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Magnetic quantum oscillations in doped antiferromagnetic insulators

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Energy spectrum of electrons (holes) doped into a two-dimensional antiferromagnetic insulator is quantized in an external magnetic field of arbitrary direction. A peculiar dependence of the de Haas–van Alphen or the Shubnikov–de Haas magneto-oscillation amplitudes on the azimuthal in-plane angle from the magnetization direction and on the polar angle from the out-of-plane direction is found, which can be used as a sensitive probe of the antiferromagnetic order in the doped Mott–Hubbard, spin-density wave, and conventional band-structure insulators.

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Quantum oscillations of magnetization and resistivity with the magnetic field are of a great experimental and theoretical value providing reliable and detailed Fermi surfaces.1–3 Specifically, interest in the de Haas–van Alphen (dHvA) and the Shubnikov–de Haas (SdH) effects in almost two-dimensional Fermi liquids has recently gone through a vigorous revival due to experimental discoveries of magneto-oscillations in a few high-temperature cuprate superconductors.4–7 Their description in the framework of the local density approximation within one sublattice and the Shubnikov–de Haas magneto-oscillation amplitudes on the azimuthal in-plane angle from the magnetization,6 somewhat inconsistent with the first-principles (local density approximation) band structures and angle-resolved photoemission spectroscopy spectra of cuprates.8 The oscillations have been observed in the superconducting (vortex) state well below the upper critical field raising a doubt concerning their normal state origin.9 While a better understanding of the dHvA/SdH effects in doped antiferromagnetic insulators is generally important, it becomes particularly vital for building an adequate theory of high-temperature superconductivity since parent cuprates are antiferromagnets.

Here, using a tight-binding Hamiltonian, we quantize the energy spectrum of electrons or holes moving on the antiferromagnetic background in a two-dimensional lattice. We find particularity vital for building an adequate theory of high-temperature superconductivity since parent cuprates are antiferromagnets.

The mean-field tight-binding Hamiltonian of carriers doped into the bipartite antiferromagnetic square lattice in the external magnetic field \( \mathbf{B} \) is written as

\[
H = \sum_{ii'} \delta_{ii'} (\Delta a_i^\dagger \sigma_i a_i + \mu_B \mathbf{B} a_i^\dagger \sigma_i a_i) + t_{ij} b_i^\dagger b_j + \sum_{ij} \delta_{ij} (\Delta b_j^\dagger \sigma_j b_j - \mu_B \mathbf{B} b_j^\dagger \sigma_i b_j) + t_{jj'} b_j^\dagger b_{j'} + \sum_{ij} t_{ij} b_j^\dagger a_i
+ \text{H.c.},
\]

where \( a_i^\dagger = (a_{i1}^\dagger, a_{i2}^\dagger) \) and \( b_i^\dagger = (b_{i1}^\dagger, b_{i2}^\dagger) \) create the carrier on sites \( i \) and \( j \) of sublattices \( A \) and \( B \), respectively, with the spin \( s = \uparrow, \downarrow, \Delta \) is the carrier spin-lattice spin exchange energy (the antiferromagnetic gap), \( \delta_{ii'} \) is the Kroneker symbol, \( t_{ij} \), \( t_{jj} \), and \( t_{ij} \) are the hopping integrals, and \( \sigma_i = (\sigma_{ix}, \sigma_{iy}) \) are the Pauli matrices.

Fourier transforming the operators from the Wannier (site) to the Bloch (momentum, \( \mathbf{k} \)) representation and assuming translational invariance, the carrier energy spectrum \( E(\mathbf{k}) \) is found by diagonalizing a \( 4 \times 4 \) matrix,

\[
\begin{pmatrix}
\epsilon_k - \Delta \sigma_0 - \mu_B B \sigma_0 & \mu_B B \sigma_0 + t_k \sigma_z & \mu_B B \sigma_0 + t_k \sigma_z \\
\mu_B B \sigma_0 + t_k \sigma_z & \epsilon_k + \Delta \sigma_0 + \mu_B B \sigma_0 & \mu_B B \sigma_0 + t_k \sigma_z \\
\mu_B B \sigma_0 + t_k \sigma_z & \mu_B B \sigma_0 + t_k \sigma_z & \epsilon_k + \Delta \sigma_0 + \mu_B B \sigma_0
\end{pmatrix},
\]

