Phase diagram of the *t-J* model on a honeycomb lattice

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We investigate the phase diagram for the *t-J* model on a two-dimensional honeycomb structure at low electronic densities. The phase diagram as a function of the interaction strength, J, consists of three phases, viz. a gas of electrons for $0 \leqslant J < 2t$, a gas of pairs for $2t \leqslant J < 3.29t$, and a fully phase-separated state for $J > 3.29t$. Further, we rigorously prove that a gas of electrons start forming pairs at $J=2t$ and the value is the same for any bipartite lattice in any dimension. We have elaborately explored the possibilities of formation of bigger clusters, i.e., bound states of three, four, and six electrons by performing exact diagonalization and perturbative analysis and ruled out formation of such clusters in the phase diagram.

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The *t-J* model has been studied extensively to investigate the phase diagram in systems where strong electronic correlations play a very crucial role. The examples of such systems are the high-T superconductors where the vital components, i.e., the copper oxide planes, are best described by a *t-J* model.[1,2] In the large J limit ($J \gg t$) the model is known to separate into a Heisenberg clusterlike phase and a hole-rich phase. The boundary that separates the phase separated state and other phases has been elaborately studied at all interaction strengths by several authors using a number of numerical and analytical techniques. These include exact diagonalization studies on small systems,[3–5] Greens function Monte Carlo,[6,7] variational Monte Carlo using Gutzwiller-Jastrow type of wave functions,[8] high temperature series expansions,[9] etc. At low densities, the critical J that signals a phase separation is found to be between 3.5 and 4.[3,9,10] At lower values of J the phase separated state becomes unstable to the formation of a gas of pairs before entering a paramagnetic phase (gas of single electrons) for small values of J.[3,7,11] At larger electronic densities the situation is less clear, though the proposed phase diagrams[7,11] indicate a significant suppression in the value of critical J (scaling almost linearly with electron density) that demarcates the phase separated state with the rest. Intuitionally the result makes sense as close to an electron filling equal to unity, an infinitesimal J should push the system towards phase separation.

While experiments provide compelling evidence for phase separation in excess oxygen and hole doped La_2CuO_4,[12] where hole-rich and hole-poor phases coexist below a certain temperature ($\sim$230 K), some of the theoretical work ruled out phase separation in the physical parameter regime for the cuprates.[13,14] Emery, Kivelson, and Lin[3,15] conjectured that the long range part of the Coulomb interaction present in physical systems prevents phase separation. Thus stripes or other charge density wave (CDW) structures may be formed as an alternative to a completely inhomogeneous phase separated state.[14,16] On a parallel ground the proximity of superconductivity to a phase separated phase is a generic feature in the correlated electronic models[17] thus rendering importance to a unified description of phase separation and superconductvity.

The survey presented thus far pertains to a square lattice. The investigation of a phase diagram in other lattice geometries is not a well-addressed problem, although it may turn out to be equally interesting. A pertinent question is how lowering of symmetry competes with the formation of different phases. In this paper, we study the phase diagram of the *t-J* model on a honeycomb lattice at low electron densities. At half filling, the model reduces to the Heisenberg model, for which the ground state is antiferromagnetically ordered.[18] In zero density limit, for large values of J/t, the electrons will condense to form a Heisenberg solid (HS) with the energy (per particle) given by $E_0 = -0.9195J$,[18] which is the same as the Heisenberg energy shifted by $-J/4$ per bond. In the $J/t \to 0$ limit, the interaction is due to the restriction of one electron per site, which act as hard scatterers. However, in the zero density limit, the electrons behave like nearly free particles with the ground state energy per particle equal to the kinetic energy of single electron $-3t$.

It is in the intermediate interaction strengths other phases may exist. In the case of a square lattice, it has been proven that the electrons start forming pairs for $J/t > 2$.[3,4] In fact, this result is true for any bipartite lattice in any dimension. In this paper we provide a rigorous proof to support our claim. Further we calculate the critical J beyond which the system phase separates into an electron rich and a vacuum phase. To explore the possibility of other phases, the critical exchange couplings for three and four electrons are calculated via exact diagonalization studies and for six electrons using a perturbative calculation. The results show that the threshold couplings for such phases are higher than the corresponding value for phase separation and hence are never formed.

