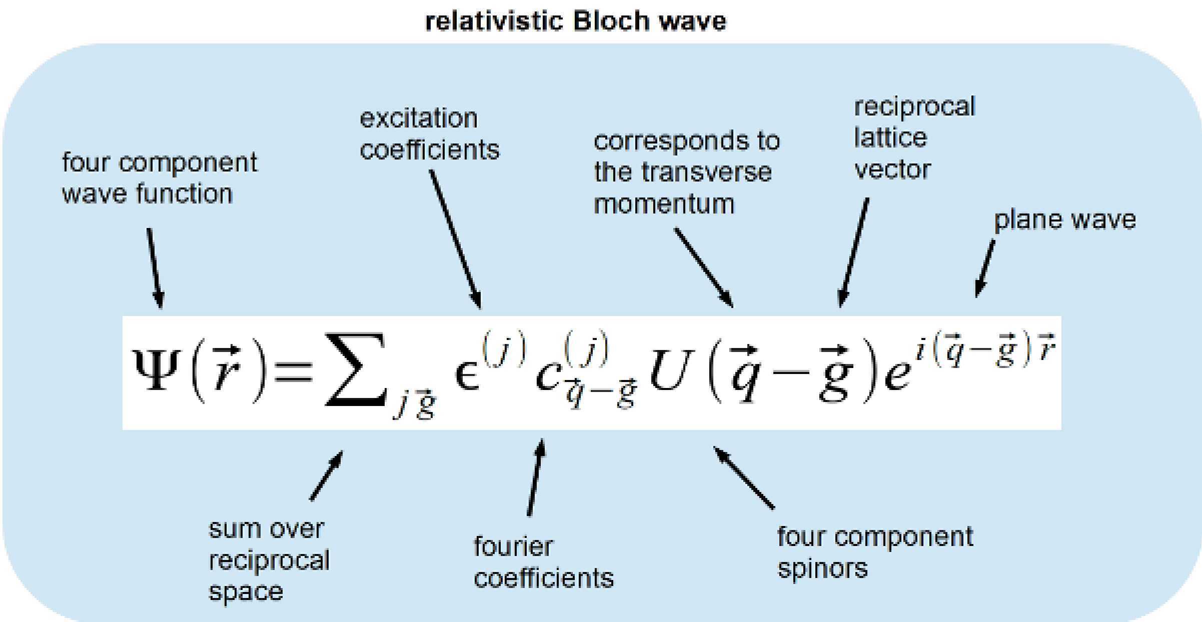

Fig. 1: Relativtistic Bloch wave

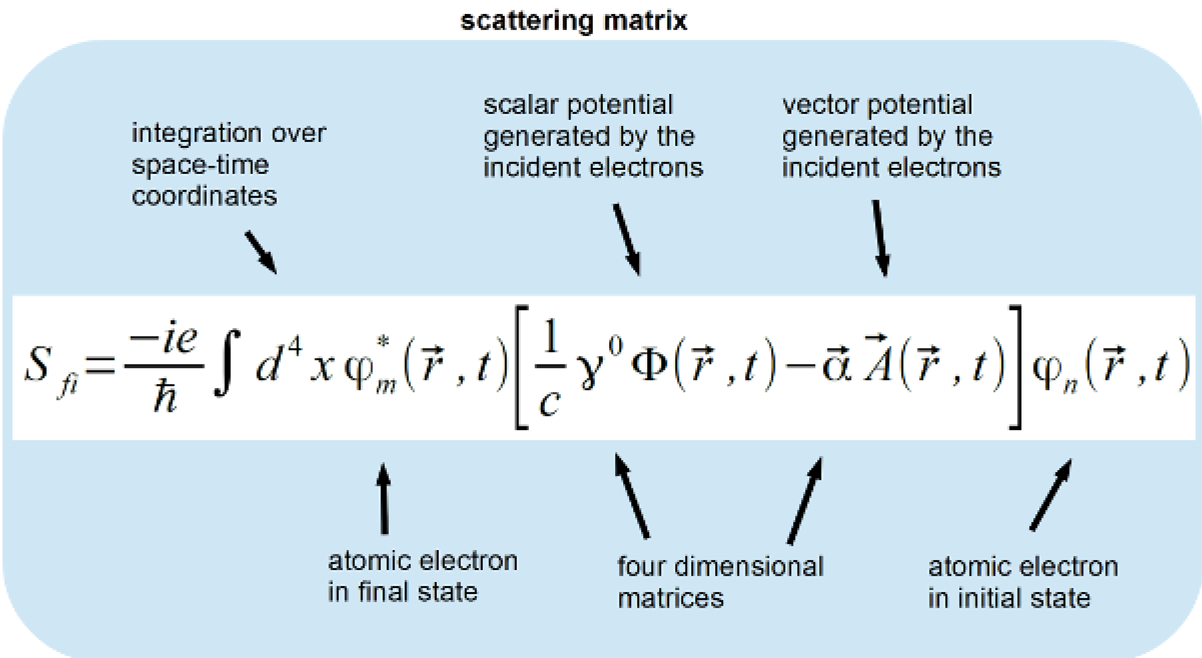

Fig. 2: Scattering Matrix