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QUANTUM PHASE TRANSITION IN A RANDOM-TILING MODEL

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Dedicated to Professor Boran Leontić on the occasion of his 70$^{\text{th}}$ birthday

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The analogue of a Mott-Hubbard transition is discussed, which appears at an incommensurate filling in a model of a two-dimensional plane, randomly tiled with CuO_4 'molecules', simulating the copper-oxide planes of high-T_c superconductors. It is shown to be a quantum phase transition, which can be crossed either in doping, at a fixed hopping overlap t, or in t, when the doping is fixed in a certain range below half-filling. It is first-order, closely analogous to a liquid-gas transition.

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1. Introduction

Quantum phase transitions are sudden changes in the nature of the ground state of a physical system, when some dynamical parameter reaches a critical value. Their theoretical mark of distinction is that they occur even when the temperature is strictly zero (as only theory can make it), so that the sampling of phase space, responsible for finding the new optimal configuration, is entirely by quantum, not thermal, fluctuations.

The main interest in these transitions is that they are triggered by quantum many-body effects, so they indicate the appearance of new 'states of matter' built by microscopic interactions. The processes involved in them have been well understood in many cases where a weak-coupling limit is appropriate, the most famous of which is BCS superconductivity. In purely electronic systems in the strong-coupling limit, to which the subsequent discussion is limited, apart from numerical simulations [1] and one-dimensional systems [2], the study of phase transitions has most often resorted to oblique approaches: drawing analogies with the one-dimensional case [3], making inferences from sophisticated weak-coupling studies [4,5], or solving essentially one-body problems, with some constraint added, which supposedly accounts for the effects of strong correlations [6,7].

The present work is of this last kind. It is motivated by the strange 'normal state' of hole-doped high-temperature superconductors, which conduct electricity in some way which has so far defied considerable efforts at explanation. These have revolved around the question, whether the conducting state can be understood by modifying a Fermi liquid picture [8], or some radically different zeroth-order approximation, involving perhaps spin-charge separation [3], is needed. In the materials themselves, a wide range of measurements, from conductivity [9] to photoemission [10], indicate a crossover, from a strange to an apparently Fermi-liquid electron system, as the doping increases from underdoped to overdoped.

Since the present model is one-body, it is unable to address these 'deep' issues directly, being, in addition, tied to a Fermi liquid language by a formal construction. However, it can still distinguish between a liquid and a gas. It turns out that the Mott-Hubbard transition in the model is a liquid-to-gas transition in the direction of *increasing* doping. The system is a liquid in the lower Hubbard band, and a gas in the in-gap band. This seems counterintuitive, because the in-gap band corresponds to a more crowded real space. It is due to the transition being provoked by hopping fluctuations, which find the spatially less ordered 'gas' beneficial for delocalization, precisely when crowding is high. The remainder of the article is a brief elaboration of these points. In particular, it will be shown that the transition is a quantum one, and can be triggered by increasing the hopping overlap at zero temperature, when the doping is fixed in a certain narrow range below half-filling.

2. *The range of the transition*

The model is the same as described previously [11]. It is a random tiling of the copper-oxide planes by CuO_4 'molecules' consisting of a copper site connected with the neighbouring oxygens by a tight-binding overlap t. The only other parameter is the copper-oxygen energy splitting, $\Delta_{pd} > 0$ in the hole picture. Only up-spins actually hop over these molecules, while the presence of the down-spins is expressed by some given concentration of forbidden sites, i.e. the absence of molecules over which the up-spins can hop. The fact that down-electrons are really not heavier than the others is simulated by annealing, so that the phase space accessible to mobile electrons includes all possible positions of the static ones, in contrast to the 'quenched' approach, which would be appropriate for real heavy impurities. The resulting translational invariance enables a k-space formulation which respects the Pauli principle, so the model effectively interpolates between quantum order in inverse space at low temperature, and classical disorder in real space at high temperature. Which temperature is 'low' is determined by the width W of the in-gap band, created by the transition:

$$W = \frac{\widetilde{\Delta}_{pd}}{1 + \Delta_{pd}/(2\widetilde{\Delta}_{pd})}, \tag{1}$$

where $\widetilde{\Delta}_{pd} = \sqrt{\Delta_{pd}^2/4 + 4t^2} - \Delta_{pd}/2$ is the distance from the oxygen band to the middle of the in-gap band.

