Quantum Mechanics of Interacting Magnetic Moments



Definitions

- Heitler–London Calculation for Ferromagnetism
- Heisenberg Model of Ferromagnets
- Néel State
- Indirect Exchange
- Spin Waves
- Schwinger Bosons
- Holstein–Primakoff Transformation
- Stoner Model
- Anderson Model
- Kondo Effect and Scaling Theory
- The Hubbard Model

$$\vec{B} = \vec{\nabla} \left[\vec{m}_1 \cdot \vec{\nabla} \frac{1}{r} \right] = \frac{3\hat{r}(\vec{m}_1 \cdot \hat{r}) - \vec{m}_1}{r^3}, \qquad (L1)$$
$$\frac{\vec{m}_1 \cdot \vec{m}_2 - 3(\vec{m}_2 \cdot \hat{r}_{12})(\vec{m}_1 \cdot \hat{r}_{12})}{(\vec{m}_1 \cdot \hat{r}_{12})} \qquad (L2)$$

$$\frac{\dot{m}_1 \cdot \dot{m}_2 - 3(\dot{m}_2 \cdot r_{12})(\dot{m}_1 \cdot r_{12})}{r_{12}^3},\tag{L2}$$

$$\frac{1}{4}\frac{m_1}{\mu_B}\frac{m_2}{\mu_B}\left(\frac{2a_0}{r_{12}}\right)^3\frac{\mu_B^2}{a_0^3} = 0.9\cdot 10^{-4}\,\mathrm{eV}\cdot\frac{m_1}{\mu_B}\frac{m_2}{\mu_B}\left(\frac{2a_0}{r_{12}}\right)^3.$$
 (L3)



Figure 1: Setting for the calculation of Heitler and London (1927).

$$l \equiv \left\| \int d\vec{r} \,\phi_1^*(\vec{r}) \phi_2(\vec{r}) \right\| \tag{L4}$$

Singlet:

$$\frac{1}{\sqrt{2}} \left(\chi_{\uparrow}(\sigma_1) \chi_{\downarrow}(\sigma_2) - \chi_{\downarrow}(\sigma_1) \chi_{\uparrow}(\sigma_2) \right), \tag{L5a}$$

Heitler–London Calculation

Triplet:

$$\chi_{\uparrow}(\sigma_{1})\chi_{\uparrow}(\sigma_{2}) \qquad S = 1 \quad ; S_{z} = 1$$

$$\frac{1}{\sqrt{2}} \left(\chi_{\uparrow}(\sigma_{1})\chi_{\downarrow}(\sigma_{2}) + \chi_{\downarrow}(\sigma_{1})\chi_{\uparrow}(\sigma_{2})\right) \qquad S = 1 \quad ; S_{z} = 0 \qquad (L6a)$$

$$\chi_{\downarrow}(\sigma_{1})\chi_{\downarrow}(\sigma_{2}) \qquad S = 1 \quad ; S_{z} = -1.$$

$$\phi_s(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2+2l^2}} [\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) + \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)], \quad (L7a)$$

$$\phi_t(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2 - 2l^2}} [\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) - \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)].$$
(L7b)

$$\left[\frac{\hat{P}_1^2}{2m} - \frac{e^2}{|\vec{r}_1 - \vec{R}_1|}\right] \phi_1(\vec{r}_1) = \mathcal{E}_0 \phi_1(\vec{r}_1).$$
(L8)

Heitler–London Calculation

$$\hat{\mathcal{H}} = \frac{\hat{P}_{1}^{2}}{2m} - \frac{e^{2}}{|\vec{r}_{1} - \vec{R}_{1}|} + \frac{\hat{P}_{2}^{2}}{2m} - \frac{e^{2}}{|\vec{r}_{2} - \vec{R}_{2}|} + \frac{e^{2}}{|\vec{r}_{1} - \vec{r}_{2}|} + \frac{e^{2}}{|\vec{R}_{1} - \vec{R}_{2}|} - \frac{e^{2}}{|\vec{r}_{1} - \vec{R}_{2}|} - \frac{e^{2}}{|\vec{r}_{2} - \vec{R}_{1}|}.$$
(L9)

$$\int d\vec{r}_{1} d\vec{r}_{2} \phi_{1}^{*}(\vec{r}_{1}) \phi_{2}^{*}(\vec{r}_{2}) \hat{\mathcal{H}} \phi_{1}(\vec{r}_{1}) \phi_{2}(\vec{r}_{2})$$

$$= \int d\vec{r}_{1} d\vec{r}_{2} \phi_{2}^{*}(\vec{r}_{1}) \phi_{1}^{*}(\vec{r}_{2}) \hat{\mathcal{H}} \phi_{2}(\vec{r}_{1}) \phi_{1}(\vec{r}_{2}) \qquad (L10)$$

$$= 2\mathcal{E}_{0} + U, \qquad (L11)$$

where

$$U = \int d\vec{r}_1 d\vec{r}_2 \begin{bmatrix} |\phi_1(\vec{r}_1)|^2 \\ |\phi_2(\vec{r}_2)|^2 \end{bmatrix} \begin{bmatrix} \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} + \frac{e^2}{|\vec{R}_1 - \vec{R}_2|} - \frac{e^2}{|\vec{r}_1 - \vec{R}_2|} - \frac{e^2}{|\vec{r}_2 - \vec{R}_1|} \end{bmatrix},$$

(L12)

