KITP Santa Barbara : New Phases, Correlated Materials, Spin-Orbit Systems 24/07/2015

Topological Phases on the Honeycomb Lattice: Spin-Orbit Coupling, Correlations & Superconductivity

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New phases of matter with electrons (fermions)



B. Douçot with the honeycomb lattice...

I) Topological Insulators Interaction Effects

iridate materials, cold atoms

II) SC on honeycomb lattices: d+id SC starting from half-filling
2 possible ground states (related to talk by Y. Ran)

New honeycomb materials Doped iridate materials (?)

Iridates: recent review (more on material aspects) J. G. Rau, E. K.-H. Lee, H.-Y. Kee, arXiv:1507.06323

Team Acknowledgements



W.-M. Liu (KITP China), Walter Hofstetter (Frankfurt), Cécile Repellin (ENS), Nicolas Regnault (Princeton/ENS) T. Maurice Rice (ETH), C. Honerkamp (Aachen), M. Scherrer, C.-H. Chung (Taiwan)

On-going work with Loic Herviou (PhD, X) and C. Mora (ENS) on Majoranas in quasi-1D Work with A. Petrescu (PRL2013, PRB 2015), M. Piraud, K. Plekhanov, G. Roux on Topo-phases with bosons

I) Topological Insulators







- Time-reversal invariant band insulator
- Strong spin-orbit interaction $\lambda \vec{L} \cdot \vec{\sigma}$
- Gapless helical edge mode (Kramers pair)



Microscopic Description: Simple Standard Model, Kane-Mele

Time reversal invariant of Haldane model (1988): Kane-Mele model

Kane & Mele, PRL 95, 226801 (2005); Fu-Kane

see also: Bernevig, Hughes, and Zhang, Science 314, 1757 (2006) + Molenkamp-experiments in three dimensions, experiments by M. Z. Hasan et al. (Bismuth materials)

Also realizations in photon systems for example: <u>M. Hafezi</u>, <u>S. Mittal</u>, <u>J. Fan</u>, <u>A. Migdall</u>, <u>J. Taylor</u> (2013) <u>Mikael C. Rechtsman</u>, <u>Julia M. Zeuner</u>, <u>Yonatan Plotnik</u>, <u>Yaakov Lumer</u>, <u>Stefan Nolte</u>, <u>Mordechai Segev</u>, <u>Alexander Szameit</u>

(2013)



strip geometry:



Phase Diagram: "Kane-Mele-Hubbard"



CDMFT

Real-space version QMC continous-time Impurity solver

QMC



Transition: 3D XY S. Rachel & KLH, 2010 Griset & C. Xu, 2011 D.-H. Lee, 2011

> M. Hohenadler et al. arXiv:1111.3949

Phys. Rev. Lett. 106, 100403 (2011)

Review: Hohenadler & Assaad, 2013

 λ/t Absence of spin liquid for Hubbard (QSL and SL Needs frustration – see later): S. Sorella et al. Scientific Reports 2012; S. R. Hassan & D. Senechal PRL 2013

Single-particle gap does not close at the Mott transition...



CDMFT

Real-space version QMC continous-time Impurity solver

Some Reviews (not full list):

G. Kotliar et al, RMP 2006 T. Maier et al, RMP 2005 A.-M. Tremblay, B.-S. Kyung, D. Senechal, 2006

DMFT:

A. Georges, G. Kotliar,W. Krauth & M. Rozenberg et al.;Metzner & Vollhardt

Wei Wu, Stephan Rachel, Wu-Ming Liu and KLH, PRB **85**, 205102 (2012) See also Yamaji & Imada, 2011; Yu, Xie & Li 2011; Zheng, Zhang & C. Wu, 2011

Edge Theory & Mott Transition

C. Xu & J. Moore; C. Wu, A. Bernevig & S.-C. Zhang;...

$$H_0 = v_F \int dx \left(\psi_{R\uparrow}^{\dagger} i \partial_x \psi_{R\uparrow} - \psi_{L\downarrow}^{\dagger} i \partial_x \psi_{L\downarrow} \right)$$

 $\psi_{R\uparrow}^{\dagger}\psi_{L\downarrow}^{\dagger} + \text{h.c.}$ (elastic) Backscattering forbidden

$$H_{I} = U \int dx \left(\psi_{R\uparrow}^{\dagger} \psi_{R\uparrow} \psi_{L\downarrow}^{\dagger} \psi_{L\downarrow} \right)$$

$$\begin{split} H = \int dx \frac{v}{2} \begin{bmatrix} \frac{1}{K} \left(\partial_x \phi\right)^2 + K \left(\partial_x \theta\right)^2 \end{bmatrix} - \frac{Um \sin \sqrt{4\pi} \phi}{(\pi a)^2} \\ & \underset{\text{for TBI/QSH phase}}{\text{With } m} = \langle \psi_{R\uparrow}^{\dagger} \psi_{L\downarrow} \rangle \end{split}$$

Technical Note on Field-Theory techniques...

