The Landscape of the Hubbard model

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Outline

1. Introduction to the Hubbard model
   * Superexchange and antiferromagnetism*

2. Coupled dimer antiferromagnet
   * CFT3: the Wilson-Fisher fixed point*

3. Honeycomb lattice: semi-metal and antiferromagnetism
   * CFT3: Dirac fermions and the Gross-Neveu model*

4. Hubbard model as a SU(2) gauge theory
   * Spin liquids, valence bond solids: analogies with SQED and SYM*

5. Quantum critical dynamics
   * AdS/CFT and the collisionless-hydrodynamic crossover*
Outline

6. Square lattice: Fermi surfaces and spin density waves
   Quantum critical theory of hot spots

7. Square lattice: d-wave superconductivity
   Instabilities to pairing and other orders
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Monday, June 7, 2010
The Hubbard Model

\[ H = -\sum_{i<j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_i c_{i\alpha}^\dagger c_{i\alpha} \]

t_{ij} \rightarrow \text{“hopping”}. U \rightarrow \text{local repulsion}, \mu \rightarrow \text{chemical potential}

\text{Spin index } \alpha = \uparrow, \downarrow

\[ n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha} \]

\[ c_{i\alpha}^\dagger c_{j\beta} + c_{j\beta} c_{i\alpha}^\dagger = \delta_{ij} \delta_{\alpha\beta} \]

\[ c_{i\alpha} c_{j\beta} + c_{j\beta} c_{i\alpha} = 0 \]

Will study on the honeycomb and square lattices
The Hubbard Model

\[ H = -\sum_{i,j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_i c_{i\alpha}^\dagger c_{i\alpha} \]

In the limit of large \( U \), and at a density of one particle per site, this maps onto the Heisenberg antiferromagnet

\[ H_{AF} = \sum_{i<j} J_{ij} S_i^a S_j^a \]

where \( a = x, y, z \),

\[ S_i^a = \frac{1}{2} c_{i\alpha}^{a\dagger} \sigma_{\alpha\beta}^a c_{i\beta}, \]

with \( \sigma^a \) the Pauli matrices and

\[ J_{ij} = \frac{4t_{ij}^2}{U} \]
therefore always appropriate, and only the critical point $g = g_c$ has genuinely different properties at $T = 0$.

5.1 Effective Hamiltonian method

We consider a Hamiltonian of the form $H = H_0 + H_1$, where the eigenstates of $H_0$ are easily determined, and we are interested in describing the influence of $H_1$ in perturbation theory. Further, we assume that the eigenvalues of $H_0$ are separated into distinct groups of closely-spaced levels, such that the energy separation between two levels within the same group is always much smaller than the separation between two levels in distinct groups. We use the symbols $\alpha, \beta, \ldots$ to denote the groups, and $i, j, \ldots$ to denote levels within each group. Thus the eigenstates of $H_0$ are $|i, \alpha\rangle$, with eigenenergies $E_{i\alpha}$, and so

$$|E_{i\alpha} - E_{j\alpha}| \ll |E_{i\alpha} - E_{j\beta}| \quad \text{for } \alpha \neq \beta$$

(5.2)

We are often interested in the structure of the levels within a given group, and would like to understand their behavior without reference to levels in other groups. However, in general, $H_1$ will have non-zero matrix elements between states belonging to different groups: consequently a conventional perturbative analysis will require repeated reference to states lying outside the group of interest. The idea of the effective Hamiltonian method is to perform a unitary transformation which eliminates these inter-group matrix elements. After the unitary transformation, we will obtain a new Hamiltonian $H_{\text{eff}}$ which has non-zero matrix elements only within each group.

We skip the straightforward, but tedious, analysis needed to obtain $H_{\text{eff}}$ order-by-order in $H_1$. We only quote here the final result to second order in $H_1$. The new Hamiltonian $H_{\text{eff}}$ is defined by the following non-zero matrix elements between any two levels, $|i, \alpha\rangle$ and $|j, \alpha\rangle$ belonging to the same group $\alpha$:

$$\langle i, \alpha|H_{\text{eff}}|j, \alpha\rangle = E_{i\alpha}\delta_{ij} + \langle i, \alpha|H_1|j, \alpha\rangle + \sum_{k, \beta \neq \alpha} \langle i, \alpha|H_1|k, \beta\rangle \langle k, \beta|H_1|j, \alpha\rangle \left( \frac{1}{E_{i\alpha} - E_{k\beta}} + \frac{1}{E_{j\alpha} - E_{k\beta}} \right)$$

(5.3)

