



2253-16

Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

24 - 29 July 2011

Synergies between quantum field theories and numerical calculations with microscopic Hamiltonians

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Future visions: Synergies between quantum field theories and numerical calculations with microscopic Hamiltonians

Talk online: sachdev.physics.harvard.edu





Yejin Huh



Matthias Punk







Erez Berg



Sunday, July 31, 2011

I. Dimerized antiferromagnets and the Wilson-Fisher CFT

- 2. J-Q model and deconfined criticality
- 3. Kagome lattice and Z_2 spin liquids
- 4. Spin liquids on the honeycomb lattice
- 5. Quantum critical points in metals: Fermi surface reconstruction

Two-dimensional Spin Dimer Models



Exploring quantum criticality in idealized 2D setups

SU(2) invariant exchange







Various non-frustrated dimer arrangements have been considered



Quantum Monte Carlo - critical exponents

Table IV: Fit results for the critical exponents ν , β/ν , and η . 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 α_c . The bottom group are results for the plaquette model. Numbers in [...] brackets denote the χ^2 /d.o.f. For comparison relevant reference values for the 3D O(3) universality class are given in the last line.

α_{c}	ν^{a}	β/ν^b	η^{c}	
$1.9096 - \sigma$	0.712(4) [1.8]	0.516(2) [0.5]	0.026(2) [0.2]	
1.9096	0.711(4) [1.8]	0.518(2) [1.1]	0.029(5) [0.8]	
$1.9096 + \sigma$	0.710(4) [1.8]	0.519(3) [2.5]	0.032(7) [1.4]	
1.9107 ^d	0.709(3) [1.7]	0.525(8) [15.3]	0.051(10) [12]	
$1.8230 - \sigma$	0.708(4) [0.99]	0.515(2) [0.84]	0.025(4) [0.15]	
1.8230	0.706(4) [1.04]	0.516(2) [0.40]	0.028(3) [0.31]	Field-theoretic RG of CFT3
$1.8230 + \sigma$	0.706(4) [1.10]	0.517(2) [1.6]	0.031(5) $[0.80]$	
P	0 7110/5)	0 518(1)	0.0975(5)	

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Staggered dimer model

Critical Field Theory



For the staggered dimer model the conventional ϕ^4 theory

$$S_{24} = \frac{1}{2} \int d^2 r d\tau \left[c_x^2 (\partial_x \vec{\varphi})^2 + c_y^2 (\partial_y \vec{\varphi})^2 + (\partial_\tau \vec{\varphi})^2 + m_0 \vec{\varphi}^2 \right] + \frac{u_0}{24} \int d^2 r d\tau (\vec{\varphi}^2)^2$$

gets supplemented by the most relevant cubic term

$$S_3 = i\gamma_0 \int d^2r d\tau \,\vec{\varphi} \cdot (\partial_x \vec{\varphi} \times \partial_\tau \vec{\varphi})$$

What is the relevance of this cubic term?

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Staggered dimer model

Classical Monte Carlo Analysis



MC data consistent with a fast algebraic decay of the correlators

 $C_{xy}(r) = \langle \mathcal{O}(r,0,0)\mathcal{O}(0) \rangle$ $C_z(r) = \langle \mathcal{O}(0,0,r)\mathcal{O}(0) \rangle$

Overall fit results in

 $[\gamma_0]_{WF} = -0.4 \pm 0.2$

Consistent with weak irrelevancy of the cubic operator at the Wilson-Fisher fixed point



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O.I. Motrunich and A. Vishwanath, *Phys. Rev. B* **70**, 075104 (2004). T. Senthil, A. Vishwanath, L. Balents, S. Sachdev and M.P.A. Fisher, *Science* **303**, 1490 (2004).

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SU(2) J-Q Model

A. W. Sandvik, PRL98, 227202 (2007)

U(1) Nature is confirmed at the critical point.



FIG. 5 (color online). Histogram of the dimer order parameter for an L = 32 system at J/Q = 0. The ring shape demonstrates an emergent U(1) symmetry, i.e., irrelevance of the Z_4 anisotropy of the VBS order parameter.