where \( t_k = \sum_{jj'} \epsilon_{jj'} \exp(ik(\mathbf{j} - \mathbf{j}')) \) is the hopping energy within one sublattice and \( t_k = \sum_{jj'} \epsilon_{jj'} \exp(ik(\mathbf{j} - \mathbf{j})) \) is the intersublattice hopping energy. This matrix corresponds to the choice of the four-dimensional vector in the spin and sublattice space at fixed \( \mathbf{k} \). Here, \( B_1 \) and \( B_2 \) are transverse and longitudinal components of the magnetic field with respect to the lattice magnetization \( \mathbf{n} \) (Fig. 1), \( \sigma_0 \) is the identity matrix, and \( \mu_B \) is the Bohr magneton. There are two electron and two hole bands dispersed as

\[
E(\mathbf{k}) = \epsilon_k \pm \left[ \Delta^2 + t_k^2 \right]^{1/2} \pm \mu_B \left[ B_1^2 + \frac{t_k^2}{\Delta} \right]^{1/2}
\]

in the lowest order with respect to the field \( \mu_B B \ll \Delta \). They are split by the external magnetic field into two subbands each with anisotropic \( g \) factor, \( g = 2[\cos^2(\phi)+\sin^2(\phi)t_k^2/\Delta^2 + t_k^2] \), depending on the angle \( \phi \) between the field and the magnetization (Fig. 1).

The anisotropic \( g \) factor differs significantly from the free electron \( g_e = 2 \) near the extremum points of the valence

FIG. 1. (Color online) The azimuthal in-plane angle \( \Phi \) from the magnetization direction \( \mathbf{n} \) and the polar angle \( \Theta \) of the magnetic field \( \mathbf{B} \) from the out-of-plane direction.
and/or conductance bands, where $t_{\perp}^2 \ll \Delta^2$. According to the general principles of quantum mechanics, deviations of the $g$ factor from its classical value are related to spin-orbit interaction. The spin-orbit interaction is not included explicitly to the Hamiltonian [Eqs. (1) and (2)]. Basically, the difference originates from the spin-orbit interaction pinning the lattice magnetization along a crystal lattice direction and implicitly present in the Hamiltonian. At a relatively low doping with the Fermi energy $E_F$ near the top (bottom) of the valence (conduction) band, one can expand Eq. (3) in powers of $t/\Delta$,

$$ E(k) \approx \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} \pm \mu_B [B_\perp^2 + \gamma^2(k)B_{\parallel}^2]^{1/2}. \quad (4) $$

Here, $m_x^{-1} = 4a^2(2t'/\Delta - t')/\hbar^2$ and $m_y^{-1} = 4a^2t'/\hbar^2$ are the components of the effective mass tensor, $a$ is the lattice constant, $t$ and $t'$ are nearest and nearest next neighbor hopping integrals, respectively, and the coefficient $\gamma(k)$ is small as $\gamma(k) \approx 2\sqrt{2}k_x^2/\Delta - (E_f/\Delta)^{1/2} \ll 1$. Here, $k_x$ and $k_y$ are deviations of the wave vector from the extremum point perpendicular and parallel to the antiferromagnetic Brillouin zone boundary, respectively, and the energy of the extremum point is taken as zero.

The anisotropic $g$ factor in doped antiferromagnetic insulators was originally derived in a weak-coupling nesting model.\textsuperscript{10} Actually, the effective mass approximation [Eq. (4)] can also be derived phenomenologically by using the symmetry arguments.\textsuperscript{11} The nonunitary group of the antiferromagnetic lattice is $G = \{D_4, R_T\}$, where $D_4$ describes all rotations which remain the system invariant. Translations $T$ by a lattice period transform from one sublattice to another, changing the sign of the magnetization. Hence, these translations are multiplied by the time inversion operator $R$. Following Brazovskii and Lukyanchuk,\textsuperscript{11} one can construct the Hamiltonian of the required symmetry as

$$ H = \left( \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} \right) \hat{a}^\dagger \sigma \hat{a} + \mu_B [(B \cdot n) \hat{a}^\dagger (n \cdot \sigma) \hat{a} + \gamma(k)(B \times n) \hat{a}^\dagger (n \times \sigma) \hat{a}], \\quad (5) $$

with the electron (hole) energy spectrum [Eq. (4)]. Here, $n$ is the magnetization unit vector and $\hat{a}^\dagger = (a_\uparrow^\dagger, a_\downarrow^\dagger)$, $\hat{a}$ are creation and annihilation operators, respectively, for the spinor describing the hole (electron) band. The coefficient $\gamma(k)$ is an odd function of $k$, which is zero at the antiferromagnetic Brillouin zone boundary, so that $\gamma(k) = \gamma_k$, where $\gamma$ does not depend on $k$. The coupling to the magnetic field in this Hamiltonian is obtained noticing that the transformation $k \rightarrow k + Q$, with $Q = \pi a/a^2$ is equivalent to the rotation in the spinor space described by the matrix $n \cdot \sigma$ (Ref. 11) (here, $a = \{a, a\}$). Direct comparison of the eigenvalues of the Hamiltonian [Eq. (5)] with the spectrum [Eq. (3)] yields $\gamma = 2\sqrt{2}/\Delta$. Importantly, the symmetry arguments are applied beyond the mean-field approximation [Eq. (1)] so that spin fluctuations just renormalize the effective mass tensor and other coefficients in Eq. (4).