Naturally, we have $\langle i, \alpha|H_{\text{eff}}|j, \beta\rangle = 0$ for all $\alpha \neq \beta$, ensuring that $H_{\text{eff}}$ is block diagonal, and we can work independently within each group $\alpha$. 
Hubbard Model and Supercell

\[ H = -t \sum \frac{c_i^\dagger c_{i+1}^\dagger + c_j^\dagger c_{j+1}^\dagger}{2} \]

\[ + U \sum \frac{n_i n_j}{2} \]  

\[ \text{Take 2 sites and 2 electrons.} \]

\[ \begin{array}{cccc}
1 \gamma &=& c_{1 \uparrow}^\dagger c_{2 \downarrow} \quad (0) & E_0 = 0 \\
2 \gamma &=& c_{1 \uparrow}^\dagger c_{2 \uparrow} \quad \langle 0 \rangle & E_0 = 0 \\
3 \gamma &=& c_{1 \downarrow}^\dagger c_{2 \downarrow} \quad \langle 0 \rangle & E_0 = 0 \\
4 \gamma &=& c_{1 \uparrow}^\dagger c_{2 \uparrow} \quad \langle 0 \rangle & E_0 = U \\
5 \gamma &=& c_{1 \downarrow}^\dagger c_{2 \downarrow} \quad \langle 0 \rangle & E_0 = U \\
6 \gamma &=& c_{1 \uparrow}^\dagger c_{2 \uparrow} \quad \langle 0 \rangle & E_0 = U \\
\end{array} \]
Eliminate states $|5\rangle$ and $|6\rangle$
by effective Hamiltonian method.

\[ H_0 = U(\eta_1 \eta_1 + \eta_2 \eta_2) \]

\[ H_1 = -t \left( c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) \]

Non-zero matrix elements

\[ \langle 6 | H_1 | 2 \rangle = -t \]

\[ \langle 5 | H_1 | 2 \rangle = -t \]

\[ \langle 6 | H_1 | 3 \rangle = t \]

\[ \langle 5 | H_1 | 3 \rangle = t. \]

So

\[ \langle 2 | H_{eff} | 2 \rangle = -\frac{2t^2}{U} = \langle 3 | H_{eff} | 3 \rangle \]

\[ \langle 2 | H_{eff} | 3 \rangle = \frac{2t^2}{U} = \langle 3 | H_{eff} | 2 \rangle. \]
For the order $E^2/\hbar$.

1)$ \rightarrow \begin{cases} 1 \text{ state} \quad \langle \psi_1 | \psi_2 \rangle \\ E = 0 \quad \rightarrow \quad E = 0 \end{cases}$

$H_{\text{eff}} = \frac{\hbar}{4 \Delta} \left( \begin{array}{cc} -2 E/\hbar & 2 E/\hbar \\ 2 E/\hbar & -2 E/\hbar \end{array} \right)$

Energy levels

$| \psi_1 \rangle \quad | \psi_2 \rangle$

$\frac{1}{\sqrt{2}}$ $\frac{1}{\sqrt{2}}$

Equivalent for $H_{\text{eff}} = J S_1 \cdot S_2$.

While $J = \frac{4 \Delta}{\hbar}$. 

$\frac{\sqrt{2}}{}$
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Square lattice antiferromagnet

\[ H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

Ground state has long-range Néel order

Order parameter is a single vector field \[ \vec{\varphi} = \eta_i \vec{S}_i \]

\[ \eta_i = \pm 1 \text{ on two sublattices} \]

\[ \langle \vec{\varphi} \rangle \neq 0 \text{ in Néel state.} \]
Square lattice antiferromagnet

\[ H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

Weaken some bonds to induce spin entanglement in a new quantum phase
Square lattice antiferromagnet

\[ H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

Ground state is a “quantum paramagnet” with spins locked in valence bond singlets

\[ \left| \uparrow \downarrow \right> - \left| \downarrow \uparrow \right> \right> = \frac{1}{\sqrt{2}} \left( \left| \uparrow \downarrow \right> - \left| \downarrow \uparrow \right> \right> \]

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Quantum critical point with non-local entanglement in spin wavefunction

Excitation spectrum in the paramagnetic phase
Excitation spectrum in the paramagnetic phase
Excitation spectrum in the paramagnetic phase
Excitation spectrum in the paramagnetic phase
Excitation spectrum in the paramagnetic phase

Sharp spin 1 particle excitation above an energy gap (spin gap)
Excitation spectrum in the Néel phase

\[ \lambda_c \rightarrow \lambda \]
Excitation spectrum in the Néel phase

Spin waves
Excitation spectrum in the Néel phase

Spin waves
1.4.2 Quantum Rotor Model

We turn to the somewhat less familiar quantum rotor models. Elementary quantum rotors do not exist in nature; rather, each quantum rotor is an effective quantum degree of freedom for the low energy states of a small number of electrons or atoms. We will first define the quantum mechanics of a single rotor and then turn to the lattice quantum rotor model. The connection to the experimental models introduced in Section 1.3 will be
described below in Section 1.4.3. Further details of this connection appear in Chapters 9, 19.

