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SPIN DELOCALIZATION PHASE TRANSITION IN A CORRELATED ELECTRONS MODEL

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ABSTRACT

In a simplified one–site model for correlated electrons systems we show the existence of a phase transition corresponding to spin delocalization. The system becomes a solvable model and zero–dimensional functional techniques are used.

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I. Introduction

In a wide variety of materials the interaction between electrons becomes important and the band theory is unable to explain physical properties. These systems pose serious difficulties, and after nearly three decades of studies only one-dimensional versions are really well understood. The most well-known example is the Hubbard model.[1] The experimental discovery of high temperature superconducting ceramics has renewed the interest on those systems.[2,3]

This paper is founded on the purpose of understanding some results concerning correlated electron systems. These results arise by applying functional techniques to the problem of determining the phases of the model. When these phases appear in discontinuous transitions some technical difficulties arise, and it is not easy to determine when the transitions occur.

We have seen that many of the interesting properties of the systems we are talking about appear in a very simplified model. The model consists of a single-site system immersed in a reservoir of electrons, such as a gas. This single-site is in a potential well with only one possible energy level, and which can trap one or two electrons (of different spins) from the surroundings. The on-site electrons repel to each other. For instance, we can think of a very definite atomic level whose occupying electrons can hop to and from a neighboring delocalized electronic band.

We will see that this model exhibits a phase transition depending on the values of the parameters involved. The order parameter will be able to be interpreted as a measure of the existence of spin delocalized electronic states.

The paper is organized as follows. The second section is dedicated to introduce the model and the formalism for doing calculations. In Sec. III we determine the phases of the model. Finally, in sec IV, we briefly discuss some further possibilities of applying these results.

II. The hamiltonian

We consider a one-site system of electrons of both up and down spin states whose Hamiltonian involves a repulsive on-site interaction:

$$H = -\mu \sum_{\sigma=\uparrow,\downarrow} c_\sigma^\dagger c_\sigma + U c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow \tag{1}$$

where σ runs over up ($\uparrow$) and down ($\downarrow$) states, and $\mu > 0$. The trapping of electrons coming from the reservoir is ruled out by the chemical potential μ. Since we can write

$$\begin{aligned} c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow &= -\frac{1}{2}\sum_\sigma c_\sigma^\dagger c_{-\sigma} c_{-\sigma}^\dagger c_\sigma + \frac{1}{2}\sum_\sigma c_\sigma^\dagger c_\sigma \\ &= -\frac{1}{2}(\sum_\sigma c_\sigma^\dagger c_{-\sigma})^2 + \frac{1}{2}\sum_\sigma c_\sigma^\dagger c_\sigma . \end{aligned} \tag{2}$$

The Hamiltonian becomes

$$H = -(\mu - \frac{U}{2})\sum_\sigma c_\sigma^\dagger c_\sigma - \frac{U}{2}(\sum_\sigma c_\sigma^\dagger c_{-\sigma})^2 . \tag{3}$$

The partition function in the path integral representation is written as

$$Z = \int \prod_{\tau,\sigma} dc_\sigma(\tau) dc_\sigma^\dagger(\tau) \exp \int_0^\beta [\,(\mu - \frac{U}{2})\sum_\sigma c_\sigma^\dagger c_\sigma + \frac{U}{2}(\sum_\sigma c_\sigma^\dagger c_{-\sigma})^2\,] \tag{4}$$

where $\beta = 1/kT$, T is the temperature. The "static" form assumed corresponds to a zeroth order strong coupling approximation.[4]

The four-fermion interaction term can be written in terms of an auxiliary bosonic field, since

$$e^{\beta(U/2)(\sum_\sigma c_\sigma^\dagger c_{-\sigma})^2} = \int d\xi e^{-\beta(1/2U)\xi^2 + \beta\xi\sum_\sigma c_\sigma^\dagger c_{-\sigma}} . \tag{5}$$

