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RESEARCH ARTICLE

Generalizing the Cooper-pair instability to doped Mott insulators

Mike GUIDRY[1], **Yang SUN** (孙扬)[2,†], **Cheng-li WU**(吴成礼)[3]

[1] *Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996–1200, USA*
[2] *Department of Physics, Shanghai Jiao Tong University, Shanghai 200240, China*
[3] *Physics Department, Chung-Yuan Christian University, Chungli, Taiwan 320, China*
E-mail: sunyang@sjtu.edu.cn

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Copper oxides become superconductors rapidly upon doping with electron holes, suggesting a fundamental pairing instability. The Cooper mechanism explains normal superconductivity as an instability of a fermi-liquid state, but high-temperature superconductors derive from a Mott-insulator normal state, not a fermi liquid. We show that precocity to pair condensation with doping is a natural property of competing antiferromagnetism and d-wave superconductivity on a singly-occupied lattice, thus generalizing the Cooper instability to doped Mott insulators, with significant implications for the high-temperature superconducting mechanism.

Keywords Cooper-pair instability, high-temperature superconductivity, $SU(4)$ model

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Understanding cuprate high-temperature superconductors is complicated by unusual properties of the normal state and how this state becomes superconducting with doping [1]. Band theory suggests that cuprates at half lattice filling should be metals, but they are instead insulators with antiferromagnetic (AF) properties. This behavior is thought to result from a Mott-insulator normal state, where the insulator properties follow from strong on-site Coulomb repulsion rather than band-filling properties. Upon doping the normal states with electron holes, there is a rapid transition to a superconducting (SC) state, with evidence for a pairing gap at zero temperature typically appearing for about 3%–5% hole density per copper site in the copper–oxygen plane. In addition, there is strong evidence at low to intermediate doping for a partial energy gap at temperatures above the SC transition temperature T_c that is termed a pseudogap (PG), with the size of the SC gap and PG having opposite doping dependence at low doping [2, 3].

Parent states of normal superconductors are fermi liquids (strongly interacting systems having excitations in one-to-one correspondence with the excitations of a non-interacting fermi gas). Normal superconductors are described by Bardeen–Cooper–Schrieffer (BCS) theory [4], and result from condensation of zero-spin, zero-momentum fermion pairs into a new collective state with long-range coherence of the wavefunction. The key to understanding normal superconductivity was the demonstration by Cooper [5] that normal fermi liquids possess a fundamental instability: an electron pair above a filled fermi sea can form a bound state for *vanishingly small attractive interaction.* In normal superconductors, the attraction is provided by interactions with lattice phonons, which bind weakly over a limited frequency range because electrons and the lattice have different response times. However, it is the Cooper instability, not the microscopic origin of the attractive interaction, that is most fundamental: a weak electron–electron interaction alone cannot produce a superconducting state, but the Cooper instability can (in principle) produce a superconducting state for *any* weakly attractive interaction.

The rapid onset of superconductivity in high-T_c compounds with hole doping suggests a fundamental instability against pair condensation, but it is difficult to understand this (and the appearance of PG states) within the standard BCS framework because the superconductor appears to derive from a Mott insulator, not a normal fermi liquid. Just as for normal superconductivity, we believe that the key to understanding high-temperature superconductivity is not the attractive interaction leading to pair binding (as important as that is), but rather the nature of the instability that produces the superconducting state. Since at larger doping the high-temperature superconducting state exhibits many properties of a normal BCS superconductor (but with d-wave pairs), this instability must reduce to the Cooper instability at larger doping, but evolve into something more complex at lower doping, where the normal state approaches a Mott insulator, and a PG exists above the SC transition temperature.

To account for rapid onset of superconductivity with hole-doping, Laughlin [6] (see also Refs. [7, 8]) proposed a modified Hamiltonian with an attractive term that partially overcomes the on-site repulsion. Then the insulator at half filling is actually a "thin, ghostly superconductor", which fails to superconduct only because its long-range order is disrupted at very low doping, ostensibly by fluctuations due to low superfluid density. This proposed new state is termed a *gossamer superconductor.* This idea might provide a justification for the resonating valence bond (RVB) state [9], which assumes implicitly that quantum antiferromagnets should exhibit superconductivity, even though cuprate ground states at half-filling appear to be best described as an insulating state with long-range AF order and no superconductivity [10–14]. In the RVB model, it is usually assumed that the long-range Néel order of the ground state at exactly half filling is replaced quickly by the RVB spin-liquid ground state upon hole-doping, with details lacking. Laughlin [6] contends that the real issue for validity of the RVB picture is not whether all quantum antiferromagnets are secretly superconductors, but whether some are. The gossamer superconductor is then proposed as a second kind of antiferromagnetism – distinguished by a small background superfluid density – that is the true normal state in the cuprates, and is the harbinger of a spin-liquid RVB ground state for low hole-doping.

