Magnetotransport in d-wave density waves

Balázs Dóra¹, Kazumi Maki²,³ and Attila Virosztek¹,⁴

¹ Department of Physics, Budapest University of Technology and Economics, H-1521 Budapest, Hungary
² Department of Physics and Astronomy, University of Southern California, Los Angeles CA 90089-0484, USA
³ Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany
⁴ Research Institute for Solid State Physics and Optics, P.O.Box 49, H-1525 Budapest, Hungary

PACS. 71.45.Lr – Charge-density-wave systems.
PACS. 72.15.Eb – Electrical and thermal conduction in crystalline metals and alloys.
PACS. 74.72.Bk – Y-based cuprates.

Abstract. – Angle dependent magnetoresistance (ADMR) and giant Nernst effect are hallmarks of unconventional density waves (UDW). Here these transport properties for d-wave density wave (d-DW) are computed for quasi-two-dimensional systems. The present theory describes ADMR observed in the pseudogap phase of Y₀.₆₈Pr₀.₃₂Ba₂Cu₃O₇ and CeCoIn₅ single crystals very satisfactorily.

Introduction. – As is well known, many electronic systems like high Tₙ cuprates, heavy fermion systems and organic conductors exhibit the pseudogap phenomenon or so-called non-Fermi liquid behaviour [1]. Further, several people proposed that the pseudogap phase in the underdoped region of high Tₙ cuprates is d-wave density wave [2–4]. We have shown recently that the giant Nernst effect seen in the pseudogap region of LSCO, YBCO and Bi2212 [5–8] can be interpreted in terms of d-wave density wave (d-DW) [9]. Also the Pauli limiting behaviour of d-DW in the c-axis resistance [10, 11] indicates that it is d-wave charge density wave and not d-wave spin density wave [12].

Also there are many parallels between organic superconductor κ-(ET)₂ salts [13], heavy fermion superconductor CeCoIn₅ and high Tₙ cuprate superconductors. In particular the quasi-two-dimensional Fermi surface, the layered structure, d-wave superconductivity [14,15] and the presence of pseudogap are noteworthy. Very recently d-DW in the pseudogap phase of CeCoIn₅ was established through the giant Nernst effect [16,17] and the angle dependent magnetoresistance [18].

As noted by Nersesyan et al. [19,20], the quasiparticle spectrum in unconventional density wave is quantized in a magnetic field. This Landau quantization gives rise to the spectacular angle dependent magnetoresistance (ADMR) and giant Nernst effect as reviewed in Ref. [21].

© EDP Sciences
These are exploited to identify the presence of UDW in α-(ET)$_2$ KH$_5$(SCN)$_4$ [22], and Bechgaard salts (TMTSF)$_2$X with X=PF$_6$ and ReO$_4$ [23, 24].

In spite of these successes earlier works are limited to quasi-one-dimensional systems. In this paper we shall first consider the Landau quantization of d-wave density waves. Then the ADMR data on Y$_{0.68}$Pr$_{0.32}$Ba$_2$Cu$_3$O$_7$ [25] and in CeCoIn$_5$ are reanalyzed. Y$_{0.68}$Pr$_{0.32}$Ba$_2$Cu$_3$O$_7$ becomes superconducting at 55 K, above it pseudogap behaviour is seen. Also the gap structure of d-DW on the quasi-two-dimensional Fermi surface can be fully exploited in CeCoIn$_5$.

