QUALITATIVE PICTURE OF A NEW MECHANISM FOR
HIGH-\(T_c\) SUPERCONDUCTORS

CHIA-REN HU

Department of Physics, Texas A\&M University,
College Station, TX 77843-4242, U.S.A.
crhu@tamu.edu

Received (16 January 2003)
Revised (31 January 2003)

Xu et al. observed enhanced Nernst effect and Iguchi et al. observed patched diamagnetism, both well above \(T_c\) in underdoped high-\(T_c\) superconductors (HTSCs). A new mechanism is proposed here, which seems to naturally explain, at least qualitatively, these observations, as well as the d-wave nature and continuity of pseudogap and pairing gap, the tunneling conductance above \(T_c\), as well as \(T^\ast(x), T_\nu(x), T_c(x)\), etc. This mechanism combines features of dynamic charged stripes, preformed pairs, and spin-bags: At appropriate doping levels, the doped holes (and perhaps also electrons) will promote the formation of anti-phase islands in short-range anti-ferromagnetic order. On the boundary of each such island reside two doped carriers; the unscreened Coulomb repulsion between them stabilizes its size. Superconductivity results when such “pre-formed pairs” Bose-condense.

Keywords: High-\(T_c\) Superconductors; new mechanism; Nernst effect; diamagnetism

Recently Xu et al.\(^1\) observed enhanced Nernst effect well above \(T_c\) in underdoped high-\(T_c\) cuprates. It occurs below an onset temperature \(T'_\nu\), which first rises sharply at very low hole concentrations \((x)\), reaching a peak well below optimal doping, and then decreases monotonically as \(x\) increases further. (For La\(_{2-x}\)Sr\(_x\)CuO\(_4\), or LSCO, the peak \(T'_\nu\) is \(\sim 128\) K whereas the maximum transition temperature \(T_c\) is below 40 K.) The Nernst effect is measured as follows: A rectangular slab of a single-crystal sample has its long edges parallel to the \(x\) and \(y\) axes. A magnetic field \(B_z\) is applied along \(z\), and a temperature gradient \(\partial_x T\) is applied along \(x\). The Nernst signal is the \(B_z\)-antisymmetric electric field \(E_y\) detected along \(y\). The Nernst coefficient is defined as

\[
\nu = \frac{1}{B_z} \frac{E_y}{\partial_x T}.
\]

It is well-known that enhanced Nernst effect can be observed around and below \(T_c\) of a low-\(T_c\), type-II superconductor. \(^2\) It has been explained in terms of the vortex lines in the superconductor. The core of each vortex line has low-lying quasiparticle states much below the superconducting gap. Thus there is extra entropy localized
inside the vortex core. A positive $\partial_x T$ then makes the vortex lines move toward $-x$, because an entropy current times $T$ is a heat current, and heat always flows from hot to cold. But a vortex line is also a flux tube, Thus as the vortex lines move toward $-x$ there is flux cutting through any line along $y$, giving rise to a positive electric field along $-y$. This “flux-flow” origin of the enhanced Nernst effect in low-$T_c$ superconductors near and below $T_c$ has been established since more than thirty years ago. Thus when Xu et al. observed enhanced Nernst effect in HTSCs, they naturally associated it with vortices also, even though this time the effect was observed well above $T_c$. (But they did carefully say “vortex or vortex-like excitations.”) Another recent experimental work, however, appears to have given direct evidence that this enhanced Nernst effect is not due to vortices. Iguchi et al., using scanning SQUID microscopy, observed vortices below $T_c$ only, and patched diamagnetism well above $T_c (=18-19 K)$ up to as high as 80K in LSCO with $x \approx 0.10$ (for which $T_c$ is above 120 K.). They also briefly stated that for a nearly optimally-doped sample, similar patched diamagnetism is also observed for about 5 K above $T_c$ ($\approx 40 K$.) Even in a slightly under-doped YBCO thin-film sample ($T_c \approx 84 K$), similar patched diamagnetism is also observed for a limited range of $T$ above $T_c$. The distinction is very unambiguous. I therefore feel that these two observations taken together are not explained by any of the high $T_c$ mechanisms proposed to date. Thus I venture to propose a new mechanism here (only a qualitative one so far).

