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Theory of quantum magneto-oscillations in underdoped cuprate superconductors

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Abstract
Solving the Gross–Pitaevskii-type equation it is shown that the magneto-oscillations observed in the superconducting state of a few underdoped cuprates originate in the quantum interference of the vortex lattice with nanoscale crystal lattice modulations of the order parameter as revealed by scanning tunneling microscopy. The commensuration of the vortex lattice and crystal lattice have $1/B^{1/2}$ periodicity, rather than the $1/B$ periodicity of conventional normal state magneto-oscillations. Experimental conditions allowing for a resolution of quantum magneto-oscillations of two different types are outlined.

(Some figures in this article are in colour only in the electronic version)

Until recently no convincing signatures of quantum magneto-oscillations have been found in the normal state of cuprate superconductors despite significant experimental efforts. The recent observations of magneto-oscillations in kinetic [1, 2] and magnetic [3, 4] response functions of underdoped $YBa_2Cu_3O_{6.5}$ and $YBa_2Cu_4O_8$ are perhaps even more striking since many probes of underdoped cuprates including ARPES [5] clearly point to a non-Fermi-liquid normal state. Their description in the framework of the standard theory for a metal [6] has led to a very small Fermi-surface area of a few percent of the first Brillouin zone [1–4], and to a low Fermi energy of only about the room temperature [3]. Clearly such oscillations are incompatible with the first-principle (LDA) band structures of cuprates, but might be compatible with a non-adiabatic polaronic normal state of charge-transfer Mott insulators [7]. Nevertheless their observation in the *superconducting* (vortex) state well below the $H_{c2}(T)$-line [1] raises a doubt concerning their normal state origin.

Here I propose an alternative explanation of the magneto-oscillations [1–4] as emerging from the quantum interference of the vortex lattice and the checkerboard or lattice modulations of the order parameter observed by STM with atomic resolution [8]. The checkerboard effectively pins the vortex lattice, when the period of the latter $\lambda = (\pi\hbar/eB)^{1/2}$ is commensurate with the period of the checkerboard lattice, a. The condition $\lambda = Na$, where N is a large integer, yields $1/B^{1/2}$ periodicity of the response functions, rather than $1/B$ periodicity of conventional normal state magneto-oscillations. To illustrate the point one can apply the Gross–Pitaevskii (GP)-type equation for the superconducting order parameter $\psi(\mathbf{r})$, generalized by us [9] for a charged Bose liquid (CBL), since many observations including a small coherence length point to a possibility that underdoped cuprate superconductors may not be conventional Bardeen–Cooper–Schrieffer (BCS) superconductors, but rather derive from the Bose–Einstein condensation (BEC) of real-space pairs, such as mobile bipolarons [10, 11],

$$\left[E(-\mathrm{i}\hbar\nabla + 2e\mathbf{A}) - \mu + \int \mathrm{d}\mathbf{r}' V(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2\right]\psi(\mathbf{r}) = 0. \tag{1}$$

Here $E(\mathbf{K})$ is the center-of-mass pair dispersion and the Peierls substitution, $\mathbf{K} \Rightarrow -\mathrm{i}\hbar\nabla + 2e\mathbf{A}$ is applied with the vector potential $\mathbf{A}(\mathbf{r})$. The integro-differential equation (1) is quite different from the Ginzburg–Landau [12] and Gross–Pitaevskii [13] equations, describing the order parameter in the BCS and neutral superfluids, respectively. In the continuum (effective mass) approximation, $E(\mathbf{K}) = \hbar^2K^2/2m^{**}$, with the long-range Coulomb repulsion between double charged bosons, $V(\mathbf{r}) = V_c(\mathbf{r}) = 4e^2/\epsilon_0 r$, this equation describes a single vortex with a *charged* core, figure 1, and the coherence length roughly the same as the screening radius, $\xi = (\hbar/2^{1/2}m^{**}\omega_p)^{1/2}$. Here $\omega_p = (16\pi n_s e^2/\epsilon_0 m^{**})^{1/2}$ is the CBL plasma frequency, ϵ_0 the static dielectric constant of the host lattice, m^{**} the boson mass, and n_s is the average