The gossamer state has desirable properties but is created by hand: a strong attractive term is added to the Hamiltonian, which justifies modifying Gutzwiller projectors such that they only partially suppress double occupancy [7]. We shall show that a model implementing competition of d-wave pairing with antiferromagnetic correlations on a lattice with no double occupancy has Mott insulator properties at half filling, but is unstable toward developing a finite singlet pairing gap under infinitesimal hole-doping. Thus, we shall argue that many features motivating the idea of gossamer superconductivity are natural consequences of AF and SC competition on a lattice having strict no double occupancy at half filling. We shall argue further that a pseudogap with correct properties is a natural consequence of the same theory, thus accounting for both the precocious onset of a pairing gap and the appearance of pseudogaps at low doping in the cuprates. Finally, we shall discuss the implications of these results for gossamer superconductivity and for the RVB model.

We wish to solve for the doping and temperature dependence of observables in a theory that incorporates on an equal footing d-wave superconductivity and antiferromagnetism. To do so, we shall employ the tools of Lie algebras, Lie groups, and generalized coherent states [15–22]. To construct a Hamiltonian embodying these degrees of freedom and expected conservation laws for charge and spin in the many-body wavefunction, we require at a minimum three staggered magnetization operators $\boldsymbol{Q}$ to describe AF, creation and annihilation operators $D^\dagger$ and D for d-wave singlet pairs and a charge operator M to describe superconductivity, and three spin operators $\boldsymbol{S}$ to impose spin conservation.

However, this set of 9 operators is physically incomplete since scattering of singlet pairs (antiparallel spins on adjacent sites) from the AF particle–hole degrees of freedom can produce triplet pairs (parallel spins on adjacent sites), which are not part of the operator set. The mathematical statement of this incompleteness is that the operator set $\{\boldsymbol{Q}, D^\dagger, D, M, \boldsymbol{S}\}$ does not close a Lie algebra under commutation. As demonstrated in Refs. [15–17, 19, 20], a (minimally) complete operator set results if we add to these operators the six triplet pair operators $\boldsymbol{\pi}^\dagger$ and $\boldsymbol{\pi}$. Then the set of 15 operators $\{\boldsymbol{Q}, D^\dagger, D, \boldsymbol{\pi}^\dagger, \boldsymbol{\pi}, M, \boldsymbol{S}\}$ closes the Lie algebra $SU(4)$. The explicit forms for these operators in both momentum and coordinate space, and the corresponding $SU(4)$ commutation algebra, may be found in Refs. [15–17, 19, 20].

A critical feature of this symmetry structure is that the $SU(4)$ algebra closes only if the 2-dimensional lattice on which the generators are defined has no doubly occupied sites [18]. Thus, the $SU(4)$ algebra embodies the minimal theory that describes AF and d-wave SC competition through a many-body wavefunction that conserves charge and spin, and that has no components corresponding to double site occupancy on the lattice. The Hamiltonian restricted to one-body and two-body terms is unique, with the general form

$$H = H_0 - G_0 D^\dagger D - G_1 \boldsymbol{\pi}^\dagger \cdot \boldsymbol{\pi} - \chi \boldsymbol{Q} \cdot \boldsymbol{Q} + \kappa \boldsymbol{S} \cdot \boldsymbol{S} \quad (1)$$

where G_0, G_1, χ, and κ are effective interaction strengths, and H_0 is the single-particle energy. The $T = 0$ ground state corresponds to a superposition of singlet and triplet fermion pairs.

We shall solve for the ground-state properties of this theory using generalized coherent states [22]. Our immediate interest is the ground-state total energy surface, which is the expectation value of the Hamiltonian in the ground coherent state (with total spin $S = 0$). The formalism for constructing the $SU(4)$ coherent state and the ground state energy surface has been developed extensively in Refs. [15–17, 19, 20], to which we refer for details. The overall $SU(4)$ symmetry may be used to eliminate the $\boldsymbol{\pi}^\dagger \cdot \boldsymbol{\pi}$ term from the Hamiltonian (1), leaving an energy surface that is a function of order parameters for singlet pairing and antiferromagnetism, with the hole-doping as a control parameter.

