Baryon chiral perturbation theory transferred to hole-doped antiferromagnets on the honeycomb lattice

Christoph P. Hofmann
In collaboration with B. Bessire, F.-J. Jiang, F. Kämpfer, U.-J. Wiese and M. Wirz

Facultad de Ciencias, UCOL

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Outline

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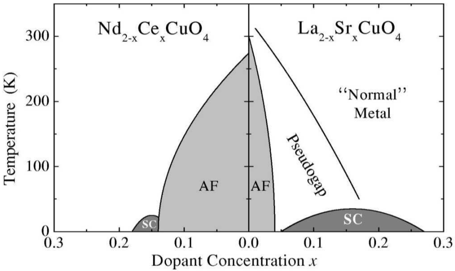
Motivation: High-T_c superconductivity in cuprates

1986: Bednorz and Müller discover high-T_c superconductivity by doping copper oxide compounds (cuprates):

$$La_2CuO_4 \longrightarrow La_{2-x}Ba_xCuO_4 \qquad (T_c = 35\text{ K})$$

- Although a lot of research has been done ever since, still, the mechanism of high-T_c superconductivity remains a mystery
- Can we learn anything from methods traditionally used particle physics?

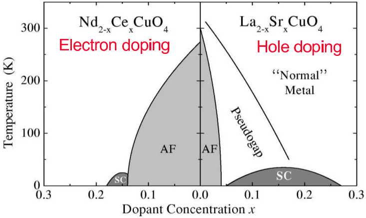
Motivation: High-T_c superconductivity in cuprates



- HTSC results from doping antiferromagnetic insulators
- Doping possible with both electrons and holes
- Electron-Hole asymmetry

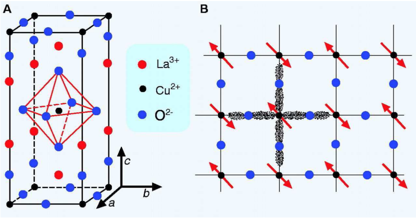
Motivation: High-T_c superconductivity in cuprates

Phase diagram of cuprates:



Damascelli, Hussain, and Shen, Rev. Mod. Phys. 75 (2003) 473

Crystal structure:



Orenstein and Millis, Science 288 (2000) 468

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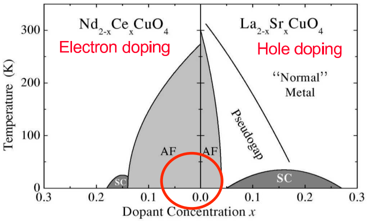

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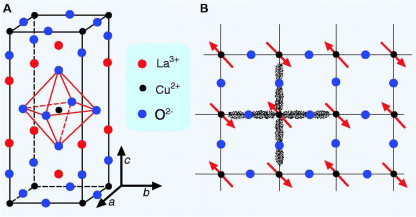
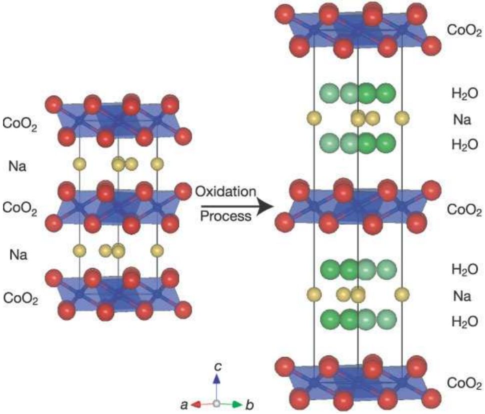


Orenstein and Millis, Science 288 (2000) 468

- HTSC results from doping antiferromagnetic insulators
- Doping possible with both electrons and holes
- Common structure: CuO_2 layers separated by spacer layers
- Concentrate on antiferromagnetic region: low doping, low T

Motivation: High-T_c superconductivity in cobaltates

Structural views of $Na_{0.7}CoO_2$ (left) and $Na_xCoO_2 \cdot H_2O$ (right), where Na and H_2O sites are partially occupied



Microscopic description: The Hubbard model

The Hubbard Hamiltonian defined on a honeycomb lattice:

$$\mathcal{H} = -t \sum_{\substack{\langle x,y \rangle \\ s=\uparrow,\downarrow}} (c_{xs}^\dagger c_{ys} + c_{ys}^\dagger c_{xs}) + U \sum_x c_{x\uparrow}^\dagger c_{x\uparrow} c_{x\downarrow}^\dagger c_{x\downarrow} - \mu' \sum_{\substack{x \\ s=\uparrow,\downarrow}} c_{xs}^\dagger c_{xs},$$

