New mechanism for current modulation in a static magnetic field in a scanning tunneling microscope

S. N. Molotkov
Institute of Solid State Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow Region, Russia

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A one-particle mechanism for a modulation of the tunneling current at the Larmor frequency in a static magnetic field is offered in an effort to explain experimental results obtained by Manassen *et al.* [Phys. Rev. Lett. **62**, 2513 (1989); Phys. Rev. B **48**, 4887 (1993)].

In a series of experiments[1,2] on a Si(111) surface containing paramagnetic centers (produced by, for example, bombardment with oxygen atoms[1]), the following effect was observed: When the sample was immersed in a static magnetic field (on the order of 200 G), measurements of frequency characteristics of the tunneling current in a scanning tunneling microscope revealed a sharp peak at the frequency corresponding to a Larmor precession of a spin localized at a center. The scale value of the frequencies in these fields was about 500 MHz. The signal was well localized in space: When the tip was moved a few angstroms away from the center along the surface, the signal disappeared.

The mechanism for the current modulation in a static magnetic field is still not completely clear. One possible mechanism was proposed in Ref. 3. It was shown that, if there is a significant spin–spin exchange interaction of itinerant electrons with a spin at a center, the coherent tunneling of pairs of itinerant electrons which have opposite spins and which have undergone a change in spin orientation via a spin at a center leads to a structural feature at the frequency of the Larmor precession of a localized spin. This is a multiparticle mechanism and stems from an exchange interaction.

That is not, however, the only possible mechanism. In the present letter we wish to call attention to the possibility of a one-particle mechanism for current modulation. We begin with a qualitative description of it.

From the standpoint of the electron spectrum, the presence of a paramagnetic center means the appearance of a spatially localized state whose energy lies in the bulk band gap of the semiconductor. Let us assume, as a starting point, that the Coulomb interaction is negligible (we will later take it into account). In a static magnetic field the states of electrons at centers with spins up and down thus differ by the Zeeman energy $E_z=\hbar\omega_L$, where $\omega_L=g\mu_B H/\hbar$, g is the g-factor, μ_B is the Bohr magneton, and H is the magnetic field. We also assume that the localized level has a finite width. This assumption, important to the discussion below, means that in the band gap there is a continuum of states: surface bands to which electrons can undergo transitions from a center. This continuum is localized near the surface. In the opposite case, we should observe a current cutoff, but a cutoff is not observed experimentally. We know that at a Si(111) 7×7 surface there is a high density of states in the band gap[4] (there is no band gap in the spectrum at the surface). Actually, for the electrons at a center there must be a reservoir which replenishes electrons to compensate for escape to the tip and vice versa. Furthermore, if in the course of tunneling, (for definiteness, from the crystal to the tip) states with a certain spin projection are not eigenstates (this is the situation observed experimentally because of the strong spin–orbit coupling in the metals used as tips: W, Au, Pt, and Ir), then these states decay in the tip into states with both spin projections. This circumstance leads to an interference of the fluxes of electrons with spins up and down. Since the energies of these states differ by an amount $\hbar\omega_L$, the interference occurs at a finite frequency and is manifested as a structural feature in the frequency spectrum of the current.

It turns out that this picture remains valid when the Coulomb interaction is strong, and there can be only a single electron at a center, with spin either up or down.

Information on the spectral characteristics of the tunneling current is embodied in the current–current correlation function. We write the Hamiltonian incorporating the basic features of the problem as follows:

$$\hat{H}=\sum_{\sigma}\epsilon_0 c_\sigma^+ c_\sigma+\sum_{k,\sigma}\epsilon_{tk} c_{tk\sigma}^+ c_{tk\sigma}+\sum_{k,\sigma}\epsilon_{ck} c_{ck\sigma}^+ c_{ck\sigma}+\sum_{k,\sigma}(T_k c_{tk\sigma}^+ c_{0\sigma}+V_k c_{ck\sigma}^+ c_{0\sigma}$$

$$+\mathrm{H.a.})+\sum_{\sigma} U n_{0\sigma} n_{0-\sigma}+\sum_{\substack{h,h'\\ \sigma,\sigma'}}\Lambda_{k,k'}^{\sigma,\sigma'} c_{tk\sigma}^+ c_{tk'\sigma'}. \qquad (1)$$