Each rotor can be visualized as a particle constrained to move on the surface of a (fictitious) \((N > 1)\)-dimensional sphere. The orientation of each rotor is represented by an \(N\)-component unit vector \(\mathbf{n}_i\) which satisfies

\[
\mathbf{n}_i^2 = 1. \tag{1.14}
\]

The caret on \(\mathbf{n}_i\) reminds us that the orientation of the rotor is a quantum mechanical operator, while \(i\) represents the site on which the rotor resides; we will shortly consider an infinite number of such rotors residing on the sites of a \(d\)-dimensional lattice. Each rotor has a momentum \(\mathbf{p}_i\), and the constraint (1.14) implies that this must be tangent to the surface of the \(N\)-dimensional sphere. The rotor position and momentum satisfy the usual commutation relations

\[
[\hat{n}_\alpha, \hat{p}_\beta] = i\delta_{\alpha\beta} \tag{1.15}
\]

on each site \(i\); here \(\alpha, \beta = 1 \ldots N\). (Here, and in the remainder of the book, we will always measure time in units in which \(\hbar = 1\), \(\text{(1.16)}\)

unless stated explicitly otherwise. This is also a good point to note that we will also set Boltzmann’s constant

\[
k_B = 1 \tag{1.17}
\]

by absorbing it into the units of temperature, \(T\).) We will actually find it more convenient to work with the \(N(N-1)/2\) components of the rotor angular momentum

\[
\hat{L}_{\alpha\beta} = \hat{n}_\alpha \hat{p}_\beta - \hat{n}_\beta \hat{p}_\alpha. \tag{1.18}
\]

These operators are the generators of the group of rotation in \(N\) dimensions, denoted \(O(N)\). Their commutation relations follow straightforwardly from (1.15) and (1.18). The case \(N = 3\) will be of particular interest to us: For this we define \(\hat{L}_\alpha = (1/2)\epsilon_{\alpha\beta\gamma} \hat{L}_{\beta\gamma}\) (where \(\epsilon_{\alpha\beta\gamma}\) is a totally antisymmetric tensor with \(\epsilon_{123} = 1\)), and then the commutation relation between the operators on each site are

\[
[\hat{L}_\alpha, \hat{L}_\beta] = i\epsilon_{\alpha\beta\gamma} \hat{L}_\gamma,
\]

\[
[\hat{L}_\alpha, \hat{n}_\beta] = i\epsilon_{\alpha\beta\gamma} \hat{n}_\gamma,
\]

\[
[\hat{n}_\alpha, \hat{n}_\beta] = 0;
\]

the operators with different site labels all commute.
The dynamics of each rotor is governed simply by its kinetic energy term; interesting effects will arise from potential energy terms that couple the rotors together, and these will be considered momentarily. Each rotor has the kinetic energy

\[ H_K = \frac{J \tilde{g}}{2} \hat{L}^2, \]  

(1.20)

where \(1/J \tilde{g}\) is the rotor moment of inertia (we have put a tilde over \(g\) as we wish to reserve \(g\) for a different coupling to be introduced below). The Hamiltonian \(H_K\) can be readily diagonalized for general values of \(N\) by well-known group theoretical methods. We quote the results for the physically important cases of \(N = 2\) and \(3\). For \(N = 2\) the eigenvalues are

\[ J \tilde{g} \ell^2 / 2 \quad \ell = 0, 1, 2, \ldots; \quad \text{degeneracy} = 2 - \delta_{\ell,0}. \]  

(1.21)

Note that there is a nondegenerate ground state with \(\ell = 0\), while all excited states are two-fold degenerate, corresponding to a left- or right-moving rotor. This spectrum will be important in the mapping to physical models to be discussed in Section 1.4.3. For \(N = 3\), the eigenvalues of \(H_K\) are

\[ J \tilde{g} (\ell + 1)^2 / 2 \quad \ell = 0, 1, 2, \ldots; \quad \text{degeneracy} = 2\ell + 1, \]  

(1.22)

corresponding to the familiar angular momentum states in three dimensions. These states can be viewed as representing the eigenstates of an even number of antiferromagnetically coupled Heisenberg spins, as will be discussed more explicitly in Section 1.4.3 and in Chapter 19, where will see that there is a general and powerful correspondence between quantum antiferromagnets and \(N = 3\) rotors.

