Hall effect of charge carriers in a correlated system

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(Received 24 September 1996)

The dynamical Hall response in a correlated electronic system is analyzed within the linear-response theory for tight-binding models. At $T=0$ the dc Hall constant for a single quasiparticle is expressed explicitly via the charge stiffness and a semiclassical result is recovered. As expected, a holelike response is found for a mobile hole introduced into a quantum antiferromagnet, as represented by the t-J model. [S0163-1829(97)04015-0]

The question of the Hall response in a system of correlated electrons has proved to be extremely difficult. Theoretical investigations of this problem in the past decade have been stimulated by experiments on superconducting cuprates where, in low-doping materials, charge carriers are holes introduced into a magnetic insulator. For cuprates in the normal state this is established by the Hall measurements,[1] which reveal a holelike dc Hall constant $R_H^0>0$. In certain cases, e.g., in $La_{2-x}Sr_xCuO_4$ at low doping $x<0.15$, the simple semiclassical result $R_H^0=1/n_h e_0$, with the hole density $n_h=x/\Omega_0$ (Ω_0 being the volume/formula unit), seems to be obeyed at low temperatures.[1] This calls for a semiconductorlike interpretation in terms of independent holelike quasiparticles (QP's) rather than the usual picture for a metal with the Fermi surface. As is well known, however, such descriptions fail to explain the strong T dependence of R_H^0, persisting down to the lowest $T>T_c$.[1–3]

A quantum-mechanical analysis of the Hall response within the linear-response theory is complicated even for a single charge carrier, as evidenced by the polaron problem[4] and a single hole in a Mott-Hubbard insulator.[5] Analogous treatments of metals with a well-defined Fermi surface[6,7] were mainly restricted to cases of nearly free electrons. Recently, the dynamical Hall response $R_H(\omega)$ for lattice models of correlated electrons, such as the t-J and the Hubbard model, has been approached within the relaxation-time[8] and other analytical approximations,[9] and evaluated in more detail by the high-ω,T analysis[10] and numerical methods.[11,12] Conclusions for these models, however, appear to be most delicate and controversial for the dc and the low-temperature limit $R_H^0(T\rightarrow 0)$, questioning even the holelike sign of R_H^0 in the regime of low hole doping.[11,12]

In this paper we consider dynamical conductivities $\widetilde{\sigma}_{\alpha\beta}(\omega)$ in the presence of a magnetic field B, whereby we perform a linearization in B.[6,7] As analyzed by Kohn,[13] at $T=0$ the usual (diagonal) dynamical conductivity (for $B=0$) is singular at low frequencies $\sigma_{\alpha\alpha}(\omega\rightarrow 0) \propto iD_{\alpha\alpha}/\omega$, where $D_{\alpha\alpha}$ is the charge stiffness parameter, representing the coherent response of the charge to the external field. It is now well established that the stiffness tensor $D_{\alpha\beta}$ in correlated systems is an important and nontrivial quantity, distinguishing, e.g., a metal and a Mott-Hubbard (magnetic) insulator.[13,14] We observe that for $B>0$ certain off-diagonal conductivities have to be singular as well, $\sigma_{\alpha\neq\beta}(\omega)\propto A/\omega^2$, in order to yield a meaningful dc Hall response $R_h^0=R_H(\omega\rightarrow 0)$. We are able to relate explicitly these quantities for the case of a single mobile carrier, a QP, where we recover the simple semiclassical relation $R_H^0=1/ne$.

Let us consider, for simplicity, a planar x-y system, with a magnetic field applied in the z direction and a uniform electric current $\vec{J}=J_x\vec{e}_x$. We follow the linear-response approach developed in Ref. 6, working with the magnetic field modulated in the y direction, $\vec{B}=Be^{iqy}\vec{e}_z$, inducing a modulated electric field $\vec{\mathcal{E}}=\mathcal{E}_y^q e^{iqy}\vec{e}_y$. At the final stage, we are interested in the limit $q\rightarrow 0$. As the corresponding vector potential we choose $\vec{A}=A^q e^{iqy}\vec{e}_x$ with $A^q=iB/q$. The dynamical Hall response $R_H(\omega)=\mathcal{E}_y^q(\omega)/J_x(\omega)B$ can be expressed as[10]