The first term describes state of electrons at centers, while the second and third describe states of electrons in the tip and in the continuous spectrum of the crystal (the reservoir). The fourth and fifth terms incorporate the tunneling coupling with the tip and the reservoir. The next-to-last term incorporates the Coulomb repulsion proper at a center and the spin–orbit interaction in the tip.

Tunneling into the tip occurs directly from a center which is replenished from the reservoir.

Our problem reduces to one of calculating the current–current correlation function. The tunneling-current operator is written in the standard form:

$$\hat{I}(t)=\frac{ie}{2}\sum_{k\sigma}(T_k c_{tk\sigma}^+ c_{0\sigma}+V_k c_{ck\sigma}^+ c_{0\sigma}-\mathrm{H.a.}). \qquad (2)$$

The spectrum of current fluctuations is determined by the correlation function

$$(II)_\Omega=\int dt e^{i\Omega t}\langle \hat{I}(t)\hat{I}(0)+\hat{I}(0)\hat{I}(t)\rangle. \qquad (3)$$

As in Ref. 5, this correlation function is expressed in terms of Keldysh Green's functions:[6]

$$(II)_\Omega = \frac{e^2}{4}\int \mathrm{Tr}\,\{(\hat{T}+\hat{V})(\omega')\hat{G}(\omega)+\hat{G}(\omega')(\hat{T}+\hat{V})(\omega)+\hat{G}(\omega')[(\hat{T}-\hat{V})$$
$$\times(\omega)\hat{G}(\omega)(\hat{T}-\hat{V})(\omega)]+[(\hat{T}-\hat{V})(\omega')\hat{G}(\omega')(\hat{T}-\hat{V})(\omega')]\hat{G}(\omega)$$
$$-[(\hat{T}-\hat{V})(\omega')\hat{G}(\omega')][(\hat{T}-\hat{V})(\omega)\hat{G}(\omega)]-[\hat{G}(\omega')(\hat{T}-\hat{V})(\omega')]$$
$$\times[\hat{G}(\omega)(\hat{T}-\hat{V})(\omega)]\}d\omega/2\pi. \quad (4)$$

The Tr here means a summation over the Keldysh contours and the spin indices. We have also introduced $\omega'=\omega+\Omega$. It is convenient to incorporate the Green's functions which are not diagonal in the spin by perturbation theory. The unperturbed spin-diagonal Green's functions $\hat{T}$ and $\hat{V}$ are defined by

$$T^{A,R}(\omega)=\sum_k |T_k|^2/(\omega-\epsilon_{tk}\pm i0),$$

$$T(\omega)=t\begin{cases} f_t(\omega), \\ f_t(\omega)+1, \end{cases}$$

$$t=\pi\sum_k |T_k|^2\delta(\omega-\epsilon_{tk}), \quad (5)$$

where $f_t(\omega)$ is a Fermi distribution function in the tip. There is a corresponding expression for $\hat{V}$, with t replaced by c, and t by v.

The Green's function of the electrons at an isolated center can be found exactly.[7] The tunneling coupling with states of the tip and the reservoir in the crystal is dealt with by perturbation theory (Ref. 8, for example). We have

$$\rho_\sigma(\omega)=\frac{\gamma\,[\omega-\epsilon_{0\sigma}-U(1-\langle n_{-\sigma}\rangle)]}{(\omega-\epsilon_{0\sigma})^2(\omega-\epsilon_{0\sigma}-U)^2+[\omega-\epsilon_{0\sigma}-U(1-\langle n_{-\sigma}\rangle)]^2\gamma^2},$$