We are ready to write down the full quantum rotor Hamiltonian, which shall be the focus of intensive study in Parts II and III. We place a single quantum rotor on the sites, \(i\), of a \(d\)-dimensional lattice, obeying the Hamiltonian

\[ H_R = \frac{J \tilde{g}}{2} \sum_i \hat{L}_i^2 - J \sum_{\langle ij \rangle} \hat{n}_i \cdot \hat{n}_j. \]  

(1.23)

We have augmented the sum of kinetic energies of each site with a coupling, \(J\), between rotor orientations on neighboring sites. This coupling energy is minimized by the simple “magnetically ordered” state in which all the rotors are oriented in the same direction. In contrast, the rotor kinetic energy is minimized when the orientation of the rotor is maximally uncertain (by the uncertainty principle), and so the first term in \(H_R\) prefers a quantum paramagnetic state in which the rotors do not have a definite orientation (i.e., \(\langle n \rangle = 0\)). Thus the roles of the two terms in \(H_R\) closely parallel those
1.4 Theoretical Models

of the terms in the Ising model $H_I$. As in Section 1.4.1, for $\tilde{g} \gg 1$, when the kinetic energy dominates, we expect a quantum paramagnet, in which following (1.9),

$$\langle 0 | \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j | 0 \rangle \sim e^{-|x_i - x_j|/\xi}. \quad (1.24)$$

Similarly, for $\tilde{g} \ll 1$, when the coupling term dominates, we expect a magnetically ordered state in which, as in (1.12),

$$\lim_{|x_i - x_j| \to \infty} \langle 0 | \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j | 0 \rangle = N_0^2. \quad (1.25)$$

Finally, we can anticipate a second-order quantum phase transition between these two phases at $\tilde{g} = \tilde{g}_c$, and the behavior of $N_0$ and $\xi$ upon approaching this point will be similar to that in the Ising case. These expectations turn out to be correct for $d > 1$, and we will show that $\tilde{g}_c = 0$ for $N \geq 3$, and so the ground state is a quantum paramagnetic state for all nonzero $\tilde{g}$. The case $N = 2, d = 1$ is special: There is a transition at a finite $\tilde{g}_c$, but the divergence of the correlation length does not obey (1.2) and the long-distance behavior of the correlation function $\tilde{g} < \tilde{g}_c$ differs from (1.25). This case will not be considered until Section 20.3 in Part III.

1.4.3 Physical realizations of quantum rotors

We will consider the $N = 3$ quantum rotors first, and expose a simple and important connection between O(3) quantum rotor models and a certain class of "dimerized" antiferromagnets, of which TlCuCl$_3$ is the example we highlighted in Section 1.3. Actually the connection between rotor models and antiferromagnets is far more general than the present discussion may suggest, as we will see later in Chapter 19. However, this discussion should enable the reader to gain an intuitive feeling for the physical interpretation of the degree of freedom of the rotor model.

Consider a dimerized system of "Heisenberg spins" $\hat{S}_1$ and $\hat{S}_2$, where $i$ now labels a pair of spins (a "dimer"). Their Hamiltonian is

$$H_d = K \sum_i (\hat{S}_1^i \cdot \hat{S}_2^i + \hat{S}_2^i \cdot \hat{S}_1^i) + \frac{J}{2} \sum_i \left( \sum_{\langle ij \rangle} (\hat{S}_1^i \cdot \hat{S}_1^j + \hat{S}_2^i \cdot \hat{S}_2^j) \right). \quad (1.26)$$

The $\hat{S}_n (n = 1, 2)$ labels the spins within a dimer. The spin operators usually representing the total spin of a set of electrons in some localized atomic states. See Fig. 1.3. On each site, the spins $\hat{S}_n$ obey the angular momentum states.
Figure 1.3 A dimerized quantum spin system. Spins with angular momentum $S$ reside on the circles, with antiferromagnetic exchange couplings as shown.

The commutation relations

$$\left[ \hat{S}_\alpha, \hat{S}_\beta \right] = i\epsilon_{\alpha\beta\gamma} \hat{S}_\gamma$$

(1.27)

(the site index has been dropped above), while spin operators on different sites commute. These commutation relations are the same as those of the $L$ operators in (1.10). However, there is one crucial difference between Hilbert space of states on which the quantum rotors and Heisenberg spins act. For the rotor models, we allowed states with arbitrary total angular momentum $\ell$ on each site, as in (1.22), and so there were an infinite number of states on each site. For the present Heisenberg spins, however, we will only allow states with total spin $S$ on each site, and we will permit $S$ to be integer or half-integer. Thus there are precisely $2S + 1$ states on each site

$$| S, m \rangle$$

(1.28)

with $m = -S, \ldots, S$.

and the operator identity

$$\hat{S}_n^2 = S(S + 1)$$

(1.29)

holds for each $n$. In addition to describing TlCuCl$_3$, Hamiltonians like $H_d$ describe spin-ladder compounds in $d = 1$ [39, 131] and "double layer" antiferromagnets in the family of the high-temperature superconductors in $d = 2$ [581, 582, 587, 402, 517, 518, 159].