I interprete Ref. 4 as to mean that the system contains localized objects which are diamagnetic and are capable of phase separation. $T_v$ is the formation temperature of these objects (as in the the formation of molecules from the constituent atoms), and the number of these objects should increase as the temperature is lowered from $T_v$, in order to account for the observed growing total area of these diamagnetic patches. Reference 1 then implies that these objects are also associated with local entropy. In order for these objects to give an enhanced Nernst effect with the same sign as that generated by vortices, these objects must be associated with local depletion of entropy rather than local excess of entropy. This is because a vortex is associated with localized flux along $B_z$, whereas a diamagnetic object has induced flux opposite to $B_z$. Thus our main aim is to find a mechanism by which such objects can be generated.

As is already widely accepted, the antiferromagnetism observed in the cuprates at zero and very low doping originates from a Mott-Hubbard insulating state. It can be described by a single-band Hubbard model. 6 At such very low doping the very low concentration of doped holes — perhaps also electrons; the difference has not yet been examined — are likely to form localized, immobile, singly-charged magnetic polarons (also known as spin-bags). 7 Such localized immobile objects clearly can not destroy long-range antiferromagnetic order (AFO). The lack of mobility of these charged objects at very low concentrations is most likely due to the inhomogeneous potential generated by the dopant ions, which keeps the well-separated charge carriers trapped to the vicinity of their parent dopant ions. As doping increases to the extend that the mean carrier separation becomes comparable to the distance
between the dopant ions and the nearest CuO$_2$ planes, the inhomogeneity of the potential becomes very weak. The doped carriers should then become mobile at $T = 0$. This should be roughly when antiferromagnetism disappears at $T = 0$, since it is well known that a moving hole leaves a trail of “wrong spins” with respect to the AFO. Indeed long-range AFO disappears in these materials at a very low hole concentration $x = x_{c1} = 0.02 - 0.03$ (and a bit larger electron concentration). Thermal energy can help carriers to become mobile at lower $x$ than $x_{c1}$, and therefore long-range AFO disappear at increasingly smaller $x$ as $T$ is increased.

As soon as some doped charge carriers become mobile, they can reorganize to form new objects. I propose that these new objects are doubly-charged anti-phase islands (DCHAPHIs) in a short-range AFO background. The boundary of such an island is like a dynamic stripe, which is known to be able to trap charges, but now bent around to form a small closed loop rather than extending from one edge of the sample to the opposite edge. The “loop” is so small that only two holes (and perhaps also electrons) can be trapped on it, in a spin-singlet state, so that the two charges can occupy the same lowest-energy orbital state on the loop. Any bound pairs formed above the superconducting transition temperature have been called “preformed pairs”. But the “preformed pair” proposed here are not bound to each other by any attractive force between them, but are rather both trapped on the same boundary of a single anti-phase island. (In this sense they resemble a doubly-charged spin bag, except that the orbital state in the present case is likely to be $d$-wave (see below), whereas the orbital state in a spin bag is likely to be $s$-wave, since the bag is presumably deepest at its center. Coulomb repulsion between the two charges may convert it to $d$-wave, but once both charge carriers avoid the center region in order to avoid each other, I expect AFO to recover in that region to turn a doubly-charged spin-bag into a DCHAPHI.) The DCHAPHIs are expected to be also associated with local depletions of magnetic entropy (at $T > 0$), because of size quantization of the antiferromagnetic magnons inside the islands. Enhanced Nernst effect can then occur. (A spin bag should also be associated with a local depletion of magnetic entropy. Only it may not be energetically as favorable if the bag size is comparable to the object shown in Fig.1, as I have argued above.) I expect energy savings when DCHAPHIs are formed from the original singly-charged objects, but the total entropy should at the same time decrease. Thus these new objects are expected to form only below some characteristic temperature which I identify as the pseudogap onset temperature $T^*$. The observed pseudogap for $T < T^*$ is identified as half of the formation energy of a DCHAPHI. I expect this energy to not change much with $T$. The main effect of rising $T$ is then to only reduce the number of such objects. This is consistent with tunneling data in the pseudogap regime where one sees a pseudogap which does not shrink in magnitude much with rising $T$, but only gradually gets filled in. (This fact is against interpreting $T^*$ as the mean-field $T_c$, the $T_c$ for incoherent pairs, or the highest of a distribution of $T_c$.)