Monopole Scaling Dimension up to $O(N^{-1})$







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Some more recent history



36 site unit cell valence bond crystal: honeycomb valence bond crystal (HVBC) (Marston and Zeng, originally)

- Key question: is it a valence bond crystal or a spin liquid? What kind of VBC or SL?
- Three key approaches support HVBC:
 - Series expansions, Singh and Huse (E=-0.433(1))
 - MERA, Evenbly and Vidal (E < -0.4322 exact bound!)</p>
 - Multiscale entanglement renormalization ansatz, a tensor product relative of DMRG capable of infinite 2D
 - High order ffective Dimer Model, Poilblanc et al (but SL close by)

S.White, seminar at Harvard, March 2011



This run had special path and edges tuned to favor HVBC.

HVBC is metastable for small m, but for $m \sim 2400$ it transitions to the spin liquid

With standard path HVBC is immediately unstable, m ~ 100

SL energy for this cylinder, bulk: -0.43824(2) XC8

S.White, seminar at Harvard, March 2011



Parton construction of Z_2 spin liquids

$$\begin{split} \vec{S}_i &= \frac{1}{2} b_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} b_{i\beta}, \\ \mathcal{H}_b &= -\sum_{i < j} Q_{ij} \varepsilon_{\alpha\beta} b_{i\alpha}^{\dagger} b_{j\beta}^{\dagger} + \text{H.c.} + \lambda \sum_i b_{i\alpha}^{\dagger} b_{i\alpha}, \\ E[\{Q_{ij}\}] &= -\sum_{i < j} \left(\alpha |Q_{ij}|^2 + \frac{\beta}{2} |Q_{ij}|^4 \right) \\ &+ K \prod_{\text{even loops}} Q_{ij} Q_{jk}^* \dots Q_{\ell i}^* \end{split}$$

N. Read and S. Sachdev, *Phys. Rev. Lett.* **66**, 1773 (1991) X.-G. Wen, *Phys. Rev. B* **44**, 2664 (1991)



A vison on the triangular lattice. The center of the vison is marked by the X. The wavy line is the 'branch-cut' where we have $\operatorname{sgn}(Q_{ij}^v) = -\operatorname{sgn}(Q_{ij})$ only on the links crossed by the line. Plotted is the minimization result of $E[\{Q_{ij}\}]$

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Parton construction of Z_2 spin liquids Field theory near a magnetic ordering transition: U(1) gauge theory with a charge 2 Higgs field:

$$\mathcal{L} = |(\partial_{\mu} - 2iA_{\mu})\Phi|^{2} + s|\Phi|^{2} + u|\Phi|^{4} + |(\partial_{\mu} - iA_{\mu})z_{\alpha}|^{2} + \widetilde{s}|z_{\alpha}|^{2} + \widetilde{u}|z_{\alpha}|^{4} + \lambda\Phi^{*}\varepsilon_{\alpha\beta}z_{\alpha}\nabla z_{\beta} + \text{H.c.}$$

This field theory has vortex solutions, with flux π , which are analogs of Abrikosov vortices in the BCS theory of superconductivity. However, here the gauge field is compact, and so $\pm \pi$ vortices are the same: these are Z_2 vortices or 'visons'.

N. Read and S. Sachdev, Phys. Rev. Lett. 66, 1773 (1991)



Periodic motion of a vison around the single site marked by the filled circle. The right state is gauge-equivalent to the left state, after the gauge transformation $b_{i\alpha} \rightarrow -b_{i\alpha}$ only for the site *i* marked by the filled circle.

 \Rightarrow Vison has a Berry phase of π upon encircling a site.



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<u>PSG of vison states</u>

The simplest case on the kagome has the visons transforming under the 48 element group $GL(2,Z_3)$: the group of invertible 2×2 matrices which elements belonging to the field Z_3 . This is *not* isomorphic to any previously studied point group in solid state physics (or in any other field of physics, as far as we know).

The low energy vison states are described by the excitations of the following field theory of a 4-component real field ψ_n

$$\mathcal{L} = \sum_{n=1...4} ((\nabla \psi_n)^2 + (\partial_\tau \psi_n)^2 + r\psi_n^2 + u\psi_n^4) + a \sum_{n < m} \psi_n^2 \psi_m^2 + b \big[\psi_1^2 (\psi_2 \psi_3 - \psi_2 \psi_4 + \psi_3 \psi_4) + \psi_2^2 (\psi_1 \psi_3 + \psi_1 \psi_4 - \psi_3 \psi_4) + \psi_3^2 (\psi_1 \psi_2 - \psi_1 \psi_4 + \psi_2 \psi_4) - \psi_4^2 (\psi_1 \psi_2 + \psi_1 \psi_3 + \psi_2 \psi_3) \big].$$

Y. Huh, M. Punk, and S. Sachdev, arXiv:1106.3330

Confinement transition from a Z_2 spin liquid to a VBS state



The diamond pattern VBC



Condensation of vison with $GL(2,Z_3)$ PSG leads to a VBS pattern similar to the "diamond" pattern favored by the DMRG studies of Steve White and collaborators.