Figure 1 illustrates the $SU(4)$ total energy surface in coherent state approximation as a function of an AF order parameter $Q = \langle \boldsymbol{\mathcal{Q}} \cdot \boldsymbol{\mathcal{Q}} \rangle^{1/2}/\Omega$ and an SC order parameter $\Delta = \langle D^\dagger D \rangle^{1/2}/\Omega$ (where Ω is the maximum number of doped holes that can form coherent pairs, assuming the half-filled lattice as vacuum), as doping $x \simeq 4P$ (for P holes per copper lattice site) is varied. The explicit expression for the energy surface is $E = -\chi\Omega^2[(1-x_q^2)\Delta^2 + Q^2]$, where [17]

$$\Delta = \frac{1}{2}\left[\frac{1}{4} - \left(Q - \frac{x}{2}\right)^2\right]^{1/2} + \frac{1}{2}\left[\frac{1}{4} - \left(Q + \frac{x}{2}\right)^2\right]^{1/2}$$

and x_q is the critical doping at which AF correlations vanish (see Fig. 1 and Refs. [19, 20]). Vertical lines bounding the curves for different doping in Fig. 1 represent the contraints

$$|Q| \leqslant \frac{1}{2}(1-x), \quad [x(1-x)]^{1/2} \leqslant 2\Delta \leqslant (1-x^2)^{1/2}$$

that result from $SU(4)$ symmetry within a finite valence space. Specifically, $|Q|$ must lie between 0 and $n/2$ (n is the electron number) because of the number of spins available, and $SU(4)$ symmetry then relates this constraint on Q to the one on Δ.

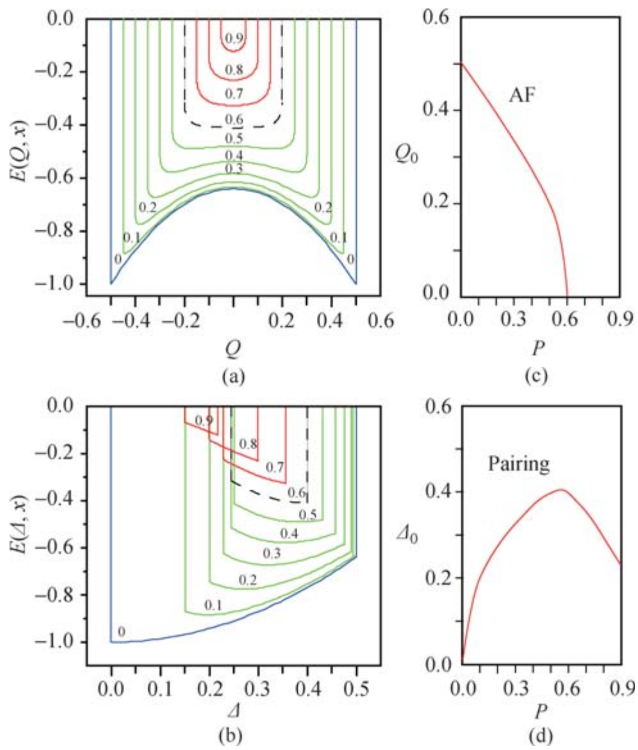

Fig. 1 Total energy vs. **(a)** AF correlation Q and **(b)** SC correlation Δ; curves labeled by hole-doping $x \simeq 4P$. Energy in units of $\chi\Omega^2/4$, with χ the AF coupling strength. The dashed line indicates the critical doping $x = x_q$ (see Refs. [19, 20]); red denotes SC; blue denotes AF; green denotes AF + SC favoring energy surfaces. **(c)** and **(d)** indicate the position of the energy minimum in Q and Δ, respectively.