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and

Heitler–London Calculation

$$\int d\vec{r}_{1} d\vec{r}_{2} \phi_{2}^{*}(\vec{r}_{1}) \phi_{1}^{*}(\vec{r}_{2}) \hat{\mathcal{H}} \phi_{1}(\vec{r}_{1}) \phi_{2}(\vec{r}_{2})$$

$$= \int d\vec{r}_{1} d\vec{r}_{2} \phi_{1}^{*}(\vec{r}_{1}) \phi_{2}^{*}(\vec{r}_{2}) \hat{\mathcal{H}} \phi_{2}(\vec{r}_{1}) \phi_{1}(\vec{r}_{2}) \qquad (L13)$$

$$= 2\mathcal{E}_{0}l^{2} + V, \qquad (L14)$$

with

$$V = \int d\vec{r}_1 d\vec{r}_2 \begin{bmatrix} \phi_1^*(\vec{r}_1)\phi_2^*(\vec{r}_2) \\ \phi_2(\vec{r}_1)\phi_1(\vec{r}_2) \end{bmatrix} \begin{bmatrix} \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} + \frac{e^2}{|\vec{R}_1 - \vec{R}_2|} - \frac{e^2}{|\vec{r}_1 - \vec{R}_1|} - \frac{e^2}{|\vec{r}_2 - \vec{R}_2|} \end{bmatrix}.$$
(L15)

$$\mathcal{E}_{s} = \langle \phi_{s} | \hat{\mathcal{H}} | \phi_{s} \rangle = 2 \frac{2\mathcal{E}_{0} + U + 2l^{2}\mathcal{E}_{0} + V}{2 + 2l^{2}} = 2\mathcal{E}_{0} + \frac{U + V}{1 + l^{2}}$$
(L16a)

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and

$$\mathcal{E}_{t} = \langle \phi_{t} | \hat{\mathcal{H}} | \phi_{t} \rangle = 2 \frac{2\mathcal{E}_{0} + U - 2l^{2}\mathcal{E}_{0} - V}{2 - 2l^{2}} = 2\mathcal{E}_{0} + \frac{U - V}{1 - l^{2}}$$
(L16b)

$$\mathcal{E}_t - \mathcal{E}_s = \frac{2l^2 U - 2V}{1 - l^4} \equiv -J.$$
 (L17)

Lieb-Mattis Theorem

$$\mathcal{F}\{\phi\} = \frac{\int d\vec{r}_1 d\vec{r}_2 \frac{\hbar^2}{2m} |\nabla_1 \phi|^2 + \frac{\hbar^2}{2m} |\nabla_2 \phi|^2 + U(\vec{r}_1, \vec{r}_2) |\phi(\vec{r}_1, \vec{r}_2)|^2}{\int d\vec{r}_1 d\vec{r}_2 |\phi(\vec{r}_1, \vec{r}_2)|^2}.$$
 (L18)

Figure 2: The energy of a wave function with a cusp is always lowered by smoothing out the cusp.

$$\hat{\mathcal{H}} = a + b\hat{S}_1 \cdot \hat{S}_2 \qquad (L19)$$

= $a + b\left(\hat{S}_1^z \hat{S}_2^z + \frac{1}{2}[\hat{S}_1^+ \hat{S}_2^- + \hat{S}_2^+ \hat{S}_1^-]\right). \qquad (L20)$

$$\hat{\mathcal{H}} = 2\mathcal{E}_0 + \frac{U - V}{1 - l^2} + \left(\frac{1}{4} - \hat{S}_1 \cdot \hat{S}_2\right) J.$$
(L21)

Heisenberg Model

$$\hat{\mathcal{H}} = -\sum_{\langle ll' \rangle} J_{ll'} \hat{S}_l \cdot \hat{S}_{l'}.$$
 (L22)

$$\sum_{l=1}^{N} \frac{\hat{P}_l^2}{2m} + \hat{U} = \hat{\mathcal{H}}_{\text{kinetic}} + \hat{\mathcal{H}}_{\text{int}}, \qquad (L23)$$

$$\hat{\mathcal{H}}_{\text{int}} = \sum_{\substack{ll'l''l'''\\\sigma\sigma'}} \langle \vec{R}_l \vec{R}_{l'} | \hat{U} | \vec{R}_{l''} \vec{R}_{l'''} \rangle \hat{c}^{\dagger}_{l\sigma} \hat{c}^{\dagger}_{l'\sigma'} \hat{c}_{l''\sigma'} \hat{c}_{l''\sigma'} \hat{c}_{l''\sigma}.$$
(L24)

$$\hat{\mathcal{H}}_{\text{int}} = \sum_{\substack{ll'\\\sigma\sigma'}} \begin{pmatrix} \langle \vec{R}_l \vec{R}_{l'} | \hat{U} | \vec{R}_l \vec{R}_{l'} \rangle \hat{c}^{\dagger}_{l\sigma} \hat{c}^{\dagger}_{l'\sigma'} \hat{c}_{l'\sigma'} \hat{c}_{l\sigma} \\ \langle \vec{R}_l \vec{R}_{l'} | \hat{U} | \vec{R}_{l'} \vec{R}_l \rangle \hat{c}^{\dagger}_{l\sigma} \hat{c}^{\dagger}_{l'\sigma'} \hat{c}_{l\sigma'} \hat{c}_{l'\sigma} \\ = \sum_{\substack{ll'\\\sigma\sigma'}} \begin{pmatrix} \langle \vec{R}_l \vec{R}_{l'} | \hat{U} | \vec{R}_l \vec{R}_{l'} \rangle \hat{c}^{\dagger}_{l\sigma} \hat{c}^{\dagger}_{l'\sigma'} \hat{c}_{l'\sigma'} \hat{c}_{l\sigma} \\ \langle \vec{R}_l \vec{R}_{l'} | \hat{U} | \vec{R}_l \vec{R}_{l'} \rangle \hat{c}^{\dagger}_{l\sigma} \delta_{ll'} - \hat{c}^{\dagger}_{l\sigma} \hat{c}_{l\sigma'} \hat{c}_{l'\sigma'} \hat{c}_{l'\sigma} \\ \end{pmatrix} .$$
(L25)