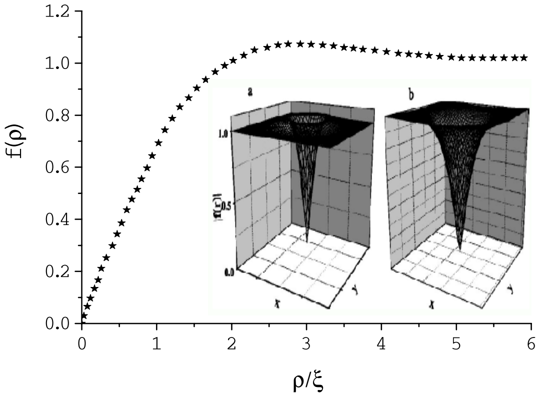

Figure 1. The order parameter profile $f(\rho) = \psi(\mathbf{r})/n_s^{1/2}$ of a single vortex in CBL [9] (symbols). Inset: CBL vortex (a) [9, 15] compared with the Abrikosov vortex (b) [14] (here $\rho = [x^2 + y^2]^{1/2}$).

condensate density. The chemical potential is zero, $\mu = 0$, if one takes into account the Coulomb interaction with a neutralizing homogeneous charge background, or defines the zero-momentum Fourier-component of $V_c(\mathbf{r})$ as zero. Each vortex carries one flux quantum, $\phi_0 = \pi\hbar/e$, but it has an unusual core, figure 1(a), [9], due to a local charge redistribution caused by the magnetic field, different from the conventional vortex [14], figure 1(b). Remarkably, the coherence length turns out very small, $\xi \approx 0.5$ nm with the material parameters typical for underdoped cuprates, $m^{**} = 10m_e$, $n_s = 10^{21}$ cm^{-3} and $\epsilon_0 = 100$. The coherence length ξ is so small at low temperatures, that the distance between two vortices remains large compared with the vortex size, $\lambda \gg \xi$, [15] in any laboratory field reached so far [1–4]. It allows us to write down the vortex-lattice order parameter, $\psi(\mathbf{r}) = \psi_{vl}(\mathbf{r})$, as

$$\psi_{vl}(\mathbf{r}) \approx n_s^{1/2}\left[1 - \sum_j \phi(\mathbf{r} - \mathbf{r}_j)\right], \qquad (2)$$

where $\phi(\mathbf{r}) = 1 - f(\rho)$, and $\mathbf{r}_j = \lambda\{n_x, n_y\}$ with $n_{x,y} = 0, \pm1, \pm2, \ldots$. (if, for simplicity, we take the square vortex lattice). The function $\phi(\rho)$ is linear well inside the core, $\phi(\rho) \approx 1$–$1.52\rho/\xi(\rho \ll \xi)$, and it has a small negative tail, $\phi(\rho) \approx -4\xi^4/\rho^4$ outside the core when $\rho \gg \xi$, figure 1 [9]. In the continuum approximation with the Coulomb interaction alone the magnetization of CBL follows the standard logarithmic law, $M(B) \propto \ln 1/B$ without any oscillations since the magnetic field profile is the same as in the conventional vortex lattice [14]. However, more often than not the center-of-mass Bloch band of preformed pairs, $E(\mathbf{K})$, has its minima at some finite wave vectors $\mathbf{K} = \mathbf{G}$ of their center-of-mass Brillouin zone [10, 16]. Near the minima the GP equation (1) is written as

$$\left[\frac{(-i\hbar\nabla - \hbar\mathbf{G} + 2e\mathbf{A})^2}{2m^{**}} - \mu\right]\psi(\mathbf{r}) + \int d\mathbf{r}' V(\mathbf{r} - \mathbf{r}')|\psi(\mathbf{r}')|^2\psi(\mathbf{r}) = 0, \qquad (3)$$

with the solution $\psi(\mathbf{r}) = \psi_{\mathbf{G}}(\mathbf{r}) \equiv e^{i\mathbf{G}\cdot\mathbf{r}}\psi_{vl}(\mathbf{r})$, if the interaction is the long-range Coulomb one, $V(\mathbf{r}) = V_c(\mathbf{r})$.