Let us examine the properties of $H_d$ for $d \sim 2$. As a first approximation, we can neglect the $J$ couplings entirely, and then $H_d$ splits into decoupled pairs of sites each with a strong antiferromagnetic coupling $K$ between two spins. The Hamiltonian for each pair can be diagonalized by noting that $S_1$ and $S_2$, couple into states with total angular momentum $0 \leq \ell \leq 2S$, and so we obtain the eigenenergies

$$(K/2)(\ell + 1) - 2S(S + 1),$$

(1.30)

Note that these energies and degeneracies are in one-to-one correspondence with those of a single quantum rotor in (1.22), apart from the difference

$$(K/2)(\ell + 1) - 2S(S + 1).$$
that the upper restriction on $\ell$ being smaller than $2S$ is absent in the rotor model case. If one is interested primarily in low energy properties, then it appears reasonable to represent each pair of spins by a quantum rotor.

We have seen that the $K/J \to \infty$ limit of $H_d$ closely resembles the $\tilde{g} \to \infty$ limit of $H_R$. To first order in $\tilde{g}$, we can compare the matrix elements of the term proportional to $J$ in $H_R$ among the low-lying states, with those of the $J$ term in $H_d$: it is not difficult to see that these matrix elements become equal to each other for an appropriate choice of couplings: see exercise 6.6.1. Therefore we may conclude that the low-energy properties of the two models are closely related for large $K/J$ and $\tilde{g}$. Somewhat different considerations in Chapter 19 will show that the correspondence also applies to the quantum critical point and to the magnetically ordered phase.

The main lesson of the above analysis is that the $O(3)$ quantum rotor model represents the low energy properties of quantum antiferromagnets of Heisenberg spins, with each rotor being an effective representation of a pair of antiferromagnetically coupled spins. The strong-coupling spectra clearly indicate the operator correspondence $\hat{L}_i = \hat{S}_1^i + \hat{S}_2^i$, and so the rotor angular momentum represents the total angular momentum of the underlying spin system. Examination of matrix elements in the large-$S$ limit shows that $\hat{n}_i \propto \hat{S}_1^i - \hat{S}_2^i$: the rotor coordinate $\hat{n}_i$ is the antiferromagnetic order parameter of the spin system. Magnetically ordered states of the rotor model with $\langle \hat{n}_i \rangle \neq 0$, which we will encounter below, are therefore spin states with long-range antiferromagnetic order and have a vanishing total ferromagnetic moment. Quantum Heisenberg spin systems with a net ferromagnetic moment are not modeled by the quantum rotor model (11.1) – these will be studied in Section 19.2 by a different approach.
Description using Landau-Ginzburg field theory

$O(3)$ order parameter $\bar{\phi}$

$$S = \int d^2r d\tau \left[ (\partial_\tau \phi)^2 + c^2 (\nabla_r \bar{\phi})^2 + (\lambda - \lambda_c) \bar{\phi}^2 + u (\bar{\phi}^2)^2 \right]$$
Excitation spectrum in the paramagnetic phase

$V(\varphi) = (\lambda - \lambda_c) \varphi^2 + u (\varphi^2)^2$

$\lambda > \lambda_c$

Spin $S = 1$

“triplon”
Excitation spectrum in the paramagnetic phase

\[ V(\vec{\varphi}) = (\lambda - \lambda_c) \varphi^2 + u (\varphi^2)^2 \]

\[ \lambda > \lambda_c \]

Spin \( S = 1 \) “triplon”
Excitation spectrum in the paramagnetic phase

\[ V(\phi) = (\lambda - \lambda_c) \phi^2 + u (\phi^2) \]

\[ \lambda > \lambda_c \]
Excitation spectrum in the paramagnetic phase

\[ V(\phi) = (\lambda - \lambda_c)\phi^2 + u(\phi^2)^2 \]

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\[ \lambda > \lambda_c \]

Spin \( S = 1 \) "triplon"
Excitation spectrum in the Néel phase

Spin waves ("Goldstone" modes) and a longitudinal "Higgs" particle

\[ V(\varphi) = (\lambda - \lambda_c)\varphi^2 + u(\varphi^2)^2 \]

\[ \lambda < \lambda_c \]
Excitation spectrum in the Néel phase

Spin waves ("Goldstone" modes) and a longitudinal "Higgs" particle

\[ V(\bar{\phi}) = (\lambda - \lambda_c)\bar{\phi}^2 + u(\bar{\phi}^2)^2 \]

\[ \lambda < \lambda_c \]
Excitation spectrum in the Néel phase

Spin waves ("Goldstone" modes) and a longitudinal "Higgs" particle

$$V(\phi) = (\lambda - \lambda_c)\phi^2 + u(\phi^2)^2$$

$$\lambda < \lambda_c$$
$S = \int d^2r d\tau \left[ (\partial_\tau \varphi)^2 + c^2 (\nabla_r \varphi)^2 + s \varphi^2 + u (\varphi^2)^2 \right]$
Quantum Monte Carlo - critical exponents

Table IV: Fit results for the critical exponents $\nu$, $\beta/\nu$, and $\eta$. We summarize results including a variation of the critical point within its error bar. For the ladder model (top group of values) fit results and quality of fits are also given at the previous best estimate of $\alpha_c$. The bottom group are results for the plaquette model. Numbers in [...] brackets denote the $\chi^2$/d.o.f. For comparison relevant reference values for the 3D $O(3)$ universality class are given in the last line.