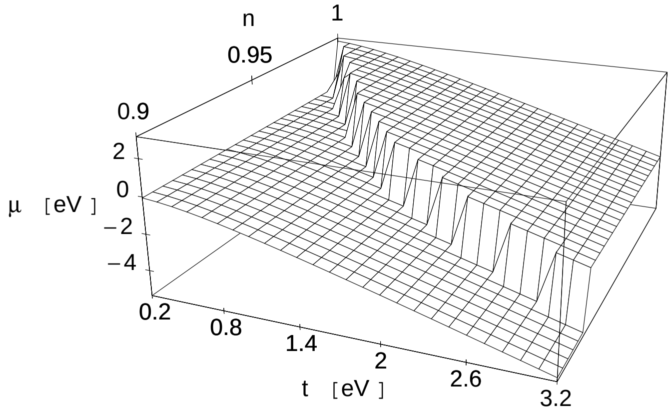

Fig. 1. The chemical potential μ of the mobile spins, as a function of the hopping overlap t and doping $n = 2n_\uparrow = 2n_\downarrow$. Electron doping is $n < 1$, and $\Delta_{pd} = 3$ eV, $T = 40$ K throughout.

Figure 1 shows the Mott-Hubbard transition in the model, as a function of concentration n and hopping overlap t. Clearly, the simple 'kinematical' expectation that it would occur at half-filling for all t is not fulfilled. Instead, the greater t is, the sooner will the transition occur in doping; however, there is also a saturation effect, so even a very large t will not pull the transition below $n \approx 0.9$. When t/Δ_{pd} is small, it occurs near half-filling.

It can be shown that at zero temperature, the transition will occur at the doping value

$$n_\uparrow + n_\downarrow = 1 + \frac{\sin^2(\varphi/2)}{2} \int_{\mathrm{BZ}} [\cos k_x + \cos k_y]\, f_\mu(\varepsilon_-), \tag{2}$$

where $\sin\varphi = 2t/\sqrt{\Delta_{pd}^2/4 + 4t^2}$, and the Fermi function is in terms of the effective bonding band dispersion ε_- of the mobile, up-spins. (The chemical potential μ refers to them, $n_\uparrow = \int_{\mathrm{BZ}} f_\mu$.) Since the band is being filled from the edge of the zone, the factor in brackets is negative, moving the transition from the classical line $n_\uparrow + n_\downarrow = 1$ to smaller values, corresponding to electron doping. If t were so large that $\sin\varphi \to 1$, the correction would be $-1/\pi^2 \approx -0.1$ at half-filling, accounting for the saturation in Fig. 1.

Equation (2) shows the transition to be controlled by the hopping overlap t. It is a quantum phase transition, with (2) giving the critical line in the plane of t and doping, at zero temperature. The physical origin of Eq. (2) is in a basic assumption of the model, that the presence of forbidden sites influences the effective dispersion of the mobile spins ε_- through a bulk parameter, the chemical potential ν of the static down-spins, schematically:

$$Z_{\mu,\nu} = Z_\mu[\varepsilon_-(\nu)] \cdot Z_\nu. \tag{3}$$

This is, essentially, a thermodynamical assumption: the energy levels of mobile up-spins depend on ν as a 'mechanical' measure of their available phase space. Equation (3) implies a contribution from $\partial\varepsilon_-(\nu)/\partial\nu$ to the counting of down-spins, which then produces a transition in the middle of the band; though not precisely in the middle, as shown above. The reason for this can be understood along the same lines: the band *narrows* as the chemical potential of down-spins increases, so that $\partial\varepsilon_-/\partial\nu$ cannot be the same for all states in the band. When it is integrated over the Brillouin zone, it gives the correction in Eq. (2).

The point of all this is that as soon as one imagines something like (3) is possible, the transition will occur at an incommensurate filling; this is a very robust consequence of the assumption (3), not the effect of some detail. As seen from Eq. (2), neglecting the correction would be like taking $\cos k_x + \cos k_y = 0$, true at half-filling, to be true for all states. The present model, by contrast, takes the Pauli principle for the mobile electrons into account exactly. The very existence of a quantum dispersion pushes the transition away from half-filling.