From Fig. 1, the energy surface at half filling ($x = P = 0$) implies a $T = 0$ ground state with AF order but no pairing order ($Q_0 \neq 0$ and $\Delta_0 = 0$, where the subscript zero denotes the value at the minimum of the energy surface). The ground state for $x = 0$ may be interpreted as an antiferromagnetic Mott insulator [15–17]. From Fig. 1(a), the energy surface retains strong AF character for small x with $Q_0 \neq 0$, but from Fig. 1(b), the ground state differs qualitatively from that at half filling even for infinitesimal hole-doping. Specifically, for any nonzero attractive pairing strength, a finite singlet d-wave pairing gap develops spontaneously for *any non-zero x*, and Δ_0 has already increased to half its value at optimal doping by the time $P \simeq 0.03$ ($x \simeq 0.12$). The rapid change in the expectation value of the pairing correlation is illustrated further in Fig. 1(d). We term this behavior *precocious pairing*.

The instability against condensing pairs displayed graphically in Fig. 1 may also be understood analytically. From the $T = 0$ solution for Δ given in Eq. (24b) of Refs. [19], we find

$$\left.\frac{\partial \Delta}{\partial x}\right|_{x\to 0} = \left.\frac{1}{4}\frac{x_q^{-1} - 2x}{[x(x_q^{-1} - x)]^{1/2}}\right|_{x\to 0} \to \infty \qquad (2)$$

displaying explicitly the pairing instability at $x = 0$.

The picture that emerges is that at half filling, the lattice is a Mott insulator with long-range AF order and no pairing gap, but upon infinitesimal hole-doping, a finite singlet pairing gap and a ground state that corresponds to strong competition between AF and SC order appear. This spontaneous development of a finite singlet pairing gap for infinitesimal hole-doping has been obtained in the coherent-state approximation subject to $SU(4)$ symmetry. Since the $SU(4)$ algebra closes only if the lattice has no double occupation, this precocious pairing has occurred without invoking double occupancy. Doping-dependent effective interactions could delay onset of SC from $P \sim 0$ to a small doping fraction, as observed, since the pair gap $G_0\Delta$ vanishes if the singlet pairing strength G_0 vanishes, even for large pair correlation Δ; weak $SU(4)$ symmetry breaking could also play a role in delaying onset of SC. However, we propose that the pair-condensation instability of the $SU(4)$ symmetry limit represents the essential physics governing the emergence of superconductors from doped Mott insulators.

Mathematically, precocious pairing results from $SU(4)$ invariance, which requires that $Q^2 + \Delta^2 + \Pi^2 = (1 - x^2)/4$, where $\Pi = \langle \boldsymbol{\pi}^\dagger \boldsymbol{\pi} \rangle^{1/2}/\Omega$ is the triplet pair correlation [19, 20]. But for a pure AF $SU(4)$ solution, $Q^2 = \frac{1}{4}(1-x)^2$, so even the AF limit has finite pair correlations Δ and π unless $x = 0$. The *physical origin* of precocious pairing is that a minimal model of antiferromagnetism, d-wave pairing, charge, and spin on a half-filled fermion lattice is unstable to condensing pairs at non-zero hole-doping under a no double occupancy constraint.

These results have several important implications. We shall discuss three: 1) the interpretation of cuprate data at low hole-doping, 2) the implications for gossamer superconductivity, and 3) the implications for models of the RVB type.

Cuprate data for low doping suggest that normal compounds at half filling are AF Mott insulators, that a finite pairing gap develops by $P \simeq 0.05$, and that a pseudogap develops in the underdoped region having opposite doping dependence than the singlet pairing gap. These results are consistent with a Mott insulator state at half filling that evolves rapidly into a state with a finite singlet pairing gap at very low hole-doping. However, since at low doping both the singlet pairing and AF correlation energies are substantial, the AF fluctuations prevent the development of strong superconductivity until near optimal doping, where the zero-temperature AF correlations are completely suppressed by a quantum phase transition at $x = x_q$. We have shown that this same coherent-state $SU(4)$ theory gives a pseudogap having the observed doping behavior, and that the pseudogap may be interpreted either as arising from competing AF and SC degrees of freedom or from fluctuations of pairing subject to $SU(4)$ constraints [19, 20].

The results presented here suggest that an inherent instability toward condensation of Cooper pairs with hole-doping is a natural consequence of a minimal model of d-wave pairing interacting with AF correlations on a lattice with no double occupancy. Thus, the rapid onset of superconductivity with hole-doping in the cuprates results from an instability that is Cooper-like (instability against condensing pairs for non-zero attractive pairing interaction), but for d-wave pairs in an AF Mott insulator. Since the $SU(4)$ coherent state reduces to a d-wave BCS state if AF interactions vanish at finite hole doping, and to an insulating state with long-range AF order if pairing and hole doping vanish [19, 20], this represents a self-consistent generalization of the Cooper instability to doped Mott insulators. Strong interactions violating no double occupancy, as in the gossamer hypothesis, are not precluded but do not seem to be necessary for the pairing instability.