**Landau quantization in d-DW.** The quasiparticle energies in a d-wave density wave are determined from the poles of the Nambu Green’s function [26]:

$$\begin{align*}
G^{-1}(\omega, \mathbf{k}) &= \omega - \xi(\mathbf{k})\rho_1 - \eta(\mathbf{k}) - \Delta(\mathbf{k})\rho_1, \\
\text{where } \rho_1 &\text{'s are the Pauli's matrices operating on the spinor space. These energies are assumed to describe the system in the pseudogap regime, above } 55 \text{ K in } Y_{0.68}\text{Pr}_{0.32}\text{Ba}_2\text{Cu}_3\text{O}_7, \text{ although similar Green's function can be obtained in the superconducting region. The basic difference between the two stems from the fact that the spinor space in superconductors consists of } (c_{k,x}, c_{k,y}^+), \text{ while in DW } (c_{k,x}, c_{-k,y}^+).\text{ For a d-wave density wave, we can further assume } \\
\Delta(\mathbf{k}) &= \Delta \cos(2\phi) \text{ or } \Delta \sin(2\phi) \text{ with } \tan(\phi) = k_y/k_x, \\
\varepsilon(\mathbf{k}) &= -2t(\cos(ak_x) + \cos(ak_y)) - \mu, \\
\eta(\mathbf{k}) &= \frac{\varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k} - \mathbf{Q})}{2} = -\mu, \\
\xi(\mathbf{k}) &= \frac{\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k} - \mathbf{Q})}{2},
\end{align*}$$

$\mu$ the chemical potential, which acts as imperfect nesting, $\mathbf{Q}$ is the best nesting vector. Since we are only interested in the low energy excitation around the nodes of gap, we can use a linearized version of the spectrum valid around these points as $\xi(\mathbf{k}) = v(k - k_0) + \theta \cos(c k_z)$ with $v$ and $v'$ the in-plane and c-axis Fermi velocities. Here dispersion perpendicular to the plane was also taken into account. In the presence of magnetic field $\mathbf{B}$ within the x'-z plane, where $x' = \hat{x} \cos(\phi) + \hat{y} \sin(\phi)$ and tilted by $\theta$ from the z axis, the effect of magnetic field is introduced in eq. (1) through the Peierls-Onsager substitution $\mathbf{k} = \mathbf{k} + e\mathbf{A}$ and

$$A = B(y \cos(\phi) - x \sin(\phi)(\hat{z} \sin(\theta) - (\hat{x} \cos(\phi) + \hat{y} \sin(\phi)) \cos(\theta)).$$

Then the quasiparticle spectrum is determined by

$$E\Psi = \left\{ \begin{array}{l}
-veB \cos(\theta)(\cos(\phi)y - \sin(\phi)x) + \frac{v'}{c} \cos(ceB \sin(\theta))(\cos(\phi)y - \sin(\phi)x) + \chi \\
-\mu - iv_2\rho_1 \partial_y \end{array} \right\} \Psi,$$

where $v_2/v = \Delta/E_F$ and we assume here $\Delta(\mathbf{k}) = \Delta \sin(2\phi)$ or $d_{xy}$-wave DW for simplicity. Further for CeCoIn$_5$ we have $c^2eH \sim 10^{-2}$ for $H=1$ T. Then $\cos(ceB \sin(\theta))(\cos(\phi)y - \sin(\phi)x) + \chi \approx \pm ceB \sin(\theta))(\cos(\phi)y - \sin(\phi)x)$ for $\gamma = \pm \pi/2$. Then the solution is easily obtained following Weisskopf [27, 28]. These are four branches of the quasiparticles; two branches around the Dirac cone $[1,0,0]$ and others at $[0,1,0]$ with

$$\begin{align*}
E_{1\uparrow}^+ &= \pm \sqrt{2neBv_2} \left| v \cos(\theta) \cos(\phi) - v' \sin(\theta) \right| \left| \cos(\phi) \right| - \mu \\
E_{2\downarrow}^+ &= \pm \sqrt{2neBv_2} \left| v \cos(\theta) \cos(\phi) + v' \sin(\theta) \right| \left| \cos(\phi) \right| - \mu \\
E_{3\downarrow}^+ &= \pm \sqrt{2neBv_2} \left| v \cos(\theta) \sin(\phi) - v' \sin(\theta) \right| \left| \sin(\phi) \right| - \mu \\
E_{4\uparrow}^+ &= \pm \sqrt{2neBv_2} \left| v \cos(\theta) \sin(\phi) + v' \sin(\theta) \right| \left| \sin(\phi) \right| - \mu.
\end{align*}$$
Here \( n = 0, 1, 2 \ldots \). Except for the \( n = 0 \) Landau level, each Landau level is double degenerated. Also the corresponding Landau wavefunctions are readily constructed as in Ref. [21]. In particular