[To derive Eq. (2), one simply adds the saddle-point equations

$$n_\uparrow = \frac{\partial \ln Z_{\mu,\nu}}{\partial \beta\mu},\; n_\downarrow = \frac{\partial \ln Z_{\mu,\nu}}{\partial \beta\nu}, \tag{4}$$

inserting at the same time the particular limit $\nu \to \varepsilon_p - 0$, which corresponds to their solution at the critical line and $T = 0$. Here ε_p is the bare energy of the oxygen level.]

3. The nature of the transition

The model transition from the lower Hubbard to the in-gap band is like from a liquid to a gas. It has been noticed previously [11] that the entropy of mobile spins suffers a discontinuous jump at the transition, and that the contribution of the interaction to the entropy abruptly rises from a fairly large negative value (≈ -0.2 k$_B$ per site) to zero. These are characteristics of a first-order liquid-gas transition. In words, as soon as the interaction has created the in-gap band, its effects are absorbed into the one-particle properties of the band states.

Indications to the same effect can be obtained studying the bulk effective mass, or, technically, the linear specific heat coefficient $\gamma = c_V/T$. First, in non-interacting band electrons, $\gamma(T)$ obeys a simple scaling relationship, when the overlap t is changed:

$$\gamma_{t'}(T) = c\gamma_t(T/c). \tag{5}$$

This is a 'law of corresponding states' for the Fermi gas: the system with an overlap reduced to $t' < t$ is the same as the 'old' system at a lower temperature and higher effective mass ($c > 1$). Figure 2 shows that this is obeyed to very high precision for states in the in-gap band. It should be noted, however, that the renormalizations involved are quantitatively much larger than in the non-interacting case. For instance, changing t from 1 eV to 0.2 eV involves a factor c of only about 10 for non-interacting electrons, while the corresponding factor in Fig. 2 is over 200.

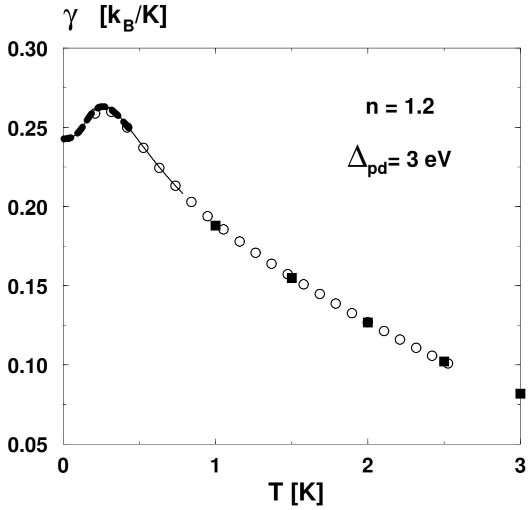

Fig. 2. Scaling property of the linear specific heat coefficient, for $n = 1.2$ *and various* t*. Squares:* $t = 0.2$ eV*. Circles:* $t = 0.3$ eV*, range to 12* K *scaled by* $c = 4.75$ *in Eq. (5). Full line:* $t = 0.8$ eV*, range to 100* K*,* $c = 127.4$*. Dashed line:* $t = 1.0$ eV*, range to 100* K*,* $c = 232.7$*.*

By contrast, in the lower Hubbard band, the scaling (5) is not obeyed. This is consistent with the behaviour of the interaction contribution to the entropy: the system being a liquid there, interactions spoil the scaling which depends only on the kinetic parameter t.

A further characteristic of a first-order transition is that the effective mass does not diverge. The same behaviour as in Fig. 2 is also observed for fillings in the immediate vicinity of the transition. The bulk mass passes through a maximum and saturates, even though for the small value $t = 0.2$ eV shown in the figure, this only happens below 0.5 K. The two minima in the free energy, corresponding to the lower Hubbard band and in-gap band, exchange place without the fluctuations around either diverging.

4. *Discussion*

The quantum transition described here differs from usual model descriptions of the Mott-Hubbard transition, in that it occurs at an incommensurate filling. This is disconcerting, since the classical 'counting' prediction for the transition point is upheld by particle-hole symmetry. However, this symmetry is broken by forbidding fluctuations onto a doubly occupied site. In the one-band model, this results in the disappearance of phase space precisely at half-filling. In the three-band model, there is still phase space associated with the oxygen sites, so there are quantum fluctuations left, even if the doubly occupied site is treated classically. This is the regime of the present model.

