

# Two-Particle Bound States in an Antiferromagnet from a Low-Energy Effective Field Theory

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September 25, 2007

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Work done in collaboration with C. Brügger, C.P. Hofmann,  
M. Pepe, and U.-J. Wiese.

# Outline

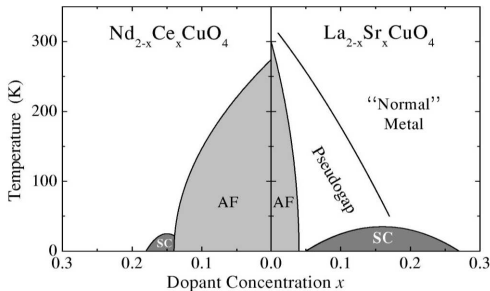
- 1 Low-energy effective field theory
  - Introduction
  - Construction of effective theory
- 2 Bound states
  - Holes
  - Electrons
- 3 Conclusions

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# Introduction

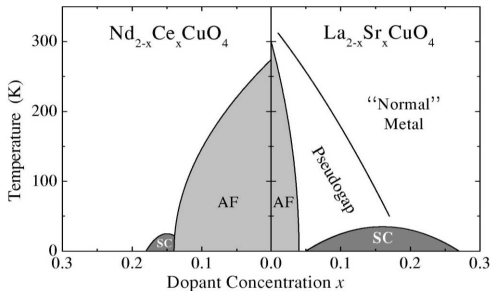
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Damascelli,  
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Rev. Mod. Phys.  
75 (2003) 473

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We primarily concentrate on the AF phase because:

- here it is possible to construct a systematic low-energy effective field theory
- Aim: systematically examine long-range forces between doped fermions

# Systematic effective field theories

Well-established example of systematic low-energy effective field theory based on symmetry considerations is:

- Chiral perturbation theory for QCD: pions  
⇒ Analogous to magnon perturbation theory

Chakravarty, Halperin, and Nelson, PRB 39 (1989) 2344

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Chakravarty, Halperin, and Nelson, PRB 39 (1989) 2344

Systematic low-energy effective theory taking into account that QCD spectrum contains massive baryons:

- Baryon chiral perturbation theory: pions + baryons  
⇒ Analog of effective theory for magnons + fermions

## Pure magnon sector: Magnon perturbation theory

General agreement:  $O(3)$ -invariant nonlinear  $\sigma$  model accurately describes low-energy magnon dynamics

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

- 2 Goldstone bosons (magnons) described by

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

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

- Low-energy magnon physics described by

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

$\rho_s$ : spin stiffness       $c$ : spin wave velocity

Chakravarty, Halperin, and Nelson, PRB 39 (1989) 2344

## State of affairs: Fermionic sector

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

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- In order to contain the correct physics, the effective theory must share the symmetries of the underlying system
- Resulting Lagrangians must contain a **complete** set of terms at each order in the derivative expansion

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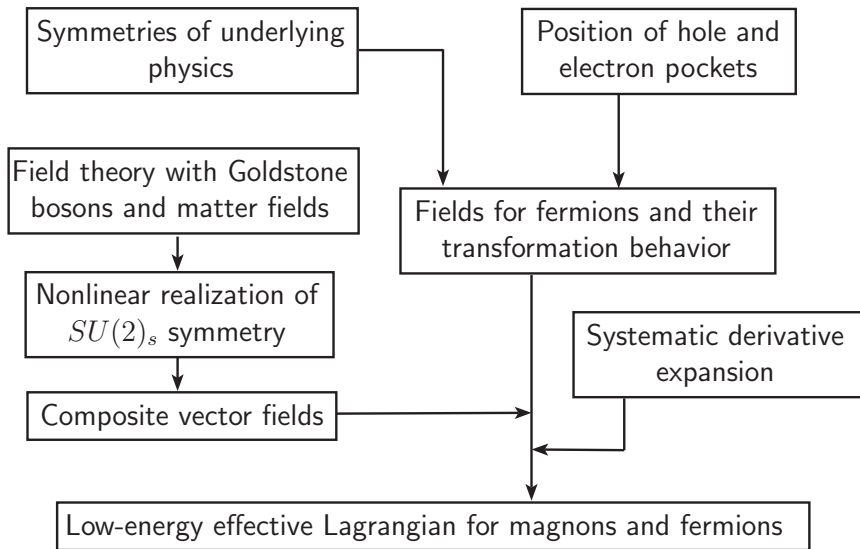
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We construct systematic low-energy effective theory based on symmetry considerations

