Disorder-induced spin polarization in restricted geometries

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We study the influence of disorder on the magnetic properties of the ground state for restricted geometries. We find that for two-dimensional systems disorder enhances the spin polarization of the system. The tendency of disorder to enhance magnetism in the ground state may be relevant to recent experimental observations of spin polarized ground states in quantum dots and small metal grains. [S0163-1829(99)05145-0]

The interplay between disorder and interactions[1] and the possibility that it leads to ground-state ferromagnetism has been the subject of much interest.[2] In several experiments in restricted geometries, such as zero-temperature transport measurements of the conductance through semiconducting quantum dots,[3] carbon nanotubes,[4] and small metal grains,[5] tantalizing hints of a weakly ferromagnetic ground state (GS) of small systems with a few hundreds of electrons have appeared. The ground-state spin polarization may be directly measured by coupling the dot or tube to external leads and measuring the differential conductance. Recent mean-field treatment of electron-electron interactions in disordered electronic systems,[6] a Hartree-Fock approximation of a random matrix theory model,[7] and geometrically confined many-electron systems,[8] as well as the study of circular and especially elliptical dots,[9] suggest the possibility of polarized GS's. In addition, a partially magnetized GS seems probable from a numerical study of such systems.[10] In this work, we suggest that the presence of disorder might enhance the possibility of magnetic GS's.

The GS spin polarization of small clean clusters is known to be highly fluctuating as a function of the number of electrons, and boundary conditions.[11] We wish to show that in some sense the situation in the disordered case is simpler. Two competing effects lead to this complex dependence of the GS spin polarization. There is a singlet favoring effect, which stems from the antisymmetric nature of the fermionic wave function. By rearranging the spin background in order to transfer some of the nodes from the spatial part of the wave function to the spin part energy is lowered.[12] On the other hand, full polarization is favored for lowering the kinetic energy of the independent holes.[13] Disorder reduces the sensitivity of the single-particle wave functions to the boundary conditions which suppress the singlet favoring effect, while the polarization favoring effect is less sensitive to disorder. Therefore, one might expect a transition from a singlet state to a polarized state, as a function of disorder. A numerical study of the $U=\infty$ Hubbard model with a nearly half-filled band supports the existence of such a transition.

In the high-density limit, *e-e* interactions contribute only a small correction to the single-particle kinetic energy, and the GS is obtained by a consecutive filling of the lowest single-particle levels possible. Thus, the GS is a singlet. However, in the low-density limit, where the Coulomb energy dominates the kinetic energy, the weight of doubly occupied states is reduced, and the possibility of a magnetic GS arises. We start by considering the simplest case of a hole in a full band. The spin comes into play since the hopping of the hole around the lattice induces permutations in the spin ordering. The hopping term is then effectively reduced by a factor proportional to the overlap of the permuted spin function with the original one, averaged with respect to the different permutations. In order to maximize the hopping term, thus minimizing the kinetic energy, this overlap should be maximal. This is achieved in the fully polarized state for which the spin wave function is unchanged by permutations of different spins. This consideration is not changed by the presence of disorder. Since the on-site potential energy is not influenced by the spin configuration, the minimization of the kinetic energy leads to a polarized GS. An exact manifestation of this argument was given by Nagaoka,[13] who showed that the GS of one hole in an otherwise half-filled band of the $U=\infty$ Hubbard model is a fully saturated ferromagnetic state, for any realization of the on-site disordered potential. Nagaoka's theorem holds for most lattices with nearest-neighbor hopping. The situation is more complicated when more than one hole exists. Although the above argument for preferring a ferromagnetic order equally applies for the case of several holes, it is known that Nagaoka's theorem cannot be extended even to the case of two holes. In fact, it was shown that the two-hole GS of the ordered $U=\infty$ Hubbard model is a singlet.[12] In order to understand the reason for this complexity, we first describe the situation in one dimension (1D).

