

Theory of spin-polarized optical potential

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We develop an approximation for the non-local spin-polarized optical potential theory for atoms in solids at intermediate and high energy. The present approximation for the optical potential builds on the GW-expression. We separate the RPA polarization propagator into a core electron and a valence electron part, and can then achieve a corresponding separation of the optical potential. For the valence electron optical potential we use a local density approximation because the charge density changes fairly slowly, whereas we use a non-local optical potential for the core electron part. Both of them depend on the spin-polarization. We apply this method to electron-Fe elastic scattering in solid, and discuss the results.

Keywords: spin-polarization; GW approximation; optical potential.

1. Introduction

In spin-polarized low-energy electron diffraction (SPLEED) (Unkuris *et al.*, 1984; Weller & Alvarado, 1988), spin-polarized photoelectron diffraction (SPPD) (Sincović & Fadley, 1985), X-ray magnetic circular dichroism (XMCD) (Schütz *et al.*, 1987), and spin-polarized EXAFS (SPEXAFS) (Schütz *et al.*, 1989) spin-dependent electron-atom elastic scattering plays an essential role.

Ankudinov and Rehr (1995, 1996) calculated the SPEXAFS and XMCD by use of the spin-polarized local density potential which is based on the von Barth-Hedin approximation (1972), and obtained much improved results compared with one-electron theory. However, we have still a question on the reliability of the local density approximation for the elastic scatterings from spin polarized systems. In our previous work, the core polarization contribution to the optical potential plays an important role (Fujikawa *et al.*, 1998, 2000)

In this work we employ the spin-polarized non-local optical potential for core parts and the spin-polarized local potential (von Barth-Hedin potential) for valence parts, and applied this theory to elastic electron-atom scatterings from a spin-polarized atom in solids.

2. Theory

In Hedin and Lundqvist (1969), p. 129, the following expression for the self-energy (optical potential) is given,

$$\begin{aligned} \Sigma_0 &= G^c W + G^v W^v P^c W^v + G^v W^v + \dots \\ &\cong V_{ex}^c + V_{pol}^c + \Sigma^v. \end{aligned} \quad (1)$$

Here $G^v W^v$ is the self-energy from the valence electrons Σ^v , $G^c W$ is the core exchange V_{ex}^c and $G^v W^v P^c W^v$ the screened polarization potential from the ion cores V_{pol}^c . The total crystal potential V^{cryst} is given by the Hartree potential plus this self-energy (Hedin,

1965a, 1965b; Hedin & Lundqvist, 1969). All these terms are spin-dependent for spin polarized systems, that is, the optical potentials for different spin are also different. The third term Σ^v can be well approximated by spin-polarized local potential (von-Barth & Hedin, 1971).

The core-polarization term $G^v W^v P^c W^v$ can be approximated by $G^v v P^c v$, where v is the bare Coulomb potential (Fujikawa *et al.*, 1993).

The spin-dependent full RPA polarization propagator is (Hedin & Lundqvist, 1969)

$$\begin{aligned} P(x, x'; \omega) &= - \sum_k^{unocc} \sum_l^{occ} \frac{2(\varepsilon_k - \varepsilon_l)}{(\varepsilon_k - \varepsilon_l)^2 - \omega^2} f_{kl}(x) f_{kl}^*(x'), \\ f_{kl}(x) &= \psi_k(x) \psi_l^*(x). \end{aligned} \quad (2)$$

Here $x = (\mathbf{r}, \xi)$ includes both space and spin variables. The sum over k runs over unoccupied electron states, while l runs over the occupied core and valence electron states. By splitting the summation over l into core and valence contributions, P can be written as a sum of core and valence parts,

$$P = P^c + P^v. \quad (3)$$

Similarly we can split the summation over k in the expression for the one-electron Green's function

$$G(x, x'; \omega) = \sum_k^{occ+unocc} \frac{\psi_k(x) \psi_k^*(x')}{\omega - \varepsilon_k} \quad (4)$$

to obtain

$$G = G^c + G^v. \quad (5)$$

The symbol $G^v v P^c v$ stands for a convolution in energy space (Fujikawa & Hedin, 1989), which can be done analytically, giving

$$\begin{aligned} [G^v v P^c v](x, x'; \omega) &= \sum_k^{unocc} \sum_l^{core} \sum_{k'}^{valence} \frac{v_{kl}(\mathbf{r}) \psi_{k'}(x) \psi_{k'}^*(x') v_{kl}^*(\mathbf{r}')}{\omega - \omega_{kl} - \varepsilon_{k'}}, \end{aligned} \quad (6)$$

where $\omega_{kl} = \varepsilon_k - \varepsilon_l$, and $v_{kl}(\mathbf{r}) = \int v(\mathbf{r} - \mathbf{r}') \psi_k^*(x') \psi_l(x') dx'$. The more tightly bound the core level l is, the smaller its contribution to $v_{kl}(x)$ due to the smaller overlap with the unoccupied function k . Thus the outermost core level will give the dominant contributions.