The $SU(4)$ symmetry-limit solutions are *exact* solutions of the original 2-D lattice problem if the effective interaction is known (see Section III of Ref. [16]). Since our primary result depends only on the *existence* of an effective interaction with a finite attractive pairing interaction (which can be checked empirically), it is exact in the dynamical symmetry limits. The coherent-state energy surface then represents an approximate mean-field solution valid for arbitrary doping, but the agreement of the general coherent-state solution with the exact solutions in the dynamical symmetry limits for ground-state properties gives confidence that the coherent state solutions carry the correct energy-surface properties over the entire physical doping range. In particular, we reiterate that the instability (2) occurs for the pure AF state ($G_0 = 0$; $x_q = 1$), which is an *exact many-body solution.*

The RVB idea has attractive features, but the observed state at half filling is not a spin liquid. Motivations of RVB models often gloss over this difficulty with the assumption that the half-filled state is, in some sense, practically a spin liquid, though it looks like an AF state. Our results give independent support for a picture similar to this, but without RVB assumptions: the $SU(4)$ ground state at half-filling has the observables of a respectable antiferromagnetic Mott insulator, but its wavefunction can reorganize spontaneously into a superconductor when perturbed by a vanishingly small hole-doping if there is a non-zero pairing interaction. For low hole-doping this superconductor is strongly modified by AF correlations. Below $T_{\rm c}$ this gives a d-wave superconducting state weakened by AF correlations; for a range of temperatures above $T_{\rm c}$, the pairing gap vanishes, but strong AF correlations in a basis of fermion pairs lead to a pseudogap that may be interpreted either in terms of preformed pairs or as competing AF and SC order. Finally, the AF competition weakens with hole-doping until the pure superconductor emerges near optimal doping.

$SU(4)$ coherent states at low doping presumably share many features with RVB states. Triplet pairs are essential for a complete set of operators in the minimal $SU(4)$ model (for example, no double occupancy is enforced by the $SU(4)$ algebra, which fails to close without triplet pairs), and a mixture of singlet and triplet pairs is essential to describe the AF states at half filling in the highly truncated $SU(4)$ fermion basis. But the significance of triplet relative to singlet pairs decreases rapidly with doping [19, 20], and underdoped $SU(4)$ ground states could have significant overlap with a singlet spin liquid. Furthermore, $SU(4)$ states at low doping lead naturally to a pseudogap that decreases in size with increased hole-doping and exhibits fermi arcs, in quantitative accord with data.

The $SU(4)$ coherent state justifies many features of RVB models, but it has a richer variational wavefunction than a singlet spin liquid because it accounts even-handedly for both AF and SC on a lattice with no double occupancy. Conversely, the $SU(4)$ coherent-state model is simpler in many respects than RVB models because SC and AF are accounted for quantitatively in a minimal theory having only (dressed) electron degrees of freedom: there are no pair bosons, no gauge fields, and no spinons or holons (which have formal justification in one dimension, but are less obviously justified in higher dimensions, and for which there is little direct evidence in cuprate superconductors). The $SU(4)$ coherent state represents a minimal extension of the BCS formalism to incorporate d-wave pairing in the presence of strong AF correlations and large effective on-site electron repulsion. It requires no Gutzwiller projection because the symmetry enforces no double occupancy on the lattice. It exhibits a type of spin–charge separation (see Ref. [23]), but not through topological spinons and holons: in the fermion basis, charge is carried both by singlet fermion hole pairs having a spin of 0 and charge −2, and triplet fermion hole pairs having a spin of 1 and charge −2, but spin is carried solely by the triplet hole pairs. As we have discussed in Refs. [15–21], these features permit a model that describes many observed features of the cuprates from half-filling to the overdoped region in a unified manner.

Finally, we comment on the newly discovered superconductivity in iron-based compounds [24], where a highest T_c of 55 K [25] has already been reached. The SC in these materials seems unconventional, competes with AF [26], and has many other similarities with the cuprates [27, 28]. The normal states are (poor) metals, though nearness to a Mott transition can be debated. It is unlikely that RVB can provide a natural unified picture of copper- and iron-based SC. However, the generalization of Cooper pairing presented in this paper can accommodate a Mott insulator normal state at half lattice filling (as appropriate for cuprates), but is consistent with a metallic normal state for valence structures characteristic of iron-based SC. Thus, a unified description of cuprate and iron-based superconductors seems possible within this framework.