Energy Vs Gauge Breaking parameter plots





FIG. 4: Comparison of trial energies per site for Dirac SL, $\mathbf{q} = \mathbf{0}$ SB wave function, and $\mathbf{q} = \mathbf{0}$ Jastrow-type magnetically ordered (MO) state. The SB state has poorer energy than Dirac SL for $J_2/J_1 \leq 0.08$, but performs better for larger J_2 and better than the Jastrow-type MO for all J_2 .

Tiamhock Tay and Olexei I. Motrunich

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The Mott transition



tU

No broken symmetries. Not adiabatically connected to a band insulating state.

Sublattice Pairing State

We find only one natural candidate spin liquid state in Schwinger-fermion representation: $\Delta e^{i\theta} \epsilon_{\alpha\beta} f^{\dagger}_{i\alpha} f^{\dagger}_{i\alpha} + h.c.$

Sublattice Pairing State



Low energy excitations:

fermionic spinons and visons (π -fluxes of Z₂ gauge field)

Yuan-Ming Lu and Ying Ran

We now understand at a microscopic level what makes a good wave function for a spin liquid on a bipartite lattice!

"Obeys" the Marshall Sign Rule + AA Singlets

We expect then that our wave function Gapped(Δ, θ) (i.e. SPS) is better then Gapless for some values of Δ and θ .



We have computed energetics over a huge manifold of possible spin liquids (including these). We find this one wins (for the qualitative reasons we discussed).

B. Clark, D. Abanin, S. Sondhi





SPS Schwinger-fermion rep.

f-spinon(fermion)+Z2 gauge field

Schwinger fermions 0-flux state Schwinger-boson rep.

z-spinon(boson)+ Z2 gauge field

Schwinger bosons (Fa Wang)

Yuan-Ming Lu and Ying Ran



Detecting the CAF phase in numerics

Two order parameters: (breaks SU(2) completely, 3 Goldstone modes)

• Vector Spin Chirality:





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Electron-doped cuprate superconductors



Electron-doped cuprate superconductors















Metal with "large" Fermi surface





Electron and hole pockets in antiferromagnetic phase with $\langle \vec{\varphi} \rangle \neq 0$







T. Helm, M.V. Kartsovnik, M. Bartkowiak, N. Bittner, M. Lambacher, A. Erb, J. Wosnitza, and R. Gross, Phys. Rev. Lett. **103**, 157002 (2009).



Photoemission in Nd_{2-x}Ce_xCuO₄



N. P.Armitage et al., Phys. Rev. Lett. 88, 257001 (2002).



Spin-fermion model: Electrons with dispersion $\varepsilon_{\mathbf{k}}$ interacting with fluctuations of the antiferromagnetic order parameter $\vec{\varphi}$.

> $\mathcal{Z} = \int \mathcal{D}c_{\alpha}\mathcal{D}\vec{\varphi}\exp\left(-\mathcal{S}\right)$ $\mathcal{S} = \int d\tau \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} \left(\frac{\partial}{\partial \tau} - \varepsilon_{\mathbf{k}} \right) c_{\mathbf{k}\alpha}$ $+\int d\tau d^2r \left| \frac{1}{2} \left(\boldsymbol{\nabla}_r \vec{\varphi} \right)^2 + \frac{s}{2} \vec{\varphi}^2 + \dots \right|$ $-\lambda \int d\tau \sum \vec{\varphi_i} \cdot (-1)^{\mathbf{r}_i} c_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta}$ Coupling between fermions and antiferromagnetic order: $\lambda^2 \sim U$, the Hubbard repulsion

A technical aside.....

Hertz-Moriya-Millis theory

Integrate out fermions and obtain an effective action for the boson field $\vec{\varphi}$ alone. Because the fermions are gapless, this is potentially dangerous, and will lead to non-local terms in the $\vec{\varphi}$ effective action. Hertz focused on only the simplest such non-local term. However, there are an infinite number of non-local terms at higher order, and these lead to a breakdown of the Hertz theory in d = 2.