The proof for the critical value of J proceeds as follows: we consider a bipartite lattice with coordination number z, and containing M points with periodic boundary conditions. The constrained $M(M-1)$ dimensional Hilbert space of two electron states with $S_z = 0$ is spanned by the basis states

$$\Phi_{mn} = c^{\dagger}_{m\uparrow} c^{\dagger}_{n\downarrow} |0\rangle, \quad m \neq n, \tag{1}$$

where $|0\rangle$ is the vacuum state. The two electron wave function is denoted by

$$\Psi = \sum_{m \neq n} \phi_{mn} \Phi_{mn}. \quad (2)$$

The t-J Hamiltonian is written in this constrained subspace of no doubly occupied sites as

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{H.c.}) + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right), \quad (3)$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) an electron of spin σ at site i, $n_i = \Sigma_\sigma c^{\dagger}_{i\sigma} c_{i\sigma}$ is the number operator, $\mathbf{S}_i$ is the spin operator, and $\langle i,j \rangle$ implies nearest-neighbor (nn) bonds. Since the interaction term is nonzero only if the electrons are on the neighboring sites, the equations of motion (EOM) can be separated in two different sets. When m and n are not neighbors, we have

$$E \phi_{mn} = -t \sum_{\delta} (\phi_{mm+\delta} + \phi_{n+\delta n}) \quad (4)$$

and for m and n to be neighbors,

$$E \phi_{mn} = -t \sum_{\delta}{}' (\phi_{mm+\delta} + \phi_{n+\delta n}) - \frac{J}{2} (\phi_{mn} + \phi_{nm}). \quad (5)$$

The sum over δ includes all neighbors, and the primed summation indicates the constraint $m + \delta \neq n$ and $n + \delta \neq m$. To obtain a lower bound for the ground state energy, we invoke the Gershgorin disk theorem from numerical linear algebra,[19] which states that all eigenvalues of a matrix are contained within the disks in a complex plane whose centers are the diagonal elements of the matrix and radii are given by the corresponding deleted row sums. From EOM it is straightforward to see that the matrix of the Hamiltonian given by Eq. (3) has the following property: for any row corresponding to ϕ_{mn}, where m and n are neighbors, the diagonal element is $-J/2$ and the deleted row sum is $-2t(z-1) - J/2$. For other rows (when m and n are not neighbors), the diagonal element is 0 and the deleted row sum is $-2tz$. Therefore the lower bound for the ground state energy $E_0^{(2)}$ is given by

$$\begin{aligned} E_0^{(2)} &\geqslant \min\{-2tz, -2t(z-1) - J\} \\ &\geqslant -2tz \quad \text{for } J \leqslant 2t \\ &\geqslant -2tz - (J - 2t) \quad \text{for } J > 2t. \end{aligned} \quad (6)$$

Since for a bound state to occur the energy of the system must lie below the noninteracting two-electron band, i.e., $-2zt$, this result proves that bound states *cannot* occur for $J < 2t$ for any lattice size. To get an upper bound on the ground state energy, we perform a variational calculation by choosing the trial state with constant amplitudes viz. $\phi_{mn} = \lambda$ (say). The ground state energy $E_0^{(2)} \leqslant \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$. The denominator, $\langle \Psi | \Psi \rangle = \lambda^2 M(M-1)$ and the numerator $\langle \Psi | H | \Psi \rangle$ is λ^2 times the sum of the elements of the Hamiltonian matrix. There are Mz rows given by Eq. (5) yielding a row sum $-2tz - (J - 2t)$ and remaining rows with the row sum $-2tz$. Therefore one can write