- Parameters of the model:

t : Hopping parameter (nearest neighbors)

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- Parameters of the model:

$$t: \text{ Hopping parameter (nearest neighbors)}$$
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- Minimal model for cobaltates: contains the relevant physics
- Away from half-filling: Hamiltonian virtually unsolvable from first principles (Neither analytically nor numerically)

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- Symmetries:

$SU(2)_s$: Global spin rotation

$U(1)_Q$: Fermion number conservation

D_i : Displacement by the two basis vectors

O : 60 degrees rotation

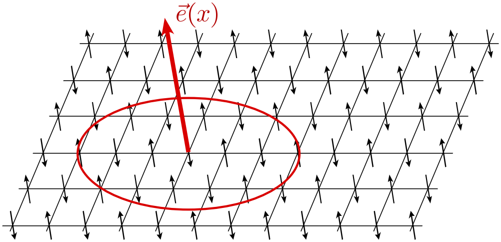
R : Reflection on a lattice axis

T : Time reversal

Antiferromagnetism: Near half-filling (1 fermion per site)

Near half-filling (shown here for square lattice):

- Antiferromagnetic alignment of spins is preferred
- Spontaneous symmetry breaking: $SU(2)_s \longrightarrow U(1)_s$
- Goldstone's theorem: 2 massless excitations $\Longrightarrow$ 2 magnons



Outline

Systematic effective field theory description

	Antiferromagnets	QCD
Spont. symm. breaking	$SU(2)_s \longrightarrow U(1)_s$	$SU(2)_L \otimes SU(2)_R \rightarrow SU(2)_{L=R}$
GB physics	Magnon perturbation theory	Chiral perturbation theory
GB + matter physics	Effective theory presented here	Baryon chiral perturbation theory

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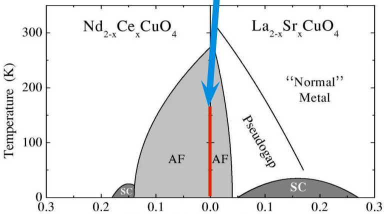

Pure magnon sector: Magnon perturbation theory

Spontaneous global $SU(2)_s \longrightarrow U(1)_s$ spin symmetry breaking:

- 2 Goldstone bosons (magnons) described by

$$\vec{e}(x) = \big(e_1(x), e_2(x), e_3(x)\big) \in S^2 = SU(2)_s/U(1)_s$$

with $x = (x_1, x_2, t)$

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- Low-energy magnon physics described by nonlinear σ-model

$$\mathcal{L} = \frac{\rho_s}{2}(\partial_i \vec{e} \cdot \partial_i \vec{e} + \frac{1}{c^2}\partial_t \vec{e} \cdot \partial_t \vec{e}) + \cdots$$

  ρ_s: spin stiffness c: spin wave velocity

Chakravarty, Halperin, and Nelson, PRB 39 (1989) 2344
Hasenfratz and Niedermayer, Phys. Lett. B268 (1991) 231

State of affairs: Fermionic sector of effective theory

Earlier attempts by: Shraiman and Siggia, Wen, Shankar, ...

General agreement:

- Magnons are coupled to fermions through composite vector fields

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- Conflicting realizations of fermion fields
- Non-unique structure of terms in Lagrangians

$\Longrightarrow$ Model Lagrangians have not been constructed systematically

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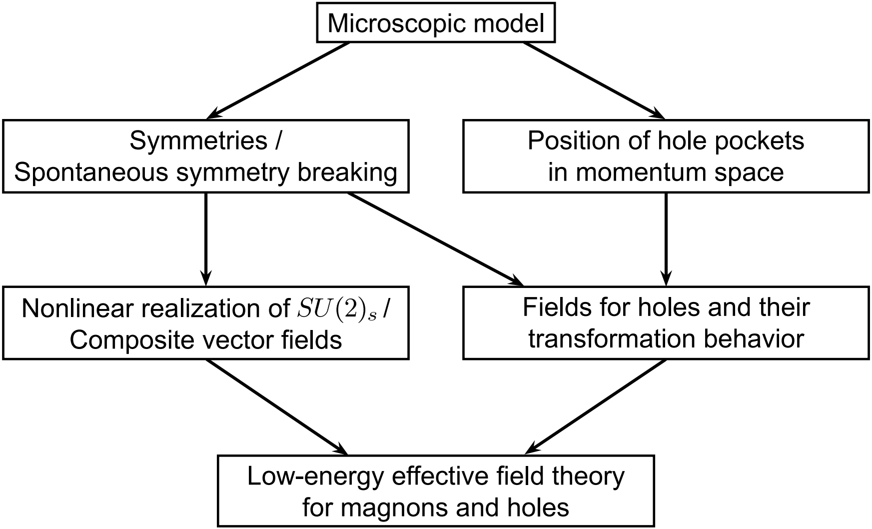
$\Longrightarrow$ Construction of a systematic low-energy effective field theory for magnons and holes analogous to baryon chiral perturbation theory