Ar. Abanov and A.V. Chubukov, Phys. Rev. Lett. 93, 255702 (2004).

A technical aside.....

We need to perform an RG analysis on a local theory of both the fermions and the $\vec{\varphi}$. It appears that such a theory can be analyzed using a 1/N expansion, where N is the number of fermion flavors. At two-loop order, the 1/N expansion is wellbehaved, and we can determine consistent RG flow equations. However, at higher loops we find corrections to the renormalizations which require summation of all planar graphs even at the leading order in 1/N, and the 1/N expansion appears to be organized as a genus expansion of random surfaces. But even this genus expansion breaks down in the renormalization of a quartic coupling of $\vec{\varphi}$. In the following, I will describe some of the two loop results.

M.A. Metlitski and S. Sachdev, Phys. Rev. B 85, 075127 (2010)











$$\mathcal{L}_{f} = \psi_{1\alpha}^{\ell\dagger} \left(\zeta \partial_{\tau} - i \mathbf{v}_{1}^{\ell} \cdot \boldsymbol{\nabla}_{r} \right) \psi_{1\alpha}^{\ell} + \psi_{2\alpha}^{\ell\dagger} \left(\zeta \partial_{\tau} - i \mathbf{v}_{2}^{\ell} \cdot \boldsymbol{\nabla}_{r} \right) \psi_{2\alpha}^{\ell}$$

Order parameter:
$$\mathcal{L}_{\varphi} = \frac{1}{2} \left(\boldsymbol{\nabla}_{r} \vec{\varphi} \right)^{2} + \frac{\widetilde{\zeta}}{2} \left(\partial_{\tau} \vec{\varphi} \right)^{2} + \frac{s}{2} \vec{\varphi}^{2} + \frac{u}{4} \vec{\varphi}^{4}$$

"Yukawa" coupling:
$$\mathcal{L}_{c} = -\lambda \vec{\varphi} \cdot \left(\psi_{1\alpha}^{\ell\dagger} \vec{\sigma}_{\alpha\beta} \psi_{2\beta}^{\ell} + \psi_{2\alpha}^{\ell\dagger} \vec{\sigma}_{\alpha\beta} \psi_{1\beta}^{\ell} \right)$$

Ar. Abanov and A.V. Chubukov, Phys. Rev. Lett. 93, 255702 (2004).



Critical point theory is strongly coupled in d = 2Results are *independent* of coupling λ



M.A. Metlitski and S. Sachdev, Phys. Rev. B 85, 075127 (2010)

 k_x





$$\left\langle c_{\mathbf{k}\alpha}^{\dagger}c_{-\mathbf{k}\beta}^{\dagger}\right\rangle = \varepsilon_{\alpha\beta}\Delta(\cos k_{x} - \cos k_{y})$$

$$\int \int \partial f dx$$
Inconventional pairing at and near hot spots

BCS theory



BCS theory



Antiferromagnetic fluctuations: weak-coupling



V. J. Emery, J. Phys. (Paris) Colloq. **44**, C3-977 (1983) D.J. Scalapino, E. Loh, and J.E. Hirsch, Phys. Rev. B **34**, 8190 (1986) K. Miyake, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **34**, 6554 (1986) S. Raghu, S.A. Kivelson, and D.J. Scalapino, Phys. Rev. B **81**, 224505 (2010)

Antiferromagnetic fluctuations: weak-coupling

 $1 + \left(\frac{U}{t}\right)^2 \log\left(\frac{E_F}{\omega}\right)$ Fermi Applies in a Fermi liquid energy as repulsive interaction $U \to 0$. Implies $T_c \sim E_F \exp\left(-\left(t/U\right)^2\right)$ V. J. Emery, J. Phys. (Paris) Collog. 44, C3-977 (1983) D.J. Scalapino, E. Loh, and J.E. Hirsch, *Phys. Rev. B* **34**, 8190 (1986) K. Miyake, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B 34, 6554 (1986) S. Raghu, S.A. Kivelson, and D.J. Scalapino, *Phys. Rev. B* 81, 224505 (2010)

Spin density wave quantum critical point

$$1 + \frac{\alpha}{\pi(1+\alpha^2)} \log^2\left(\frac{E_F}{\omega}\right)$$

M.A. Metlitski and S. Sachdev, Phys. Rev. B 85, 075127 (2010)

Spin density wave quantum critical point

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M.A. Metlitski and S. Sachdev, Phys. Rev. B 85, 075127 (2010)