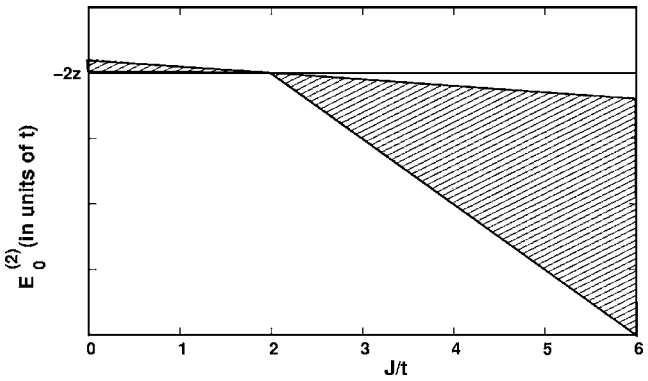

FIG. 1. Bounds for the ground state energy, $E_0^{(2)}$, of the two electron system. The energy must lie in the shaded region.

$$E_0^{(2)} \leqslant -2zt + \frac{(2t - J)z}{M - 1}. \quad (7)$$

We have plotted these bounds in Fig. 1. $E_0^{(2)}$ must lie in the shaded region. Thus, for any M, two electron bound states are formed for $J > 2t$. It is interesting to note that for $J < 2t$, in the $M \to \infty$ limit, the upper bound coincides with the lower bound, and hence $E_0^{(2)} = -2zt$ on an infinite lattice. In this case, the electrons are nearly free, since the average distance between the electrons is too large compared to the range of the interaction. At $J = 2t$, independent of the lattice size, the ground state is given by $\phi_{mn} =$ constant and hence is not a bound state. This is a very important result and is most generally applicable to any bipartite lattice in any dimension. It also provides an explanation for the corresponding result ($J_{2c} = 2t$) known in the context of one-dimensional chains,[20,21] two-leg ladder,[22] and two-dimensional square lattice.[4,6,11,23]

However, for $J > 2t$, the ground state energy depends on the lattice. Hereafter, our calculations are done for the honeycomb lattice. For two electrons, we have obtained the ground state energy $E_0^{(2)}$ by exact diagonalization. Figure 2, among other things, shows the energy per particle for two electrons on an infinite lattice. Now consider an electronic system at near-zero density in the thermodynamic limit. For

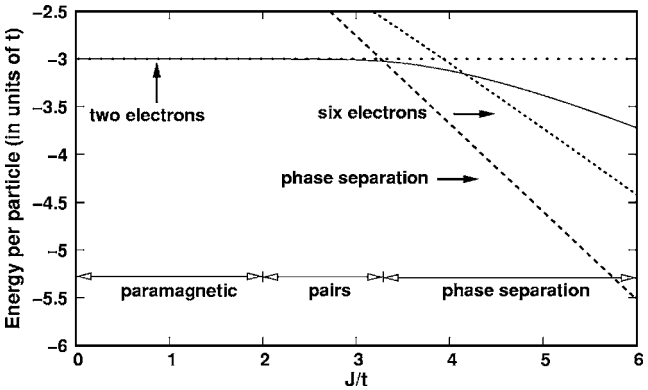

FIG. 2. The phase diagram in zero density limit for a honeycomb lattice. Energy per particle for six electrons is obtained by perturbative analysis.

very large values of J/t, the system condenses into an antiferromagnetic phase separated state with energy per particle $E^{(PS)}=E_0=-0.9195J$. This is represented by a dashed line in Fig. 2. As J is decreased below a critical value $J_{PS}=3.29t$ (the intersection between $E_0^{(2)}$ and $E^{(PS)}$), pairs of electrons become energetically more stable. Thus, for $J<3.29t$, the system consists of a dilute gas of pairs, which is nonmagnetic. When J is decreased further below $J_{2c}=2t$ (the threshold value for pair formation), the gas of pairs becomes unstable and the pairs dissociate into single electrons, thereby signaling paramagnetism. These results are summarized in Fig. 2. However, the possibility of other intervening phases with clusters of three or more electrons cannot be ruled out. We show that none of these phases are stable at any value of J. At low temperatures, the dilute gas of pairs may condense to become a BCS-like superconductor.