The above order parameter is a measure of the tendency of the system to form combined up and down states. That is roughly so, because the only states which can produce a nonzero expectation value for ξ are combinations of spin up and down electrons. In order to integrate out fermionic fields it is useful to introduce the bi-spinor $\psi = (c_\uparrow, c_\downarrow)$. Then, from (5), we obtain for the partition function

$$Z = \int d\xi d\psi d\psi^\dagger \exp(\int_0^\beta \psi^\dagger[(\mu - \frac{U}{2})\mathrm{I} + \xi\sigma_1]\psi - \frac{\beta}{2U}\xi^2\,). \tag{6}$$

We now introduce a temperature-independent form for the order parameter. This is justified since we will be looking for its saddle-point value. We now integrate out the ψ fields to obtain

$$Z = \int d\xi \exp(-\frac{\beta}{2U}\xi^2)(\det|(\mu - \frac{U}{2})\mathrm{I} + \xi\sigma_1|)^{\frac{\beta\Lambda}{\pi}} . \tag{7}$$

An exponent for the resulting determinant is obtained since the fermionic integral in ψ is a product of one-dimensional integrals at each temperature point τ. The number of integrals is regularized by dividing the temperature interval $(0,\beta)$ into cells of length π/Λ, where Λ is a cutoff for the temperature[5]. On the other hand, the multiplicative factor in the partition function, β^2, can be dropped out. The determinant is easily computed to be

$$\begin{aligned} \det[(\mu - \frac{U}{2})\mathrm{I} + \xi\sigma_1] &= \det[(\mu - \frac{U}{2})I]\det[1 + (\mu - \frac{U}{2})^{-1}\xi\sigma_1] \\ &= (\mu - \frac{U}{2})^2[1 - \frac{\xi^2}{(\mu - U/2)^2}] \\ &= (\mu - \frac{U}{2})^2 \mathrm{sgn}(1 - \frac{\xi^2}{(\mu - U/2)^2}) \exp \ln|1 - \frac{\xi^2}{(\mu - U/2)^2}| . \end{aligned} \tag{8}$$

Therefore, the partition function finally becomes

$$Z = \int d\xi sgn(\mu^2 - \xi^2)) \exp(-\frac{\beta}{2U}\xi^2 + \frac{\beta\Lambda}{\pi}\ln|(\mu - \frac{U}{2})^2 - \xi^2|). \tag{9}$$

The presence in the partition function of a sign function depending on fields is important and signals a difficulty in high dimensional models. It implies a disconnected configuration space for the ξ field, and the partition function acquires an anomalous form. Then, we have to consider each sector separately[6].

III. The phases of the model

The action, as we have seen, separates itself into two disconnected sectors for the order parameter ξ (see fig. 1). We will consider each sector separately. Also, to simplify expresions we will assume[7] $\Lambda = \pi$.

(i) $|\xi| < |\mu - U/2|$.

The effective action is

$$S[\xi] = \frac{1}{2U}\xi^2 - \ln[1 - \frac{\xi^2}{(\mu - \frac{U}{2})^2}] \tag{10}$$

and we only find one extremum, for $\xi = 0$, which is a minimum since $S''[0] = 1/U + 2/(\mu - U/2)^2 > 0$.

(ii) $|\xi| > |\mu - u/2|$.

Now we have

$$S[\xi] = \frac{1}{2U}\xi^2 - \ln[\frac{\xi^2}{(\mu - \frac{U}{2})^2} - 1] \tag{11}$$

and there is also a minimum for $\xi_0^2 = 2U + (\mu - U/2)^2$, since $S''[\xi_0] = 2/U + (\mu - U/2)^2/U^2 > 0$.