# Symmetry-based construction of effective theory



# Symmetries

Symmetries of the underlying model (Hubbard model):

$SU(2)_S$  : Global spin rotation

$SU(2)_Q$  : Non-Abelian fermion number (pseudo spin)

$D_i$  : Displacement

$O$  : 90 degrees rotation

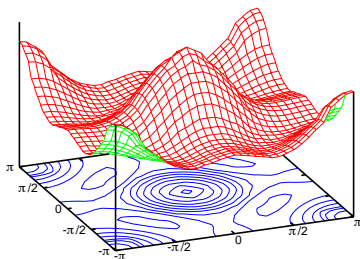
$R$  : Reflection about a lattice axis

$T$  : Time reversal

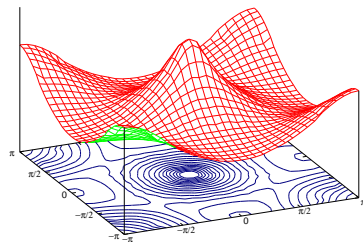
# Fields for holes and electrons

## Single particle dispersion relations

Holes:



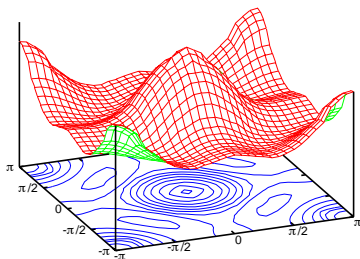
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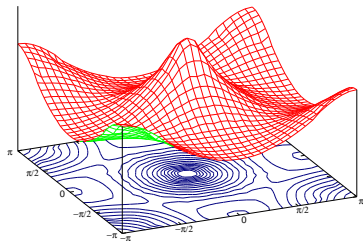
# Fields for holes and electrons

## Single particle dispersion relations

Holes:



Electrons:



$$\psi_{\pm}^{\alpha}(x) \quad \psi_{\pm}^{\beta}(x) \quad \psi_{\pm}^{\alpha\dagger}(x) \quad \psi_{\pm}^{\beta\dagger}(x)$$

$$\psi_{\pm}(x) \quad \psi_{\pm}^{\dagger}(x)$$

Index  $\pm$ : spin relative to local staggered magnetization  $\vec{e}(x)$

# Nonlinear realization of the $SU(2)_s$ symmetry

We expand in the magnon fluctuations  $m_1(x)$ ,  $m_2(x)$  around the ordered staggered magnetization  $\vec{e} = (0, 0, 1)$

$$\vec{e}(x) = \left( \frac{m_1(x)}{\sqrt{\rho_s}}, \frac{m_2(x)}{\sqrt{\rho_s}}, \sqrt{1 - \frac{m_1(x)^2}{\rho_s} - \frac{m_2(x)^2}{\rho_s}} \right)$$

Using the infinitesimal parameters  $m_1(x)$  and  $m_2(x)$  to define

$$v_\mu^\pm(x) = \frac{1}{2\sqrt{\rho_s}} \partial_\mu [m_2(x) \pm im_1(x)] + \mathcal{O}(m^3)$$

$$v_\mu^3(x) = \frac{1}{4\rho_s} [m_1(x) \partial_\mu m_2(x) - m_2(x) \partial_\mu m_1(x)] + \mathcal{O}(m^4)$$