$$G_\sigma^{>}(\omega)=i\rho_\sigma(\omega)\begin{cases} F(\omega), \\ F(\omega)+1, \end{cases} \quad (6)$$

$$F(\omega)=[tf_t(\omega)+vf_c(\omega)]/(t+v),$$

$$\gamma=t+v.$$

The distribution function at a center is formed through a tunneling coupling with reservoir and the tip. The spin-dependent contribution to the spectrum of the tunneling current against the background of the ordinary shot noise stems from the temporal correlation of the fluxes of tunneling electrons with spins up and down. Using (4)–(6), we can write this contribution as follows:

$$\delta(II)_\Omega \simeq \frac{|t_{\uparrow\downarrow}|^2}{\pi}\int G_\uparrow(\omega)G_\downarrow(\omega+\Omega)[F(\omega)+F(\omega+\Omega)$$
$$-2F(\omega)F(\omega+\Omega)]d\omega/2\pi, \quad (7)$$

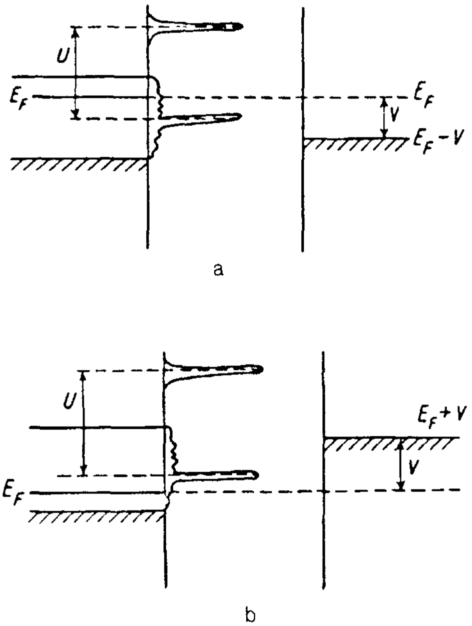

FIG. 1.

where $t_{\uparrow\downarrow}$ is the correction to the Green's function of the tip which is not diagonal in the spin, given by

$$|t_{\uparrow\downarrow}|^2=\frac{1}{\pi}\,\mathrm{Im}\left\{\sum_{k,k'}|T_k|^2\,\Lambda_{k,k}^{\uparrow\downarrow}|T_{k'}|^2/[(\omega-\epsilon_{tk\uparrow}+i0)(\omega-\epsilon_{tk'\downarrow}+i0)]\right\}. \tag{8}$$

Two different situations are possible. The Fermi level (in the absence of an applied voltage) is higher than the level at the center. The second level is always empty, since it lies high in the conduction band, because of the strong Hubbard repulsion (Fig. 1a). An excess spin noise with a structural feature at the frequency $\Omega\simeq\omega_L$ should therefore be observed when there is a positive voltage on the tip. It is given by

$$\delta(II)_\Omega\simeq e^2\frac{\gamma}{\pi[(\Omega-\omega_L)^2+\gamma^2]}|t_{\uparrow\downarrow}|^2[(v+t)/(2v+t)]^2. \tag{9}$$

In the opposite case, in which the Fermi level lies below the level at the center (Fig. 1b), a structural feature in the current spectrum should be observed when there is a negative voltage on the tip.

In summary, the noise predicted in the tunneling current is a shot noise, in contrast with the coherent noise discussed previously.[3] Experimentally, both mechanisms may operate.

It is interesting to estimate how narrow the localized level can be before the current cuts off. Typical values of the tunneling current are lnA. These values correspond to a tunneling rate of 10^{10} e/s. This result means that the reservoir should replenish electrons in the level or remove electrons from the level with a time scale

$\tau \simeq 10^{-10}$ s. The width of the level must be $\gamma \gg \hbar/\tau \simeq 10^{-5}$ eV. The level is thus quite narrow, and in ordinary ESR experiments it would behave as a genuinely localized level.

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