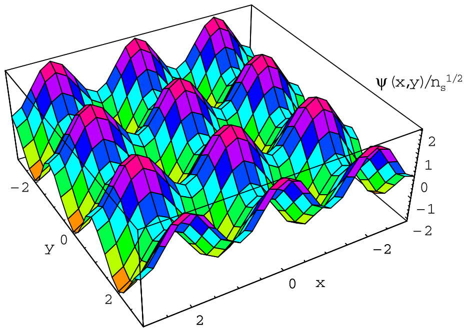

Figure 2. The checkerboard d-wave order parameter of CBL [17] on the square lattice in zero magnetic field (coordinates x, y are measured in units of a).

In particular, a nearest-neighbor (nn) approximation for the hopping of intersite bipolarons between oxygen p-orbitals on the CuO_2 2D lattice yields four generate states $\psi_{\mathbf{G}}$ with $\mathbf{G}_i = \{\pm2\pi/a_0, \pm2\pi/a_0\}$, where a_0 is the lattice period [16]. Their positions in the Brillouin zone move towards Γ point beyond the nn approximation. The true ground state is a superposition of four degenerate states, respecting time-reversal and parity symmetries [17],

$$\psi(\mathbf{r}) = An_s^{1/2}\left[\cos(\pi x/a) \pm \cos(\pi y/a)\right]\psi_{vl}(\mathbf{r}). \qquad (4)$$

Here we use the reference frame with x and y axes along the nodal directions and $a = 2^{-3/2}a_0$. Two 'plus/minus' coherent states, equation (4), are physically identical since they are related via a translation transformation, $y \Rightarrow y + a$. Normalizing the order parameter by its average value $\langle\psi(\mathbf{r})^2\rangle = n_s$ and using $(\xi/\lambda)^2 \ll 1$ as a small parameter yield the following 'minus' state amplitude, $A \approx 1 - N\sum_{n=0}^{\infty} 2[\tilde{\phi}_1(2^{1/2}\pi/a) + \tilde{\phi}_2(2^{1/2}\pi/a)]\delta_{n,R/2} + [\tilde{\phi}_1(2\pi/a) + \tilde{\phi}_2(2\pi/a)]\delta_{n,R}$ for the square vortex lattice[1] with the reciprocal vectors $\mathbf{g} = (2\pi/\lambda)\{n_x, n_y\}$. Here $\delta_{n,R}$ is the Kroneker symbol, $R = \lambda/a$ is the ratio of the vortex-lattice period to the checkerboard period ($n = 0, 1, 2, \ldots$.), $N = BS/\phi_0$ is the number of flux quanta in the area S of the sample, and $\tilde{\phi}_k(q) = (2\pi/S)\int_0^\infty d\boldsymbol{\rho}\, \rho J_0(\rho q)\phi^k(\rho)$ is the Fourier transform of k's power of $\phi(\rho)$, where $J_0(x)$ is the zero-order Bessel function.

The order parameter $\psi(\mathbf{r})$, equation (4) has the d-wave symmetry changing sign in real space, when the lattice is rotated by $\pi/2$. This symmetry is due to the pair center-of-mass energy dispersion with the four minima at $\mathbf{K} \neq 0$, rather than due to a specific symmetry of the pairing potential. It also reveals itself as a *checkerboard* modulation of the carrier density with two-dimensional patterns in zero magnetic field, figure 2, as predicted by us [17] prior to their observations [8]. Solving the Bogoliubov–de Gennes equations with the order parameter, equation (4), yields the real-space checkerboard modulations of the single-particle density of states [17], similar to those observed by STM in cuprate superconductors.