For large J, we have calculated the energy per particle of a cluster of three and four electrons which are $-0.5J$ and $-0.5915J$, respectively. The more interesting case is that for six electrons, which can form a ring and have an energy of $-0.7171J$ per particle. To show that clusters of three electrons are not formed, we calculate the ground state energy $E_0^{(3)}$ for a three electron system via exact diagonalization. The critical J, viz. J_{3c}, is defined as the value at which the energy of the three electron system satisfies $E_0^{(3)}=E_0^{(2)}-3t$, the right-hand side being the energy of a bound pair and a free electron. J_{3c} depends on the lattice size. We have calculated these values for $4\times4\times2$, $6\times6\times2$, and $8\times8\times2$ lattices (the factor of 2 is due to two lattice sites per unit cell) and hence extrapolated it to infinite lattice. These results are shown in Fig. 3. The extrapolated value of J_{3c} is $3.75t$. Since $J_{3c}>J_{PS}$, the phase separation occurs before the formation clusters of three electrons. For a cluster of four electrons, J_{4c} is obtained in an exactly similar manner except for the ground state energy of the four electron system is now compared with that of two bound pairs. J_{4c} is found to be $4.32t$.

However, for six electrons, it is not possible to exactly diagonalize the Hamiltonian matrix as it is too large. We estimate the critical value of the interaction term, J_{6c}, using a perturbative analysis similar to Lin.[4] For $J\gg t$, the Hamiltonian reduces to that of the Heisenberg model. The ground state of the model is a ring of six electrons, which is calculated to be having an energy of $-4.302776J$. We obtain the correction to this ground state by treating the hopping term (t) as perturbation. The hopping term connects the ground state with 120 ($6\times{}^6C_3$) (Ref. 24) excited states comprising a chain of five and a free electron. We have numerically calculated the correction to the ground state energy up to second order in t/J (first order yields zero) and is given by

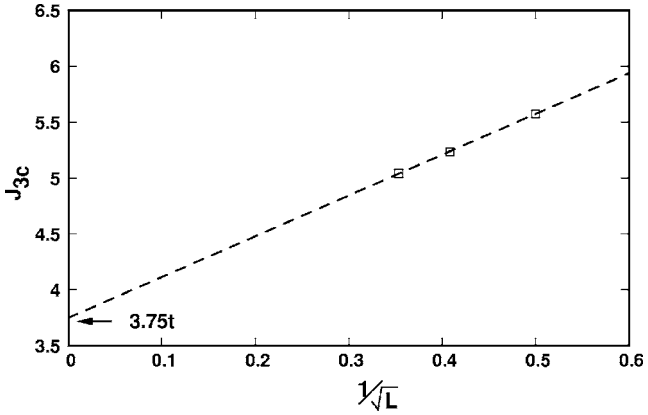

FIG. 3. The critical value J_{3c} as a function of L, where the number of sites in the lattice is $L\times L\times 2$. The extrapolated value of J_{3c} is $3.75t$.

$$E_0^{(6)}=J\left[-4.302776-4.266608\left(\frac{t}{J}\right)^2\right]. \tag{8}$$

By comparing $E_0^{(6)}$ with the energy of three pairs, we get $J_{6c}=4.16t$ which indicates that the cluster of six electrons is not a stable configuration and hence does not figure in the phase diagram.

It may be noted that, in addition to the value of J_{2c}, the qualitative features of the phase diagram in zero density limit seem to be independent of the lattice and dimensionality. The representative values for J_{ps}, known by now, are $2.5t$ for one-dimensional chains ($z=2$),[21] $3.29t$ for a honeycomb lattice in two dimensions ($z=3$), and $3.43t$ for a square lattice ($z=4$).[3,7] It will be interesting to investigate the validity of this phase diagram for all bipartite lattices and to obtain the dependence of J_{ps} on coordination number and dimensionality.