In summary, we have examined a minimal theory of cuprate d-wave superconductivity and antiferromagnetism on a lattice with no double occupancy. Total energy surfaces imply ground states that are antiferromagnetic Mott insulators at half filling, but are unstable against developing singlet d-wave pairing gaps upon hole-doping, thereby generalizing the Cooper instability to doped Mott insulators. Many properties motivating gossamer superconductivity are explained naturally, without invoking the gossamer hypothesis. We find support for the assumption of resonating valence bond models that the state with AF order at half filling would really like to be a spin-singlet liquid. However, the $SU(4)$ coherent state is simpler to implement, yet contains richer physics, than a spin-singlet liquid, and accounts systematically for many cuprate properties across the entire physical doping range. Finally, we suggested that these ideas have the potential to unify descriptions of cuprate and new iron-based superconductivity.

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References

1. D. A. Bonn, Nature Physics, 2006, 2: 159, and references therein
2. T. Timusk and B. Statt, Rep. Prog. Phys., 1999, 62: 61
3. M. Norman, D. Pines, and C. Kollin, Adv. Phys., 2005, 54: 715
4. J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev., 1957, 108: 1175
5. L. N. Cooper, Phys. Rev., 1956, 104: 1189
6. R. B. Laughlin, arXiv: cond-mat/0209269, 2002
7. F. C. Zhang, Phys. Rev. Lett., 2003, 90: 207002
8. P. Coleman, Nature, 2003, 424: 625
9. P. W. Anderson, Science, 1987, 235: 1196
10. D. Vaknin, S. K. Sinha, D. E. Moncton, D. C. Johnston, J. M. Newsam, C. R. Safinya, and H. E. King Jr., Phys. Rev. Lett., 1987, 58: 2802
11. J. M. Tranquada, D. E. Cox, W. Kunnmann, H. Moudden, G. Shirane, M. Suenaga, P. Zolliker, D. Vaknin, S. K. Sinha, M. S. Alvarez, A. J. Jacobson, and D. C. Johnston, Phys. Rev. Lett., 1988, 60: 156
12. S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett., 1988, 60: 1057
13. J. D. Reger and A. P. Young, Phys. Rev. B, 1988, 37: 5978
14. E. Dagotto, Rev. Mod. Phys., 1994, 66: 763
15. M. W. Guidry, Rev. Mex. de Fisica, 1999, 45 Suplemento 2: 132
16. M. W. Guidry, L. A. Wu, Y. Sun, and C. L. Wu, Phys. Rev. B, 2001, 63: 134516
17. L. A. Wu, M. W. Guidry, Y. Sun, and C. L. Wu, Phys. Rev. B, 2003, 67: 014515
18. M. W. Guidry, Y. Sun, and C. L. Wu, Phys. Rev. B, 2004, 70: 184501
19. Y. Sun, M. W. Guidry, and C. L. Wu, Phys. Rev. B, 2006, 73: 134519
20. Y. Sun, M. W. Guidry, and C. L. Wu, Phys. Rev. B, 2007, 75: 134511
21. M. W. Guidry, Y. Sun, and C. L. Wu, New J. Phys., 2009, 11: 123023
22. W. M. Zhang, D. H. Feng, and R. Gilmore, Rev. Mod. Phys., 1990, 62: 867
23. P. W. Anderson, Physics Today, 1997, October: 42
24. Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc., 2008, 130: 3296
25. Z. A. Ren, W. Lu, J. Yang, W. Yi, X. L. Shen, Z. C. Li, G. C. Che, X. L. Dong, L. L. Sun, F. Zhou, and Z. X. Zhao, Chin. Phys. Lett., 2008, 25: 2215
26. C. de la Cruz, Q. Huang, J. W. Lynn, J. Li, W. Ratcliff II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and P. C. Dai, Nature (London), 2008, 453: 899
27. Y. Sun, M. Guidry, and C. L. Wu, Chin. Sci. Bull., 2008, 53: 1617
28. M. Guidry, Y. Sun, and C. L. Wu, Front. Phys. China, 2009, 4(4): 433