## Transformation behavior of hole fields

$$SU(2)_s : \quad \psi_{\pm}^f(x)' = \exp(\pm i\alpha(x))\psi_{\pm}^f(x)$$

$$U(1)_Q : \quad Q\psi_{\pm}^f(x) = \exp(i\omega)\psi_{\pm}^f(x)$$

$$D_i : \quad D_i\psi_{\pm}^f(x) = \mp \exp(ik_i^f a) \exp(\mp i\varphi(x))\psi_{\mp}^f(x)$$

$$O : \quad O\psi_{\pm}^{\alpha}(x) = \mp \psi_{\pm}^{\beta}(Ox) \quad O\psi_{\pm}^{\beta}(x) = \psi_{\pm}^{\alpha}(Ox)$$

$$R : \quad R\psi_{\pm}^{\alpha}(x) = \psi_{\pm}^{\beta}(Rx) \quad R\psi_{\pm}^{\beta}(x) = \psi_{\pm}^{\alpha}(Rx)$$

$$T : \quad T\psi_{\pm}^f(x) = \mp \exp(\mp i\varphi(Tx))\psi_{\pm}^{f\dagger}(Tx)$$

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# Effective Lagrangian for magnons and holes

Lagrangian to leading order:

$$\begin{aligned}
 \mathcal{L} = & \rho_s (\partial_i \vec{e} \cdot \partial_i \vec{e} + \frac{1}{c^2} \partial_t \vec{e} \cdot \partial_t \vec{e}) \\
 & + \sum_{\substack{f=\alpha,\beta \\ s=+,-}} \left[ M \psi_s^{f\dagger} \psi_s^f + \psi_s^{f\dagger} D_t \psi_s^f \right. \\
 & + \frac{1}{2M'} D_i \psi_s^{f\dagger} D_i \psi_s^f + \sigma_f \frac{1}{2M''} (D_1 \psi_s^{f\dagger} D_2 \psi_s^f + D_2 \psi_s^{f\dagger} D_1 \psi_s^f) \\
 & + \Lambda (\psi_s^{f\dagger} v_1^s \psi_{-s}^f + \sigma_f \psi_s^{f\dagger} v_2^s \psi_{-s}^f) \\
 & \left. + N_1 \psi_s^{f\dagger} v_i^s v_i^{-s} \psi_s^f + \sigma_f N_2 (\psi_s^{f\dagger} v_1^s v_2^{-s} \psi_s^f + \psi_s^{f\dagger} v_2^s v_1^{-s} \psi_s^f) \right]
 \end{aligned}$$

with

$$\begin{aligned}
 D_\mu \psi_\pm^f(x) &= [\partial_\mu \pm i v_\mu^3(x)] \psi_\pm^f(x) \\
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Let us have a look at the Lagrangian for holes:

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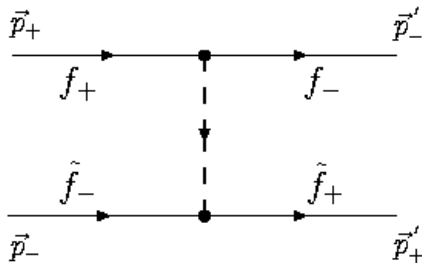
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- Holes flip spin by emitting/absorbing a single magnon
- The two holes must have antiparallel spins:  $+$  and  $-$

# Feynman diagram for one-magnon exchange



$\vec{p}_\pm$ : momenta of incoming holes

$\vec{p}'_\pm$ : momenta of outgoing holes

# One-magnon exchange potentials in coordinate space

Evaluating the corresponding Feynman diagrams, integrating out the magnons, and transforming to coordinate space...

