Determination of the spin-polarized surface density of states in strongly correlated metals by field emission: Theory

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It is shown that the combination of spin-polarization and field-emission energy distribution measurements on ferromagnetic transition metals will provide direct information about the one-dimensional surface density of states in a direction normal to the metal surface for a given spin.

We have recently shown[1] (in a paper hereafter referred to as I) that field-emission energy distribution (FEED) measurements of a metal surface yield direct information about the one-dimensional surface density of states in the direction normal to the surface. This result was based on the independent-particle model for the metal electrons. Recent tunneling[2] and photoemission[3-5] experiments on ferromagnetic transition metals have measured the polarization of the emitted electrons. The observed polarization provided evidence that the independent-particle model may not be valid for these materials presumably because of strong electron-electron corrections.[6-8] The only field-emission measurements performed on these metals were total current measurements.[9] They did not show any anomalous polarization of the emitted electrons, however the validity of these experiments is not generally accepted, particularly since their subsequent field-emission measurements on W indicated a polarization of about 10%.[10] This same group has also reported field-emission measurements on Ge in high magnetic fields.[11] Müller *et al.*[12] have found a polarization of about 89% in the current field emitted from EuS-coated W tips. Politzer and Cutler[13] have carried out an independent electron calculation for the field emission from Ni. Some of their conclusions are consistent with the theory of I; for example, the factor in I denoted by N_m can vanish by reason of symmetry for a d-band electron traveling along a symmetry axis so that the theory in I takes account of the sensitivity of the tunneling probability to the metal wave-function symmetry. Similarly, the smaller probability of d electron tunneling compared to s electron tunneling[14] is reflected in the factor N_m. In this paper we extend our previous work to the case of the ferromagnetic transition metals by discarding the assumption that the independent-particle model is valid for the metal.

Appelbaum and Brinkman[15] (AB) have derived a general expression for the tunneling current between two normal metals which can be adapted to the case of field emission:

$$j_\sigma(\omega)=\frac{2}{\pi\hbar}\left(\frac{\hbar^2}{2m}\right)^2\int\int d^3r\,d^3r'\left[\operatorname{Im}G^{(R)}(\vec{r}\,',\vec{r};\omega)\times\left(\frac{\vec{\partial}}{\partial x}-\frac{\overleftarrow{\partial}}{\partial x}\right)_{x_0}\left(\frac{\vec{\partial}}{\partial x'}-\frac{\overleftarrow{\partial}}{\partial x'}\right)_{x_0}\operatorname{Im}G^{(L)}(\vec{r},\vec{r}\,',\sigma,\omega)\right], \tag{1}$$

where $j_\sigma(\omega)$ is the FEED current of spin σ at energy ω. $G^{(L)}$ is the Green's function of the left system which is essentially the metal and is defined more precisely in I. $G^{(R)}$ is the Green's function of the right system which is essentially the external electric field and x_0 is a point within the tunneling barrier as described in I.

In order to evaluate $j_\sigma(\omega)$ we must know $G^{(L)}$ and $G^{(R)}$ near $x=x'=x_0$ as indicated by Eq. (1). $G^{(R)}$ is the Green's function for the one-particle Hamiltonian of the right system and may be written

$$G^{(R)}(\vec{r},\vec{r}\,';\omega)=\sum_R\frac{\psi_R^*(\vec{r})\psi_R(\vec{r}\,')}{\omega-E_R}, \tag{2}$$

where $\psi_R(\vec{r})$ is given by Eq. (14) of Ref. 1 for $x\sim x'\sim x_0$ and E_R is an eigenvalue of the right-system Hamiltonian.

The left system consists of the metal plus the electric field in the region between the metal surface and x_0 as shown in Ref. 1, Fig. 2(a). The left system is described by a many-electron Hamiltonian, thus the Green's function $G^{(L)}$ satisfies

$$[\omega-H_L(\vec{r})]G^{(L)}(\vec{r},\vec{r}\,',\sigma,\omega)-\int d^3r''\,\Sigma_L^\sigma(\vec{r},\vec{r}\,'')G^{(L)}(\vec{r}\,'',\vec{r}\,',\sigma,\omega)-\int d^3r''\,\Sigma_L^{\sigma\bar{\sigma}}(\vec{r},\vec{r}\,'')G^{(L)}(\vec{r}\,'',\vec{r}\,',\bar{\sigma}\sigma,\omega)=\delta(\vec{r}-\vec{r}\,'), \tag{3}$$

where $H_L(\vec{r})$ is the one-particle part of the left-system Hamiltonian, $G^{(L)}(\bar{\sigma}\sigma)$ is the spin-flip Green's function and Σ_L^σ, $\Sigma^{\sigma\bar{\sigma}}$ are appropriate self-energies. It is assumed that the image potential is contained in $H_L(\vec{r})$. For $\vec{r}$ or $\vec{r}'$ in the tunneling barrier we expect $\Sigma_L(\vec{r}, \vec{r}') = 0$ and the left-system Hamiltonian may be taken to be the independent-particle Hamiltonian, H_L.[8] Consequently, it follows from AB (3.11)–(3.14) that for $x \sim x' \sim x_0$,

$$G^{(L)}(\vec{r}, \vec{r}', \sigma; \omega) = \sum_L \frac{\psi_L^*(\vec{r})\psi_L(\vec{r}')}{\omega - E_{L,\sigma}}, \qquad (4)$$

where ψ_L is given by Ref. 1, Eq. (18) with N_L replaced by N_L^σ, a spin-dependent normalization factor. $E_{L,\sigma}$ is the excitation energy required to remove an electron spin σ from the left system. Use of Eqs. (2) and (4) in (1) yields Eq. (22) of Ref. 1.

Proceeding as in I leads directly to the equivalent[16] of Eq. (32) of Ref. 1,

$$j_\sigma(\omega)/j_0(\omega) = A_\sigma(\omega)\rho^{\perp}_{m,\sigma}(\omega, x_m), \qquad (5)$$

where $j_0(\omega)$ is the current per spin that would be observed if the metal were free-electron-like. $A_\sigma(\omega)$ is a slowly varying function of ω that includes $j_0(\omega)^{-1}$, and

$$\rho^{\perp}_{m,\sigma}(\omega, x_m) = \sum_m{}' |\alpha_m^\sigma(x_m)|^2 \delta(\omega - \epsilon_m), \qquad (6)$$

where $\sum_m'$ denotes a sum over metal states with momentum normal to the metal surface. $\alpha_m^\sigma(x_m)$ is the component of the metal wave function for spin σ that has total momentum parallel to the surface equal to zero:

$$\alpha_m^\sigma(x_m) = \int_{x = x_m} dS\, \psi_{m,\sigma}(\vec{r}), \qquad (7)$$

where $\psi_{m,\sigma}(\vec{r})$ is the metal wave function and the integral is over a plane parallel to the metal surface and a distance x_m away from it. Similarly, in Eq. (32) of Ref. 1, $\psi_m(x_m)$ should be replaced by $\alpha(x_m) = \int_{x=x_m} dS\, \psi_m(\vec{r})$ because α is the component of ψ_m with zero total momentum parallel to the surface and it is just that component which determines the tunneling probability. The mathematical details will be included in a later publication.[17] In Eq. (7), x_m is taken to be the classical turning point located 2–3 Å outside the metal surface. Thus combined FEED and spin-polarization measurements will provide direct information about the one-dimensional "surface" density of states for a given spin.

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