<table>
<thead>
<tr>
<th>$\alpha_c$</th>
<th>$\nu^a$</th>
<th>$\beta/\nu^b$</th>
<th>$\eta^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.9096 $- \sigma$</td>
<td>0.712(4) [1.8]</td>
<td>0.516(2) [0.5]</td>
<td>0.026(2) [0.2]</td>
</tr>
<tr>
<td>1.9096</td>
<td>0.711(4) [1.8]</td>
<td>0.518(2) [1.1]</td>
<td>0.029(5) [0.8]</td>
</tr>
<tr>
<td>1.9096 $+ \sigma$</td>
<td>0.710(4) [1.8]</td>
<td>0.519(3) [2.5]</td>
<td>0.032(7) [1.4]</td>
</tr>
<tr>
<td>1.9107$^d$</td>
<td>0.709(3) [1.7]</td>
<td>0.525(8) [15.3]</td>
<td>0.051(10) [12]</td>
</tr>
<tr>
<td>1.8230 $- \sigma$</td>
<td>0.708(4) [0.99]</td>
<td>0.515(2) [0.84]</td>
<td>0.025(4) [0.15]</td>
</tr>
<tr>
<td>1.8230</td>
<td>0.706(4) [1.04]</td>
<td>0.516(2) [0.40]</td>
<td>0.028(3) [0.31]</td>
</tr>
<tr>
<td>1.8230 $+ \sigma$</td>
<td>0.706(4) [1.10]</td>
<td>0.517(2) [1.6]</td>
<td>0.031(5) [0.80]</td>
</tr>
<tr>
<td>Ref. 49</td>
<td>0.7112(5)</td>
<td>0.518(1)</td>
<td>0.0375(5)</td>
</tr>
</tbody>
</table>

$^aL > 12.$

$^bL > 16.$

$^cL > 20.$

$^d$Previous best estimate of Ref. 19.


Quantum Monte Carlo - critical exponents

Table IV: Fit results for the critical exponents $\nu$, $\beta/\nu$, and $\eta$. We summarize results including a variation of the critical point within its error bar. For the ladder model (top group of values) fit results and quality of fits are also given at the previous best estimate of $\alpha_c$. The bottom group are results for the plaquette model. Numbers in [...] brackets denote the $\chi^2$/d.o.f. For comparison relevant reference values for the 3D $O(3)$ universality class are given in the last line.

<table>
<thead>
<tr>
<th>$\alpha_c$</th>
<th>$\nu^a$</th>
<th>$\beta/\nu^b$</th>
<th>$\eta^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.9096 $- \sigma$</td>
<td>0.712(4) [1.8]</td>
<td>0.516(2) [0.5]</td>
<td>0.026(2) [0.2]</td>
</tr>
<tr>
<td>1.9096</td>
<td>0.711(4) [1.8]</td>
<td>0.518(2) [1.1]</td>
<td>0.029(5) [0.8]</td>
</tr>
<tr>
<td>1.9096 $+ \sigma$</td>
<td>0.710(4) [1.8]</td>
<td>0.519(3) [2.5]</td>
<td>0.032(7) [1.4]</td>
</tr>
<tr>
<td>1.9107</td>
<td>0.709(3) [1.7]</td>
<td>0.525(8) [15.3]</td>
<td>0.051(10) [12]</td>
</tr>
<tr>
<td>1.8230 $- \sigma$</td>
<td>0.708(4) [0.99]</td>
<td>0.515(2) [0.84]</td>
<td>0.025(4) [0.15]</td>
</tr>
<tr>
<td>1.8230</td>
<td>0.706(4) [1.04]</td>
<td>0.516(2) [0.40]</td>
<td>0.028(3) [0.31]</td>
</tr>
<tr>
<td>1.8230 $+ \sigma$</td>
<td>0.706(4) [1.10]</td>
<td>0.517(2) [1.6]</td>
<td>0.031(5) [0.80]</td>
</tr>
<tr>
<td>Ref. 49</td>
<td>0.7112(5)</td>
<td>0.518(1)</td>
<td>0.0375(5)</td>
</tr>
</tbody>
</table>


Field-theoretic RG of CFT3
E. Vicari et al.