\[
\Psi_0 \sim \exp \left[ \frac{1}{2} eBv}{v_2} \cos(\theta) \pm g \sin(\theta) \right] \left( y \cos(\phi) - x \sin(\phi) \right)^2 \tag{11}
\]

from the Dirac cone at \([1,0,0]\) and

\[
\Psi_0 \sim \exp \left[ \frac{1}{2} eBv}{v_2} \cos(\theta) \pm g \sin(\theta) \right] \left( y \cos(\phi) - x \sin(\phi) \right)^2 \tag{12}
\]

from the one at \([0,1,0]\).

From these Landau levels, the thermodynamics as well as the magnetotransport properties are readily deduced.

**Angular dependent magnetoresistance.** We shall limit ourselves to two limiting cases: A. \( \sigma_{xx} \) in a magnetic field in the \( z-y \) plane.

Here we take the angle \( B \) makes from the \( c \)-axis is \( \theta \). Then the quasiparticle spectra are given by eqs. \[10\] with \( \phi = \pi/2 \). So \( E_{1n}^\pm \) and \( E_{2n}^\pm \) reduces to \( -\mu \), the same as the \( n = 0 \) Landau levels, while \( E_{13n}^\pm \) and \( E_{4n}^\pm \) are given by

\[
E_{3n}^\pm = \pm \sqrt{2neBv^2 \left| v \cos(\theta) - v' \sin(\theta) \right| - \mu} \tag{13}
\]

\[
E_{4n}^\pm = \pm \sqrt{2neBv^2 \left| v \cos(\theta) + v' \sin(\theta) \right| - \mu}. \tag{14}
\]

Then the electric conductivity is given by

\[
\sigma(B, \theta) = \sum_n \sigma_n \text{sech}^2 \left( \frac{1}{2} \beta E_n \right), \tag{15}
\]

where \( E_n \)'s are the energy of all the Landau levels. The above equation can be obtained by following the reasoning of ref. [29]. This expression is somewhat different from the one we proposed earlier [21], but we think more appropriate when \( \mu \neq 0 \). When \( \beta|E_{31}| \gg 1 \) and \( \beta|E_{41}| \gg 1 \), only the lowest levels contribute significantly, and eq. \[15\] is simplified as

\[
\sigma(B, \theta) = 6\sigma_0 \text{sech}^2 \left( \frac{1}{2} \zeta_0 \right) + 2\sigma_1 \left( \text{sech}^2 \left( \frac{1}{2} (x_1 - \zeta_0) \right) + \text{sech}^2 \left( \frac{1}{2} (x_2 - \zeta_0) \right) + \right.
\]

\[
\left. \text{sech}^2 \left( \frac{1}{2} (x_1 + \zeta_0) \right) + \text{sech}^2 \left( \frac{1}{2} (x_2 + \zeta_0) \right) \right) = 4\sigma_0 (1 + \cosh(\zeta_0))^{-1} +
\]

\[
+ 8\sigma_1 \left[ 1 + \cosh(x_1) \cosh(\zeta_0) \right] + 1 + \cosh(x_2) \cosh(\zeta_0) \left( \frac{\cosh(x_1) + \cosh(\zeta_0)}{\cosh(x_1) + \cosh(\zeta_0)} \right)^2, \tag{16}
\]

where \( \zeta_0 = \beta \mu, x_1 = \beta \sqrt{2eBv^2 \left| v \cos(\theta) - v' \sin(\theta) \right|} \) and \( x_2 = \beta \sqrt{2eBv^2 \left| v \cos(\theta) + v' \sin(\theta) \right|} \). In figs. \[10\] we show the in-plane and out of plane angle dependent magnetoresistance data from \( \text{Y}_0.68\text{Pr}_{0.32}\text{Ba}_2\text{Cu}_3\text{O}_7 \) by Sandu et al. [25] together with our fitting based on eq. \[16\]. At 52 K, the applied magnetic field (14 T) can be strong enough to destroy superconductivity and drive the systems into the pseudogap regime, while at 105 K the presence of pseudogap is still felt.