Lieb and Mattis have proven for the 1D Hubbard model with an even number of electrons, interaction strength $U<\infty$, and open boundary conditions (BC's), that the GS is a singlet.[14] In the limit of $U=\infty$, the GS is degenerate with respect to all possible spin values. This is plausible in terms of the above argument, since in this limit the electrons cannot bypass each other, and therefore no spin permutation is induced, thus there is no preference to the spin polarized GS. However, when periodic BC's are imposed in 1D, electrons can change their ordering by hopping through the boundaries. It was shown[15] that the problem of m interacting electrons (at $U=\infty$) can be mapped onto a system of m noninteracting spinless fermions on a 1D ring, where the effect of the spin is replaced by a fictitious flux Φ_j, $\Phi_j/\Phi_0 = 2\pi j/m$ $(j=0,1,\ldots,m-1)$, where the fully spin polarized state corresponds to $\Phi_{j=0}=0$. The GS energy is obtained by minimization of the GS energies with respect to the possible ''flux'' values j. A detailed analysis of the j values

which can be generated by the spin background can be done using group representation theory. The flux value which minimizes the GS energy of two spinless particles on a ring is $\Phi=\pi$. This is so even in the presence of disorder.[15] Therefore, the 1D two-hole GS is minimized when a nontrivial spin background is formed, such that a fictitious flux π is generated. The one-hole energy, in turn, is minimized in the absence of flux. Therefore, a trivial spin background, such as the one generated by the fully polarized state, is preferred. On the other hand, when a (real) flux π is applied to the ring, the situation is the opposite. The two-hole GS is accompanied by a trivial spin background, while the one-hole GS is obtained by creating a spin background which forms a fictitious flux $-\pi$, which masks the real flux.

In terms of this picture, we now suggest an explanation to the 2D behavior. In 2D particles can bypass each other, and change their ordering, in many ways (even for hard wall, or open, BC's). For each couple of holes, the hopping of one hole around the other one is equivalent to a hopping of that hole around a flux π, since a phase π accompanies winding of each fermion around another. Since it might be energetically favorable to screen these fluxes, a nontrivial spin background may be generated. The situation is even more complex, since there are many paths in which each hole can circulate its neighbors, and there are, in general, many such couples. In short, we can say that the spin background in the 2D GS is due to the need to optimally mask the fermionic BC's between the holes. One should remember, however, that while in the 1D case, the Nagaoka effect was not relevant, as explained above, in the 2D case there is a competition between these effects. For the case of two holes, it was shown using a special variational wave function, that the energy gain resulting from a complex spin background, supersedes the energy increase at the bottom of the band, coming from the reduction of the hopping amplitude due to the Nagaoka effect.[12] However, in general, one obtains a complex dependence on the details of small clean clusters,[11] due to these competing effects. On the other hand, for bosons the above consideration is not relevant, resulting in the fact that the Nagaoka effect wins for any number of holes and the GS is always ferromagnetic.

Let us now consider the effect of disorder on the tendency towards a complex spin background. As disorder increases, the single-particle functions become less sensitive to the boundary conditions, and thus the fermionic BC constraint becomes less important. Therefore, one may expect that the incentive for reordering of the spin background decreases, while, as in the one-hole case, there still is a contribution from the hopping amplitude leading to a Nagaoka state. We note that while one might expect the effects of disorder in 2D to be smaller than in 1D, this is not the case here. The insensitivity of the 1D GS spin structure to disorder is accounted for by the fact that the spin permutation subgroup induced by the 1D hopping terms is cyclic.[15] Hence, spin background effects in 1D are not major. On the other hand, the permutation subgroup induced by the 2D hopping terms is non-Abelian, and therefore the spin background has nontrivial effects on the dynamics of the holes. Thus we might expect an interplay between disorder and the behavior of the spin background in 2D.