TlCuCl$_3$
An insulator whose spin susceptibility vanishes exponentially as the temperature $T$ tends to zero.
Pressure in TICuCl$_3$
**TlCuCl$_3$ at ambient pressure**


**FIG. 1.** Measured neutron profiles in the $a^*c^*$ plane of TlCuCl$_3$ for $i=(1.35,0,0)$, $ii=(0,0,3.15)$ [r.l.u]. The spectrum at $T=1.5$ K.
TlCuCl$_3$ at ambient pressure

Sharp spin 1 particle excitation above an energy gap (spin gap)

Observation of $3 \rightarrow 2$ low energy modes, emergence of new longitudinal mode (the “Higgs boson”) in Néel phase, and vanishing of Néel temperature at quantum critical point.

Prediction of quantum field theory

Potential for $\bar{\phi}$ fluctuations: $V(\bar{\phi}) = (\lambda - \lambda_c)\bar{\phi}^2 + u(\bar{\phi}^2)^2$

Paramagnetic phase, $\lambda > \lambda_c$

Expand about $\bar{\phi} = 0$:

$$V(\bar{\phi}) \approx (\lambda - \lambda_c)\bar{\phi}^2$$

Yields 3 particles with energy gap $\sim \sqrt{(\lambda - \lambda_c)}$
**Prediction of quantum field theory**

Potential for $\varphi$ fluctuations: $V(\varphi) = (\lambda - \lambda_c)\varphi^2 + u(\varphi^2)^2$

**Paramagnetic phase, $\lambda > \lambda_c$$**

Expand about $\varphi = 0$:

$$V(\varphi) \approx (\lambda - \lambda_c)\varphi^2$$

Yields 3 particles with energy gap $\sim \sqrt{(\lambda - \lambda_c)}$

**Néel phase, $\lambda < \lambda_c$$**

Expand $\varphi = (0, 0, \sqrt{(\lambda_c - \lambda)/(2u)}) + \varphi_1$:

$$V(\varphi) \approx 2(\lambda_c - \lambda)\varphi^2_{1z}$$

Yields 2 gapless spin waves and one Higgs particle with energy gap $\sim \sqrt{2(\lambda_c - \lambda)}$
**Prediction of quantum field theory**

\[
\frac{\text{Energy of Higgs particle}}{\text{Energy of triplon}} = \sqrt{2}
\]

\[
V(\varphi) = (\lambda - \lambda_c)\varphi^2 + u(\varphi^2)^2
\]

- **TLCuCl$_3$**
  - $p_c = 1.07$ kbar
  - $T = 1.85$ K

**Figure:**
- Energy $\sqrt{2}E(p < p_c), E(p > p_c)$ [meV]
- Pressure $|p - p_c|$ [kbar]
- $Q=(0 \ 4 \ 0)$
- $Q=(0 \ 0 \ 1)$
- $E(p < p_c)$ unscaled

**References:**
- S. Sachdev, arXiv:0901.4103

Monday, June 7, 2010
Graphene
Graphene

Semi-metal with massless Dirac fermions

\[ \varepsilon_{\vec{k}} = \hbar v_F |\vec{k}| \]

Semi-metal with massless Dirac fermions

Brillouin zone

Monday, June 7, 2010
Graphene

Dirac semi-metal

Insulating antiferromagnet with Neel order

$U/t$
I. HONEYCOMB LATTICE AT HALF FILLING

We define the unit length vectors
\[ e_1 = (1, 0), \quad e_2 = (-1/2, \sqrt{3}/2), \quad e_3 = (-1/2, -\sqrt{3}/2). \] (1)

Note that \( e_i \cdot e_j = -1/2 \) for \( i \neq j \), and \( e_1 + e_2 + e_3 = 0 \).

We take the origin of co-ordinates of the honeycomb lattice at the center of an empty hexagon. The A sublattice sites closest to the origin are at \( e_1, e_2, \) and \( e_3 \), while the B sublattice sites closet to the origin are at \( -e_1, -e_2, \) and \( -e_3 \).

The reciprocal lattice is generated by the wavevectors
\[ G_1 = \frac{4\pi}{3} e_1, \quad G_2 = \frac{4\pi}{3} e_2, \quad G_3 = \frac{4\pi}{3} e_3 \] (2)

The first Brillouin zone is a hexagon whose vertices are given by
\[ Q_1 = \frac{1}{3}(G_2 - G_3), \quad Q_2 = \frac{1}{3}(G_3 - G_1), \quad Q_3 = \frac{1}{3}(G_1 - G_2), \] (3)

and \(-Q_1, -Q_2,\) and \(-Q_3\).

We define the Fourier transform of the fermions by
\[ c_A(k) = \sum_r c_A(r)e^{-ik \cdot r} \] (4)
and similarly for \( c_B \).

