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Decay of electronic excitations in bulk metals and at surfaces

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Abstract

We present a brief survey of the contemporary state of theoretical study of quasiparticles (excited electrons and holes) dynamics in bulk metals and at metal surfaces. Quasiparticle decay mechanisms are discussed in terms of electron–electron (e–e) and electron–phonon (e–ph) interactions. The e–ph decay channel is shown to be important for all materials considered. It is especially important for systems with the thickness of one monolayer. In the e–e decay channel the quasiparticle decay can be realized via one-electron transfer processes, via creation of electron–hole pairs, and via plasmon excitation. In ferromagnetic systems the electron (hole) decay via the Stoner pair excitation or/and magnon excitation is made possible.

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1. Introduction

The last decade enormous progress in the study of electron and hole dynamics at clean metal surfaces has been achieved both theoretically and experimentally [1–17]. Interest in this study is motivated by an essential role which excited electrons and holes play in many processes, e.g. in the energy and charge transfer or in the spin transport at surfaces. The key quantity for these processes is the lifetime of the excited electron (hole) which sets the duration of the excitation and in combination with the velocity determines the mean free path of the excited particle. The decay (lifetime broadening or linewidth of the corresponding quantum state) of the excited electron can mainly occur via electron–electron (e–e), electron–phonon (e–ph) or/and electron–defect (e–def) scattering. The latter type of scattering can be, in principle, avoided in scanning tunneling spectroscopy (STS) measurements [7,14,16] and strongly reduced (minimized) in photoemission spectroscopy (PES) study [8,13]. Therefore we present here the calculation results and give analysis of decay mechanisms of excited electrons and holes for different systems in terms of e–e and e–ph interactions only. These results (published and new) are used here to demonstrate the excited particles decay mechanisms. We also give a brief sketch of the theory which is necessary for understanding the decay mechanisms.

In the e–e channel the decay can be realized via one-electron energy conserving transfer processes (one-electron scattering) or inelastic scattering. For instance, one-electron scattering dominates decay of electrons in resonance image-potential (IS) and surface states (SS) [18], as well as in resonance quantum-well states (QWS) [19]. This scattering also plays important role in the decay of excited electrons at single alkali adatoms on noble metals surfaces [20,21].

Inelastic e–e scattering being related with energy relaxation is normally accompanied by the creation of an electron–hole (e–h) pair. This is the most common

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mechanism of the decay of excited electrons (holes) in bulk metal electron states [22–26], in surface [7], image potential [1,4,27–29], and quantum-well [30] states located inside the energy gap of the projected bulk band structure. This mechanism also works well for excited electrons in ISs in an external electric field [31,32]. Another mechanism related with energy relaxation is the quasiparticle decay accompanied by excitation of plasmon. This occurs when plasmon (collective) excitations are in the range of energies accessible for the electron (hole) decay. This is the case for image states on silver surfaces [33].

Additional mechanisms of quasiparticle decay related with energy relaxation arise in ferromagnetic metals. In these materials the decay of an electron with certain direction of spin (up or down) can be accompanied by the creation of Stoner pair (an electron with one direction of spin and a hole with opposite spin direction) or/and magnon excitation. These mechanisms (perhaps together with electron–magnon scattering mechanism) may be responsible for the spin-dependent electron (hole) dynamics in ferromagnetics [34–38].

In the e–ph channel energy relaxation is realized via e–ph scattering. This mechanism is the only one which describes the temperature dependence of the electron (hole) decay [39,40]. The e–ph scattering mechanism was carefully examined both theoretically and experimentally for bulk electron states [42,43], SSs on metal surfaces [5,44–53], and QWSs as well [40,41,54–56].

The paper is organized as follows. In Section 2, we briefly describe GW approximation commonly used to study electron (hole) dynamics in bulk materials and at surfaces. We also give brief outline of the theory used for the description of e–ph scattering. As to theoretical methods employed for the study of one-electron scattering at metal surfaces and inelastic e–e scattering in ferromagnetic materials we refer the reader to current literature. In this section we use atomic units, i.e., $\hbar = e^2 = m = 1$. In Section 3, we discuss excited electrons (holes) decay mechanisms in different systems including clean surfaces, adlayers on metals, free standing monolayers, and bulk metals. In Section 4, the results of this work are summarized.