A numerical study of this effect was done in the framework of the $U=\infty$ Hubbard model, a canonical model for the study of itinerant ferromagnetism.[16] This model is described by the Hamiltonian

$$H=\sum_{i\sigma}\varepsilon_i n_{i\sigma}-t\sum_{\langle ij\rangle\sigma}a^{\dagger}_{i\sigma}a_{j\sigma}+\text{c.c.}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}, \quad (1)$$

where $a^{\dagger}_{i\sigma}$ is the fermionic creation operator on site i with spin σ, $n_{i\uparrow}=a^{\dagger}_{i\uparrow}a_{i\uparrow}$, and the on-site energies ε_i are drawn randomly according to a uniform distribution between $-W/2$ and $W/2$. The large U regime of the model has attracted much interest due to its relevance to the theory of high-T_c superconductivity.[17]

Although the model clearly does not contain many of the physical attributes of the typical experimental system such as a quantum dot (especially at the infinite U limit), nevertheless, it is important to gain insight into the complicated problem of the influence of disorder on the spin structure of interacting electrons in restricted geometries by studying simplified models. Moreover, the infinite U limit has the attractive feature of suppressing antiferromagnetic correlations which are clearly not relevant to quantum dots, even in the clean limit.[9]

Exact diagonalization for the full many-particle Hamiltonian of Eq. (1) was used to test the above arguments. Although we have used small systems one may expect that due to the chaotic nature of the dots[10] the dependence on the number of electrons or the BC's will play a less important role for disordered systems than in clean ones.[11] Thus, the study of a small number of electrons is still useful in understanding the properties of dots which are populated by an order of magnitude more electrons. We have used up to 14 electrons on up to 4×4 lattices. The size of the Hilbert space is then 471 435 600, which is far beyond exact diagonalization capabilities. Fortunately one can omit the double occupied states for $U=\infty$ and use the spin symmetry of the Hamiltonian to reduce this number considerably. The number of spatial functions in this case is 120, and the number of total spin configurations in the $S_z=0$ sector is 3432, yielding a total of 411 840 states. We have used group theory to construct the definite S states, and to decompose the space into subspaces of definite S and S_z. The largest sectors ($S=1,2$) consisted of 1001 spin functions and a total of 120 120 basis functions. Group theory was used for constructing the matrices describing the effect of hopping on the different spin functions. We then employed the Lanczos algorithm to find the exact GS for 600 realizations at every disorder value. In the ordered case, the GS was a singlet, in accordance with Ref. 12.

Figure 1 presents the GS-spin distributions as a function of W, for 14 electrons on a hard-wall 4×4 lattice. The average spin $\langle S\rangle$ is also plotted against W, and one can see that it increases significantly with W. In the presence of disorder, one gets a distribution of GS-spin values. For weak disorder, the main effect is smearing the peak at $S=0$ to low S values. Thus, a tendency towards weak ferromagnetism is clearly demonstrated even for weak disorder ($W=3t$), which corresponds to a ballistic (mean free path larger than the system size) regime. Moreover, as disorder increases, high S values

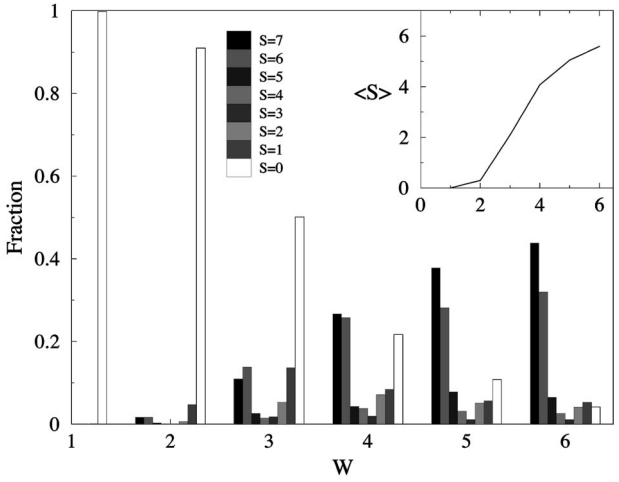

FIG. 1. The spin distributions as a function of disorder W for a 4×4 lattice with 14 electrons. For each W, the bar chart represents the probability of finding the GS of the system at a particular value of S. The inset presents the average spin $\langle S\rangle$ as a function of W.

dominate the distribution. For $W=6t$ corresponding to a diffusive regime a clear dominance of the high spin state appears.