In summary, we have obtained the phase diagram of a system described by the t-J model on a two-dimensional honeycomb lattice in zero density limit. For $J\leqslant 2t$, the system behaves like free electrons. For $2t<J<3.29t$, we have a dilute gas of pairs. Finally, for $J>3.29t$, the system is fully phase separated with an "electron rich" (HS) and a "no electron" phase. We have also rigorously shown that the pair formation begins at $J=2t$ for a $t-J$ model on any bipartite lattice in any dimension.

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[1] P. W. Anderson, Science **235**, 1196 (1987).
[2] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, R3759 (1988).
[3] V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).
[4] H. Q. Lin, Phys. Rev. B **44**, 4674 (1991).
[5] V. Waas, H. Fehske, and H. Büttner, Phys. Rev. B **48**, 9106 (1993).
[6] C. S. Hellberg and E. Manousakis, Phys. Rev. B **52**, 4639 (1995).
[7] C. S. Hellberg and E. Manousakis, Phys. Rev. Lett. **78**, 4609 (1997).
[8] H. Yokoyama and M. Ogata, J. Phys. Soc. Jpn. **65**, 3615 (1996).
[9] W. O. Putikka, M. U. Luchini, and T. M. Rice, Phys. Rev. Lett.

68, 538 (1992); W. O. Putikka and M. U. Luchini, Phys. Rev. B **62**, 1684 (2000).
[10] M. Marder, N. Papanicolaou, and G. C. Psaltakis, Phys. Rev. B **41**, 6920 (1990).
[11] M. Yu Kagan and T. M. Rice, J. Phys.: Condens. Matter **6**, 3771 (1994).
[12] J. D. Jorgensen, B. Dabrowski, S. Pe, D. G. Hinks, L. Soderholm, B. Morosin, J. E. Schirber, E. L. Venturini, and D. S. Ginley, Phys. Rev. B **38**, 11337 (1988); P. C. Hammel, A. P. Reyes, Z. Fisk, M. Takigawa, J. D. Thompson, R. H. Heffner, S. W. Cheong, and J. E. Schirber, *ibid.* **42**, R6781 (1990); J. H. Cho, F. C. Chou, and D. C. Johnston, Phys. Rev. Lett. **70**, 222 (1993).
[13] M. Calandra, F. Becca, and S. Sorella, Phys. Rev. Lett. **81**, 5185 (1998).
[14] C. S. Hellberg and E. Manousakis, Phys. Rev. Lett. **83**, 132 (1999).
[15] S. A. Kivelson, V. J. Emery, and H. Q. Lin, Phys. Rev. B **42**, 6523 (1990); S. A. Kivelson and V. J. Emery, in *Strongly Correlated Electronic Materials: The Los Alamos Symposium, 1993*, edited by K. S. Bedell *et al.* (Addison-Wesley, Reading, MA, 1994).
[16] V. J. Emery and S. A. Kivelson, Physica C **209**, 597 (1993).
[17] E. Dagotto, J. Riera, Y. C. Chen, A. Moreo, A. Nazarenko, F. Alcaraz, and F. Ortolani, Phys. Rev. B **49**, 3548 (1994).
[18] J. D. Reger, J. A. Riera, and A. P. Young, J. Phys.: Condens. Matter **1**, 1855 (1989).
[19] *Matrix Computations*, 3rd ed., edited by G. H. Golub and Charles F. Van Loan, (The John Hopkins University Press, Baltimore, 1996) p. 320
[20] Li Chen and C. Mei, Phys. Rev. B **39**, 9006 (1989); X. Zotos, *ibid.* **37**, 5594 (1988).
[21] M. Ogata, M. U. Luchini, S. Sorella, and F. F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).
[22] S. Basu, R. J. Gooding, and P. W. Leung, Phys. Rev. B **63**, 100506(R) (2001).
[23] A. G. Petukhov, J. Galán, and J. A. Vergés, Phys. Rev. B **46**, 6212 (1992).
[24] Three each of up and down spins can be arranged on six sites in ${}^6C_3$ ways, and the factor of 6 accounts for all the configurations rotated by 30°.