At any $x > x_{c1}$ the singly-charged object is a linear combination of a singly-charged magnetic polaron and a bare charge carrier, because short-range AFO fluc-
tuates in and out of existence. But the DCHAPHIs can exist only when local short-
range AFO is present. Thus the so-identified \( T^* \) is a monotonically decreasing function of \( x \) (as is observed,) because the average formation energy of a DCHAPHI should be a decreasing function of \( x \), due to the fact that in any given region of space, short-range AFO fluctuates into existence for smaller fraction of the time when \( x \) is larger. This view is consistent with the fact that the observed pseudogap decreases with \( x \). 9

Figure 1 gives a snapshot of such a DCHAPHI, but it should be emphasized that the size and shape of a DCHAPHI are actually both fluctuating. So Fig. 1 gives only its typical size and shape. Later I will argue why the average size of such an object is actually smaller than shown here.

![Fig. 1. A snapshot of a doubly-charged anti-phase island in a short-range antiferromagnetic background. An up (down) arrow indicates a spin-up (down) electron at that site. Filled circle indicates an electron at that site but \( < s_z > = 0 \). Open circle indicates a hole, or no electron at that site.](image)

If these DCHAPHIs are not trapped, they should be mobile objects through de-
formations of their boundaries. HTSC in the cuprates can then be identified as the Bose-Einstein condensation (BEC) of these “preformed pairs”. The observed contin-
uity of the tunneling gap across \( T_c \) supports this view. One can also qualitatively understand why \( T_c \) first rises from zero at \( x_{c2} \approx 0.05 \), reaches a peak at \( x = x_{opt} \) for optimum doping, and then falls to zero at \( x = x_{c3} \geq 0.25 \). 11 The initial rise is because BEC temperature is a rising function of boson concentration, which in our case is the concentration of the DCHAPHIs, which at \( T = 0 \) clearly is an increasing function of \( x \) for small \( x \). (See later discussion for \( x > \) about 0.1.) The downward bending of \( T_c \) to reach a peak and the fall of \( T_c \) after the peak can be understood as due to the fall of \( T^* \), which leads to reduced number of “preformed pairs” at a given temperature.

A common difficulty in this type of theories, including this theory, the spin-bag theory, and all preformed-pair theories, is the size of the objects involved, since these objects generally can not exist near and beyond close packing. Fig. 2 shows a close packing density for the DCHAPHIs, and it only corresponds to \( x = 0.125 \). This is far below the observed \( x_{c3} \approx 0.25 \). Even at this density the DCHAPHIs are
Qualitative Picture of a New Mechanism for High-$T_c$ Superconductors

Fig. 2. Close packing of the DCHAPHIs shown in Fig. 1. The dotted square can be repeated to generate the whole structure. It encloses sixteen sites and two holes. Hence this configuration corresponds to $x = 0.125$.

probably no longer energetically favored to form, since there is little AFO outside their boundaries. We conclude that at $T = 0$ and for $x$ beyond some $x$ value around 0.1, the number of DCHAPHIs can not continue to increase with $x$. The remaining charge carriers, — there are more of them for larger $x$, — must exist in another form, such as the singly-charged objects mentioned earlier. These singly-charged objects can weaken short-range AFO, contributing to the lowering of the DCHAPHI formation energy, $T^*, T_\nu$, and $T_c$, more for larger $x$ in this region. (Note that at $T$ substantially above zero, there are less DCHAPHIs, so the close-packing limitation is less stringent. Thus for a limited range of $x$ beyond about 0.1, the number of DCHAPHIs can still increase with $x$. This might account for the continued rise of $T_c$ with $x$ until the latter reaches $x_{\text{opt}} \simeq 0.15$. The fact that even at $T = 0$ not all doped charges form DCHAPHIs is not as serious as it might appear to be, since already in the BCS theory, only a small fraction of the electrons near the Fermi surface form Cooper pairs. Yet it does not prevent a BCS superconductor from exhibiting strong superconducting properties such as perfect or nearly perfect diamagnetism.)