Similar behavior was obtained for smaller lattices and periodic BC's. Figure 2 presents the results for the same conditions as in Fig. 1 employing periodic BC's. Clearly, the tendency towards ferromagnetic behavior persists, although higher values of W are needed to obtain similar values of spin polarization. This is the result of the fact that for periodic BC's, higher values of W are needed to generate the same value of dimensionless conductance. One sees that, in contrast with the situation in the ordered case, the qualitative behavior of the system is not sensitive to the lattice size or the BC's. This manifests the chaotic nature of the dot, which suppress dependencies on the details of the system. A clear manifestation of this point is presented by the results for 13 electrons on a 5×3 lattice. In the ordered case, the behavior of this cluster depends dramatically on the BC's. For hard-wall BC's, the GS is fully polarized (i.e., $S=\frac{13}{2}$), while for periodic BC's, the GS has the minimal spin $S=\frac{1}{2}$. On the other hand, once the system is diffusive the GS-spin polarization distributions become closer and when the dimensionless conductance is of order 1, both distributions are quite similar, where $\langle S\rangle=5.90$ for hard-wall BC's and $\langle S\rangle=3.96$ for periodic BC's.

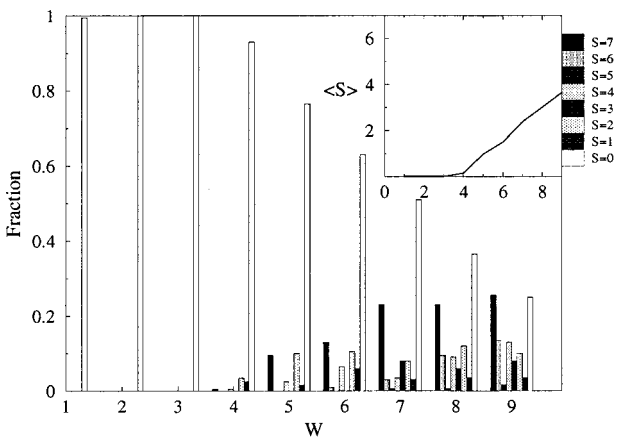

FIG. 2. Same as Fig. 1 for periodic BC's.

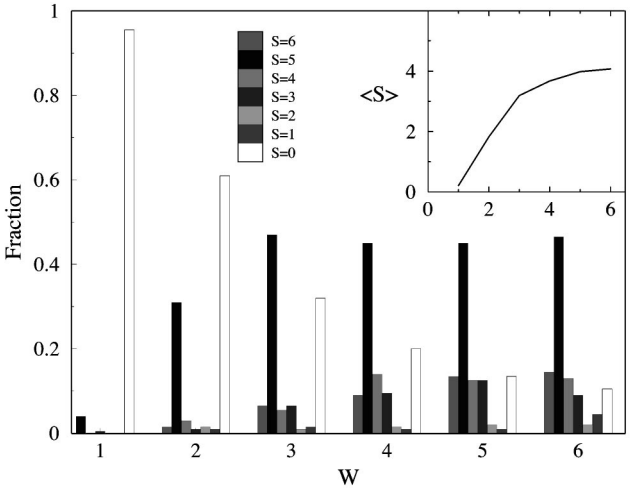

FIG. 3. The spin distributions as a function of disorder W for a 5×3 lattice with 12 electrons.

Exact diagonalization also confirms the tendency towards nonzero ground-state spin values even for a higher number of holes. In Fig. 3 we depict the spin distribution for 12 electrons on a hard-wall 5×3 lattice (3 holes). The GS spin is significantly enhanced as function of disorder, although the most probable spin state is not fully ferromagnetic. This tendency towards partial polarization of the ground state persists in higher hole ratios.