We replace ω_{kl} by a constant Δ , the average excitation energy, and we can then use closure and avoid the summation over the unoccupied states. The screened polarization potential can be written by use of this approximation and the different orbital for different spins (DODS) approximation,

$$\begin{aligned} V_{pol}^{c, \sigma}(\mathbf{r}, \mathbf{r}'; \omega) &= [G^v v P^c v]^\sigma(\mathbf{r}, \mathbf{r}'; \omega) \\ &= A(\mathbf{r}, \mathbf{r}') G^{v, \sigma}(\mathbf{r}, \mathbf{r}'; \omega - \Delta). (\sigma = \text{up or down}). \end{aligned} \quad (7)$$

This optical potential is non-local, spin-dependent and can be solved self-consistently. We define a function $A(\mathbf{r}, \mathbf{r}')$,

$$\begin{aligned} A(\mathbf{r}, \mathbf{r}') &= \sum_k^{unocc} \sum_l^{core} v_{kl}(\mathbf{r}) v_{kl}^*(\mathbf{r}') \\ &= \int v(\mathbf{r} - \mathbf{r}_1) v(\mathbf{r}' - \mathbf{r}_2) \\ &\quad \times [\delta(x_1 - x_2) - \rho(x_1, x_2)] \rho^c(x_2, x_1) dx_1 dx_2, \end{aligned} \quad (8)$$

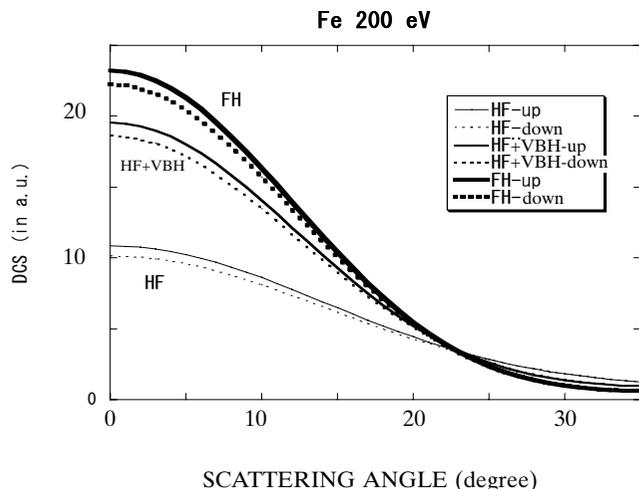


Figure 1
Differential cross section (DCS) in a.u. as a function of scattering angle for electron elastic scattering from Fe atom in solids at 200 eV. Solid (dotted) line shows spin-up (-down) results. Three potentials are used for comparison; HF (Hartree-Fock), HF+VBH (von Barth-Hedin) and FH (present method).

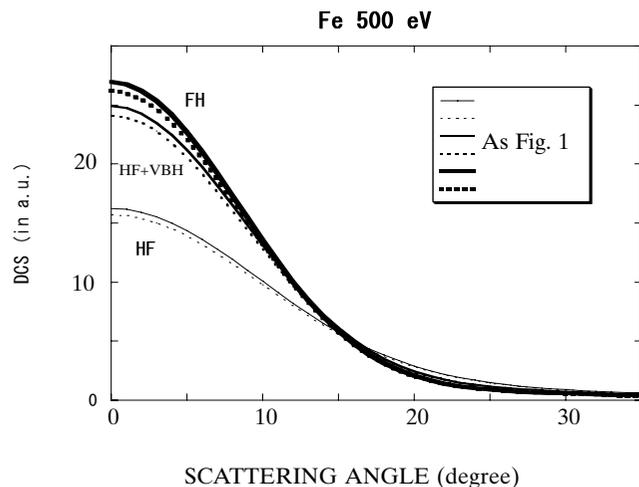


Figure 2
The same type of results as in Fig. 1, but for 500 eV.

where ρ and ρ^c are the one-electron density matrices for all electrons and for core electrons respectively. As far as we consider the spin-polarized systems within DODS approximation, the polarization function A does not depend on spin-polarization. On the other hand the Green's function G^v depends on the spin-polarization through the spin-polarized potentials $V_{ex}^c + V_{pol}^c + \Sigma^v$.

3. Results and discussion

Figure 1 shows the differential cross section (DCS) as a function of scattering angle for elastic electron scattering from a spin-polarized Fe atom in solids using different potentials, Hartree-Fock (HF), HF for core electrons and von Barth-Hedin for valence electrons (HF+VBH) and the present (FH) potentials. Here, we use an electron configuration of the Fe atom in ferromagnetic iron metal proposed by Mizumaki (1996), $3d^{\uparrow 4.946} 3d^{\downarrow 1.682} 4s^{\uparrow 0.690} 4s^{\downarrow 0.644}$. The kinetic energy of the incident electrons is assumed to be 200 eV.