$$R_H(\omega)=\frac{1}{B}\,\frac{-\widetilde{\sigma}_{yx}^q(\omega)}{\widetilde{\sigma}_{xx}^q(\omega)\widetilde{\sigma}_{yy}^q(\omega)-\widetilde{\sigma}_{xy}^q(\omega)\widetilde{\sigma}_{yx}^q(\omega)}\Bigg|_{B,q\rightarrow 0}, \quad (1)$$

where $\widetilde{\sigma}_{\alpha\beta}$ denote components of the conductivity tensor, evaluated at finite $B\neq 0$. Models for strongly correlated electrons are usually analyzed within the tight-binding framework where the magnetic field enters (only) the kinetic energy H_{kin} via the Peierls phase, i.e.,

$$H_{\mathrm{kin}}=-t\sum_{\langle ij\rangle s}(e^{i\theta_{ij}}c_{js}^{\dagger}c_{is}+\mathrm{H.c.}), \quad (2)$$

where $\theta_{ij}=e\vec{r}_{ij}\cdot\vec{A}(\vec{r}=\vec{R}_{ij})$, $\vec{r}_{ij}=\vec{r}_j-\vec{r}_i$, and $\vec{R}_{ij}=(\vec{r}_i+\vec{r}_j)/2$. The operators for the particle current $\widetilde{j}$ and for the stress tensor τ can now be given by

$$\widetilde{j}_\alpha^k=-\frac{1}{e}\frac{\partial H_{\mathrm{kin}}}{\partial A_\alpha^{-k}}=t\sum_{\langle ij\rangle s} r_{ij}^\alpha e^{i\vec{k}\cdot\vec{R}_{ij}}(ie^{i\theta_{ij}}c_{js}^{\dagger}c_{is}+\mathrm{H.c.}),$$

$$\tau_{\alpha\beta}^k=-\frac{1}{e^2}\frac{\partial^2 H_{\mathrm{kin}}}{\partial A_\alpha^{-k}\partial A_\beta^{-k}}=t\sum_{\langle ij\rangle s} r_{ij}^\alpha r_{ij}^\beta e^{i\vec{k}\cdot\vec{R}_{ij}}(e^{i\theta_{ij}}c_{js}^{\dagger}c_{is}+\mathrm{H.c.}). \quad (3)$$

The conductivity tensor at $B\neq 0$ can be expressed as[6,10]

$$\widetilde{\sigma}_{\alpha\beta}^q(\omega)=\frac{ie^2}{\Omega\omega^+}[\phi_{\alpha\beta}^q(0^+)-\phi_{\alpha\beta}^q(\omega^+)],$$

$$\phi_{\alpha\beta}^q(\omega_m)=\int_0^\beta d\tau e^{\omega_m\tau}\langle T_\tau \widetilde{j}_\alpha^q(\tau)\widetilde{j}_\beta^0(0)\rangle_B, \quad (4)$$

where $\omega_m=2\pi imT$, $\omega^+=\omega+i\delta,\delta>0$, Ω is the volume of the system, T_τ is the time ordering operator, and $\langle\,\rangle_B$ denotes an average for $B\neq 0$.

Next we perform a linearization in B, in analogy to the treatment of a Fermi gas.[6,7] From Eqs. (3) it follows that

$$\tilde{j}^k_\alpha=j^k_\alpha-e\tau^{k-q}_{\alpha x}A^q,\quad j^k_\alpha=\tilde{j}^k_\alpha(B=0). \tag{5}$$

Taking into account the linear coupling term $H'=-ej_x^{-q}A^q$, we can express the off-diagonal components ϕ^q_{yx}, linearized in A^q, in the form

$$\phi^q_{yx}=eA^qK^q_{yx},\quad K^q_{yx}=K^I_{yx}+K^{II}_{yx},$$

$$K^I_{yx}(\omega_m)=-\int_0^\beta d\tau e^{\omega_m\tau}\langle T_\tau j^q_y(\tau)\tau^{-q}_{xx}(0)\rangle_0, \tag{6}$$

$$K^{II}_{yx}(\omega_m)=\frac{1}{\beta}\int_0^\beta d\tau\int_0^\beta d\tau' e^{\omega_m\tau}\langle T_\tau j^q_y(\tau)j^{-q}_x(\tau')j^0_x(0)\rangle_0,$$

where we have taken into account that some averages, such as $\langle\tau^q_{yx}(\tau)j^0_x(0)\rangle_0$ and $\langle j^q_y(\tau)j^0_x(0)\rangle_0$, vanish by symmetry. We can then rewrite Eq. (1) as

$$R_H(\omega)=\left.\frac{e^3[K^q_{yx}(0^+)-K^q_{yx}(\omega^+)]}{q\Omega\omega^+\sigma^0_{xx}(\omega)\sigma^0_{yy}(\omega)}\right|_{q\to 0}, \tag{7}$$

where $\sigma_{\alpha\alpha}$ now refers to the case $B=0$.