The method of exact diagonalization is restricted to small lattices. In order to learn whether the tendency towards ferromagnetism persists for larger systems we turn to a variational method. Many authors have considered various variational wave functions to study the instability of the Nagaoka state of the $U=\infty$ model for a thermodynamic concentration of holes.[18–22] Since the reliability of these functions for an accurate calculation of the phase boundary of ferromagnetism is doubtful, we only use this method to get a hint about disorder influence of the stability. For this purpose, we use the most simple of these functions,[18] which is one of a single-particle excitation. An up-spin electron is removed from the occupied states and placed with flipped spin into another state. The explicit wave function is given by

$$|\psi\rangle=N_s^{-1/2}\sum_m e^{iqr_m}a^\dagger_{m\downarrow}(1-n_{m\downarrow})C_{k_F\uparrow}|F\rangle, \tag{2}$$

where $C_k^\dagger$ is the fermionic creation operator with momentum k, and $|F\rangle$ is the ferromagnetic Nagaoka state

$$|F\rangle=\prod_{0\le|k|\le k_F}C^\dagger_{k\uparrow}|vac\rangle. \tag{3}$$

Direct calculation of the excitation energy yields[18]

$$\lambda(q)=\langle\psi|H-E_0|\psi\rangle/\langle\psi|\psi\rangle=(\hat{\mu}-\epsilon_F)+\epsilon_q\delta(1-\hat{\mu}^2/z^2t^2), \tag{4}$$

where E_0 is the energy of the Nagaoka state, $\hat{\mu}=-E_0/(N\delta)$, and z is the coordination number. The excitation energy is thus the energy of the new state, corrected for the reduction in the hopping of the down electron due to its neighboring up electrons, plus the energy gain of the up electrons which have to avoid the down electron, minus the energy on the flipped electron.

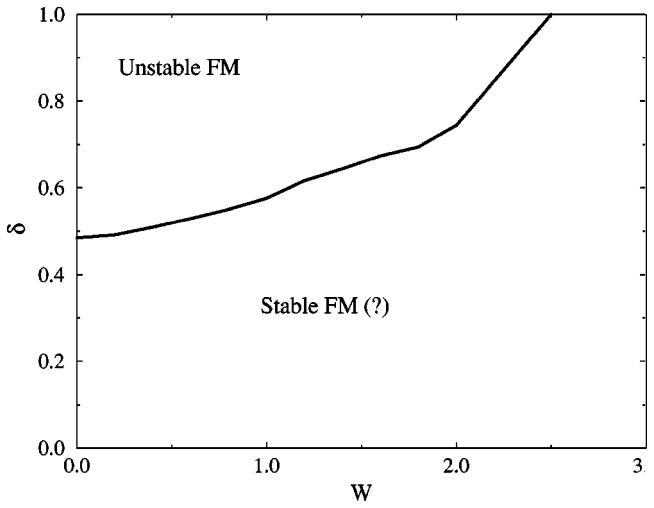

FIG. 4. Stability curve for the single flip excitation: the critical hole density δ vs the disorder distribution width W.

Clearly the lowest value of $\lambda(q)$ is obtained by setting ϵ_q as the bottom of the band energy. This excitation energy is an upper bound to the lowest excitation of the Nagaoka state. Whenever this energy becomes negative, the Nagaoka state is unstable. It was shown in Ref. 18 that this happens for $\delta = 0.49$ (for a square lattice), while for smaller hole concentration, the Nagaoka state remains stable with respect to this excitation. More complicated variational functions were used to further improve this bound.