The orbital quantization of the spectrum [Eq. (3)] is readily obtained via the Peierls substitution,\textsuperscript{12} $k \rightarrow -i \nabla + eA$, ...
with the vector potential \( \mathbf{A}(r) \) in Eq. (2). In the lowest order with respect to \( E_F/\Delta \), we can use the effective mass approximation [Eq. (4)], which yields the conventional Fock–Landau level, with

\[
E_n = \hbar \omega \cos(\Theta)(n + 1/2) \pm \mu_s B_1,
\]

where \( \omega = eB/(m_3)^{1/2} \) is the cyclotron frequency, \( n = 0, 1, 2, \ldots \), and \( \Theta \) is the polar angle between the magnetic field and the out-of-plane direction (Fig. 1).

Now, the oscillating part of the magnetization per unit volume \( \tilde{M} \) is calculated following the standard route by applying the Poisson summation:

\[
\tilde{M} = \sum_{n=1}^{\infty} M_r \sin \frac{2\pi n F}{B}.
\]

Here,

\[
M_r = A_r(\Theta) \cos \left( \frac{\pi r (m_3)^{1/2} \tan(\Theta) \cos(\Theta)}{m_e} \right)
\]

is the amplitude of \( r \) harmonic, with

\[
A_r(\Theta) = (-1)^{n+1} \frac{eE_F \cos(\Theta)}{2\pi \hbar dr} \times R_T \left( \frac{2\pi r k_F T}{\hbar \omega \cos(\Theta)} \right) R_p \left( \frac{2\pi \Gamma}{\hbar \omega \cos(\Theta)} \right).
\]

\( F = (m_3)^{1/2} E_F/\hbar \cos(\Theta) \) is the fundamental frequency of oscillations, \( R_T(z) = z/\sinh(z) \) and \( R_p(z) = \exp(-z) \) are conventional temperature and the Dingle reduction factors, \( \Gamma/\hbar \) is the scattering rate, \( m_e \) is the free electron mass, \( d \) is the interplane distance, and \( \Phi \) is the azimuthal in-plane angle from the magnetization direction (Fig. 1). Both angles \( \Theta \) and \( \Phi \) in Eq. (8) are changing in the interval 0 \( \lesssim \Theta, \Phi \lesssim \pi/2 \). Three-dimensional corrections to the energy spectrum can be accounted for by the additional Yamaji factor, \( R_y = J_0(4\pi r T_{\perp}/\hbar \omega \cos(\Theta)) \) in Eq. (9), where \( J_0(x) \) is the zero-order Bessel function, \( T_{\perp} = t_1 J_0[k_F d \tan(\Theta)] \), \( r_1 \) is the out-of-plane hopping integral, and \( \hbar k_F \) is the Fermi momentum.

As follows from Eq. (8), the essential anisotropy of the \( g \) factor causes a strong dependence of the oscillation amplitude on the azimuthal in-plane angle of the field from the magnetization direction [Fig. 2(a)], which is absent in the ordinary nonmagnetic layered metals [Fig. 2(b)], where the magnetization amplitudes are found as

\[
M'_r = A_r(\Theta) \cos \left[ \frac{\pi r (m_3)^{1/2}}{m_e \cos(\Theta)} \right].
\]

The dependence on \( \Phi \) and \( \Theta \) [Eq. (8)] is extremely pronounced at low temperatures (compare upper panel and lower panel of Fig. 2), as also shown in Fig. 3 for some fixed azimuthal angles.