In high \( T_c \) cuprates, \( v'/v \ll 1 \), so we have assumed \( x_1 = x_2 \). From the fittings, using the universal Fermi velocity \[30\] \( v = 2.3 \times 10^7 \text{ cm/s} \), we obtain \( v_2 = 1.6 \times 10^6 \text{ cm/s} \) and \( \mu = 40 - \)
Fig. 1 – The relative change of the in-plane magnetoresistance of Y$_{0.68}$Pr$_{0.32}$Ba$_2$Cu$_3$O$_7$ [25] is plotted as a function of angle $\theta$ at $H=14$ T for $T=52$ K. The solid line is fit based on eq. 16.

Fig. 2 – The relative change of the in-plane magnetoresistance of Y$_{0.68}$Pr$_{0.32}$Ba$_2$Cu$_3$O$_7$ [25] is plotted as a function of angle $\theta$ at $H=14$ T for $60$ K (circles), $65$ K (pentagrams) together with our fit based on eq. 16.

60 K. Since $E_F \sim 5000$ K in high $T_c$ cuprate we extract $\Delta = 360$ K for Y$_{0.68}$Pr$_{0.32}$Ba$_2$Cu$_3$O$_7$ from $v_2/v = \Delta/E_F$. This value is consistent with a recent c-axis optical conductivity data on underdoped YBCO [31]. Here $\Delta$ is the maximal gap of d-DW in the non-Fermi liquid or pseudogap phase of Y$_{0.68}$Pr$_{0.32}$Ba$_2$Cu$_3$O$_7$. The small deviations of the theory from the experimental results around $\theta = 90^\circ$ originates from the collapse of all the Landau levels in the $v'/v \ll 1$ limit, as seen from eqs. 13 and 14.

B. ADMR in a magnetic field in the x-y plane.

For a d-DW it is of crucial importance to see if $d_{x^2-y^2}$-wave density wave or $d_{xy}$-wave density waves are realized. For the d-DW in the pseudogap phase in high $T_c$ cuprates the angle resolved photoemission spectra (ARPES) [32] tells it is $d_{x^2-y^2}$-wave in high $T_c$ cuprates. On the other hand $d_{xy}$-wave appears to be more consistent with CeCoIn$_5$, as suggested by Aoki et al. [33]. $\sigma_{zz}(B, \phi)$ in a rotating field within the a-b plane is given by

$$\sigma_{zz}(B, \phi) = 16\sigma_0 (1 + \cosh(\zeta_0))^{-1} + 8\sigma_1 \left[ \frac{1 + \cosh(x_1) \cosh(\zeta_0)}{(\cosh(x_1) + \cosh(\zeta_0))^2} + \frac{1 + \cosh(x_2) \cosh(\zeta_0)}{(\cosh(x_2) + \cosh(\zeta_0))^2} \right],$$

(17)

where $x_1 = \beta \sqrt{2eBv_2v'\sin(\phi)}$ and $x_1 = \beta \sqrt{2eBv_2v'\cos(\phi)}$ In fig. 3 the $\phi$ dependence of eq. 17 is shown for parameters typical for CeCoIn$_5$ [18]. Here we assumed $d_{xy}$-wave DW. For $d_{x^2-y^2}$-wave DW, the same expression applies if we shift $\phi$ to $\phi + \pi/4$. By varying the parameters, the small dip at $90^\circ$ can be sharpened, and the broad bump at $45^\circ$ can be weakened, but these two features always remain present.
Fig. 3 – The relative change of the in-plane magnetoresistance of \( Y_{0.68}Pr_{0.32}Ba_2Cu_3O_7 \) [25] is plotted as a function of angle \( \theta \) at \( H=14 \) T for \( T=75 \) K. The solid line is fit based on eq. 16.