- Apply (Slave)-Rotor theory of Florens & Georges, PRB 70, 035114 (2004)
- See review E. Zhao & A. Paramekanti
- Rewrite fermions as rotors (charge degrees of freedom) and spinons



$$c_{i\sigma} = e^{i\theta_i} f_{i\sigma}$$

Introduce constraint

$$\sum_{\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} + L_i = 1$$
$$\frac{U}{2} \sum_{i} \left(\sum_{\sigma} n_{i\sigma} - 1 \right)^2 \longrightarrow \frac{U}{2} \sum_{i} L_i^2$$

Hubbard interaction simplifies

$$L = (i/U)\partial_{\tau}\theta$$

Interaction affects rotor only

) weak U: rotor condense,
$$\,f_\sigma \propto c_\sigma$$



S. Rachel & KLH, PRB **82**, 012405 2010 Application to QSH phenomena

[+ other theory arguments]

Presence of spin orbit coupling

More Slave-Rotor: use sigma-model representation
At the Blue transition, "spin-charge" separation

$$X = e^{i\theta} \quad |X|^2 = 1$$

- mean-field decoupling or Hubbard Stratonovich
- Gap of the rotor-field (zero at the transition)

$$\Delta_g = 2\sqrt{U(\rho + \min \xi_k)}$$



See also S.S. Lee & P. Lee PRL 2005 Young, S. S. Lee, C. Kallin, PRB 2008 Pesin & Balents, Nat. Phys. 2010 Y.-B. Kim & et al. 2010 + many recent works



S. Rachel & KLH, PRB 82, 075106 (2010); arXiv:1003.2238, 20 pages

Mean-Field Solution allows TMI phase:

- Mott gap
- Spin degrees of freedom form a topological Kane-Mele phase

Analogue of S=1 spin Haldane chain NOT STABLE in 2D, here 3D: Pesin-Balents (OK); WHY?

2D: Direct Transition from TBI to XY

Kane-Mele Spinon model

$$\mathcal{L}_{MF} = m \sum_{a=\pm} \left(f_{\uparrow a}^{\dagger} \tau^{z} f_{\uparrow a} - f_{\downarrow a}^{\dagger} \tau^{z} f_{\downarrow a} \right)$$

Monopole insertion = "spin flip" operator

Localized $+2\pi$ flux of the gauge field implies that a single extra spin-up spinon will be Induced along with the gauge flux, while one spin-down spinon will be depleted

Fermions are gapped:

$$\mathcal{L}_{Maxwell} = (1/2e^2) \sum_{\mu} (\epsilon_{\mu\nu\lambda} \partial_{\nu} a_{\lambda})^2$$

Monopoles only cost a finite action: monopole propagator is long-ranged

Here, this implies magnetic order in the XY plane: <S⁺> is finite

Polyakov's gauge field argument: see also S. S. Lee & P. Lee; Y. Ran et al; M. Hermele...

Connection to reality?

• Na₂IrO₃: anisotropic spin-orbit coupling (<u>thin films</u>: arXiv:1303:5245, M. Jenderka et al)

Shitade et al. PRL 102 256402 (2009); G. Jackeli & G. Khaliullin, PRL 102, 017205 (2009)

H.-C. Jiang, Z.-C. Gu, X.-L. Qi and S. Trebst, Phys. Rev. B 83, 245104 (2011);

S. Bhattacharjee, Sung-Sik Lee and Yong-Baek Kim, New J. Phys. 14, 073015 (2012)

Y. Singh et al. 2012; Z. Nussinov & J. van den Brink, arXiv:1303.5922 ...



α Lithium Iridates and Spiral order R. Coldea

Talk next week G. Cao



D. Pesin & L. Balents, Nature Phys. 2010 Krempa, Choy, Y.-B. Kim & L. Balents Spin Ice physics: N. Shannon; S. Onoda R. Coldea, Titanate Pyrochlores...