In the following we restrict our analysis to $T=0$. Let us assume, for simplicity, that the absolute ground state $|0\rangle$, having the energy E_0 and the wave vector $\vec{Q}=0$, is nondegenerate. For the diagonal conductivity $\sigma^q_{\alpha\alpha}$ we can perform the $q\to 0$ limit. Strictly at $q=0$, we take into account the sum rule $\phi^q_{\alpha\alpha}(0)\to\langle\tau^0_{\alpha\alpha}\rangle$, while $\phi^0_{\alpha\alpha}(\omega\to 0)<\phi^q_{\alpha\alpha}(0^+)$. One can separate the response into a coherent (singular) part[13,14] and an incoherent (regular) part, expressed in terms of eigenstates,

$$\sigma^0_{\alpha\alpha}(\omega)=\frac{2ie^2}{\Omega\omega^+}D_{\alpha\alpha}+\sigma^{\rm reg}_{\alpha\alpha}(\omega),$$

$$D_{\alpha\alpha}=\frac{\langle\tau^0_{\alpha\alpha}\rangle}{2}-\sum_{m>0}\frac{|(j^0_\alpha)_{0m}|^2}{\epsilon_m}, \tag{8}$$

$$\sigma^{\rm reg}_{\alpha\alpha}(\omega)=\frac{ie^2}{\Omega}\sum_{m>0}\frac{|(j^0_\alpha)_{0m}|^2}{\epsilon_m}\left[\frac{1}{\omega^++\epsilon_m}+\frac{1}{\omega^+-\epsilon_m}\right],$$

where we use the notation $(j^0_\alpha)_{0m}=\langle 0|j^0_\alpha|m\rangle$ and $\epsilon_m=E_m-E_0$.

Expressing K^q_{yx} in terms of eigenstates (at $T=0$) is also straightforward, although more tedious. Due to the q character of operators entering Eqs. (6), it is convenient to distinguish eigenstates $|m\rangle,|\tilde{m}\rangle$, and $|\hat{m}\rangle$, corresponding to wavevectors $\vec{Q}$, $\vec{Q}-\vec{q}$, and $\vec{Q}+\vec{q}$, respectively. So we obtain from Eqs. (6)

$$K^q_{yx}(\omega^+)=\sum_{\tilde{m}}\left[\frac{\gamma_{\tilde{m}}}{\omega^+-\epsilon_{\tilde{m}}}+\frac{\tilde{\gamma}_{\tilde{m}}}{\omega^++\epsilon_{\tilde{m}}}\right]+\sum_{m>0}\left[\frac{\delta_m}{\omega^+-\epsilon_m}+\frac{\tilde{\delta}_m}{\omega^++\epsilon_m}\right], \tag{9}$$

where it follows from $\tilde{\sigma}_{\alpha\beta}(-\omega)=\tilde{\sigma}^*_{\alpha\beta}(\omega)$ and Eqs. (4), (6), and (9) that $\tilde{\gamma}_{\tilde{m}}=\gamma_{\tilde{m}}$ (real), $\tilde{\delta}_m=\delta_m$ (real), and

$$\gamma_{\tilde{m}}=(j^q_y)_{0\tilde{m}}\left[(\tau^{-q}_{xx})_{\tilde{m}0}-\sum_l\frac{(j^{-q}_x)_{\tilde{m}l}(j^0_x)_{l0}}{\epsilon_l-\epsilon_{\tilde{m}}}-\sum_{\tilde{l}}\frac{(j^{-q}_x)_{\tilde{l}0}(j^0_x)_{\tilde{m}\tilde{l}}}{\epsilon_{\tilde{l}}}\right], \tag{10}$$

$$\delta_m=-(j^0_x)_{m0}\left[\sum_{\tilde{l}}\frac{(j^q_y)_{0\tilde{l}}(j^{-q}_x)_{\tilde{l}m}}{\epsilon_{\tilde{l}}-\epsilon_m}+\sum_{\hat{l}}\frac{(j^q_y)_{\hat{l}m}(j^{-q}_x)_{0\hat{l}}}{\epsilon_{\hat{l}}}\right].$$