Heisenberg Model

$$\hat{S}^{z} = \frac{1}{2} [\hat{c}^{\dagger}_{\uparrow} \hat{c}_{\uparrow} - \hat{c}^{\dagger}_{\downarrow} \hat{c}_{\downarrow}] = \frac{1}{2} [\hat{n}_{\uparrow} - \hat{n}_{\downarrow}]$$
(L27a)

$$\hat{S}^+ = \hat{c}^{\dagger}_{\uparrow} c_{\downarrow}; \quad \hat{S}^- = \hat{c}^{\dagger}_{\downarrow} c_{\uparrow}.$$
 (L27b)

$$\hat{n}_{l\uparrow}\hat{n}_{l'\uparrow} + \hat{n}_{l\downarrow}\hat{n}_{l'\downarrow} \tag{L28}$$

$$= \frac{1}{2} \left\{ (\hat{n}_{l\uparrow} + \hat{n}_{l\downarrow}) (\hat{n}_{l'\uparrow} + \hat{n}_{l'\downarrow}) + (\hat{n}_{l\uparrow} - \hat{n}_{l\downarrow}) (\hat{n}_{l'\uparrow} - \hat{n}_{l'\downarrow}) \right\}$$
(L29)

$$= \frac{1}{2} \left\{ 1 + 4\hat{S}_{l}^{z} \cdot \hat{S}_{l'}^{z} \right\}.$$
(L30)

$$\hat{\mathcal{H}}_{\text{exch}} = -\langle \vec{R}_{l}\vec{R}_{l'}|\hat{U}|\vec{R}_{l'}\vec{R}_{l}\rangle \begin{cases} \hat{n}_{l\uparrow}\hat{n}_{l'\uparrow} + \hat{c}_{l\uparrow}^{\dagger}\hat{c}_{l\downarrow}c_{l'\downarrow}^{\dagger}\hat{c}_{l'\uparrow} \\ + \hat{c}_{l\downarrow}^{\dagger}\hat{c}_{l\uparrow}c_{l'\downarrow}^{\dagger}\hat{c}_{l'\downarrow} + \hat{n}_{l\downarrow}\hat{n}_{l'\downarrow} \end{cases}$$

$$= -2\langle \vec{R}_{l}\vec{R}_{l'}|\hat{U}|\vec{R}_{l'}\vec{R}_{l}\rangle \left\{ \frac{1}{4} + \hat{S}_{l}^{z}\hat{S}_{l'}^{z} + \frac{1}{2}[\hat{S}_{l}^{+}\hat{S}_{l'}^{-} + \hat{S}_{l}^{-}\hat{S}_{l'}^{+}] \right\}$$
(L31)
(L32)

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Heisenberg Model

$$= -2\langle \vec{R}_{l}\vec{R}_{l'}|\hat{U}|\vec{R}_{l'}\vec{R}_{l}\rangle \left\{\frac{1}{4} + \hat{S}_{l}\cdot\hat{S}_{l'}\right\}, \qquad (L33)$$

$$-4\sum_{\langle ll'\rangle} \langle \vec{R}_l \vec{R}_{l'} | \hat{U} | \vec{R}_{l'} \vec{R}_l \rangle \hat{S}_l \cdot \hat{S}_{l'}$$
(L34)

Ground State

$$\langle \uparrow \uparrow \uparrow \dots | \hat{\mathcal{H}} | \uparrow \uparrow \uparrow \dots \rangle = -\sum_{\langle ll' \rangle} \frac{J_{ll'}}{4}.$$
 (L35)

$$\hat{S}^{\alpha} = \frac{1}{2} \sum_{ll'} a_l^{\dagger} \sigma_{ll'}^{\alpha} a_{l'}.$$
(L36)

$$\hat{S}^{z} = \frac{1}{2} \left(\hat{a}_{1}^{\dagger} \hat{a}_{1} - \hat{a}_{2}^{\dagger} \hat{a}_{2} \right)$$
 (L37a)

$$\hat{S}^{x} = \frac{1}{2} \left(\hat{a}_{1}^{\dagger} \hat{a}_{2} + \hat{a}_{2}^{\dagger} \hat{a}_{1} \right)$$
 (L37b)

$$\hat{S}^{y} = i \frac{1}{2} \left(\hat{a}_{2}^{\dagger} \hat{a}_{1} - \hat{a}_{1}^{\dagger} \hat{a}_{2} \right).$$
 (L37c)

$$\begin{bmatrix} \hat{S}^{x}, \hat{S}^{y} \end{bmatrix} = i\frac{1}{4} \begin{bmatrix} \hat{a}_{1}^{\dagger}\hat{a}_{2} + \hat{a}_{2}^{\dagger}\hat{a}_{1}, \hat{a}_{2}^{\dagger}\hat{a}_{1} - \hat{a}_{1}^{\dagger}\hat{a}_{2} \end{bmatrix}$$