Tianhan Liu, Benoit Doucot, Karyn Le Hur, PRB 2013 A. Ruegg and G. Fiete, PRL 2012 J. Reuther, R. Thomale & S. Rachel, PRB 2012 M. Kargarian, A. Langari, G. Fiete PRB 2012

Phase diagram 3D: L. Balents

Shitade model and Mott transition

A. Shitade, H. Katsura, J. Kunes, X.-L. Qi, S.-C. Zhang, and N. Nagaosa, PRL 2009

$$H_0 = \sum_{\langle i,j \rangle} t c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{\ll i,j \gg} i t' \sigma^w_{\sigma\sigma'} c^{\dagger}_{i\sigma} c_{j\sigma'}$$

- Criticial U identical to Kane-Mele-Hubbard model
- Spin Polarization when inserting a localized Flux

Insertion of monopoles in the slave-rotor U(1) representation: dilute gaz of instantons

Spin Polarization: Linear Response At one Site

Spin Texture...

Tianhan Liu, Benoit Doucot, Karyn Le Hur, PRB 2013

Possible spin liquid? A. Ruegg & G. Fiete PRL 2012



Large-U: Magnetism depends on the Kitaev-Heisenberg models

Talk by N. Perkins

J. Chaloupka, G. Jackeli and G. Khaliullin Phys. Rev. Lett. 105, 027204 (2010).



T. Liu, C. Reppelin, N. Regnault, B. Douçot & KLH (check with ED)



Cold Atoms:

Ways to implement magnetic fields & gauge fields

A. L. Fetter RMP 2009; J. Dalibard, F. Gerbier, G. Juzeliunas, P. Ohberg RMP 2011; M. Aidelsburger et al. Nature (2012); Juzeliunas & Spielman NJP (2012);...

One model proposed by N. Goldman et al. arXiv:1011.3909 (PRL)

Example of non-Abelian Gauge Fields here on square lattice

$$H_{0} = -\sum_{j} \left\{ t_{x} c_{j+\hat{x}}^{\dagger} e^{-i2\pi\gamma\sigma^{x}} c_{j} + t_{y} c_{j+\hat{y}}^{\dagger} e^{i2\pi\alpha x\sigma^{z}} c_{j} \right.$$
$$\left. + \text{h.c.} \right\} + \lambda_{x} \sum_{j} (-1)^{x} c_{j}^{\dagger} c_{j} ,$$

INTERACTION EFFECTS & PHASE DIAGRAM?

P. Orth, D. Cocks, S. Rachel, M. Buchhold, KLH & W. Hofstetter, review 1212.5607

D. Cocks, P. P. Orth, S. Rachel, M. Buchhold, K. Le Hur, W. Hofstetter, PRL 2012

Interacting spinful Hofstadter-Harper model $\Upsilon = \lambda_x = 0$

Interaction Effects

At weak U and half-filling, semi-metal (SM), graphene **Number of Dirac points vary** with $\alpha = 1/q$ (q even)

Application of I. Herbut's theory For transition SM to ordered state

The transition occurs for $U_c = 1/q^2$

Magnetism depends on γ

See also M. Scheurer, S. Rachel, P. P. Orth Sci. Rep. 5, 8386 (2015)



DMFT in Real space

II) BCS superconductor: zero modes

The BCS superconductors can be described using mean field theory (1957)

$$\mathcal{H}_{\text{BCS}} = \sum_{ab} \left[f_a^{\dagger} T_{ab} f_b - f_b T_{ab} f_a^{\dagger} + f_a \Delta_{ab} f_b + f_b^{\dagger} \Delta_{ab}^* f_a^{\dagger} \right] ,$$

 $T^{\dagger}=T$ Hermitian $\Delta_{ab}=-\Delta_{ba}$ Anti-symmetric

Quasiparticle spectrum
$$~\gamma^{\dagger}=u_{a}f_{a}^{\dagger}+v_{a}f_{a}$$

found as Eigenvalues of Bogoliubov-de-Gennes equations

$$\begin{pmatrix} T & \Delta \\ \Delta^{\dagger} & -T^T \end{pmatrix} \cdot \psi = E\psi = \mathcal{H}\psi \qquad \psi = \begin{pmatrix} u \\ v \end{pmatrix} \text{.Gurarie, Radzihovsky, 2007}$$