In order to estimate the effect of disorder on the stability of the ferromagnetic phase, we look into the behavior of the single-flip excitation energy in disordered systems. A natural way to incorporate disorder would have been to replace the plane waves expansion in Eq. (2) with the random vector (RVM) single-particle wave functions of the disordered system.[23] Such a naive replacement results in

$$\lambda^{\mathrm{dis}}(q) = \langle \psi | H - E_0 | \psi \rangle / \langle \psi | \psi \rangle = (\hat{\mu} - \epsilon_F) + \epsilon_q \delta, \qquad (5)$$

i.e., the same as Eq. (4), except for the last term which vanishes in the RVM limit (here q denotes the state index). Since ϵ_F and $\hat{\mu}$ are not influenced by the disorder and the lowest single-electron energy is lowered by disorder, the RVM prediction leads to a destabilization of the ferromagnetic state, in contrast with our above arguments.

However, the results of the actual calculation were different. We have taken different realizations of disorder of a 24×24 system, diagonalizing the single-particle (noninteracting) Hamiltonian to find its eigenvalues and eigenvectors, then calculating directly the excitation energy of the single flip variational wave function. Figure 4 shows the stability regime in the δ-W plane, as follows from this excitation calculation. For an ordered system we get the result of Ref. 18 that the ferromagnetic state is stable for $\delta \leqslant 0.49$. However, as disorder increases, the stability regime grows, in contradiction with RVM predictions. This stems from the fact that RVM ignores correlations between the wave functions and the eigenvalues which are important in this case. It therefore seems that the exact results for small systems characterize the behavior in larger systems as well.

An extensive work was done in order to find whether Nagaoka's theorem can be extended to higher hole density, or to finite U. Various variational wave functions were suggested to test the stability of the Nagaoka state in the thermodynamic limit (see Refs. 18–22 and 24, and references therein). Bounds were given to the holes density for which stability may remain. The best bound to date is $\delta_{cr} \leqslant 0.2514$ (Ref. 20) (where δ is the number of holes per site). Still, the stability of the Nagaoka state, and the possibility of explaining ferromagnetism by it, is an unresolved problem.[24] As we have seen, the behavior of the disordered model might be simpler. Regardless of the behavior of the ordered model, it might be expected that the Nagaoka effect will certainly dominate in the strongly localized regime where the average distance between holes is more then ξ, i.e., $\delta^{-1/d} \gg \xi/L$, where L is the system linear size.

We would like to add a remark about the $U=\infty$ limit. The Nagaoka effect and the decrease in the singlet favoring effect described here, are not unique to the $U=\infty$ limit. However, for the Hubbard model, ferromagnetism arises (even for one hole) only for $U \gg t$, since due to the perfect nesting property of the lattice model, the GS of the almost half-filled case tends to be antiferromagnetic (AFM). In order to wash out this tendency, the limit $U=\infty$ is taken. However, real quantum dots do not show AFM behavior, since they are not described by a perfect lattice. One then might expect formation of larger magnetic moments due to disorder to show in real quantum dots even for moderate values of U.

In conclusion, the influence of disorder on the magnetic properties of the GS was studied. For an ordered system, large magnetic moments are generally suppressed, and the spin structure of the GS, if any, is very complicated. On the other hand, we have shown that disorder plays an important role in determining the spin polarization of 2D systems described by the infinite U Hubbard model. Weak disorder tends to create a partially polarized ground state, while stronger disorder tends to stabilize a fully ferromagnetic GS. This behavior clearly indicates that there is a basis to expect that for more realistic descriptions of the experimental systems ($U \neq \infty$) disorder will play an important role in creating a spin polarized ground state.

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[1] See, for example, B. L. Altshuler and A. G. Aronov, in *Electron-Electron Interactions in Disordered Systems*, edited by A. J. Efros and M. Pollak (North-Holland, Amsterdam, 1985), pp. 1–153; H. Fukuyama, *ibid.*, pp. 153–230.

[2] A. M. Finkelstein, Z. Phys. B: Condens. Matter **56**, 189 (1984); C. Castellani, C. DiCastro, P. A. Lee, M. Ma, S. Sorella, and E. Tabet, Phys. Rev. B **30**, 1596 (1984); M. Milovanović, S. Sachdev, and R. N. Bhatt, Phys. Rev. Lett. **63**, 82 (1989); D. Belitz and T. R. Kirkpatrick, Rev. Mod. Phys. **66**, 261 (1994).