Symmetry-based construction of effective theory



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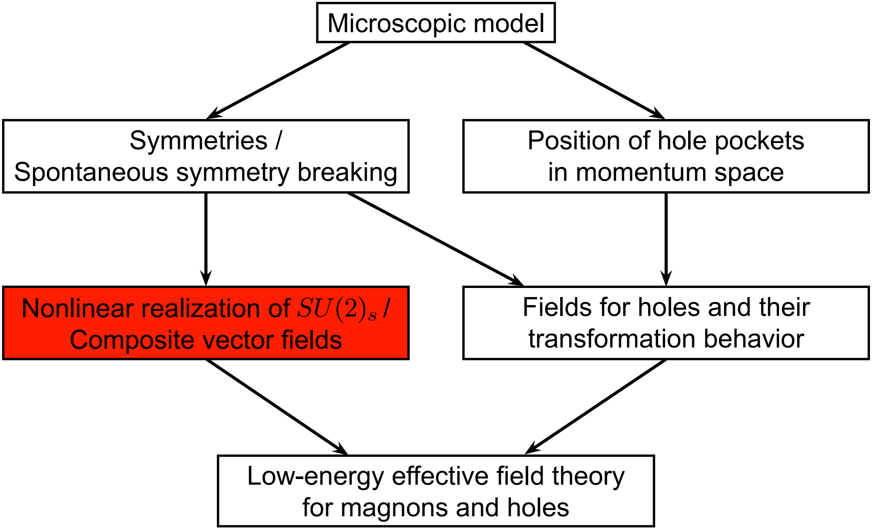

Nonlinear realization of $SU(2)_s$ symmetry

- $\mathbb{C}P(1)$ representation of magnon field

$$P(x) = \frac{1}{2}\left(\mathbb{1} + \vec{e}(x) \cdot \vec{\sigma}\right) \in \mathbb{C}P(1)$$

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Global $SU(2)_s$ rotation manifests itself as local $U(1)_s$ transformation!

Composite vector fields

- We introduce an anti-Hermitean field

$$v_\mu(x) = u(x)\partial_\mu u(x)^\dagger = \begin{pmatrix} v_\mu^3(x) & v_\mu^+(x) \\ v_\mu^-(x) & -v_\mu^3(x) \end{pmatrix}$$

  with $\mu \in \{1, 2, t\}$

- Components used to couple magnons to holes

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- Components used to couple magnons to holes

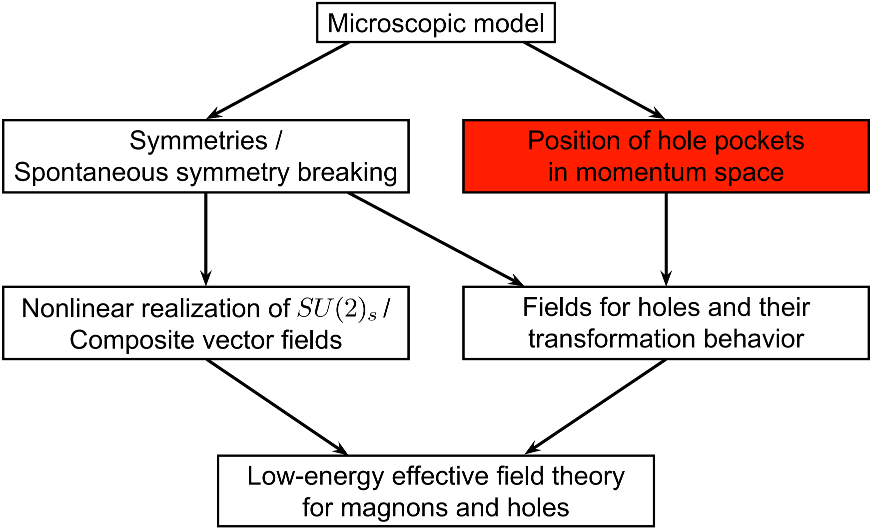
- Under global $SU(2)_s$ the components transform as

$$v_\mu^3(x)' = v_\mu^3(x) - \partial_\mu \alpha(x), \qquad v_\mu^\pm(x)' = v_\mu^\pm(x) \exp\left(\pm 2i\alpha(x)\right)$$