= $i\hat{S}^{z}$. (L38)

$$\hat{S}^{+} = \hat{a}_{1}^{\dagger} \hat{a}_{2}; \ \hat{S}^{-} = \hat{a}_{2}^{\dagger} \hat{a}_{1}.$$
(L39)

$$\frac{1}{2}\left(\hat{a}_{1}^{\dagger}\hat{a}_{1}+\hat{a}_{2}^{\dagger}\hat{a}_{2}\right)=S.$$
 (L40)

$$\hat{a}_{2}^{\dagger}\hat{a}_{2} = 2S - \hat{a}_{1}^{\dagger}\hat{a}_{1} \tag{L41}$$

$$\hat{a}_2 = \sqrt{2S - \hat{a}_1^{\dagger} \hat{a}_1}.$$
 (L42)

$$\hat{S}^+ = a_1^\dagger \sqrt{2S - \hat{a}_1^\dagger \hat{a}_1} \tag{L43a}$$

$$\hat{S}^{-} = \sqrt{2S - \hat{a}_{1}^{\dagger} \hat{a}_{1} \hat{a}_{1}}$$
 (L43b)

$$\hat{S}^z = (\hat{a}_1^{\dagger} \hat{a}_1 - S).$$
 (L43c)

$$\hat{S}^+, \hat{S}^-] = 2\hat{S}^z.$$
 (L44)

$$\hat{S}_{l} \cdot \hat{S}_{l'} = \frac{1}{2} \left(\hat{S}_{l}^{+} \hat{S}_{l'}^{-} + \hat{S}_{l'}^{+} \hat{S}_{l}^{-} \right) + \hat{S}_{l}^{z} \hat{S}_{l'}^{z} \qquad (L45)$$

$$= \frac{1}{2} \hat{a}_{l}^{\dagger} \sqrt{2S - \hat{a}_{l}^{\dagger} \hat{a}_{l}} \sqrt{2S - \hat{a}_{l'}^{\dagger} \hat{a}_{l'}} \hat{a}_{l'} + \frac{1}{2} \hat{a}_{l'}^{\dagger} \sqrt{2S - \hat{a}_{l}^{\dagger} \hat{a}_{l'}} \sqrt{2S - \hat{a}_{l'}^{\dagger} \hat{a}_{l}} \hat{a}_{l} + (S - \hat{a}_{l}^{\dagger} \hat{a}_{l})(S - \hat{a}_{l'}^{\dagger} \hat{a}_{l'}).$$

$$(L46)$$

$$\hat{a}_l = \sqrt{S}b_l + \left(\hat{a}_l - \sqrt{S}b_l\right),\tag{L47}$$

$$\hat{\mathcal{H}} = -\sum_{ll'} J_{ll'} S^2 \begin{bmatrix} \frac{1}{2} \left(b_l b_{l'}^* + b_{l'} b_l^* \right) \sqrt{2 - |b_l|^2} \sqrt{2 - |b_{l'}|^2} \\ + \left(1 - |b_l|^2 \right) \left(1 - |b_{l'}|^2 \right) \end{bmatrix}.$$
(L48)

$$\mathcal{E}_0 = -JNzS^2 \left(|b|^2 (2 - |b|^2) + (1 - |b|^2)^2 \right) = -JNzS^2, \tag{L49}$$

$$\hat{\mathcal{H}} \approx -NJzS^2 - 2J\sum_{\langle ll'\rangle} S\left(\hat{a}_l^{\dagger}\hat{a}_{l'} + \hat{a}_{l'}^{\dagger}\hat{a}_l - \hat{a}_l^{\dagger}\hat{a}_l - \hat{a}_{l'}^{\dagger}\hat{a}_{l'}\right).$$
(L50)

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$$\hat{a}_l = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \hat{a}_k e^{-i\vec{k}\cdot\vec{r}_l} \tag{L52}$$

$$\hat{\mathcal{H}} = -NJzS^2 - 2JS\sum_{\vec{k}}\sum_{\vec{\delta}}\left[\cos\left(\vec{k}\cdot\vec{\delta}\right) - 1\right]\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{k}}$$
(L53)
$$= -NJzS^2 + \sum_{\vec{k}}\hbar\omega_{\vec{k}}\hat{n}_{\vec{k}},$$
(L54)

where

$$\hbar\omega = 2SJ \sum_{\vec{\delta}} \left(1 - \cos(\vec{\delta} \cdot \vec{k}) \right), \tag{L55}$$

Spin Waves in Antiferromagnets



Figure 3: The Néel state.

$$S_{l'}^{\pm} \to S_{l'}^{\mp} \quad S_{l'}^{z} \to -S_{l'}^{z}. \tag{L56}$$

Spin Waves in Antiferromagnets

$$\begin{aligned} \hat{\mathcal{H}} &= 2|J| \sum_{\langle ll' \rangle} \frac{1}{2} \left[\hat{S}_{l}^{+} \hat{S}_{l'}^{+} + \hat{S}_{l}^{-} \hat{S}_{l'}^{-} \right] - \hat{S}_{l}^{z} \hat{S}_{l'}^{z} \end{aligned} \tag{L57} \\ &= 2|J| \sum_{\langle ll' \rangle} \frac{\frac{1}{2} \hat{a}_{l}^{\dagger} \sqrt{2S - \hat{a}_{l}^{\dagger} \hat{a}_{l}} \hat{a}_{l'}^{\dagger} \sqrt{2S - \hat{a}_{l'}^{\dagger} \hat{a}_{l'}} \\ &+ \frac{1}{2} \sqrt{2S - \hat{a}_{l}^{\dagger} \hat{a}_{l}} \hat{a}_{l} \sqrt{2S - \hat{a}_{l'}^{\dagger} \hat{a}_{l'}} (L58) \end{aligned}$$

$$\hat{\mathcal{H}} \approx -Nz|J|S^2 \Big[(1-b^2)^2 - b^2 (2-b^2) \Big],$$
 (L59)

$$b = 0. \tag{L60}$$

$$\hat{\mathcal{H}} \approx 2|J| \sum_{\langle ll' \rangle} \left[-S^2 + S \left\{ \hat{a}_l^{\dagger} \hat{a}_l + \hat{a}_{l'}^{\dagger} \hat{a}_{l'} + \hat{a}_l^{\dagger} \hat{a}_{l'}^{\dagger} + \hat{a}_l \hat{a}_{l'} \right\} \right].$$
(L61)
$$\hat{a}_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{l} e^{i\vec{k}\cdot\vec{R}_l} \hat{a}_l$$
(L62)