Now we define the continuum limit by the fields
\[ \Psi_{A1} = c_A(Q_1), \quad \Psi_{B1} = c_B(Q_1), \quad \Psi_{A2} = c_A(-Q_1), \quad \Psi_{B2} = c_B(-Q_1) \] (5)

The hopping Hamiltonian is
\[ H_0 = -t \sum_{\langle ij \rangle} \left( c^\dagger_{A\alpha} c_{B\alpha} + c^\dagger_{B\alpha} c_{A\alpha} \right) \] (6)

where \( \alpha \) is a spin index. If we introduce Pauli matrices \( \tau^a \) in sublattice space, this Hamiltonian can be written as
\[ H_0 = \int \frac{d^2k}{4\pi^2} c^\dagger(k) \left[ -t \left( \cos(k \cdot e_1) + \cos(k \cdot e_2) + \cos(k \cdot e_3) \right) \tau^x \right. \]
\[ \left. + t \left( \sin(k \cdot e_1) + \sin(k \cdot e_2) + \sin(k \cdot e_3) \right) \tau^y \right] \] (7)
The low energy excitations of this Hamiltonian are near \( k \approx \pm Q_1 \). In terms of the fields near \( Q_1 \) and \(-Q_1\), we define

\[
\begin{align*}
\Psi_{A1\alpha}(k) & = c_{A\alpha}(Q + k) \\
\Psi_{A2\alpha}(k) & = c_{A\alpha}(-Q + k) \\
\Psi_{B1\alpha}(k) & = c_{B\alpha}(Q + k) \\
\Psi_{B2\alpha}(k) & = c_{B\alpha}(-Q + k)
\end{align*}
\]

We consider \( \Psi \) to be an 8 component vector, and introduce Pauli matrices \( \rho^a \) which act in the 1, 2 valley space. Then the Hamiltonian is

\[
H_0 = \int \frac{d^2k}{4\pi^2} \Psi^\dagger(k) \left( v\tau^y k_x + v\tau^x \rho^z k_y \right) \Psi(k),
\]

where \( v = 3t/2 \); below we set \( v = 1 \). Now define \( \overline{\Psi} = \Psi^\dagger \rho^z \tau^z \). Then we can write the imaginary time Lagrangian as

\[
L_0 = -i \overline{\Psi} \left( \omega \gamma_0 + k_x \gamma_1 + k_y \gamma_2 \right) \Psi
\]

where

\[
\begin{align*}
\gamma_0 & = -\rho^z \tau^z \\
\gamma_1 & = \rho^z \tau^x \\
\gamma_2 & = -\tau^y
\end{align*}
\]

So the low energy theory has 4 2-component Dirac fermions.

### A. Antiferromagnetism

We use the operator equation (valid on each site \( i \)):

\[
U \left( n_\uparrow - \frac{1}{2} \right) \left( n_\downarrow - \frac{1}{2} \right) = -\frac{2U}{3} S_i^{a2} + \frac{U}{4}
\]

Then we decouple the interaction via

\[
\exp \left( \frac{2U}{3} \sum_i \int d\tau S_i^{a2} \right) = \int \mathcal{D} J_i^a(\tau) \exp \left( -\sum_i \int d\tau \left[ \frac{3U}{8} J_i^{a2} - J_i^a S_i^a \right] \right)
\]

We now integrate out the fermions, and look for the saddle point of the resulting effective action for \( J_i^a \). At the saddle-point we find that the lowest energy is achieved when the vector has opposite orientations on the A and B sublattices. Anticipating this, we look for a continuum limit in terms of a field \( \varphi^a \) where

\[
J^a_A = \varphi^a, \quad J^a_B = -\varphi^a
\]
The coupling between the field $\varphi^a$ and the $\Psi$ fermions is given by

$$\sum_i J^a_i c^\dagger_{i\alpha} \sigma^a_{\alpha\beta} c_{i\beta} = \varphi^a \left( c^\dagger_{A\alpha} \sigma^a_{\alpha\beta} c_{A\beta} - c^\dagger_{B\alpha} \sigma^a_{\alpha\beta} c_{B\beta} \right) = \varphi^a \Psi^\dagger \tau^z \sigma^a \Psi = -\varphi^a \overline{\Psi} \rho^z \sigma^a \Psi$$

(15)

From this we motivate the low energy theory

$$\mathcal{L} = \overline{\Psi} \gamma_\mu \partial_\mu \Psi + \frac{1}{2} \left[ (\partial_\mu \varphi^a)^2 + \varphi^{a2} \right] + \frac{u}{24} (\varphi^{a2})^2 - \lambda \varphi^a \overline{\Psi} \rho^z \sigma^a \Psi$$

(16)

Note that the matrix $\rho^z \sigma^a$ commutes with all the $\gamma_\mu$; hence $\rho^z \sigma^a$ is a matrix in “flavor” space. This is the Gross-Neveu model, and it describes the quantum phase transition from the Dirac semi-metal to an insulating Néel state. In the Néel state, we have $\varphi^a = N_0 \delta_{az}$ (say), and so the dispersion of the electrons is

$$\omega_k = \pm \sqrt{k^2 + \lambda^2 N_0^2}$$

(17)

near the points $\pm Q_1$. These form the conduction and valence bands of the insulator.