[1] Results for the square vortex lattice are also applied to the triangular lattice. Moreover there is a crossover from triangular to square coordination of vortices with increasing magnetic field in the mixed phase of cuprate superconductors [18].

Now we take into account that the interaction between composed pairs includes a short-range repulsion along with the long-range Coulomb one, $V(\mathbf{r}) = V_c(\mathbf{r}) + v\delta(\mathbf{r})$ [16]. At sufficiently low carrier density the short-range repulsion is a perturbation to the ground state, equation (4), if the corresponding characteristic length, $\xi_h = \hbar/(2m^{**}n_s v)^{1/2}$ is large compared with the coherence length ξ, related to the long-range Coulomb repulsion, $\xi_h \gg \xi$. The short-range repulsion constant v is roughly the pair bandwidth w of the order of 100 meV times the unit cell volume, $v \approx wa_0^3$ [16]. Using this estimate one can readily show that the perturbation treatment of the short-range interaction is justified for any relevant density of pairs, if $\epsilon_0 \lesssim 10^3$. On the other hand, a strong short-range interaction could affect both the checkerboard and the vortex lattices, if ξ_h is comparable with ξ and a. Importantly the short-range repulsion energy of CBL, $U = (v/2)\langle\psi(\mathbf{r})^4\rangle$, has a part, ΔU, oscillating with the magnetic field as

$$\frac{\Delta U}{U_0} \approx N \sum_{n=0}^{\infty} \left[A_1\delta_{n,R/2} + A_2\delta_{n,R} + A_3\delta_{n,2R}\right], \qquad (5)$$

where $U_0 = vn_s^2/2$ is the hard-core energy of a homogeneous CBL, and the amplitudes are proportional to the Fourier transforms of $\phi(\rho)$ as

$$A_1 = 15\tilde{\phi}_1(2^{1/2}\pi/a) - 45\tilde{\phi}_2(2^{1/2}\pi/a) + 24\tilde{\phi}_3(2^{1/2}\pi/a) - 6\tilde{\phi}_4(2^{1/2}\pi/a) + 8\tilde{\phi}_1(10^{1/2}\pi/a) - 12\tilde{\phi}_2(10^{1/2}\pi/a) + 8\tilde{\phi}_3(10^{1/2}\pi/a) - 2\tilde{\phi}_4(10^{1/2}\pi/a),$$

$$A_2 = -(23/2)\tilde{\phi}_1(2\pi/a) + (57/2)\tilde{\phi}_2(2\pi/a) - 16\tilde{\phi}_3(2\pi/a) + 4\tilde{\phi}_4(2\pi/a) - 12\tilde{\phi}_1(2^{3/2}\pi/a) + 9\tilde{\phi}_2(2^{3/2}\pi/a) - 6\tilde{\phi}_3(2^{3/2}\pi/a) + 3\tilde{\phi}_4(2^{3/2}\pi/a),$$

and

$$A_3 = -\tilde{\phi}_1(4\pi/a) + (3/2)\tilde{\phi}_2(4\pi/a) - \tilde{\phi}_3(4\pi/a) + (1/4)\tilde{\phi}_4(4\pi/a).$$

Unavoidable disorder in cuprates and temperature fluctuations induce some randomness in the vortex-lattice period, λ. Hence one has to average ΔU over R with the Gaussian distribution, $G(R) = \exp[-(R - \bar{R})^2/\gamma^2]/\gamma\pi^{1/2}$ around an average $\bar{R}$ with the width $\gamma \ll \bar{R}$, which could depend on temperature. Then using the Poisson summation formula yields

$$\frac{\Delta U}{U_0} = N \sum_{k=0}^{\infty} A_1 \mathrm{e}^{-\pi^2k^2\gamma^2/16}\cos(\pi k\bar{R}) + A_2\mathrm{e}^{-\pi^2k^2\gamma^2/4}\cos(2\pi k\bar{R}) + A_3\mathrm{e}^{-\pi^2k^2\gamma^2}\cos(4\pi k\bar{R}). \quad (6)$$