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Spin Waves in Antiferromagnets

$$\hat{\mathcal{H}} = -|J|NzS^2 + |J|S\sum_{\vec{k}\vec{\delta}} \left[\left(\hat{a}^{\dagger}_{\vec{k}}\hat{a}^{\dagger}_{-\vec{k}} + \hat{a}_{\vec{k}}\hat{a}_{-\vec{k}} \right) \cos(\vec{k}\cdot\vec{\delta}) + 2\hat{a}^{\dagger}_{\vec{k}}\hat{a}_{\vec{k}} \right].$$
(L63)

$$\hat{a}_{\vec{k}} = \cosh \alpha_{\vec{k}} \,\hat{\gamma}_{\vec{k}} + \sinh \alpha_{\vec{k}} \,\hat{\gamma}_{-\vec{k}}^{\dagger}, \qquad (L64)$$

$$\tanh 2\alpha_{\vec{k}} = -\frac{1}{z} \sum_{\vec{\delta}} \cos(\vec{k} \cdot \vec{\delta}). \tag{L65}$$

$$\hat{\mathcal{H}} = -Nz|J|S(S+1) + 2|J|zS\sum_{\vec{k}} \left(\hat{\gamma}_{\vec{k}}^{\dagger}\hat{\gamma}_{\vec{k}} + \frac{1}{2}\right)\sqrt{1 - \tanh^2 2\alpha_{\vec{k}}}.$$
 (L66)

$$-NS^2|J|z\left(1+\frac{\Gamma}{zS}\right).\tag{L67}$$

$$\mathcal{E}_{\vec{k}} = 2|J|S\sqrt{z^2 - (\sum_{\vec{\delta}}\cos\vec{k}\cdot\vec{\delta})^2}.$$
 (L68)

Comparison with Experiment



Figure 4: (A) Dispersion relation for ferromagnetic magnons in iron. [Yethiraj et al. (1991), and Lynn (1975),.] (B) Dispersion relation for antiferromagnetic magnons in CuO. [Aïn et al. (1989).]

Stoner Model

$$\mathcal{E} = \int_{0}^{\mathcal{E}_{F}-\Delta} d\mathcal{E}' D(\mathcal{E}')\mathcal{E}' + \frac{1}{2} \int_{\mathcal{E}_{F}-\Delta}^{\mathcal{E}_{F}+\Delta} d\mathcal{E}' D(\mathcal{E}')\mathcal{E}' - \frac{1}{2}nJ\langle S \rangle^{2}, \qquad (L69)$$

$$\langle S \rangle = \frac{1}{2n} \int_{\mathcal{E}_F - \Delta}^{\mathcal{E}_F + \Delta} d\mathcal{E}' \frac{1}{2} D(\mathcal{E}') = \frac{1}{2n} D(\mathcal{E}_F) \Delta.$$
(L70)

$$\frac{\partial \mathcal{E}}{\partial \Delta}\Big|_{\mathcal{E}_F} = \Delta D(\mathcal{E}_F) - \frac{J}{4n} D(\mathcal{E}_F)^2 \Delta, \qquad (L71)$$

$$\frac{\partial \mathcal{E}}{\partial \Delta}\Big|_{\mathcal{E}_F} = 0 \Rightarrow \frac{J}{n} D(\mathcal{E}_F) = 4.$$
 (L72)

$$\mathcal{E} = \int_{0}^{\mathcal{E}_{F} - \Delta_{1}} d\mathcal{E}' D(\mathcal{E}') \mathcal{E}' + \frac{1}{2} \int_{\mathcal{E}_{F} - \Delta_{1}}^{\mathcal{E}_{F} + \Delta_{2}} d\mathcal{E}' D(\mathcal{E}') \mathcal{E}' - \frac{1}{2} Jn \langle S \rangle^{2}, \qquad (L73)$$

$$\frac{\partial \Delta_2}{\partial \Delta_1} = \frac{D(\mathcal{E}_F - \Delta_1)}{D(\mathcal{E}_F + \Delta_2)},\tag{L74}$$

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Stoner Model

$$\frac{\partial \mathcal{E}}{\partial \Delta_{1}} \leq 0 \qquad (L75)$$
$$\Rightarrow \Delta_{1} + \Delta_{2} \leq \frac{J}{4n} \int_{\mathcal{E}_{F} - \Delta_{1}}^{\mathcal{E}_{F} + \Delta_{2}} d\mathcal{E}' D(\mathcal{E}'). \qquad (L76)$$