Eigenvalues comes in pairs $\pm E$ since $\omega^x \mathcal{H} \omega^x = -\mathcal{H}^*$ where $\omega^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. This implies $\omega^x \psi^*$ is an eigenstate with -E

Zero energy Modes: Majorana fermions

$$\omega^{x}\Psi^{*}=\Psi \rightarrow^{v=u^{*}}$$

Zero modes have these two states *degenerate*, and can take a superposition of the form

$$\psi = \begin{pmatrix} u \\ u^* \end{pmatrix}$$
. $\gamma^{\dagger} = u\psi^{\dagger} + v\psi = u\psi^{\dagger} + u^*\psi = \gamma$

The quasiparticle at E=O is a Majorana fermion! Example: p+ip superconductor or 5/2 FQH state (N. Read & Green) Topological SCs (Fu-Kane) 1D p-wave Superconductor (A. Kitaev; InAs wires Y. Oreg, G. Refael, F. von Oppen and J. Sau, R. Lutchyn, S. Tewari and S. das Sarma)...

Application for topological quantum computation, quantum error correction codes C. Nayak, S. Simon, A. Stern, M. Freedman, S. das Sarma RMP 2008 Barbara Terhal, RMP 2015

Example: p+ip SC

excitations (quasiparticles) are described via the Bogoliubov-de-Gennes (BdG) equations

$$\Delta(q) = (q_x + iq_y)\,\Delta$$

$$\begin{pmatrix} -\frac{\nabla^2}{2m} - \mu & -i\frac{1}{2}\{\Delta, (\partial_x + i\partial_y)\} \\ -i\frac{1}{2}\{\Delta^*, (\partial_x - i\partial_y)\} & \frac{\nabla^2}{2m} + \mu \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

The quasiparticles are gapped in the bulk,

$$E = \pm \sqrt{\left(-\mu + \frac{q^2}{2m}\right)^2 + |\Delta|^2 q^2}$$

but the Gap is reduced and eventually vanishes at the system boundary or in vortices.

Quasiparticle bound states in cores...



Majorana zero energy states

In s-wave condensates, the spectrum of bound states has no zero modes (Caroli, de Gennes, Matricon, 1964).

In p+ip condensate, zero modes exist (Kopnin and Salomaa 1991, G. E. Volovik).

Neglect the quadratic kinetic energy term, and we have the structure of a <u>Dirac equation</u>.

$$egin{pmatrix} -\mu & -irac{1}{2}\{\Delta, (\partial_x + i\partial_y)\} \ -irac{1}{2}\{\Delta^*, (\partial_x - i\partial_y)\} & \mu \end{pmatrix} egin{pmatrix} u \ u^* \end{pmatrix} = 0 \ .$$

Two solutions – exponential decay, and exponentially growing. In infinite system – only exponential decay normalizable (physical) so only <u>one bound state zero mode</u> (Green and Read 2000, Tewari et al 2007, Gurarie+Radzihovsky 2006 and others...)

Honeycomb lattice & s-wave case:

BdG equations

Notations J. Alicea & M. Fisher 2006

$$\frac{1}{2} \begin{pmatrix} \left[\mu - iv \left(\eta \cdot \nabla \right) \right] & +i\Delta_0 \eta^y \sigma^y \tau^y \\ -i\Delta_0^* \eta^y \sigma^y \tau^y & - \left[\mu + iv \left(\eta^T \cdot \nabla \right) \right] \end{pmatrix} \phi = E\phi$$

Choose states that are spin and "valley" (Dirac node index) eigenstates – 4 fold degeneracy of the entire quasiparticle spectrum.

Exact solution can be built: prove the existence of 4 zero energy modes

D. Bergman & KLH, PRB 2009

$$e^{-\frac{1}{v}\int_0^r f(r')dr'} \ \Delta = -ie^{i\phi}f(r)$$

<u>Near</u>-zero energy modes

At <u>exactly</u> half filling, Ghaemi and Wilczek 2007 showed explicitly that zero modes exist, and invoked a result from high energy physics – the existence of zero modes bound to vortex cores in this case is guaranteed by an <u>index theorem</u> (E. Weinberg 1981)

Problem: As pointed out by Ghaemi+Wilzcek

Zeeman splitting from a magnetic field splits the spin-degeneracy, and endows these states with non-zero energy (therefore named <u>near</u>-zero modes)

$$\left(\mathcal{H}+B\sigma^{y}\right)\phi=\pm B\phi=E\phi$$



Exact Diagonalization: No protection

Beyond Dirac approximation



In general : Fully Gapped...