The potentials are given by:

$$V^{\alpha\alpha}(\vec{r}) = \gamma \frac{\sin(2\varphi)}{r^2} \quad V^{\beta\beta}(\vec{r}) = -\gamma \frac{\sin(2\varphi)}{r^2}$$
$$V^{\alpha\beta}(\vec{r}) = V^{\beta\alpha}(\vec{r}) = \gamma \frac{\cos(2\varphi)}{r^2}$$

$\vec{r} = \vec{r}_+ - \vec{r}_-$ : Distance vector between holes

$\varphi$ : Angle between  $\vec{r}$  and  $x$ -axis

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

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- The resulting Schrödinger equation:

$$\begin{pmatrix} -\frac{1}{M'} \Delta & V^{\alpha\beta}(\vec{r}) \\ V^{\alpha\beta}(\vec{r}) & -\frac{1}{M'} \Delta \end{pmatrix} \begin{pmatrix} \Psi_1(\vec{r}) \\ \Psi_2(\vec{r}) \end{pmatrix} = E \begin{pmatrix} \Psi_1(\vec{r}) \\ \Psi_2(\vec{r}) \end{pmatrix}$$

$\Psi_1(\vec{r})$ : Prob' amplitude for flavor-spin combination  $\alpha_+ \beta_-$

$\Psi_2(\vec{r})$ : Prob' amplitude for flavor-spin combination  $\alpha_- \beta_+$

# Solving the Schrödinger equation I

- Making a separation ansatz:

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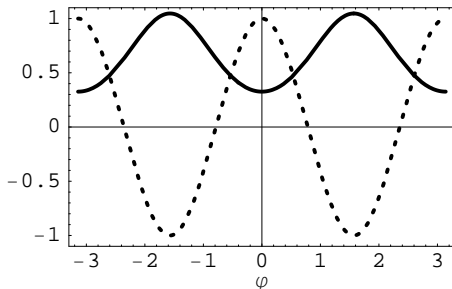
$$-\frac{d^2\chi_{\pm}(\varphi)}{d\varphi^2} \pm M'\gamma \cos(2\varphi)\chi_{\pm}(\varphi) = -\lambda\chi_{\pm}(\varphi)$$

- Solution with the lowest eigenvalue  $-\lambda$  is:

$$\chi_{\pm}(\varphi) = \frac{1}{\sqrt{\pi}} \text{ce}_0(\varphi \pm \frac{1}{2}M'\gamma) \quad \lambda = \frac{1}{8}(M'\gamma)^2 + \mathcal{O}(\gamma^4)$$

# Solving the Schrödinger equation II

As an illustration:



Dotted curve:  $\cos(2\varphi)$

Solid curve:  $ce_0(\varphi, \frac{1}{2}M'\gamma)$

# Solving the Schrödinger equation III

- The radial Schrödinger equation takes the form

$$-\left[\frac{d^2R(r)}{dr^2} + \frac{1}{r}\frac{dR(r)}{dr}\right] - \frac{\lambda}{r^2}R(r) = M'ER(r)$$

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- Energy determined from:  $K_\nu(\sqrt{M'|E_n|}r_0) = 0$

## Some things to note

- The energy spectrum for large  $n$

$$E_n \sim -\frac{1}{M' r_0^2} \exp(-2\pi n / \sqrt{\lambda})$$

⇒ Binding energy is exponentially small

⇒ Infinite number of bound states

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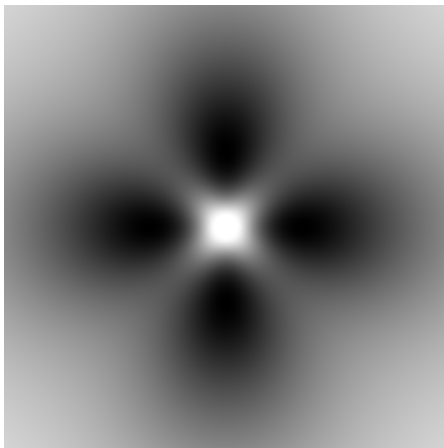
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- Note:  $\chi_+(\varphi)$  and  $\chi_-(\varphi)$  have the same eigenvalue  $-\lambda$
- We build an eigenstate of the rotation  $O$

$$\Psi_{\pm}(\vec{r}) = R(r) \begin{pmatrix} \chi_+(\varphi) \mp i\chi_-(\varphi) \\ \chi_+(\varphi) \pm i\chi_-(\varphi) \end{pmatrix}$$