Fig. 3. The eight boundary sites, numbered 1 through 8, of the anti-phase island shown in Fig. 1.

To understand the experiment of Iguchi et al., we first show that these DCHAPHIs are diamagnetic. Figure 3 shows the eight boundary sites of an anti-phase island shown in Fig. 1, labeled 1 through 8, on which a doped charge carrier reside. (Actually there are two such charges on them, but we need only consider
The hopping matrix elements between sites 1 and 2, 3 and 4, 5 and 6, and 7 and 8 are just the hopping matrix element $-t$ (with $t > 0$) in the usual $t - J$ model, which has been shown to be equivalent to the Hubbard model for large $U$. However, the effective hopping matrix elements between sites 2 and 3, 4 and 5, 6 and 7, and 8 and 1, denoted as $-t'$, should satisfy $t' < 0$, because they are the result of third-order processes with one illustrated in Fig. 4, (and another one which is just this one in a different order,) involving two negative energy denominators and three matrix elements in the numerator, two of which are $-t < 0$, and one of which is $J > 0$.

\begin{equation}
\mathcal{H} = -t(c_2^\dagger c_1 + c_3^\dagger c_2 + c_5^\dagger c_4 + c_7^\dagger c_7) + |t'| (c_3^\dagger c_2 + c_4^\dagger c_4 + c_6^\dagger c_6 + c_8^\dagger c_8) + h.c.
\end{equation}

The non-degenerate ground state of this Hamiltonian is $(1, 1, -1, -1, 1, 1, -1, -1)^T$, i.e., a $d$-wave state, with energy $-(t + |t'|)$. It is filled by two holes (or electrons) forming a singlet state, so there is clearly no spin contribution to the magnetic susceptibility. This eigen-vector is real, so its angular momentum expectation value is zero. The state is then diamagnetic. (This is basically Larmar diamagnetism, also known as Langevin susceptibility.) Extending the above 8-site model to include the effect of an external magnetic field has confirmed this conclusion. The parameter $t'$ should be left as an independent parameter of the theory, since any next-nearest-neighbor hopping term in the original Hubbard model can also contribute to $t'$ directly. These DCHAPHIs can probably undergo phase separation, since the phase-separation argument of Emery et al. should apply to these objects as well as the charged objects they considered. (An alternative possibility is

![Fig. 4. A third order process which allows a doped charge to hop from site 2 to site 3 defined in Fig. 3.](image-url)
a phase separation of the two types of charged objects without creating an inhomogeneous charge distribution.) The diamagnetic patches observed by Iguchi et al. are then qualitatively explained. The increased total area of such patches as \( T \) is lowered from \( T^* \) is then simply due to the formation of more such diamagnetic objects. Figure 4 also shows that the size of a DCHAPHI is smaller than is shown in Fig. 1 at any transient moment when a doped charge carrier is hopping between such two sites as 2 and 3. (If a third-order process were to involve a site outside the boundary, two neighboring spins would become parallel. Such intermediate states would have higher energy.)

Finally, let us look at the enhanced Nernst effect observed by Xu et al.\(^1\) Vortices can give rise to such an effect, since each vortex carries a magnetic flux along \( B_z \), and also carries excess entropy inside its core. These are the two essential ingredients for generating an enhanced Nernst effect. Another situation can also give rise to this effect with the same sign: That is when there are localized diamagnetic objects in the system with a depletion of entropy in the spatial regions occupied by them. This is precisely the present situation, since the DCHAPHIs must also be associated with a depletion of entropy inside the spatial regions occupied by them because of size quantization of the antiferromagnetic magnons inside the islands. Xu et al. found that \( T_\nu \) first rises sharply at an \( x \) value very close to \( x_{c1} \), reaching a peak at an \( x \) larger than \( x_{c2} \) but below \( x_{opt} \) (i.e., at \( \sim 0.1 \) for LSCO), and then to fall gradually as \( x \) is increased further. The gradual fall is simply due the gradual fall of \( T^* \) in this \( x \) range. In this range \( T_\nu \) is below \( T^* \) probably because a small \( x \)-dependent number of these DCHAPHIs are trapped by inhomogeneous potential to become immobile, and therefore can not contribute to the Nernst effect. Another possible contributing factor is that the two types measurements may have different sensitivity on a very low concentration of such objects. The patching of a low concentration of DCHAPHIs may also be at least partially responsible for the difference. The initial sharp rise of \( T_\nu \) is most-likely also due to the potential traps: A very low concentration of such objects can become all trapped and immobile, and therefore can not contribute to the Nernst effect, even though they can still give rise to a pseudogap in tunneling with deeper center dip at lower \( T \), because their number still increases with lower \( T \). The number of such traps is a rapidly decreasing function of \( x \) for reasons already given. Clearly \( T_\nu \) has to increase sharply so that the number of DCHAPHIs at \( T > T_\nu \) can still be so low that they can be all trapped. Since raising \( T \) can further release some trapped objects, this sharp rise of \( T_\nu \) can only be even sharper. We thus have a qualitative understanding of the initial rapid rise of \( T_\nu \).