Fig. 4 – The relative change of the in-plane magnetoresistance of \( Y_{0.68}Pr_{0.32}Ba_2Cu_3O_7 \) [25] is plotted as a function of angle \( \theta \) at \( H=14 \) T for \( 105 \) K together with our fit based on eq. 16.

Fig. 5 – The relative change of the c-axis magnetoresistance of \( Y_{0.68}Pr_{0.32}Ba_2Cu_3O_7 \) [25] is shown as a function of angle \( \theta \) at \( H=14 \) T for 60 K (circles) and 65 K (pentagrams). The solid line represents our fit based on eq. 16.

**Conclusion.** We have extended the early analysis of the Landau quantization [19, 20] to d-wave density wave. Then the quasiparticle spectrum in a magnetic field describes the ADMR in \( Y_{0.68}Pr_{0.32}Ba_2Cu_3O_7 \) [25] and in \( \text{CeCoIn}_5 \) [18] very well. Though the present...
The predicted $\phi$ dependence of $\sigma_{zz}$ in CeCoIn$_5$ is plotted for H=4 T, 6 T, 8 T and 10 T (from bottom to top).

analysis suggests $d_{xy}$-wave density wave in CeCoIn$_5$, it is possible to discriminate $d_{x^2-y^2}$-wave and $d_{xy}$-wave DW through the ADMR where the magnetic field is rotated within the a-b plane. Also the present results will be used for further exploration of d-wave DW in CeCu$_2$Si$_2$, URu$_2$Si$_2$, $\kappa$-(ET)$_2$ salts and many other compounds.

We are thankful to V. Sandu and C. C. Almasan for helpful discussion and for providing us with the data of ref. [25]. We have benefitted from useful discussions with C. Capan, P. Gegenwart and P. Thalmeier. B. D. acknowledges the hospitality and support of the Max Planck Institute for Chemical Physics of Solids, Dresden, where part of this work was done. This work was supported by the Magyary Zoltán postdoctoral program of Foundation for Hungarian Higher Education and Research (AMFK) and by the Hungarian Scientific Research Fund under grant numbers OTKA TS040878, TS049881 T046269.

REFERENCES

[1] P. Thalmeier and G. Zwicknagl, in Handbook on the Physics and Chemistry of Rare Earth, edited by K. Gschneidner, J.-C. Bünzli, and V. Pecharsky (Elsevier, Amsterdam, 2005), volume 34, chap. 219.
[2] E. Capelluti and R. Zeyher, Phys. Rev. B 59, 6475 (1999).
[3] L. Benfatto, S. Caprara, and C. Di Castro, Eur. Phys. J. B 17, 95 (2000).
[4] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B 63, 094503 (2001).
[5] Z. A. Xu, N. P. Ong, Y. Wang, T. Kakeshita, and S. Uchida, Nature 87, 486 (1998).
[6] Y. Wang, Z. A. Xu, T. Kakeshita, S. Uchida, S. Ono, Y. Ando, and N. P. Ong, Phys. Rev. B 64, 224519 (2001).
[7] Y. Wang, N. P. Ong, Z. A. Xu, T. Kakeshita, S. Uchida, D. A. Bonn, R. Liang, and W. N. Hardy, Phys. Rev. Lett. 87, 257003 (2002).
[8] C. Capan, K. Behnia, J. Hinderer, A. G. M. Jansen, W. Lang, C. Marcenat, C. Marin, and J. Flouquet, Phys. Rev. Lett. 88, 056601 (2002).
[9] K. Maki, B. Dóra, A. Virosztek, and A. Ványolos, Curr. Appl. Phys. 4, 693 (2004).
[10] T. Shibauchi, L. Krusin-Elbaum, M. Li, M. P. Maley, and P. H. Kee, Phys. Rev. Lett. 86, 5763 (2001).