$v_\mu^3(x)$: Abelian gauge field

$v_\mu^\pm(x)$: Vector field ("charged" under $U(1)_s$)

Symmetry-based construction of effective theory



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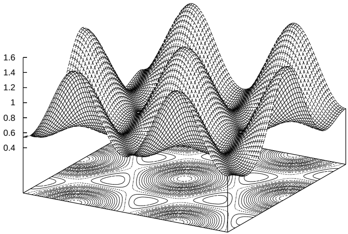
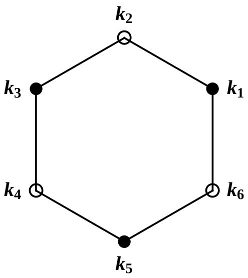
Single hole (away from half-filling) dispersion relation in the first Brillouin zone:



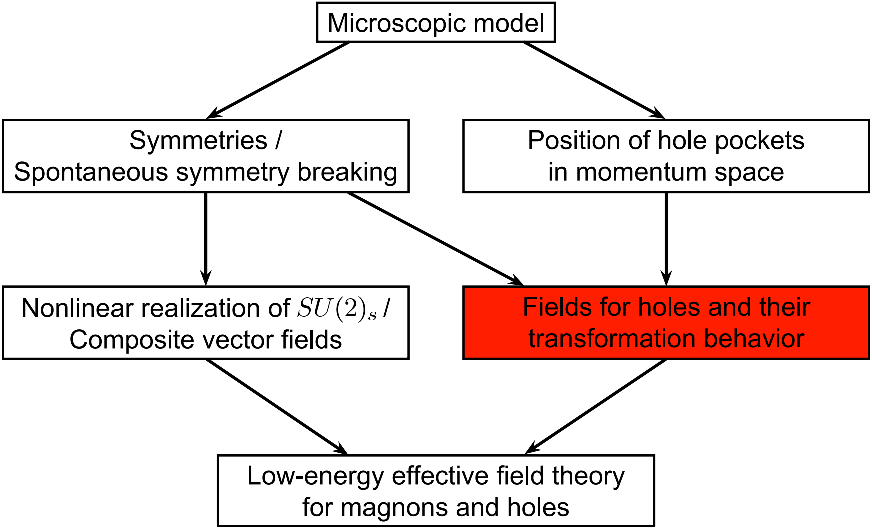
Minima at lattice momenta $\vec{k} = (\pm\frac{2\pi}{3a}, \pm\frac{2\pi}{3\sqrt{3}a})$ and $\vec{k} = (0, \pm\frac{4\pi}{3\sqrt{3}a})$

Location of hole pockets



The six corners of the first Brillouin zone of the Honeycomb lattice with three sets of pairs of inequivalent points

Symmetry-based construction of effective theory



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U(1)_Q: &\quad {}^Q\psi^f_\pm(x) = \exp(i\omega)\psi^f_\pm(x), \\
D_i: &\quad {}^{D_i}\psi^f_\pm(x) = \exp(ik^f a_i)\psi^f_\pm(x), \\
O: &\quad {}^O\psi^\alpha_\pm(x) = \mp\exp(\pm i\tfrac{2\pi}{3} \mp i\varphi(Ox))\psi^\beta_\mp(Ox), \\
R: &\quad {}^R\psi^f_\pm(x) = \psi^{f'}_\pm(Rx), \\
T: &\quad {}^T\psi^f_\pm(x) = \exp(\mp i\varphi(Tx))\psi^{f'\dagger}_\pm(Tx), \\
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\end{aligned}
$$

- Systematic derivative expansion: Construct the most general Lagrangian which respects all the symmetries