We again separate $K^q_{yx}(\omega)$ into a regular and a singular part. The latter should cancel the singular terms $\sigma^0_{\alpha\alpha}\propto 1/\omega$ in Eq. (7), in order to yield a meaningful $R_H(\omega\to 0)$. It is evident that the relevant contribution to K^q_{yx} in Eq. (9) comes from terms with vanishing $\epsilon_m,\epsilon_{\tilde{m}}$. By analogy with free fermions we can speculate on several possibilities for low-lying excitations. For example, in a metal with a Fermi surface one has to consider electron-hole pairs as the relevant excited states. At present we are not able to treat Eq. (9) in a meaningful way for the analogous regime in a correlated metal.

It is, however, feasible to consider the nontrivial response of a single charge carrier, a QP, e.g., the one introduced by doping a Mott-Hubbard insulator or an antiferromagnet (AFM). For a well-defined QP we require a quadratic dispersion $\epsilon_{q\to 0}\propto q^2$ and a pseudogap in the optical response $\sigma^{\rm reg}_{\alpha\alpha}(\omega\to 0)\to 0$, hence $(j^0_\alpha)_{0m}\to 0$ for $\epsilon_m\to 0$. Such assumptions seem to hold, e.g., for a mobile hole introduced into a two-dimensional quantum AFM.[15–17]

Under these restrictions we note that δ_m terms contribute only to $(\tilde{\sigma}^q_{yx})^{\rm reg}$ because the prefactor $(j^0_\alpha)_{0m}$ vanishes for $m\to 0$. In contrast, the essential contribution to the $\tilde{m}$ sum in Eq. (9) comes from the QP excited state $|\tilde{0}\rangle$ with $\epsilon_{\tilde{0}}=\epsilon_q\gtrsim 0$. It is possible to simplify $\gamma_{\tilde{0}}$, since we can at the same time perform the limit $q\to 0$ for certain matrix elements (note that $\vec{q}$ points in the y direction), i.e., $(\tau^{-q}_{xx})_{\tilde{0}0}\to(\tau^0_{xx})_{00}$, while for $l\neq 0$ and $\tilde{l}\neq\tilde{0}$, $\epsilon_{\tilde{l}},\epsilon_l-\epsilon_{\tilde{0}}\to\epsilon_l$ and $(j^{-q}_x)_{\tilde{0}l},(j^{-q}_x)_{\tilde{l}0},(j^0_x)_{\tilde{0}\tilde{l}}\to(j^0_x)_{0l}$. Comparing Eqs. (8) and (10) we recognize

$$\gamma_{\tilde{0}}=2(j^q_y)_{0\tilde{0}}D_{xx}. \tag{11}$$

There is no analogous simple $q\to 0$ limit for $(j^q_y)_{0\tilde{0}}$. A useful relation is obtained when we consider, for $B=0$, the current response j^q_y to the external field $\mathcal{E}^q_y$. Such a response has been invoked for finite systems in order to enforce the validity of the sum rule for $\sigma^{\rm reg}_{\alpha\alpha}$.[19] The corresponding conductivity σ^{qq}_{yy} can be expressed, by analogy to the $q=0$ one in Eqs. (8), as

$$\sigma_{yy}^{qq}(\omega)=\frac{ie^2}{\Omega}\sum_{\tilde{m}}\frac{|(j_y^q)_{0\tilde{m}}|^2}{\epsilon_{\tilde{m}}}\left[\frac{1}{\omega^+-\epsilon_{\tilde{m}}}+\frac{1}{\omega^++\epsilon_{\tilde{m}}}\right]. \quad (12)$$