One needs one-1/4 graphene: Topological Insulators (Fu-Kane; Beenakker) to ensure Majorana protection

Still Chirality from Hubbard...

Possibility of gapped spin liquid

J₁-J₂ model; Tran & Kim, arXiv:1011.1700 & Clark, Abanin & Sondhi PRL 2010;... Other variants of spin liquid: C. Xu & S. Sachdev; Vaezi et al; ...

Let's start from Néel half-filled phase and dope the system



Wei Wu, Michael M. Scherer, Carsten Honerkamp & KLH, PRB 2013 (RMFT, fRG: t-J1-J2)
 A. Black-Schaffer, W. Wu and KLH, PRB 2014 (RMFT t-J, QMC on Hubbard)
 A. Black-Schaffer & KLH, arXiv:1503.02509 (topological phase transition due to SDW)

d+id Pairing: RMFT & QMC

2.5

1.5

Renormalized mean-field theory

2)

1/2

filling

k_y

 E_{2a}

- F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Tech. 1, 36 (1988).
- P. W. Anderson, P. A. Lee, M. Randeria, T. M. Rice, N. Trivedi, and F. C. Zhang, J. Phys.: Condens. Matter 16, R755 (2004).
- B. Edegger, V. N. Muthukumar, and C. Gros, Adv. Phys. 56, 927 (2007).
- M. Ogata and H. Fukuyama, Rep. Prog. Phys. **71**, 036501 (2008).
- K. Le Hur and T. M. Rice, Ann. Phys. 324, 1452 (2009).



See also results from L. Balents, X. G. Wen : Z. G. Gu et al. Phys. Rev. B **88**, 155112 (2013) Grassmann Tensor Network Approach, DMRG

 $(k_x^2 - k_y^2, 2k_x k_y)$

SDW and SC: Two chiral Superconductors



Universality class C (2 co-propagating edge modes)

Counter-propagating helical edge modes (class A)

chiral d-wave SCs: honeycomb

Doping $In_3Cu_2VO_9$ possible with Zn (Copper gives spin-1/2)

A. Möller, U. Löw, T. Taetz, M. Kriener, G. André, F. Damay,
O. Heyer, M. Braden, and J. A. Mydosh, Phys. Rev. B 78, 024420 (2008).
Y. J. Yan, Z. Y. Li, T. Zhang, X. G. Luo, G. J. Ye, Z. J. Xiang,
P. Cheng, L. J. Zou, and X. H. Chen, Phys. Rev. B 85, 085102 (2012).
D.-Y. Liu, Y. Guo, X.-L. Zhang, J.-L. Wang, Z. Zeng, H.-Q. Lin, and L.-J. Zou, EPL 103, 47010 (2013).

Experimental works

Chiral d-wave SCs have also been suggested in SrPtAs, MoS2, graphene and silicene

Possibility of Majorana fermions adding spin-orbit coupling

S.-J. Sun, C.-H. Chung, Y.-Y. Chang, W.-F. Tsai and F.-C. Zhang, arXiv:1506.02584

SC in doped Heisenberg-Kitaev models: exotic p+ip triplet states

On-going work T. Liu, C. Repellin, N. Regnault, B. Douçot, KLH (PhD thesis of T. Liu) See also Y. Z. You, I. Kimchi & A. Vishwanath, PRB 2012; Daniel D. Scherer et al PRB 2014 **Talk next week G. Khaliullin**

Summary

Two-dimensional correlated TBIs

Not yet confirmed in experiments (effort in material aspects)

Magnetism in Mott phase depends on the Kitaev-Heisenberg models (relevant for 2D iridates); **not Kitaev alone** ...

Boson Systems are also interesting (cold atoms; photons) Review on photons (see refs inside); **arXiv May 2015** – submitted to CRAS Karyn Le Hur¹, Loïc Henriet¹, Alexandru Petrescu^{2,1}, Kirill Plekhanov¹, Guillaume Roux³, Marco Schiró⁴ Another Workshop in parallel at KITP on « photons » next Fall 2015

Topological SC close to Mott state:

d+id chiral (class C) – stay until ¼ filling at large U... Mixed d+id/d-id (class A) possible when coexistence with SDW