(see also Ar. Abanov, A.V. Chubukov, and A. M. Finkel'stein, *Europhys. Lett.* **54**, 488 (2001)) M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)





Enhancement of pairing susceptibility by interactions Spin density wave quantum critical point

$$1 + \frac{\alpha}{\pi(1+\alpha^2)} \log^2\left(\frac{E_F}{\omega}\right)$$

- \log^2 singularity arises from Fermi lines; singularity *at* hot spots is weaker.
- Interference between BCS and quantum-critical logs.
- Momentum dependence of self-energy is crucial.
- Not suppressed by 1/N factor in 1/N expansion.

Ar. Abanov, A.V. Chubukov, and A. M. Finkel'stein, *Europhys. Lett.* **54**, 488 (2001) M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)



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Spin-fermion model: Electrons with dispersion $\varepsilon_{\mathbf{k}}$ interacting with fluctuations of the antiferromagnetic order parameter $\vec{\varphi}$.

$$\begin{split} \mathcal{Z} &= \int \mathcal{D}c_{\alpha}\mathcal{D}\vec{\varphi}\exp\left(-\mathcal{S}\right) \\ \mathcal{S} &= \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{\dagger} \left(\frac{\partial}{\partial\tau} - \varepsilon_{\mathbf{k}}\right) c_{\mathbf{k}\alpha} \\ &+ \int d\tau d^{2}r \left[\frac{1}{2} \left(\boldsymbol{\nabla}_{r}\vec{\varphi}\right)^{2} + \frac{s}{2}\vec{\varphi}^{2} + \ldots\right] \\ &- \lambda \int d\tau \sum_{i} \vec{\varphi}_{i} \cdot (-1)^{\mathbf{r}_{i}} c_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta} \end{split}$$

Spin-fermion model: Electrons with dispersions $\varepsilon_{\mathbf{k}}^{(x)}$ and $\varepsilon_{\mathbf{k}}^{(y)}$ interacting with fluctuations of the antiferromagnetic order parameter $\vec{\varphi}$.

$$\begin{split} \mathcal{Z} &= \int \mathcal{D}c_{\alpha}^{(x)} \mathcal{D}c_{\alpha}^{(y)} \mathcal{D}\vec{\varphi} \exp\left(-\mathcal{S}\right) \\ \mathcal{S} &= \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{(x)\dagger} \left(\frac{\partial}{\partial \tau} - \varepsilon_{\mathbf{k}}^{(x)}\right) c_{\mathbf{k}\alpha}^{(x)} \\ &+ \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{(y)\dagger} \left(\frac{\partial}{\partial \tau} - \varepsilon_{\mathbf{k}}^{(y)}\right) c_{\mathbf{k}\alpha}^{(y)} & \underset{\text{S. Sachdev, to}}{\overset{\text{S. Sachdev, to}}{\overset{\text{appear}}{\overset{\text{appear}}{\overset{\text{green}}{\overset{green}}}}}}} } } } } } } } } \\ + \int d\tau d\tau d^2 r \left[\frac{1}{2} \left(\boldsymbol{\nabla}_{r}\vec{\varphi}\right)^2 + \frac{s}{2} \vec{\varphi}^2 + \ldots \right]}} } \frac{s}{2} \vec{\varphi}^2 + \ldots \right]} } } } \\ \\ - \lambda \int d\tau \sum_{i} \vec{\varphi}_{i} \vec{\varphi}_{i} \cdot (-1)^{r_{i}} c_{i} (\alpha)} \dagger {\overset{green}}{\overset{green}}} } } \\ } \\ } \\ \\ - \lambda \int d\tau \sum_{i} \vec{\varphi}_{i} \vec{\varphi}_{i} \cdot (-1)^{r_{i}} {\overset{green}}{\overset{green}}} } } \\ \\ \\ \end{array}{greenn}} } \\ \\ \\ \end{array}{greenn}} } \\ \\ \\ \end{array}{greenn}} } \\ \\ \end{array}{greenn}} } \\ \\ \end{array}{greenn}} } \\ \\ \end{array}{greenn}} \\ \\ \end{array}{greenn}} \\ \\ \end{array}{greenn}} \\ \\ \end{array}{greennn}} \\ \\ \end{array}{greennn}} } \\ \\ \end{array}{greennn}} \\ \\ \end{array}{greennn}}$$



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