The essential difference between Eqs. (8) and (12) is that the coherent peak at $\omega=0$ in Eq. (12) now splits into two peaks at $\omega=\pm\epsilon_{\tilde{0}}$, respectively. Since the sum rule is not changed,[19] we can equate their intensities,[17]

$$D_{yy}=(j_y^q)_{0\tilde{0}}^2/\epsilon_q. \quad (13)$$

Moreover, for a single QP also the coherent mass is directly related to the stiffness,[18], i.e., $\epsilon_q=D_{yy}q^2$. Hence, from Eq. (13) we get $|(j_y^q)_{0\tilde{0}}|=D_{yy}q$. From Eqs. (7) and (9), with $K_{yx}^q(\omega>\epsilon_{\tilde{0}})\sim 2\gamma_{\tilde{0}}/\omega^+$, we finally obtain

$$R_H^0=\mathrm{sgn}(\zeta)\frac{\Omega}{e}, \quad \zeta=\langle 0|j_y^q|\tilde{0}\rangle. \quad (14)$$

This is a semiclassical result for the single QP, since $Z=\mathrm{sgn}(\zeta)=\pm 1$.

The remaining question of the sign of ζ is not trivial; at least we did not find a simple argument that would yield the expected plausible answer. While it is easy to show that $Z=1$ for a single free electron at the bottom of the band (note that $e=-e_0<0$), for a more general case the calculation of Z requires the knowledge of the ground-state wave function $|\Psi^q\rangle$ at finite $q\neq 0$, which can be quite involved within a correlated system. For a single QP it is convenient to represent $|\Psi^q\rangle$ in terms of localized functions

$$|\Psi^q\rangle=\sum_l e^{i(\vec{Q}+\vec{q})\cdot\vec{r}_l}|\psi_l^q\rangle. \quad (15)$$

Then one can express ζ via Eq. (3) for $q\ll 1$, assuming a local character of $|\psi_l^q\rangle$,

$$\zeta=\frac{qt}{2}\sum_{i,j,l}e^{-i\vec{Q}\cdot\vec{r}_l}\langle\psi_l^q|(r_i^y+r_j^y)(j_{y+}^{ij}-j_{y-}^{ij})|\psi_0^q\rangle. \quad (16)$$

$j_{y\pm}^{ij}=\Sigma_s r_{ij}^y c_{js}^\dagger c_{is}$, where we have chosen $\vec{r}_0=0$, and $j_{y\pm}^{ij}=\Sigma_s r_{ij}^y c_{js}^\dagger c_{is}$ are forward (backward) hopping operators in Eq. (3), corresponding to $r_{ij}^y=\pm 1$, respectively. It now seems plausible that the charge signature should come from the sign of the dominating forward hopping $r_i^y+r_j^y$ in Eq. (16), which should be positive for an electron (e.g., for a free electron the only forward term is $\vec{r}_i=0$, $\vec{r}_j=\vec{r}_l=\vec{e}_y$) and negative for holes due to the opposite direction of the electron hopping (at least for free fermions). However, as shown below for a concrete example, the evaluation and the result are not so evident in general.

Let us consider the problem of a spin polaron, i.e., a single hole inserted into an AFM,[15] as relevant to cuprates and described within the t-J model,

$$H=-t\sum_{\langle ij\rangle s}(\tilde{c}_{js}^\dagger\tilde{c}_{is}+\mathrm{H.c.})+J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j, \quad (17)$$

where $\tilde{c}_{is},\tilde{c}_{is}^\dagger$ are projected operators, not allowing double occupancy of sites. Although the projection introduces an interaction also in the kinetic term, the analysis of the Hall response presented above remains valid, provided that operators $\tilde{j}$ and τ in Eqs. (3) are redefined accordingly.

The quantity ζ for a single hole in the t-J model has been considered in another context in Ref. 17. Since, in general, $|\psi_l^q\rangle$ are complicated, we evaluate ζ using the perturbation expansion. We start with a static hole in the Néel AFM, taking into account only the Ising-type spin interaction $JS_i^zS_j^z$. Corrections due to the hopping term H_{kin} with $t/J\ll 1$ and the spin flip part H_γ with $\gamma=J_\perp/J\ll 1$ are treated at $T=0$ perturbatively.[16] As noted in Ref. 17, nonzero contributions in Eq. (16) can arise only from nonlocal $l\neq 0$ terms, since for $l=0$ contributions of j_{y-} and j_{y+} cancel. The ground state of one hole in the t-J model is at $\vec{Q}=(\pm\pi/2,\pm\pi/2)$.[15,16] Although such a ground state is clearly degenerate, this should not change our results for R_H^0.