[11] L. Krusin-Elbaum, T. Shibauchi, and C. H. Mielke, Phys. Rev. Lett. 92, 097005 (2004).

[12] B. Dóra, A. Virosztek, and K. Maki, Phys. Rev. B 65, 155119 (2002).

[13] M. Pinteric, S. Tomic, and K. Maki, Physica C 408-410, 75 (2004).

[14] K. Izawa, H. Yamaguchi, Y. Matsuda, H. Shishido, R. Settai, and Y. Onuki, Phys. Rev. Lett. 87, 057002 (2001).

[15] K. Izawa, H. Yamaguchi, T. Sasaki, and Y. Matsuda, Phys. Rev. Lett. 88, 027002 (2002).

[16] R. Bel, K. Behnia, Y. Nakajima, K. Izawa, Y. Matsuda, H. Shishido, R. Settai, and Y. Onuki, Phys. Rev. Lett. 92, 217002 (2004).

[17] B. Dóra, K. Maki, A. Ványolos, and A. Virosztek, Phys. Rev. B 71, 172502 (2005).

[18] T. Hu, H. Xiao, C. C. Almasan, K. Maki, B. Dóra, T. Sayles, and B. Maple, unpublished.

[19] A. A. Nersesyan and G. E. Vachnadze, J. Low Temp. Phys. 77, 293 (1989).

[20] A. A. Nersesyan, G. I. Japaridze, and I. G. Kimeridze, J. Phys. Cond. Mat. 3, 3353 (1991).

[21] B. Dóra, K. Maki, and A. Virosztek, Mod. Phys. Lett. B 18, 327 (2004).

[22] K. Maki, B. Dóra, M. V. Kartsovnik, A. Virosztek, B. Korin-Hamzić, and M. Basletić, Phys. Rev. Lett. 90, 256402 (2003).

[23] W. Kang, H.-Y. Kang, Y. J. Jo, and S. Uji, Synth. Met. 133-134, 15 (2003).

[24] B. Dóra, K. Maki, A. Ványolos, and A. Virosztek, Europhys. Lett. 67, 1024 (2004).

[25] V. Sandu, E. Cimpoiasu, T. Katuwal, S. Li, M. B. Maple, and C. C. Almasan, Phys. Rev. Lett. 93, 177005 (2004).

[26] Y. Nambu, Phys. Rev. 117, 648 (1960).

[27] V. S. Weisskopf, in Quantum Electrodynamics, edited by J. Schwinger (Dover, New York, 1958).

[28] R. Jackiw, Phys. Rev. D 29, 2375 (1984).

[29] see for example A. A. Abrikosov, Fundamentals of the Theory of Metals (North-Holland, Amsterdam, 1998).

[30] X. J. Zhou, T. Yoshida, A. Lanzara, P. V. Bogdanov, S. A. Kellar, K. M. Shen, W. L. Yang, F. Ronning, T. Sasagawa, T. Kakeshita, T. Noda, H. Eisaki, et al., Nature 423, 398 (2003).

[31] A. V. Pimenov, A. V. Boris, L. Yu, V. Hinkov, T. Wolf, J. L. Tallon, B. Keimer, and C. Bernhard, Phys. Rev. Lett. 94, 227003 (2005).

[32] H. Ding, T. Yokoya, J. C. Campuzano, T. Takahashi, M. Randeria, M. Norman, T. Mochiku, K. Kadowaki, and J. Giapintzakis, Nature 382, 51 (1996).

[33] H. Aoki, T. Sukakibara, H. Shishido, R. Settai, Y. Onuki, P. Miranovic, and K. Machida, J. Phys. Cond. Mat 16, L13 (2004).