The absolute minimum, and therefore the phase the system adopts, is determined by evaluating the action in these extrema. We have $S[0] = 0$, and

$$\begin{aligned} S[\xi_0] &= \frac{1}{2U}\xi_0^2 - \ln(\frac{\xi_0^2}{(\mu - U/2)^2} - 1) \\ &= 1 + \frac{\mu^2}{2U} - \ln\frac{2U}{(\mu - U/2)^2}. \end{aligned} \tag{12}$$

Define $\Delta_\beta(U) \equiv S[\xi_0] - S[0]$, representing the difference of the free energy between nonzero and zero phases, respectively. We see that there is a region bounded above and below, where $\Delta_\beta(U)$, for fixed μ and β, becomes negative (fig. 2). This region includes the singular point $U = 2\mu$.

The dependence on temperature comes from the chemical potential μ, which is determined by the characteristics of the external reservoir. For a gas of electrons we have

$$n_{\mathbf{k}} = \frac{1}{\exp(\beta\omega_{\mathbf{k}}) + 1} \tag{13}$$

where $\omega_{\mathbf{k}} = \epsilon(\mathbf{k}) - \mu$. Then

$$< n >= \frac{2}{V}\sum_{\mathbf{k}} \frac{1}{\exp(\beta\omega_{\mathbf{k}}) + 1} \tag{14}$$

determines μ in terms of a given fixed density of electrons, $< n >$. For the simplest case of a constant dispersion relation, and low temperature approximation, we have $\mu = \epsilon - A/\beta$ where A can be positive or negative depending on the density of electrons. Also the strong coupling restriction imposes that $(\mu - U/2) << U \Rightarrow (\epsilon - U/2) << U$, for low temperatures. All these considerations imply the graph in fig. 3.

Conclusions.

We have studied a simplified correlated electrons model, whose features we expect to be qualitatively correct. The reason for the simplification is, of course, the possibility of getting a solvable theory. However, we have to pay a price, for instance, an explicit dependence on the cutoff A. Although, this dependence does not alter the results qualitatively and, on the other hand, this temperature cutoff could be estimated for realistic models. We also think that this model has something to say about the

Hubbard model. In that case, the reservoir would correspond to a sea of localized electrons, coming to the single site from its neighboring positions. The mechanism of the hopping is, in some sense, averaged, and the larger is the coordination number of a site the better will be the approximation.

An important open problem is to go to quantitative predictions. Also we can intend to remove some restrictions, for example, the strong coupling approximation. Work in those directions is in progress now.

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† *On leave of absence from P. Universidad Catolica de Chile.*

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4. The $\int d\tau c^{\dagger}\partial_{\tau}c$ term is taken as the perturbative part of the action. See, for instance, F. Guerin and R. D. Kenway, Nucl. Phys. **B176** (1980) 168.

5. See ref. 4.

6. We have that

$$Z = \int_{|\xi|<|\mu-\frac{U}{2}|} d\xi e^{-\frac{1}{2U}\xi^2+\ln[(\mu-\frac{U}{2})^2-\xi^2]} - \int_{|\xi|>|\mu-\frac{U}{2}|} d\xi e^{-\frac{1}{2U}\xi^2+\ln[\xi^2-(\mu-\frac{U}{2})^2]}$$

and it is not correct to consider this two-sector model in a unified theory. Actually, the entire approach rests on the existence of a minimum for $S[\xi]$ and it will become meaningful only for the configurations in a neighborhood of that minimum.

7. This explicit dependence on the cutoff does not modify the results qualitatively.

FIGURE CAPTIONS

Fig. 1. The free energy $S[\xi]$ for the order parameter ξ. There are two disconnected domains, each one with a minimum.In the figure the system is in the zero phase.

Fig. 2. The difference in the free energy, $\Delta_\beta(U)$, between the nonzero and zero phases, for fixed μ and β. The region between the zeros corresponds to the dominance of the spin delocalization phase.

Fig. 3. The difference in the free energy between the nonzero and zero phases in terms of the temperature, for low temperatures.