Calculations Within Band Theory

$$\mathcal{E} = \mathcal{E}_{\uparrow} + \mathcal{E}_{\downarrow} \tag{L77}$$

where

$$\mathcal{E}_{\uparrow} = N_{\uparrow} \left[\frac{3}{5} \mathcal{E}_{F\uparrow} - \frac{3}{4} \frac{e^2 k_{F\uparrow}}{\pi} \right], \qquad (L78)$$

$$\mathcal{E}_{F\uparrow} = \frac{\hbar^2 k_{F\uparrow}^2}{2m}$$
, and $\frac{4\pi}{3} \frac{1}{(2\pi)^3} k_{F\uparrow}^3 = \frac{N_{\uparrow}}{\mathcal{V}}$. (L79)

$$\mathcal{E}_{\text{polarized}} = N \left[\frac{3}{5} \frac{\hbar^2}{2m} \left(6\pi^2 n \right)^{2/3} - \frac{3}{4\pi} e^2 \left(6\pi^2 n \right)^{1/3} \right], \quad (L80)$$

$$\mathcal{E}_{\text{unpolarized}} = N \left[\frac{3}{5} \frac{\hbar^2}{2m} \left(3\pi^2 n \right)^{2/3} - \frac{3}{4\pi} e^2 \left(3\pi^2 n \right)^{1/3} \right].$$
(L81)

$$\frac{2\pi\hbar^2}{5m} \left(\frac{1}{2^{1/3}} + 1\right) < e^2 (6\pi^2 n)^{-1/3} \tag{L82}$$

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Calculations Within Band Theory

$$\Rightarrow \quad \frac{r_W}{a_0} > \frac{2\pi}{5} \left(\frac{1}{2^{1/3}} + 1\right) \left(\frac{9\pi}{2}\right)^{1/3} = 5.45. \tag{L83}$$

Element:	Sc	Ti	V	Cr	Mn	Fe	Co	Ni
Calculated m/μ_B (bcc):	0	0	0	0	0.70	2.15	1.68	0.38
Experimental m/μ_B (bcc):				0		2.12		
Calculated m/μ_B (fcc):	0	0	0	0	0	0	1.56	0.60
Experimental m/μ_B (fcc):							1.61	0.61

Kondo Effect



Figure 5: Resistivity data for $Mo_x Nb_{1-x}$ alloys. [Source: Sarachik et al. (1964).]

 $\hat{\mathcal{H}} = \epsilon_0 [\hat{n}_{0\uparrow} + \hat{n}_{0\downarrow}] + U \hat{n}_{0\uparrow} \hat{n}_{0\downarrow} + \sum_{\vec{k}\sigma} [\epsilon_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} + v_{\vec{k}} \hat{c}^{\dagger}_{0\sigma} \hat{c}_{\vec{k}\sigma} + v_{\vec{k}}^* \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{0\sigma}].$ (L84)



Figure 6: Conduction electrons placed in contact with an impurity site.

$$\hat{P}_0 = (1 - \hat{n}_{0\downarrow})(1 - \hat{n}_{0\uparrow}),$$
 (L85)

$$|\psi_0\rangle = \hat{P}_0|\psi\rangle, \ |\psi_1\rangle = \hat{P}_1|\psi\rangle, \text{and}|\psi_2\rangle = \hat{P}_2|\psi\rangle.$$
 (L86)

$$\hat{\mathcal{H}}_{ll'} = \hat{P}_l \hat{\mathcal{H}} \hat{P}_{l'} \qquad (L87)$$

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so $\hat{\mathcal{H}}|\psi\rangle = \mathcal{E}|\psi\rangle$ can be rewritten as

$$\begin{pmatrix} \hat{\mathcal{H}}_{00} & \hat{\mathcal{H}}_{01} & 0\\ \hat{\mathcal{H}}_{10} & \hat{\mathcal{H}}_{11} & \hat{\mathcal{H}}_{12}\\ 0 & \hat{\mathcal{H}}_{21} & \hat{\mathcal{H}}_{22} \end{pmatrix} \begin{pmatrix} |\psi_0\rangle\\ |\psi_1\rangle\\ |\psi_2\rangle \end{pmatrix} = \mathcal{E} \begin{pmatrix} |\psi_0\rangle\\ |\psi_1\rangle\\ |\psi_2\rangle \end{pmatrix}$$
(L88)

$$\hat{\mathcal{H}}_{00}|\psi_0\rangle + \hat{\mathcal{H}}_{01}|\psi_1\rangle = \mathcal{E}|\psi_0\rangle \tag{L89}$$

$$\Rightarrow \qquad |\psi_0\rangle = \left(\mathcal{E} - \hat{\mathcal{H}}_{00}\right)^{-1} \hat{\mathcal{H}}_{01} |\psi_1\rangle \tag{L90}$$

and
$$|\psi_2\rangle = \left(\mathcal{E} - \hat{\mathcal{H}}_{22}\right)^{-1} \hat{\mathcal{H}}_{21} |\psi_1\rangle;$$
 (L91)

$$\left\{\hat{\mathcal{H}}_{10}\left(\mathcal{E}-\hat{\mathcal{H}}_{00}\right)^{-1}\hat{\mathcal{H}}_{01}+\left(\hat{\mathcal{H}}_{11}-\mathcal{E}\right)+\hat{\mathcal{H}}_{12}\left(\mathcal{E}-\hat{\mathcal{H}}_{22}\right)^{-1}\hat{\mathcal{H}}_{21}\right\}|\psi_{1}\rangle=0.$$
 (L92)

$$\sum_{\vec{k}\sigma} v_{\vec{k}} \hat{c}^{\dagger}_{0\sigma} \hat{c}_{\vec{k}\sigma}.$$
 (L93)

$$\hat{\mathcal{H}}_{10} = \sum_{\vec{k}\sigma} v_{\vec{k}} \hat{c}^{\dagger}_{0\sigma} \hat{c}_{\vec{k}\sigma} \hat{P}_0 \qquad (L94)$$

$$= \sum_{\vec{k}\sigma} v_{\vec{k}} \hat{c}^{\dagger}_{0\sigma} \hat{c}_{\vec{k}\sigma} (1 - \hat{n}_{0\downarrow}) (1 - \hat{n}_{0\uparrow})$$
(L95)