One can readily generalize our results to any shape of the Fermi surface and calculate corrections to amplitudes and fundamental frequencies of higher order in \( E_F/\Delta \) and in the magnetic field by applying the Lifshits–Kosevich quasiclassical approximation.\footnote{Within the approximation, dHvA frequencies \( F_\perp \) are determined by the extremal cross-section areas, with \( S_{\perp} \) of the two spin-split electron (or hole) Fermi surfaces, \( F_\perp = \hbar S_{\perp}/2\pi e \). Following Ref. 17, one can expand the extremal cross-section area in powers of the magnetic field, so that \( F_\perp = F \pm \alpha B \pm \beta B^2 \pm \epsilon B^3 \). Here, the second term describes the Zeeman splitting of the bands with the anisotropic \( g \) factor. It does not shift the frequency but affects the amplitude. The third term describes a small shift of the fundamental frequency \( F \) depending on the magnetic field. The last term describes a small field-dependent correction to the \( g \) factor. For example, when the field is perpendicular to the magnetization, \( B_1 = 0 \), and the effective mass approximation is applied near the X point, \( (\pi/2a, \pi/2a) \), of the antiferromagnetic Brillouin zone, one finds \( F = \hbar k_F^2/2e, \alpha = (m_3)^{1/2} y k_F/\mu_s m_e, \beta = m_3/8m_e^2 \gamma e/8 \pi^2 \hbar, \) and \( \epsilon = m_3/8m_e \gamma \pi^2 e^2/12 \pi^2 \hbar^2 k_F \), with \( \hbar k_F = [2(m_3)^{1/2} E_\perp]^{1/2} \).}

For an arbitrary field direction, one obtains, using Eq. (4) with \( \gamma = y k_F \leq 1 \),

\[
M'_r = \cos \left[ \frac{2\pi \gamma m_3 \cos^2(\Phi) + \gamma^2 k_F^2 \sin^2(\Phi)}{m_e \cos(\Theta)} \right] E[\kappa(\Phi)].
\]

Here, \( \Phi \) is the angle between the magnetic field and the magnetization (Fig. 1), \( E(\kappa) \) is the elliptic integral of the second kind, and

\[
\kappa(\Phi) = \sqrt{\frac{\gamma^2 k_F^2 \sin^2(\Phi)}{\cos^2(\Phi) + \gamma^2 k_F^2 \sin^2(\Phi)}}^{1/2}.
\]

Taking \( y = 0 \) in Eq. (11), one obtains Eq. (8), since \( \cos^2(\Phi) = \sin^2(\Theta) \cos^2(\Phi) \) and \( E[0] = \pi/2, E[1] = 1 \). The finite transverse spin susceptibility, \( y k_F = (2E_F/\Delta)^{1/2} \), only slightly blurs the strong \( \Phi \) dependence of the amplitudes (Fig. 3) if
dependence is quite different, as in Eq. (12) yields

\[ M_z = A_z(\Theta) \cos \left( \frac{2r(2m_\ell m_\ell E_p/\Delta)^{1/2}}{m_e \cos(\Theta)} \right) \]

where with a small transverse \( g \) factor. On the other hand, if the magnetic field is rotating in the \((\hat{z}, \mathbf{n})\) plane, the angular dependence is quite different,

\[ M_z = A_z(\Theta) \cos \left( \frac{\pi r(m_\ell m_\ell)^{1/2} \tan(\Theta)}{m_e} \right) \]

as in Eq. (8) with \( \Phi = 0 \).

Real antiferromagnetic solids, such as cuprates, could be disordered or twinned, so that the magnetization direction \( \mathbf{n} \) within the plane is random. Nevertheless, the dependence of \( \Delta H^2 \) amplitudes on the polar angle \( \Theta \) remains rather unconventional. Indeed, averaging Eq. (8) over all directions of \( \Phi \) from 0 to \( \pi/2 \) yields

\[ \langle M_z \rangle = A_z(\Theta) J_0 \left( \frac{\pi r(m_\ell m_\ell)^{1/2} \tan(\Theta)}{m_e} \right) \]

which is distinguishably different from the amplitudes in a nonmagnetic metal [Eq. (10)] (Fig. 4). There are known relations between oscillations in transport and thermodynamic quantities \( 1 \) at least in nonmagnetic substances. Relying on them, we expect the similar nontrivial angle dependences also in the \( \Delta H^2 \) magneto-oscillations.

In summary, we have derived the energy spectrum of electrons (holes) doped into a two-dimensional antiferromagnetic insulator in terms of all-neighbor hopping integrals of nonmagnetic lattice [Eq. (3)] and quantized it in the external magnetic field of arbitrary direction. The peculiar dependence of \( \Delta H^2 \)/\( \Delta \) magneto-oscillation amplitudes on the azimuthal in-plane angle from the magnetization direction and on the polar angle from the out-of-plane direction is found, which could be instrumental as a sensitive probe of the antiferromagnetic order in the doped Mott–Hubbard, spin-density wave, and conventional band-structure insulators.

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