Effective Lagrangian for magnons and holes

$$
\begin{aligned}
\mathcal{L}_2 = \sum_{\substack{f=\alpha,\beta \\ s=+,-}} \Big[& M\psi_s^{f\dagger}\psi_s^f + \psi_s^{f\dagger} D_t \psi_s^f + \frac{1}{2M'} D_i \psi_s^{f\dagger} D_i \psi_s^f \\
& + \Lambda \psi_s^{f\dagger}(isv_1^s + \sigma_f v_2^s)\psi_{-s}^f \\
& + iK\big[(D_1 + is\sigma_f D_2)\psi_s^{f\dagger}(v_1^s + is\sigma_f v_2^s)\psi_{-s}^f \\
& \qquad - (v_1^s + is\sigma_f v_2^s)\psi_s^{f\dagger}(D_1 + is\sigma_f D_2)\psi_{-s}^f\big] \\
& + \sigma_f L \psi_s^{f\dagger}\epsilon_{ij} f_{ij}^3 \psi_s^f + N_1 \psi_s^{f\dagger} v_i^s v_i^{-s} \psi_s^f \\
& + is\sigma_f N_2 \left(\psi_s^{f\dagger} v_1^s v_2^{-s} \psi_s^f - \psi_s^{f\dagger} v_2^s v_1^{-s} \psi_s^f\right)\Big],
\end{aligned}
$$

with field strength

$$f_{ij}^3(x) = \partial_i v_j^3(x) - \partial_j v_i^3(x),$$

covariant derivatives

$$D_t \psi_\pm^f(x) = \left[\partial_t \pm i v_t^3(x) - \mu\right] \psi_\pm^f(x),$$
$$D_i \psi_\pm^f(x) = \left[\partial_i \pm i v_i^3(x)\right] \psi_\pm^f(x),$$

and

$$\sigma_\alpha = +1, \quad \sigma_\beta = -1$$

Outline

1. Motivation
   - High-T_c superconductivity
   - Condensed matter analog of baryon chiral perturbation theory
2. Construction of Effective Field Theory for Holes and Magnons
   - Effective field theory for magnons
   - Effective field theory for holes and magnons
3. Spiral Phases
4. Two-Hole Bound States
5. Conclusions

Assumptions

To describe the antiferromagnet with finite doping, we assume

- Fermions experience a homogeneous magnon background field $v_i = (x)$
- The magnetic background does not vary in time: $v_t = 0$
- Fermion contact interactions are small

Uniform Background Field

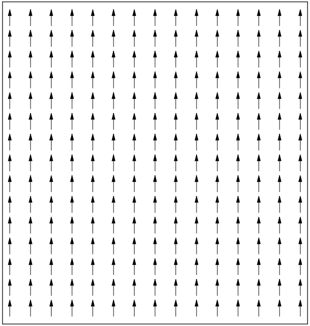
- The homogeneous doping of fermions requires a homogeneous magnetic background.
  $\Rightarrow \quad v_i = const.$ up to a $U(1)_s$ "gauge" transformation:

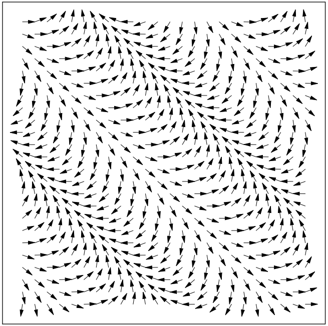
$$\begin{aligned}
v_i^3(x)' &= v_i^3(x) - \partial_i\alpha(x) = \sin^2\frac{\theta(x)}{2}\partial_i\varphi(x) - \partial_i\alpha(x) = c_i^3, \\
v_i^{\pm}(x)' &= v_i^{\pm}(x)\exp(\pm 2i\alpha(x)) \\
&= \frac{1}{2}\left[\sin\theta(x)\partial_i\varphi(x) \pm i\partial_i\theta(x)\right]\exp(\mp i(\varphi(x) - 2\alpha(x))) \\
&= c_i^{\pm}
\end{aligned}$$

Theorem

The staggered magnetization $\vec{e}(x)$ configuration formed for uniform background fields c_i, c_i^3 is either homogeneous or a spiral

Phases of Hole-Doped Antiferromagnets





Homogeneous phase with constant staggered magnetization
Four hole pockets occupied

Spiral phase with helical structure
Two hole pockets occupied

Phases of Hole-Doped Antiferromagnets

All **four** hole pockets populated:

$$\epsilon_4 = \epsilon_0 + Mn + \frac{\pi n^2}{4M'}$$

Two hole pockets populated:

$$\epsilon_2 = \epsilon_0 + Mn + \left(\frac{\pi}{2M'} - \frac{\Lambda^2}{8\rho_s} \right) n^2$$