$$= \sum_{\vec{k}\sigma} v_{\vec{k}} \hat{c}^{\dagger}_{0\sigma} \hat{c}_{\vec{k}\sigma} (1 - \hat{n}_{0,-\sigma}).$$
(L96)

$$\hat{\mathcal{H}}_{01} = \hat{\mathcal{H}}_{10}^* = \sum_{\vec{k}\sigma} (1 - \hat{n}_{0,-\sigma}) v_{\vec{k}}^* \hat{c}_{\vec{k}\sigma}^\dagger \hat{c}_{0\sigma}.$$
 (L97)

$$\hat{\mathcal{H}}_{11} = \hat{P}_1[\epsilon_0 + \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma}]; \\ \hat{\mathcal{H}}_{00} = \hat{P}_0 \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma}$$
(L98)

and

$$\hat{\mathcal{H}}_{21} = \hat{\mathcal{H}}_{12}^* = \sum_{\vec{k}\sigma} v_{\vec{k}} \hat{c}_{0\sigma}^{\dagger} \hat{c}_{\vec{k}\sigma} \hat{n}_{0,-\sigma}.$$
(L99)

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$$\hat{\mathcal{H}}_{10} \left(\mathcal{E} - \hat{\mathcal{H}}_{00} \right)^{-1} \hat{\mathcal{H}}_{01} |\psi_1\rangle \tag{L100}$$

$$= \hat{\mathcal{H}}_{10} \sum_{\vec{k}\sigma} (1 - \hat{n}_{0,-\sigma}) v_{\vec{k}}^* \hat{c}_{\vec{k}\sigma}^\dagger \hat{c}_{0\sigma} \left(\mathcal{E} - [\hat{\mathcal{H}}_{11} - \epsilon_0 + \epsilon_{\vec{k}}] \right)^{-1} |\psi_1\rangle.$$
(L101)

$$\frac{\hat{\mathcal{H}}_{10}}{\epsilon_0 - \mathcal{E}_F} \sum_{\vec{k}\sigma} v_{\vec{k}}^* (1 - \hat{n}_{0,-\sigma}) \hat{c}_{\vec{k}\sigma}^\dagger \hat{c}_{0\sigma} |\psi_1\rangle \tag{L102}$$

$$= \sum_{\vec{k}\vec{k}'\sigma\sigma'} \frac{v_{\vec{k}'}v_{\vec{k}}^*}{\epsilon_0 - \mathcal{E}_F} \hat{c}_{0\sigma'}^{\dagger} \hat{c}_{\vec{k}'\sigma'} (1 - \hat{n}_{0,-\sigma'}) (1 - \hat{n}_{0,-\sigma}) \hat{c}_{\vec{k}\sigma}^{\dagger} \hat{c}_{0\sigma} |\psi_1\rangle \qquad (L103)$$

$$= \sum_{\vec{k}\vec{k}'\sigma\sigma'} \frac{v_{\vec{k}'}v_{\vec{k}}^*}{\mathcal{E}_F - \epsilon_0} \hat{c}_{0\sigma'}^{\dagger} \hat{c}_{\vec{k}\sigma}^{\dagger} \hat{c}_{\sigma'} \hat{c}_{0\sigma} |\psi_1\rangle.$$
(L104)

$$\hat{n}_{0\uparrow}\hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}_{\vec{k}'\uparrow} + \hat{n}_{0\downarrow}\hat{c}^{\dagger}_{\vec{k}\downarrow}\hat{c}_{\vec{k}'\downarrow} \tag{L105}$$

$$= \frac{1}{2} (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}) (\hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}'\uparrow} - \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{k}'\downarrow}) + \frac{1}{2} (\hat{n}_{0\uparrow} + \hat{n}_{0\downarrow}) (\hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}'\uparrow} + \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{k}'\downarrow})$$
(L106)
$$= \hat{S}^{z} (\hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}'\uparrow} - \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{k}'\downarrow}) + \frac{1}{2} \sum_{\sigma} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}'\sigma}.$$
(L107)

$$\sum_{\vec{k}\vec{k}'} \frac{v_{\vec{k}'}v_{\vec{k}}^*}{\mathcal{E}_F - \epsilon_0} \left[\hat{S}^+ \hat{c}_{\vec{k}\downarrow}^\dagger \hat{c}_{\vec{k}'\uparrow} + \hat{S}^- \hat{c}_{\vec{k}\uparrow}^\dagger \hat{c}_{\vec{k}'\downarrow} + \hat{S}^z (\hat{c}_{\vec{k}\uparrow}^\dagger \hat{c}_{\vec{k}'\uparrow} - \hat{c}_{\vec{k}\downarrow}^\dagger \hat{c}_{\vec{k}'\downarrow}) + \frac{1}{2} \sum_{\sigma} \hat{c}_{\vec{k}\sigma}^\dagger \hat{c}_{\vec{k}'\sigma} \right] |\psi_1\rangle.$$
(L108)

$$\hat{\mathcal{H}}_{\text{eff}} = \hat{\mathcal{H}}_{11} + \sum_{\vec{k}\vec{k}'} J_{\vec{k}\vec{k}'} \left[\hat{S}^{+} \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{k}'\uparrow} + \hat{S}^{-} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}'\downarrow} + \hat{S}^{z} (\hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}'\uparrow} - \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{k}'\downarrow}) \right]
+ K_{\vec{k}\vec{k}'} \sum_{\sigma} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}'\sigma} \qquad (L109a)
J_{\vec{k}\vec{k}'} = v_{\vec{k}'} v_{\vec{k}}^{*} \left[\frac{1}{\mathcal{E}_{F} - \epsilon_{0}} + \frac{1}{U + \epsilon_{0} - \mathcal{E}_{F}} \right].$$
(L109b)