The oscillating correction to the magnetic susceptibility, $\Delta\chi(B) = -\partial^2\tilde{\Omega}/\partial B^2$, is strongly enhanced due to high oscillating frequencies in equation (6). Since the superfluid has no entropy we can use ΔU as the quantum correction to the thermodynamic potential $\tilde{\Omega}$ even at finite temperatures below $T_c(B)$. Differentiating twice the first harmonic ($k = 1$) of the first lesser damped term in equation (6) we obtain

$$\Delta\chi(B) \approx \chi_0 \mathrm{e}^{-\delta^2 B_0/16B}\left(\frac{B_0}{B}\right)^2 \cos(B_0/B)^{1/2}, \qquad (7)$$

where $\chi_0 = U_0SA_1e^2a^2/4\pi^4\hbar^2$ is a temperature-dependent amplitude, proportional to the condensate density squared, $B_0 = \pi^3\hbar/ea^2 = 8\pi^3\hbar/ea_0^2$ is a characteristic magnetic field, which is approximately 1.1×10^6 T for $a_0 \approx 0.38$ nm, and γ is replaced by $\gamma \equiv \delta\bar{R}$ with the relative distribution width δ. Assuming that $\xi \gtrsim a$, so that the amplitude A_1 is roughly a^2/S, the quantum correction $\Delta\chi$, equation (7), is of the order of wx^2/B^2, where x is the density of holes per unit cell. It is smaller than the conventional normal state (de Haas-van Alphen) correction, $\Delta\chi_{\mathrm{dHvA}} \sim \mu/B^2$ [6], for a comparable Fermi-energy scale $\mu = wx$, since $x \ll 1$ in the underdoped cuprates.

Different from normal state dHvA oscillations, which are periodic versus $1/B$, the vortex-lattice oscillations, equation (7) are periodic versus $1/B^{1/2}$. They are quasiperiodic versus $1/B$ with a field-dependent frequency $F = B_0(B/B_0)^{1/2}/2\pi$, which is strongly reduced relative to the conventional-metal frequency ($\approx B_0/2\pi$) since $B \ll B_0$, as observed in the experiments [1–3]. The quantum correction to the susceptibility, equation (7) fits well the oscillations in $YBa_2Cu_3O_{6.5}$ [4], figure 3 (upper panel). Importantly, if the vortex lattice has two domains with different coordination of vortices (see footnote 1), then there are two resonating fields, B_0 of the square lattice and $B_1 = 2B_0/3$ of the triangular lattice, causing beats in the oscillations, as observed in [3] at low temperatures in $YBa_2Cu_4O_8$ (figure 3, middle panel). A pinning force on the vortex lattice, F_p, due to the checkerboard modulations is proportional to $\partial U/\partial a$. Hence the oscillating part of the Hall and longitudinal resistivity is proportional to $F_p/B \propto \exp(-\delta^2B_0/16B)(B_0/B)^{1/2}\sin(B_0/B)^{1/2}$, which fits the oscillatory part of the Hall resistance [1] rather well, figure 3 (lower panel). The oscillations amplitudes, proportional to $n_s^2\exp(-\delta^2B_0/16B)$ decay with increasing temperature since the randomness of the vortex lattice, δ, increases, and the Bose-condensate evaporates.