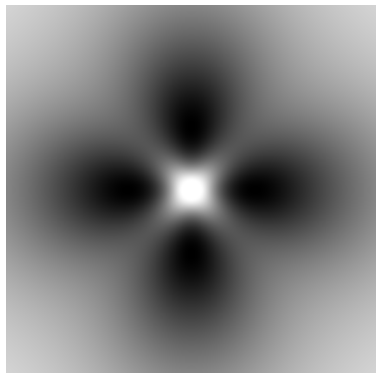
## Probability distribution for the ground state: $\alpha\beta$

Ground state probability distribution for a bound pair of two holes with different flavors:



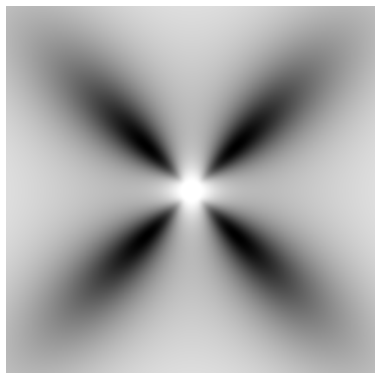
# Probability distribution for the ground state

$\alpha\beta$



resembles  $d_{x^2-y^2}$  symmetry

$\alpha\alpha, \beta\beta$



resembles  $d_{xy}$  symmetry

Kuchiev and Sushkov  
Physica C218 (1993) 197

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Let us have a look at the Lagrangian:

$$\mathcal{L} = \sum_{s=+,-} \left[ \cdots + iK (D_1 \psi_s^{\dagger} v_1^s \psi_{-s} - \psi_s^{\dagger} v_1^s D_1 \psi_{-s} \right. \\ \left. - D_2 \psi_s^{\dagger} v_2^s \psi_{-s} + \psi_s^{\dagger} v_2^s D_2 \psi_{-s}) + \cdots \right]$$

# One-magnon exchange potential between electrons I

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One-magnon exchange between electrons is weaker than between holes: **Additional derivatives!**

# One-magnon exchange potentials in coordinate space

Evaluating the corresponding Feynman diagram, integrating out the magnons, and transforming to coordinate space...

The potential is given by:

$$V(\vec{r}, \vec{P}) = \frac{K^2}{2\pi\rho_s} \left[ 12 \frac{\cos(4\varphi)}{r^4} + \frac{P^2}{2} \frac{\cos(2(\varphi + \chi))}{r^2} \right]$$

$\vec{r} = \vec{r}_+ - \vec{r}_-$ : Distance vector between electrons

$\vec{P}$ : Total momentum of pair

$\varphi$ : Angle between  $\vec{r}$  and  $x$ -axis

$\chi$ : Angle between  $\vec{P}$  and  $x$ -axis

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Note:

- The potential depends on the total momentum  $\vec{P}$ !
- The potential falls off as  $1/r^4$

# Schrödinger equation for two electrons

- Problem is not Galilean invariant
- Distance vector  $\vec{r}$  changes its direction

# Schrödinger equation for two electrons

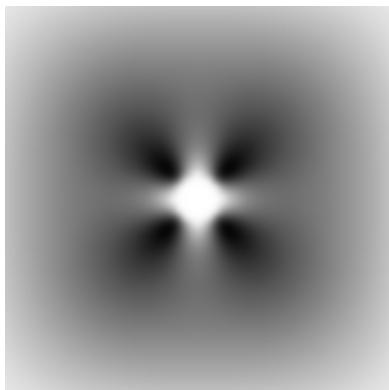
- Problem is not Galilean invariant
- Distance vector  $\vec{r}$  changes its direction
- The resulting Schrödinger equation:

$$\begin{aligned} -\frac{1}{M'} \Delta \Psi(\vec{r}) + \frac{K^2}{2\pi\rho_s} \left[ 12 \frac{\cos(4\varphi)}{r^4} + \frac{P^2}{2} \frac{\cos(2(\varphi + \chi))}{r^2} \right] \Psi(-\vec{r}) \\ = \left[ E - \frac{P^2}{2M'} \right] \Psi(\vec{r}) \end{aligned}$$