2. Theory

2.1. Electron–electron interaction

Within many-body theory the inelastic e–e scattering contribution to the decay rate Γ, i.e. inverse lifetime, of an electron with momentum $(\mathbf{k}, i)$ and energy $\epsilon_{\mathbf{k},\mathrm{i}} > E_\mathrm{F}$ is obtained in the "on energy-shell" approximation as the projection of the imaginary part of the self-energy operator onto the electron state $\psi_{\mathbf{k},\mathrm{i}}(\vec{r})$ (see, for instance Refs. [6,57])

$$\Gamma_{\mathrm{e\text{-}e}}(\epsilon_{\mathbf{k},\mathrm{i}}) = \tau^{-1}_{\mathrm{e\text{-}e}}(\epsilon_{\mathbf{k},\mathrm{i}}) = -2\int \mathrm{d}\vec{r}\int \mathrm{d}\vec{r}'\psi^*_{\mathbf{k},\mathrm{i}}(\vec{r})\,\mathrm{Im}\,\Sigma(\vec{r},\vec{r}';\epsilon_{\mathbf{k},\mathrm{i}})\psi_{\mathbf{k},\mathrm{i}}(\vec{r}'), \quad (1)$$

where $\psi_{\mathbf{k},\mathrm{i}}(\vec{r})$ and $\epsilon_{\mathbf{k},\mathrm{i}}$ are the eigenfunctions and eigenvalues of the one-electron Hamiltonian. We consider here paramagnetic systems and thus omit spin index. The imaginary part of the self-energy is evaluated in the commonly used GW approximation in terms of the screened electron–electron interaction $W(\vec{r},\vec{r}';w_{i,\mathrm{f}})$ and the allowed final states $\psi_{\mathbf{k},\mathrm{f}}(\vec{r})$ for the decay process

$$\mathrm{Im}\,\Sigma(\vec{r},\vec{r}',\epsilon_{\mathbf{k},\mathrm{i}}) = \sum_{\epsilon_{\mathbf{k},\mathrm{f}}}^{\epsilon_{\mathbf{k},\mathrm{i}}\geqslant\epsilon_{\mathbf{k},\mathrm{f}}\geqslant E_F} \psi^*_{\mathbf{k},\mathrm{f}}(\vec{r}')\,\mathrm{Im}\,W(\vec{r},\vec{r}';w_{i,f})\psi_{\mathbf{k},\mathrm{f}}(\vec{r}). \quad (2)$$

Here $w_{i,f} = \epsilon_{\mathbf{k},\mathrm{i}} - \epsilon_{\mathbf{k},\mathrm{f}}$ and the summation is performed over the final-state energies which are between the initial state and the Fermi energy, E_F. For the holes these energies are below the Fermi energy. The final expression for the inverse lifetime then becomes

$$\tau^{-1}_{\mathrm{e\text{-}e}}(\epsilon_{\mathbf{k},\mathrm{i}}) = -2\sum_{\epsilon_{\mathbf{k},\mathrm{f}}}\int \mathrm{d}\vec{r}\int \mathrm{d}\vec{r}'\psi^*_{\mathbf{k},\mathrm{i}}(\vec{r})\psi^*_{\mathbf{k},\mathrm{f}}(\vec{r}')\,\mathrm{Im}\,W(\vec{r},\vec{r}';w_{i,f}) \times \psi_{\mathbf{k},\mathrm{i}}(\vec{r}')\psi_{\mathbf{k},\mathrm{f}}(\vec{r}). \quad (3)$$

The screened interaction W is given by

$$W(\vec{r},\vec{r}';w) = v(\vec{r}-\vec{r}') + \int \mathrm{d}\vec{r}_1\int \mathrm{d}\vec{r}_2 v(\vec{r}-\vec{r}_1) \times \chi(\vec{r}_1,\vec{r}_2;w)v(\vec{r}_2-\vec{r}'), \quad (4)$$

where $v(\vec{r}-\vec{r}')$ is the bare Coulomb interaction, $\chi(\vec{r},\vec{r}';w)$ is the linear density–density response function.

In the case of ferromagnetic materials it is important to go beyond the GW approximation considering also multiple e–h scattering effects within T-matrix formalism. This more general method, GW + T, represents a generalization of the GW approximation by including the higher-order self-energy terms that allow one to calculate the quasiparticle decay in ferromagnetic systems on the same footing as in paramagnetics. We do not give the outline of this theory here and refer the reader to the description of the theory and its different applications in Refs. [38,58–60]. For the description of the one-electron scattering contribution to the quasiparticle decay in terms of wave packet propagation we refer the reader to Refs. [21,61].

2.2. Electron–phonon interaction

The phonon–induced lifetime broadening $\Gamma_{\mathrm{e\text{-}ph}}(\epsilon_{\mathbf{k},\mathrm{i}})$ of an electron state with momentum $(\mathbf{k}, i)$ and energy $\epsilon_{\mathbf{k},\mathrm{i}}$ is related to the Eliashberg $\alpha^2F_{\mathbf{k},i}(\omega)$ spectral function through the integral over all the scattering events that conserve energy and momentum [39]

$$\Gamma_{\mathrm{e\text{-}ph}}(\epsilon_{\mathbf{k},\mathrm{i}}) = 2\pi\int_0^{\omega_m}\alpha^2F_{\mathbf{k},\mathrm{i}}(\omega)[1 - f(\epsilon_{\mathbf{k},\mathrm{i}}-\omega) + f(\epsilon_{\mathbf{k},\mathrm{i}}+\omega) + 2n(\omega)]\mathrm{d}\omega \quad (5)$$

Here, f and n are the Fermi and Bose distribution functions and ω_m is the maximum phonon frequency. The spectral function is given by

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