It is convenient to represent the localized wave functions $|\psi_l^q\rangle$ in terms of a basis of string states $|\varphi_{lm}^q\rangle$, which are obtained by applying the operations of H_{kin} and H_γ on the ground state $|\varphi_{l0}^0\rangle$ (the Néel state with a static hole on the site l). Finally, we want to express $|\psi_l^q\rangle$ in the form

$$|\psi_l^q\rangle=\sum_m c_m^q|\varphi_{lm}^q\rangle. \quad (18)$$

Although the calculation of allowed $|\varphi_{lm}^q\rangle$ and the corresponding c_m^q can be quite involved (and not unique), it is straightforward to lowest orders of the perturbation series in t,γ.[16,17] The lowest nonzero contribution in Eq. (14) comes, e.g., from $\vec{r}_l=-2\vec{e}_y$. Let us evaluate the term starting with $|\varphi_{00}^0\rangle$. The operator j_{0j}^+ with $\vec{r}_j=-\vec{e}_y$ moves the hole in the $-y$ direction and leaves behind one flipped spin (relative to the Néel state). The resulting state can be represented also as an excited state $|\varphi_{lm}^q\rangle$, reached within the perturbation expansion from $|\varphi_{l0}^0\rangle$ by applying H_{kin} and H_γ once. This particular contribution of perturbation expansion is thus

$$\zeta_{ijl}=e^{-i\vec{Q}\cdot\vec{r}_l}\frac{qt^2}{2\Delta_1\Delta_2}<0, \quad (19)$$

where $\Delta_1,\Delta_2>0$ are energies of intermediate excited states. There are more nonzero contributions within the same order of perturbation theory, but they are negative as well, confirming the holelike character of the QP. Although the result $Z=-1$ is strictly valid in the t-J model for $\gamma\ll 1$, $J/t\ll 1$, we do not expect any change in the sign of Z when entering the relevant regime $\gamma=1$, $J<t$.[16]

The obtained results are not surprising. The charge carrier in an interacting system, obeying the properties of the QP, behaves in the dc Hall response at $T=0$ according to the semiclassical relation. The main difference is that no particular assumptions, such as the relaxation-time approximation, are needed to derive this result. This should hold not only for correlated systems, but also for electrons interacting with phonons, etc. We presented also the calculation that confirms a holelike Hall response for a single hole in the t-J model.

It is tempting to generalize the above results in several directions in order to be applicable to more realistic situations in correlated systems, and in cuprates in particular. At low hole doping $n_h\ll 1$, we expect that holes in cuprates behave as independent QP-spin polarons. Then $\tilde{\sigma}_{\alpha\beta} \propto n_h$, which leads to $R_H^0 = 1/n_h e_0$ in this regime. Such behavior indeed seems to be found at lowest T in underdoped $La_{2-x}Sr_xCuO_4$ (Refs. 1 and 3) (although there seem to be quantitative discrepancies between various data), but not quite so in other underdoped cuprates.[1] Approaching the ''optimum''-doping regime, the scenario of an independent QP is clearly not applicable since the electrons reveal a rather well-defined large Fermi surface, while R_H^0 can even change sign. The evaluation of R_H^0 in this intermediate regime can, in principle, be treated with Eqs. (7)–(10), taking into account, in Eq. (9), all relevant low-lying excited states $|\tilde{m}\rangle$. Whereas the stiffness $D_{\alpha\alpha}$ has been examined in detail before,[14] the central quantity for R_H^0, as inferred from Eq. (11), appears to be $\langle (j_y^q)_{0\tilde{m}} \rangle_{av}$, averaged over low-lying excitations satisfying $\epsilon_{\tilde{m}}(q \to 0) \to 0$. Analyzing the latter quantity in a doped system, one could possibly gain more insight into the change of the charge-carrier character on doping, so far understood theoretically only in the high-frequency limit $R_H^* = R_H(\omega \to \infty)$.[10,12] Another challenging question is clearly the anomalous $R_H^0(T)$ dependence, which, however, is beyond our $T=0$ analysis.

The author acknowledges the financial support and the hospitality of the Max-Planck Institut für Festkörperforschung, Stuttgart, as well as of the Institut Romand des Recherches Numérique en Physiques des Matériaux (IRRMA), EPFL, Lausanne, where part of this work was performed. The author also thanks P. Horsch, A. Ramšak, and X. Zotos for fruitful discussions.

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