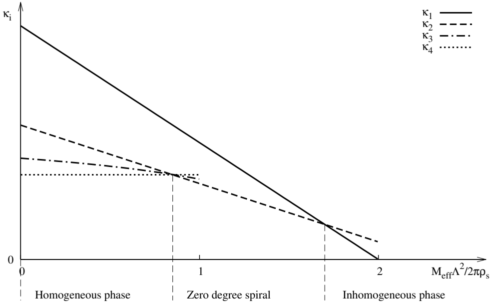
$$\epsilon_i = \epsilon_0 + Mn + \frac{1}{2}\kappa_i n^2$$

ϵ_0: Energy density at half filling

n: Total fermion density

κ: Compressibility

Stability of Phases for Hole Doping

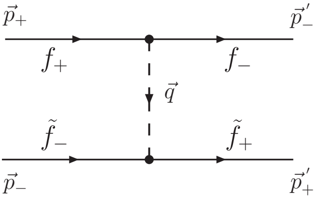


- A homogeneous phase, a spiral phase or an inhomogeneous phase are energetically favorable, for large, intermediate, and small values of ρ_s, respectively

Outline

One-magnon exchange potentials

- At low energies holes interact with each other via magnon exchange
- Two holes can exchange a single magnon only if they have antiparallel spins, which are both flipped in the magnon-exchange process



Formation of two-hole bound states

The magnon-exchange potential is attractive and magnon mediated forces thus lead to bound states if the low-energy constant Λ is larger than the critical value

$$\Lambda_c = \sqrt{\frac{2\pi\rho_s}{M'}}.$$

- Binding energy depends on low energy effective constants
- As long as the binding energy is small compared to the relevant high-energy scales our effective result is valid

f-wave symmetry of two-hole bound states

The Schrödinger equation describing the relative motion of the hole pair is a two-component equation

$$\begin{pmatrix} -\frac{1}{M'}\Delta & \gamma\frac{1}{\vec{r}^{\,2}}\exp(-2i\varphi) \\ \gamma\frac{1}{\vec{r}^{\,2}}\exp(2i\varphi) & -\frac{1}{M'}\Delta \end{pmatrix} \begin{pmatrix} \Psi_1(\vec{r}\,) \\ \Psi_2(\vec{r}\,) \end{pmatrix} = E \begin{pmatrix} \Psi_1(\vec{r}\,) \\ \Psi_2(\vec{r}\,) \end{pmatrix}, \tag{1}$$

with

$$\gamma = \frac{\Lambda^2}{2\pi\rho_s}, \tag{2}$$

and probability amplitudes $\Psi_1(\vec{r}\,)$ and $\Psi_2(\vec{r}\,)$ which represent the two flavor-spin combinations $\alpha_+\beta_-$ and $\alpha_-\beta_+$. The distance vector $\vec{r}$ points from the β to the α hole.

Under 60 degrees rotation the wavefunction transforms as

$$^{O}\Psi(r,\varphi) = -\Psi(r,\varphi) \tag{3}$$

The wave function for the ground state of two holes of flavors α and β bound by magnon exchange exhibits f-wave symmetry.

Outline

Conclusions

- High-T superconductors represent the condensed matter analog of baryon chiral perturbation theory
- We have constructed a systematic low-energy effective field theory for lightly hole-doped antiferromagnets on the honeycomb lattice
- Using the effective theory we have investigated spiral phases in hole-doped cobaltates
- We have calculated the one-magnon-exchange potential and investigated the formation of two-hole bound states
- Free, relativistic, massless fermions emerge naturally as a consequence of the symmetries

Outlook

- Analysis of materials with other lattice geometries: Triangular and Kagomé lattice
- Incorporation of Phonons as low-energy degrees of freedom
- Systematic treatment of loop graphs
- Towards the elusive mechanism of high-T superconductivity

Some basic facts about graphene

- Low-energy excitations of graphene are free, massless and relativistic Dirac fermions
- Undoped graphene is described by the Hubbard model at half-filling in the weak coupling limit ($U \ll t$)
- Remember: In the strong coupling limit ($U \gg t$) we have an antiferromagnetic phase, characterized by the spontaneously broken symmetry $\mathrm{SU}(2) \to \mathrm{U}(1)$
- The effective machinery also applies if there are no Goldstone bosons present in the low-energy spectrum

