Spectroscopic TEM/STEM, EELS, EFTEM

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The influence of the self-interaction correction on the calculation of differential cross-sections

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Electron energy loss spectroscopy (EELS) allows to determine the chemical composition of a specimen quantitatively, if the ionization cross section is known. These are calculated via transition matrix elements between atomic bound and free electron wave functions. Using the approximation of a spherical symmetric atomic potential these wavefunctions can be separated into a radial and an angular part [1]. The latter can be determined analytically, whereas the radial part is challenging. A numerical calculation of the radial electron wave function has already been performed by Frigge [2] using a program to solve the Kohn-Sham equation within the linear density approximation to obtain the radial wave functions. Due to the exponential behavior of the central potential within the standard LDA approach one can describe the asymptotic behavior of the final free electrons wave functions by a combination of Bessel and Neumann functions.

To avoid this unphysical exponential decay of the potential, we have used a self-interaction correction in the Kohn-Sham potential [3]. This potential shows the physically correct decay proportional to -1/r in the outer region. In order to normalize the free electron one now has to fit the function to regular and irregular Coulomb wave functions, which are the correct radial functions for a free charged particle in a Coulomb potential. This procedure leads to a non-negligible phase shift of the free electron wave function.

The modification of the atomic potential due to the self interaction correction is even more significant in the inner atomic region. The correction results in a potential being by far more attractive than the standard one. This is particularly important for the free electrons with an orbital angular momentum $l>0$. Here the difference of the Kohn-Sham potential results in a shift of the centrifugal barrier around the center of the atom [Fig. 1]. This leads to a drastic shift and a change in amplitude of the free wave function [Fig. 2]. Due to the strong overlap to bound electron wave functions in this region this also has an effect on the differential cross section.

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3 J.P. Perdew and A. Zunger, Phys. Rev. B 23 (1981), 5048
4. We thank Prof. Dr. Peter Krüger (Institut für Festkörpertheorie, Universität Münster) for valuable discussions and for providing the program to calculate the self interaction corrected Kohn-Sham potentials.

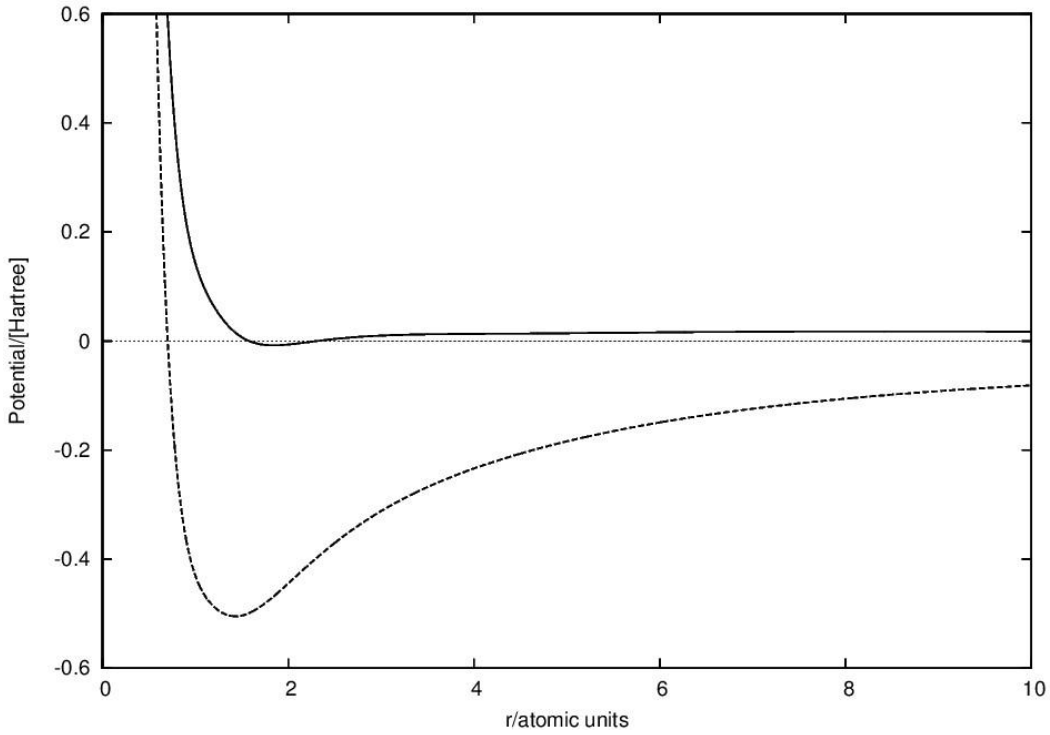

Figure 1. Effective potential calculated within standard LDA (solid line) and self interaction correction (dashed line)

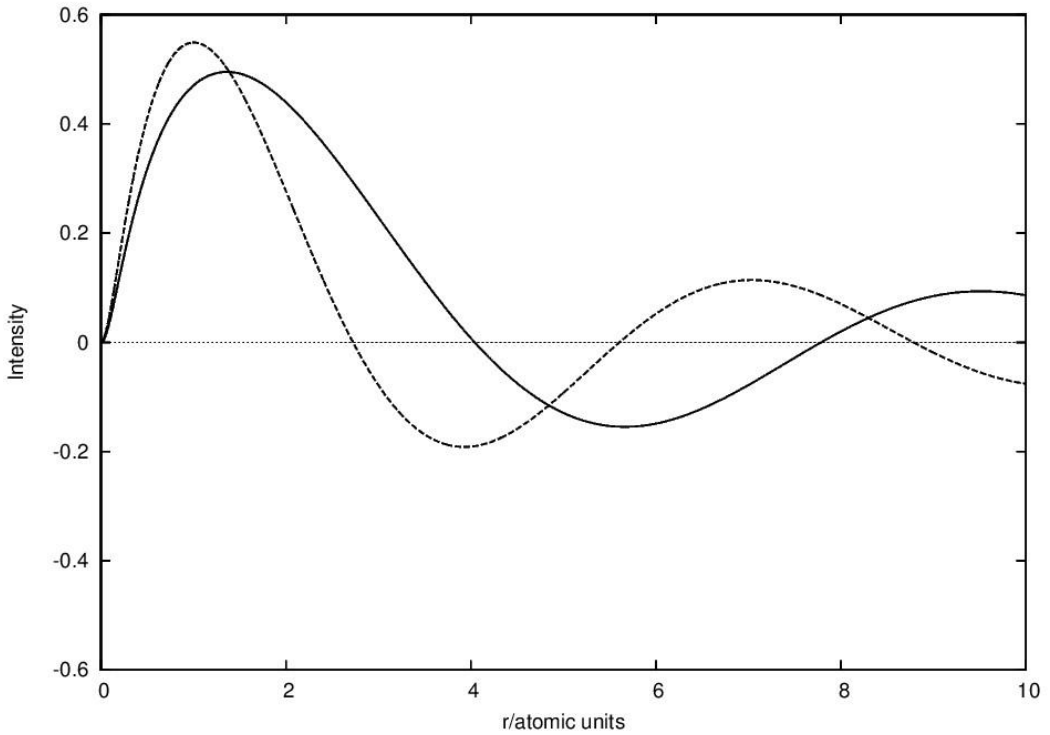

Figure 2. Free electron wave function (l=2,E=10eV) for a standard LDA (solid line) and a self interaction corrected (dashed line) potential