The quantum fluctuations are due to projected hopping, which plays the role of an interaction. It creates the in-gap band, which explains why it corresponds to a 'gas' phase: this is where hopping has won! Once particle-hole symmetry is broken, the criterion for the transition becomes quantitative, as expressed by Eq. (2). Such a situation is generic for a phase transition, whose position is usually determined by a competition of energy scales, not arguments of symmetry. Magnetic interactions, for instance, also cause a transition in some incommensurate range, around half-filling. In their absence, no long-range order is expected in the preset model, although a significant tendency to order may be inferred from the interaction entropy in the lower Hubbard band, as the transition is approached [11].

Charge correlations prefer the less ordered 'gas' phase when space becomes crowded, and so their effect is opposite to that of magnetic interactions. The in-gap states are called a gas because, as discussed in Sect. 3, they are characterized by an absence of residual interactions. As opposed to these qualitative considerations, their quantitative parameters may indicate states very close to localization, as shown in Fig. 2. An interpretation of the gas in terms of the underlying fermions is not possible directly within the model, because it uses a trick to count the fermion phase space correctly: the k-space states which diagonalize the grand potential are based on the translational invariance of the ensemble as a whole, not of an individual member of it. The states in a *given* sample could be different from a Fermi liquid. The 'gas' probably means that annealment by quantum fluctuations has moved the forbidden sites out of the way, for hopping to occur down (quantum) percolation channels, which extend across the system, giving rise to some effective band-width. This gives an appealing picture, how mean free paths can be shorter than the lattice spacing: at low t/Δ_{pd}, few of these channels remain open at any finite temperature, because hopping is then inefficient against the even larger entropy associated with complete site disorder. Simulations should help confirm this interpretation, but very steep increases of the entropy with temperature have been obtained [11] in the model at $t/\Delta_{pd} \approx 1/10$.

Finally, one may wonder how much of this picture would remain, if both kinds of electrons were allowed to hop. It is easy to imagine some kind of mutual compromise along the lines sketched above, but the physical question is, would such a network survive on time scales much longer than those associated with the traversal of a single electron across the crystal. If so, this would give a picture of conduction in real space, in which a given electron moves as a single particle, but all electrons of one spin present themselves as a quasi-static collective (the network) to those of the other spin. The present model is essentially a realization 'by hand' of this intriguing symmetry breaking, first proposed by Gutzwiller for the Hubbard model: that one kind of spin sees the other 'as if occupying a band of width zero' [12]. Interestingly enough, the model construction implies a direct experimental consequence of this assumption. Namely, the chemical potential of these 'other' spins, the ν in Eq. (3), is independent of doping throughout the in-gap band (because they are dispersionless), so the dispersion $\varepsilon(\nu)$ should not vary with doping either. Experimentally, positions of dispersive peaks along typical cuts in the Brillouin zone vary by a rough, but still unexpectedly uniform, 0.2 eV in a wide class of materials [13,14], from optimally doped to insulators [15], but again, this changes for overdoping [15].

To conclude, a model quantum phase transition has been described, caused by hopping fluctuations in the presence of a classical on-site repulsion. It is analogous to a liquid-gas transition, and is not associated with a divergence of the effective mass, even though it may appear otherwise for all but the lowest temperatures.

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KVANTNO-FAZNI PRIJELAZ U MODELU NASUMIČNOG POPLOČENJA

Raspravlja se analogon Mott-Hubbardovom prijelazu koji se pojavljuje kod nesumjerljivog popunjavanja u modelu dvodimenzijske ravnine nasumično popločene "molekulama" CuO_4, oponašajući ravnine bakarnog oksida u visoko-temperaturnim supravodičima. Pokazuje se da je to kvantni prijelaz koji nastupa bilo dopiranjem uz nepromijenjen parametar preskoka t, bilo promjenom t, pri čemu doping ostaje nepromijenjen u nekom rasponu ispod polovične popunjenosti. Prijelaz je prvog reda, analogan prijelazu tekućina – plin.