In summary, I propose that the magneto-oscillations in underdoped cuprate superconductors [1–3] result from the quantum interference of the vortex lattice and the lattice modulations of the order parameter, figure 2, playing a role of the periodic pinning grid. The magnetic length, $\lambda \gtrsim 5$ nm, remains larger than the zero-temperature in-plane coherence length, $\xi \lesssim 2$ nm, measured independently, in any field reached in [1–3]. Hence the magneto-oscillations are observed in the vortex (mixed) state well below the upper critical field, rather than in the normal state, as also confirmed by the *negative* sign of the Hall resistance [1]. It is well known, that in 'YBCO' the Hall conductivities of vortexes and quasiparticles have opposite sign causing the sign change in the Hall effect in the mixed state [19]. Also there is a substantial magnetoresistance [2], which is a signature of the flux flow regime rather than of the normal state. Hence it would be rather implausible if such oscillations have a normal state origin due to small electron Fermi-surface pockets [4] with the characteristic wavelength of electrons larger than the widely accepted coherence length. In any case our expression (7), describes the oscillations as well as the standard Lifshitz–Kosevich formula of dHvA and SdH effects [1–4]. The difference of these two dependences could be resolved in

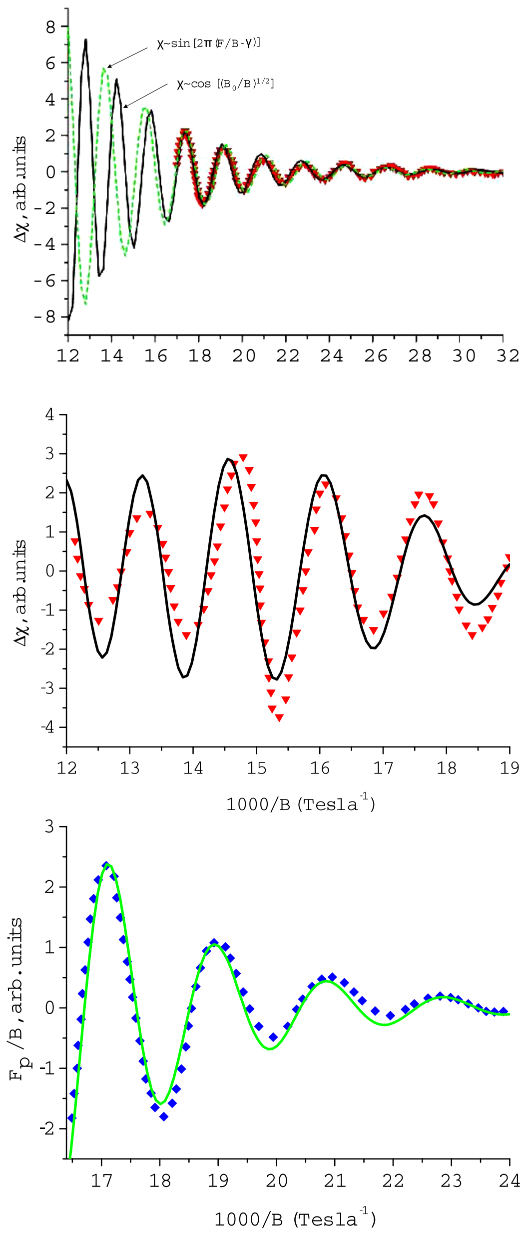

Figure 3. Quantum corrections to the vortex-lattice susceptibility versus $1/B$, equation (7) (solid line, $B_0 = 1.000 \times 10^6$ T, $\delta = 0.06$) compared with oscillating susceptibility of $YBa_2Cu_3O_{6.5}$ (symbols) and with the conventional normal state oscillations (dashed line) [4] at $T = 0.4$ K, upper panel. Middle panel: oscillating susceptibility of $YBa_2Cu_4O_8$ (symbols [3]) at $T = 0.53$ K compared with the theory (solid line, $B_0 = 1.190 \times 10^6$ T, $\delta = 0.07$), where 20% of the triangular vortex-lattice susceptibility added to the square lattice one. Lower panel: quantum corrections to the current, proportional to F_p/B ($B_0 = 0.853 \times 10^6$ T and $\delta = 0.1$, solid line) compared with the oscillatory part of the Hall resistance in the mixed state of $YBa_2Cu_3O_{6.5}$ (symbols [1]) at 1.5 K.

ultrahigh magnetic fields as shown in figure 3, upper panel. In case it turns out that the magneto-oscillations are conventional dHvA normal state oscillations, then the low Fermi energy will support the polaronic non-adiabatic superconductivity in cuprates [7].