Effective Lagrangian for free fermions

$$\mathcal{L}_2^{free} = \sum_{\substack{f=\alpha,\beta \\ X=A,B}} \Big[\psi^{X,f\dagger}\partial_t\psi^{X,f} + v_F(\sigma_X\psi^{X,f\dagger}\partial_1\psi^{X',f} + i\sigma_f\psi^{X,f\dagger}\partial_2\psi^{X',f}) \Big],$$

$$\sigma_X = \begin{cases} 1 & X = A \\ -1 & X = B \end{cases}, \quad \text{and} \quad \sigma_f = \begin{cases} 1 & f = \alpha \\ -1 & f = \beta \end{cases}.$$

X': Other sublattice than X $\qquad v_F$: Fermion velocity

- Strength of systematic effective field theory approach: Free, massless, relativistic Dirac fermions as an immediate consequence of a systematic symmetry analysis

Comparison with Dirac Lagrangian in (2+1)-dimensions

Combining the fermion fields to the spinors

$$\Psi^{\alpha}(x) = \begin{pmatrix} \psi^{A,\alpha}(x) \\ \psi^{B,\alpha}(x) \end{pmatrix}, \qquad \Psi^{\beta}(x) = \begin{pmatrix} \psi^{A,\beta}(x) \\ \psi^{B,\beta}(x) \end{pmatrix},$$

one shows that the effective Lagrangian for free fermions is equivalent to

$$\mathcal{L}_2^{free} = v_F \left(\bar{\Psi}^{\alpha} \gamma_{\mu} \partial_{\mu} \Psi^{\alpha} + \bar{\Psi}^{\beta} \gamma_{\mu} \partial_{\mu} \Psi^{\beta} \right),$$

which represents the Dirac Lagrangian in $(2+1)$-dimensions for a free and massless particle with Euclidean metric

Nonlinear Realization of $SU(2)_s$ on the fermions

$$u(x)' = h(x)u(x)g^{\dagger} \quad C_x' = gC_x$$

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$$\Psi^X(x)' = h(x)u(x)C_x = h(x)\Psi^X(x)$$

$$\Psi^X(x) = \begin{pmatrix} \psi_+^X(x) & \psi_-^{X\dagger}(x) \\ \psi_-^X(x) & -\psi_+^{X\dagger}(x) \end{pmatrix}, \quad x \in \textit{even sublattice}$$

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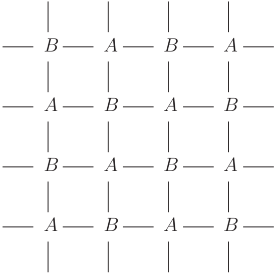
The global spin rotation symmetry is also realized locally on the fermions.

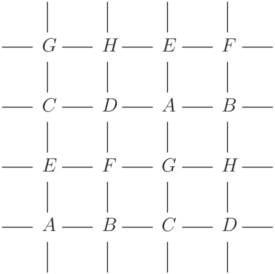
Sublattice Structure 1



$$k = (k1, k2) \in \left\{(0,0); \left(\frac{\pi}{a}, \frac{\pi}{a}\right)\right\}$$

Sublattice Structure 2

$$k = (k_1, k_2) \in \left\{ (0,0)\,, \left(\frac{pi}{a}, \frac{\pi}{a}\right)\,, \left(\frac{\pi}{a}, 0\right)\,, \left(0, \frac{\pi}{a}\right)\,, \left(\pm\frac{\pi}{2a}, \pm\frac{\pi}{2a}\right) \right\}$$



From Charge Carriers to Grassmann numbers

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Hubbard model in manifestly $SU(2)_{\vec{Q}}$ invariant form (at half filling)

$$\mathcal{H} = -\frac{t}{2} \sum_{x,i} \text{Tr}[C_x^\dagger C_{x+\hat{i}} + C_{x+\hat{i}}^\dagger C_x] + \frac{U}{12} \sum_x \text{Tr}[C_x^\dagger C_x C_x^\dagger C_x].$$

$$C_x = \begin{pmatrix} c_{x\uparrow} & (-1)^x c_{x\downarrow}^\dagger \\ c_{x\downarrow} & -(-1)^x c_{x\uparrow}^\dagger \end{pmatrix}$$

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$$\Psi^X(x) = u(x) C_x \quad X := sublatticeindex$$