In this figure we show the spin polarization of the incident electrons by "up" and "down". The calculated results show that the DCS for the FH potential is the largest, and is quite different from the HF+VBH result in small-angle scattering ($\theta \leq 35^\circ$). This result shows that the non-local core polarization potential has large influence on the elastic scatterings in the small-angle region. We also find that these optical potentials give quite different DCS from the HF potential. These findings are similar to those for the spin-independent cases (Fujikawa *et al.*, 2000). The spin splitting in the DCS is not so sensitive to the potential, however the optical potential give a larger splitting than the HF potential.

Figure 2 shows the same type of results as in Fig. 1, but for 500 eV. With increasing energy the contribution from the optical potentials tend to zero, and we can see that the difference between the FH and the HF, and the difference between the HF+VBH and the FH potentials become smaller when we go from 200 to 500 eV. We still find a larger spin splitting with the optical potential than with the HF potential.

In EXAFS back scattering amplitudes play an important role. So far several calculations of SPEXAFS have been done based on the spin-polarized local density approximations, for example Ankudinov *et al.* used a crude approximation for the von Barth-Hedin potential for all electrons (Ankudinov, 1996; Ankudinov & Rehr, 1995). The back scattering amplitudes in the plane wave approximation are written as

$$f(\pi, k) = |f(\pi, k)| \exp\{i\psi(k)\}. \quad (9)$$

Figure 3 shows the back scattering amplitude $|f(\pi, k)|$ for the spin-polarized Fe atom in solids. In general the back scattering is mainly affected by the potential from inner electrons, and the core polarization potential has a large influence on the backscattering amplitudes. In the low energy region the difference of $|f(\pi; k)|$ for different spins is larger than that in high energy region as expected. The difference in $|f(\pi; k)|$ for different spins decays slightly more rapidly with k for the FH and HF+VBH potentials in comparison with the result for the HF potential.

Figure 4 shows the phase of the back scattering amplitude $\psi(k)$ for the spin-polarized Fe atom in solids. This figure shows that the spin-polarization effect is much larger in the phase $\psi(k)$ than in the backscattering intensity $|f(\pi; k)|$. Similar effect is observed for

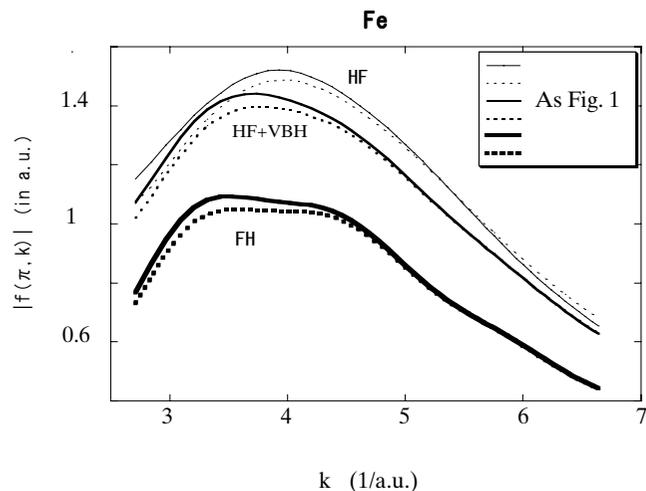


Figure 3
The back scattering amplitude $|f(\pi, k)|$ as function of the photoelectron wave vector k for a spin-polarized Fe atom in solids. Three different potentials, HF, HF+VBH and FH, are used.

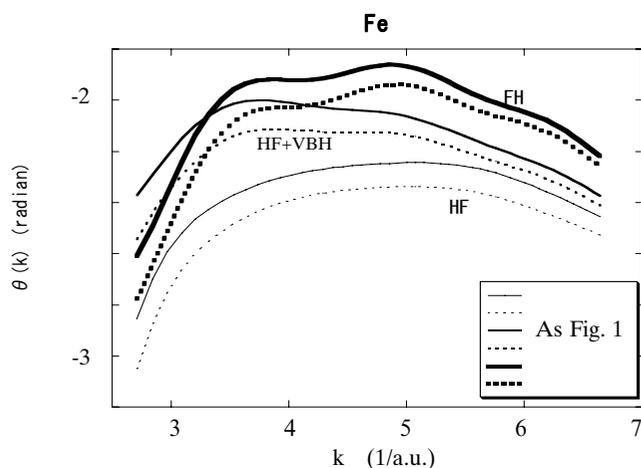


Figure 4

The phase of the back scattering amplitude $\psi(k)$ as function of photoelectron wave vector k for a spin-polarized Fe atom in solids. Three different potentials, HF, HF+VBH and FH, are used.

the back scattering from non-magnetic systems; the potential has a larger influence on the phase than on the back scattering intensity (Fujikawa *et al.*, 2000).

4. Conclusion

We present here the spin-polarized non-local optical potential theory and some calculated results. In the small-angle scattering the difference of the scattering intensity for different spin is larger for

the optical potentials than for the HF potential. In the back scattering that is also the case, and the spin effect is much larger in the phase $\psi(k)$ than in the intensity $|f(\pi; k)|$. These results are important to analyze SPEXAFS on the basis of Fourier transform technique. Unfortunately the computation time is quite large in comparison with HF+VBH potential calculation (about 10 times larger).

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