While our theory utilizes GP-type equation for hard-core charged bosons [9], the quantum interference of vortex and crystal lattice modulations of the order parameter is quite universal extending well beyond equation (1) independent of a particular pairing mechanism. It can also take place in the standard BCS superconductivity at $B < H_{c2}$, but hardly be observed because of much lower value of H_{c2} in conventional superconductors resulting in a very small damping factor, $\propto \exp(-\delta^2 B_0/16B) \lll 1$.

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References

[1] Doiron-Leyraud N, Proust C, LeBoef D, Levalois J, Bonnemaison J-B, Liang R, Bonn D A, Hardy W N and Taillefer L 2007 *Nature* **447** 565
[2] Bangura A F, Fletcher J D, Carrington A, Levallois J, Nardone M, Vignolle B, Heard P J, Doiron-Leyraud N, LeBoeuf D, Taillefer L, Adachi S, Proust C and Hussey N E 2008 *Phys. Rev. Lett.* **100** 047004
[3] Yelland E A, Singleton J, Mielke C H, Harrison N, Balakirev F F, Dabrowski B and Cooper J R 2008 *Phys. Rev. Lett.* **100** 047003
[4] Jaudet C, Vignolles D, Audouard A, Levallois J, LeBoeuf D, Doiron-Leyraud N, Vignolle B, Nardone M, Zitouni A, Liang R, Bonn D A, Hardy W N, Taillefer L and Proust C 2007 *Preprint* 0711.3559
[5] Damascelli A, Hussain Z and Shen Z-X 2003 *Rev. Mod. Phys.* **75** 473
[6] Schoenberg D 1984 *Magnetic Oscillations in Metals* (Cambridge: Cambridge University Press)
[7] Alexandrov A S 2001 *Physica* C **363** 231
[8] Vershinin M, Misra S, Ono S, Abe Y, Ando Y and Yazdani A 2004 *Science* **303** 1995
[9] Alexandrov A S 1999 *Phys. Rev.* B **60** 14573
[10] Alexandrov A S 1996 *Phys. Rev.* B **53** 2863
[11] Devreese J T 1996 *Encyclopedia of Applied Physics* vol 14 (New York: VCH) p 383
[12] Ginzburg V L and Landau L D 1950 *Zh. Eksp. Teor. Fiz.* **20** 1064
[13] Gross E P 1961 *Nuovo Cimento* **20** 454
Pitaevskii L P 1961 *Zh. Eksp. Teor. Fiz.* **40** 646
Pitaevskii L P 1961 *Sov. Phys.—JETP* **13** 451 (Engl. Transl.)
[14] Abrikosov A A 1957 *Zh. Eksp. Teor. Fiz.* **32** 1442
Abrikosov A A 1957 *Sov. Phys.—JETP* **5** 1174 (Engl. Transl.)
[15] Kabanov V V and Alexandrov A S 2005 *Phys. Rev.* B **71** 132511
[16] Alexandrov A S and Kornilovitch P E 2002 *J. Phys.: Condens. Matter* **14** 5337
[17] Alexandrov A S 1998 *Physica* C **305** 46
[18] Gilardi R *et al* 2002 *Phys. Rev. Lett.* **88** 217003
Brown S P *et al* 2004 *Phys. Rev. Lett.* **92** 067004
[19] Harris J M, Krishana K, Ong N P, Cagnon R and Taillefer L 1996 *J. Low Temp. Phys.* **105** 877