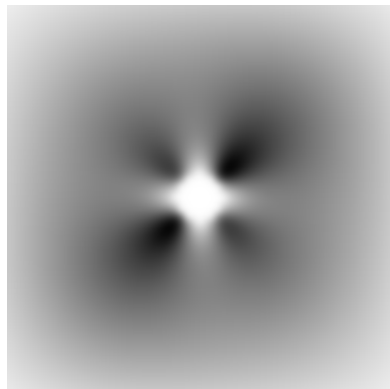
⇒ Solve numerically!

# Probability distributions for the ground state

Ground state probability distributions for a bound pair of electrons:



$$\vec{P} = 0$$



$$\vec{P} = \frac{1}{\sqrt{2}}(P, P)$$

# Outline

- 1 Low-energy effective field theory
  - Introduction
  - Construction of effective theory
- 2 Bound states
  - Holes
  - Electrons
- 3 Conclusions

# Conclusions

- We have constructed a systematic low-energy effective field theory for lightly doped cuprates
- Using the effective theory we have analytically derived the one-magnon exchange potentials between two holes or electrons
- We have shown that in both cases bound states exist and we have gained insight into the nature of the ground state wave functions
- The presented low-energy effective theory is a powerful tool for the investigation of various phenomena in lightly doped antiferromagnets
- **The low-energy effective theory has the advantage of being model independent**  $\implies$  it describes all models which share the symmetries of the Hubbard model

## Recent work done in our collaboration: References

- *Two-hole bound states from a systematic low-energy effective theory for magnons and holes in an antiferromagnet: PRB 74 (2006) 224432*
- *Systematic low-energy effective field theory for electron-doped antiferromagnets: PRB 75 (2007) 214405*
- *Homogeneous versus spiral phases of hole-doped antiferromagnets: A systematic effective field theory investigation: PRB 75 (2007) 014421*

## Nonlinear realization of $SU(2)_s$ symmetry

Write  $CP(1)$  representation of magnon field

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

Diagonalize the magnon field

$$u(x)P(x)u(x)^\dagger = \frac{1}{2}(\mathbb{1} + \sigma_3) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$u(x) \in SU(2)_s \quad u_{11}(x) \geq 0$$

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Under global  $SU(2)_s$  spin transformations

$$P(x)' = gP(x)g^\dagger \quad g \in SU(2)_s$$

$$u(x)' = h(x)u(x)g^\dagger \quad h(x) \in U(1)_s \quad u_{11}(x)' \geq 0$$

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

## Gauge and vector fields

We introduce an anti-Hermitian field

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

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

$$v_\mu^3(x)' = v_\mu^3(x) - \partial_\mu \alpha(x) \quad v_\mu^\pm(x)' = v_\mu^\pm(x) \exp(\pm 2i\alpha(x))$$

$v_\mu^3(x)$ : Gauge field-like

$v_\mu^\pm(x)$ : Vector field-like

## Relating microscopic operators to effective fields I

With the matrix-valued operator

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

the Hubbard Hamiltonian can be written

$$H = -\frac{t}{2} \sum_{x,i} \text{Tr}[C_x^\dagger C_{x+i} + C_{x+i}^\dagger C_x] + \frac{U}{12} \sum_x \text{Tr}[C_x^\dagger C_x C_x^\dagger C_x] \\ - \frac{\mu}{2} \sum_x \text{Tr}[C_x^\dagger C_x \sigma_3]$$

## Relating microscopic operators to effective fields II

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

$$\psi_x^{A,B,\dots,H} = u(x)C_x, \quad x \in A, B, \dots, H$$

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- Postulate: Transformation properties are inherited!