We can not make any quantitative predictions for testing purpose at the present stage. Nevertheless, there can still exist additional qualitative signatures of this theory besides the ones already discussed. One important confirmation of this theory would be the observation of singlet or triplet excited states of the DCHAPHIs. But they may not exist as stable objects. Thus for strong support of this theory one should look for patched pseudogap using STM, in the same sample type, spatial
and temperature regions where patched diamagnetism is observed. Another strong support would be if the noise spectrum in the Nernst signal is found to be drastically different above and below $T_c$. (The flux in a vortex is fixed, but the number of vortices is proportional to $B_z$. The flux in a DCHAPHI is proportional to $B_z$, but its number should be essentially independent of $B_z$.)

Note added after refereeing process: We have completed a mean-field study of the Hubbard model which confirms the existence and stability of a DCHAPHI and the conversion of a doubly-charged spin-bag to a DCHAPHI when the Coulomb repulsion between the two charges are turned on. [Q. Wang and C.-R. Hu, unpublished.]

The author would like to acknowledge support from the Texas Center for Superconductivity and Advanced Materials at the University of Houston.

References

1. Z.A. Xu, N.P. Ong, Y. Wang, T. Kakeshita, and S. Uchida, Nature 406, 486 (2000). See also Y. Wang et al., Phys. Rev. B64, 224519 (2001); Phys. Rev. Lett. 88, 257003 (2002).
2. R. P. Huebener, Magnetic Flux Structures in Superconductors (Springer Verlag, Berlin, Heidelberg, 1979) Chap. 9.
3. See also P. A. Lee, Nature 406, 467 (2000), particularly its title “Some vortices like it hot”. But even this work warned against vortex interpretation near its end.
4. I. Iguchi, T. Yamaguchi, and A. Sugimoto, Nature 412, 420 (2001); Physica C367, 9 (2002).
5. V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. 64, 475 (1990), and Physica B163, 306 (1990); V. J. Emery and S. A. Kivelson, Physics 209, 597 (1993).
6. P. W. Anderson, Science 235, 1196 (1987).
7. J. R. Schrieffer, X.-G. Wen, and S.-C. Zhang, Phys. Rev. Lett. 60, 944 (1988). W. P. Su, Phys. Rev. B37, 9904 (1988).
8. J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura, and S. Uchida, Nature 375, 561 (1995); J. Orenstein and A. J. Millis, Science 288, 468 (2000); and references cited therein.
9. T. Timusk and B. Statt, Rep. Prog. Phys. 62, 61 (1999).
10. T. Ekino, S. Hashimoto, T. Takasaki, and H. Fujii, Phys. Rev. B64, 092510 (2001); M. Kugler, O. Fischer, Ch. Renner, S. Ono, and Y. Ando, Phys. Rev. Lett. 86, 4911 (2001).
11. H. Takagi, T. Ido, S. Ishibashi, M. Uota, S. Uchida, and Y. Tokura, Phys. Rev. B40, 2254 (1989).
12. N. W. Ashcroft and N. D. Mermin, Solid State Physics (Saunders College Publishing, 1st ed., 1976), Chap. 31.
13. V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. 64, 475 (1990); and Physica B163, 306 (1990); C. S. Hellberg and E. Manousakis, Phys. Rev. Lett. 78, 4609 (1997).