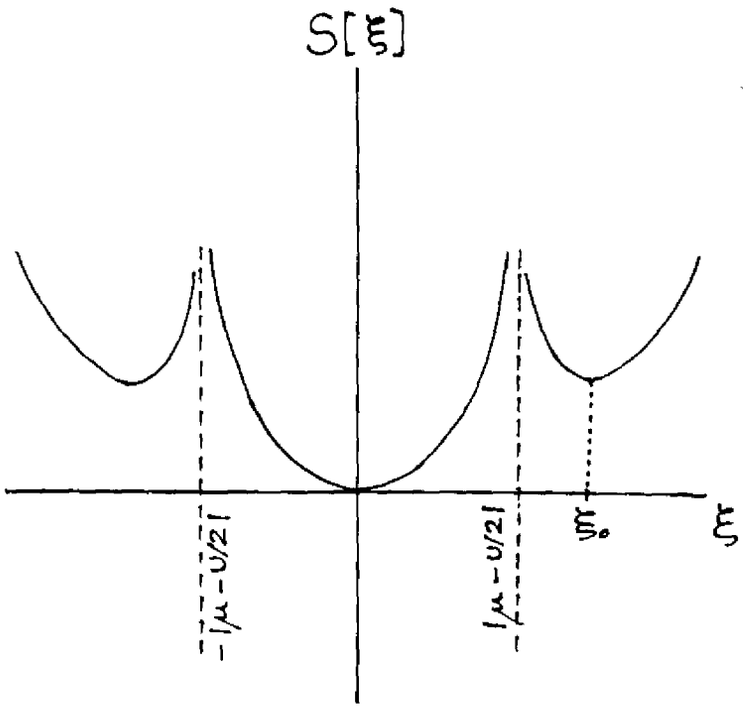

Fig.1

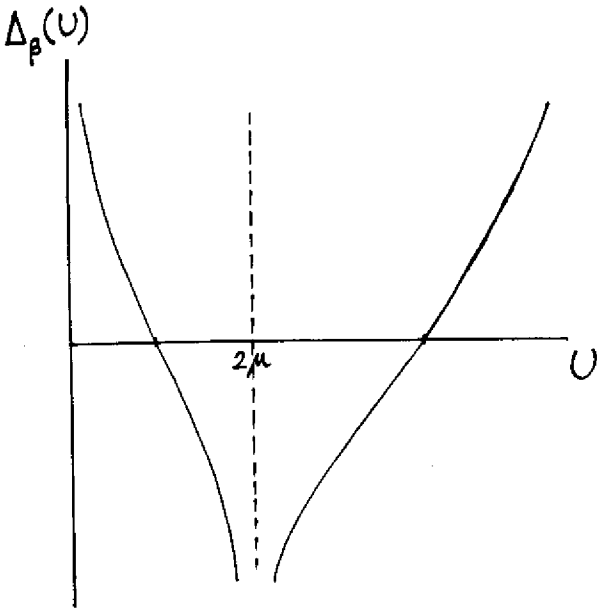

Fig.2

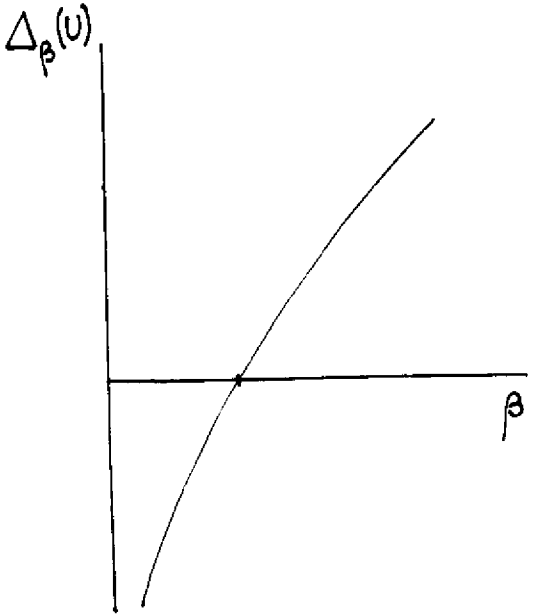

Fig.3