[3] U. Sivan, R. Berkovits, Y. Aloni, O. Prus, A. Auerbach, and G.

Ben-Yoseph, Phys. Rev. Lett. **77**, 1123 (1996); F. Simmel, T. Heinzel, and D. A. Wharam, Europhys. Lett. **38**, 123 (1997); S. R. Patel, S. M. Cronenwett, D. R. Stewart, A. G. Huibers, C. M. Marcus, C. I. Duruoz, J. S. Harris, K. Campman, and A. C. Gossard, Phys. Rev. Lett. **80**, 4522 (1998); F. Simmel, D. Abusch-Magder, D. A. Wharam, M. A. Kastner, and J. P. Kotthaus, Phys. Rev. B **59**, R10 441 (1999).

[4] S. J. Tans, M. H. Devoret, R. J. A. Groeneveld, and C. Dekker, Nature (London) **394**, 761 (1998).

[5] D. Dacidović and M. Tinkham (unpublished).

[6] A. V. Andreev and A. Kamenev, Phys. Rev. Lett. **81**, 3199 (1998).

[7] P. W. Brouwer, Y. Oreg, and B. I. Halperin, Phys. Rev. B **60**, 13 977 (1999).

[8] H. U. Baranger, D. Ullmo, and L. I. Glazman, Phys. Rev. B (to be published 15 Dec. 1999).

[9] K. Hirose and N. S. Wingreen, Phys. Rev. B **59**, 4604 (1999); R. Egger, W. Hausler, C. H. Mak, and H. Grabert, Phys. Rev. Lett. **82**, 3320 (1999); M. Koshinen, M. Manninen, and S. M. Reimann, *ibid.* **79**, 1389 (1997).

[10] R. Berkovits, Phys. Rev. Lett. **81**, 2128 (1998).

[11] E. Dagotto, A. Moreo, F. Ortolani, D. Poilblanc, and J. Riera, Phys. Rev. B **45**, 10 741 (1992); G. Chiappe, E. Louis, J. Galan, F. Guinea, and J. A. Verges, *ibid.* **48**, 16 539 (1993).

[12] B. Doucot and X. G. Wen, Phys. Rev. B **40**, 2719 (1989).

[13] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[14] E. Lieb and D. C. Mattis, Phys. Rev. **125**, 164 (1962).

[15] E. Eisenberg and R. Berkovits, J. Phys. A **32**, 3599 (1999).

[16] J. Hubbard, Proc. R. Soc. London, Ser. B **276**, 238 (1963); M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963); J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).

[17] P. W. Anderson, Science **235**, 1196 (1987).

[18] B. S. Shastry, H. R. Krishnamurthy, and P. W. Anderson, Phys. Rev. B **41**, 2375 (1990).

[19] W. von der Linden and D. M. Edwards, J. Phys.: Condens. Matter **3**, 4917 (1991).

[20] P. Wurth, G. S. Uhrig, and E. Müller-Hartmann, Ann. Phys. (Leipzig) **5**, 148 (1996).

[21] T. Hanisch, G. S. Uhrig, and E. Müller-Hartmann, Phys. Rev. B **56**, 13 960 (1997).

[22] T. Okabe, Phys. Rev. B **57**, 403 (1998).

[23] N. Ullah, Nucl. Phys. **58**, 65 (1964).

[24] For recent results, see S. Liang and H. Pang, Europhys. Lett. **32**, 173 (1995); R. O. Zaitsev and Yu. V. Mikhailova, Fiz. Nizk. Temp. **22**, 1281 (1996) [Low Temp. Phys. **22**, 974 (1996)]; E. V. Kuz'min, Fiz. Tverd. Tela (St. Petersburg) **39**, 193 (1997) [Phys. Solid State **39**, 169 (1997)].