Solution for $\vec{e}(x)$ for constant background fields

$$\vec{e}(x) = \left(sin\theta(x) cos\varphi(x), \sin\theta(x) sin\varphi(x), \cos\theta(x)\right)$$

$$\cos\theta(x) = \frac{1}{\sqrt{1+\left(\frac{c_i}{c_i^3}\right)^2}} \left[\cos\eta + \frac{c_i}{c_i^3}\sin\eta\cos\left(2\sqrt{1+\left(\frac{c_i}{c_i^3}\right)^2} c_i^3 x_i\right)\right].$$

$$\varphi(x) = \mathrm{atan}\left(\frac{\frac{c_i}{c_i^3}\sin\left(2\sqrt{1+\left(\frac{c_i}{c_i^3}\right)^2} c_i^3 x_i\right)}{\sin\eta - \frac{c_i}{c_i^3}\cos\eta\cos\left(2\sqrt{1+\left(\frac{c_i}{c_i^3}\right)^2} c_i^3 x_i\right)}\right).$$

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Four possible states at each lattice site: $|0\rangle, \quad |\uparrow\rangle, \quad |\downarrow\rangle, \quad |\uparrow\downarrow\rangle$

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How does the ground state order?

- By hopping system can lower its energy
- Hopping only possible for antiparallel spins

$\Longrightarrow$ Antiferromagnetic spin alignment is favored!

Relating microscopic operators to effective fields I

With the matrix-valued operator

$$C_x = \begin{pmatrix} c_{x\uparrow} & (-1)^x \ c^\dagger_{x\downarrow} \\ c_{x\downarrow} & -(-1)^x c^\dagger_{x\uparrow} \end{pmatrix}$$

the Hubbard Hamiltonian can be written

$$H = -\frac{t}{2} \sum_{x,i} \mathrm{Tr}[C^\dagger_x C_{x+\hat{i}} + C^\dagger_{x+\hat{i}} C_x] + \frac{U}{12} \sum_x \mathrm{Tr}[C^\dagger_x C_x C^\dagger_x C_x] - \frac{\mu}{2} \sum_x \mathrm{Tr}[C^\dagger_x C_x \sigma_3]$$

Relating microscopic operators to effective fields II

- Defining new lattice operators with the help of the diagonalizing matrix $u(x)$:

$$\Psi_x^{A,B,\ldots,H} = u(x) C_x, \qquad x \in A, B, \ldots, H$$

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$$\Psi_x^{A,B,\dots,H} \quad \longrightarrow \quad \Psi^{A,B,\dots,H}(x)$$

- Postulate: Transformation properties are inherited!

Accidental Galilean boost invariance

$$G: \quad {}^G P(x) = P(Gx), \qquad Gx = (\vec{x} - \vec{v}\ t, t),$$
$$ {}^G\psi^f_\pm(x) = \exp\left(\vec{p}^f \cdot \vec{x} - \omega^f t\right) \psi^f_\pm(Gx),$$
$$ {}^G\psi^{f\dagger}_\pm(x) = \psi^{f\dagger}_\pm(Gx) \exp\left(-\vec{p}^f \cdot \vec{x} + \omega^f t\right),$$

with $\vec{p}^f = (p^f_1, p^f_2)$ and ω^f given by

$$p^f_1 = \frac{M'}{1-(M'/M'')^2}\left[v_1 - \sigma_f \frac{M'}{M''} v_2\right],$$
$$p^f_2 = \frac{M'}{1-(M'/M'')^2}\left[v_2 - \sigma_f \frac{M'}{M''} v_1\right],$$
$$\omega^f = \frac{{p^f_i}^2}{2M'} + \sigma_f \frac{p^f_1 p^f_2}{M''} = \frac{M'}{1-(M'/M'')^2}\left[\frac{1}{2}(v_1^2 + v_2^2) - \sigma_f \frac{M'}{M''} v_1 v_2\right]$$

Transformation behavior of electron fields

$$
\begin{aligned}
SU(2)_s : &\quad \psi_\pm(x)' = \exp(\pm i\alpha(x))\psi_\pm(x) \\
U(1)_Q : &\quad {}^Q\psi_\pm(x) = \exp(i\omega)\psi_\pm(x) \\
D_i : &\quad {}^{D_i}\psi_\pm(x) = \mp\exp(ik_i a)\exp(\mp i\varphi(x))\psi_\mp(x) \\
O : &\quad {}^O\psi_\pm(x) = \pm\psi_\pm(Ox) \\
R : &\quad {}^R\psi_\pm(x) = \psi_\pm(Rx) \\
T : &\quad {}^T\psi_\pm(x) = \exp(\mp i\varphi(Tx))\psi^\dagger_\pm(Tx) \\
&\quad {}^T\psi^\dagger_\pm(x) = -\exp(\pm i\varphi(Tx))\psi_\pm(Tx)
\end{aligned}
$$