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$$\hat{\mathcal{H}}_{12} = J \sum_{\vec{k}\vec{q}} \hat{S}^{-} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{q}\downarrow} + \hat{S}^{+} \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{q}\uparrow} + \hat{S}^{z} \left[\hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{q}\uparrow} - \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{q}\downarrow} \right], \qquad (L111a)$$

$$\hat{\mathcal{H}}_{21} = J \sum_{\vec{k}'\vec{q}'} \hat{S}^{-} \hat{c}^{\dagger}_{\vec{q}'\uparrow} \hat{c}_{\vec{k}\downarrow} + \hat{S}^{+} \hat{c}^{\dagger}_{\vec{q}'\downarrow} \hat{c}_{\vec{k}'\uparrow} + \hat{S}^{z} \left[\hat{c}^{\dagger}_{\vec{q}'\uparrow} \hat{c}_{\vec{k}'\uparrow} - \hat{c}^{\dagger}_{\vec{q}'\downarrow} \hat{c}_{\vec{k}'\downarrow} \right].$$
(L111b)

$$\hat{\mathcal{H}}_{12}(\mathcal{E}-\hat{\mathcal{H}}_{22})^{-1}\hat{\mathcal{H}}_{21}|\psi_1\rangle \tag{L112}$$

$$\approx \hat{\mathcal{H}}_{12}\hat{\mathcal{H}}_{21}(\mathcal{E}-\hat{\mathcal{H}}_{22}-[\mathcal{W}-\mathcal{E}_F])^{-1}|\psi_1\rangle \qquad (L113)$$

$$\approx \hat{\mathcal{H}}_{12}\hat{\mathcal{H}}_{21}(-\mathcal{W})^{-1}|\psi_1\rangle.$$
 (L114)

$$\hat{\mathcal{H}}_{12}\hat{\mathcal{H}}_{21} = J^2 D(\mathcal{W}) \left[-\delta \mathcal{W}\right] \sum_{\vec{k}\vec{k}'} \frac{3}{4} \sum_{\sigma} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}'\sigma} - \begin{cases} \hat{S}^- \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}'\downarrow} + \hat{S}^+ \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{k}'\uparrow} \\ + \hat{S}^z \left[\hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}'\uparrow} - \hat{c}^{\dagger}_{\vec{k}\downarrow} \hat{c}_{\vec{k}'\downarrow} \right] \end{cases}$$
(L115)

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$$J + \delta J = J - 2\frac{J^2}{W}D(W)\delta W, \qquad (L116)$$

$$\frac{3}{2}J^2 D(\mathcal{W}) \frac{\delta \mathcal{W}}{\mathcal{W}} \sum_{\vec{k}\vec{k}'\sigma} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}'\sigma}.$$
 (L117)

$$\frac{dJ}{d\mathcal{W}} = -2\frac{J^2}{\mathcal{W}}D(\mathcal{W}). \tag{L118}$$

$$W \exp\left[-\frac{1}{2D_0 J}\right] = \text{constant} \equiv k_B T_K,$$
 (L119)

$$\rho = \mathcal{F}\left(\frac{T}{T_K}\right). \tag{L120}$$

$$\mathcal{F}(x) = \left[\frac{1}{\ln(x)}\right]^2 \tag{L121}$$

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$$\Rightarrow \mathcal{F}\left(\frac{T}{T_{K}}\right) = \rho = \left[\frac{2D_{0}J}{1+2D_{0}J\ln(k_{B}T/\mathcal{W})}\right]^{2} \qquad (L122)$$
$$\sim 4D_{0}^{2}J^{2}\left(1-4D_{0}J\ln(k_{B}T/\mathcal{W})\right). \qquad (L123)$$

$$\rho \sim \mathcal{A}T^5 - \mathcal{B}n_{\rm mi}\ln(k_BT/\mathcal{W}), \qquad (L124)$$

$$\frac{d\rho}{dT} = 0 \Rightarrow T_{\min} = \left(\frac{\mathcal{B}n_{\min}}{5\mathcal{A}}\right)^{1/5}.$$
 (L125)

$$\mathcal{F}\left(\frac{T}{T_K}\right) = \left[\frac{1}{\cosh^{-1}(T/T_K)}\right]^2,\tag{L126}$$

$$C_{\mathcal{V}} \propto n \frac{T}{T_K} = n \frac{k_B T}{\mathcal{W}} \exp\left[\frac{1}{2D_0 J}\right].$$
 (L127)



Figure 8: Low-temperature specific heat of the heavy fermion compound UBe₁₃. [Source Ott et al. (1983, 1984).]

Hubbard Model

$$\hat{\mathcal{H}} = \sum_{\substack{\langle ll' \rangle \\ \sigma}} -\mathfrak{t} \left[\hat{c}^{\dagger}_{l\sigma} \hat{c}_{l'\sigma} + \hat{c}^{\dagger}_{l'\sigma} \hat{c}_{l\sigma} \right] + U \sum_{l} \hat{c}^{\dagger}_{l\uparrow} \hat{c}_{l\uparrow} \hat{c}^{\dagger}_{l\downarrow} \hat{c}_{l\downarrow}, \qquad (L128)$$

Mean-Field Solution

$$\hat{\mathcal{H}} = \sum_{\substack{\langle ll' \rangle \\ \sigma}} -\mathfrak{t} \left[\hat{c}_{l\sigma}^{\dagger} \hat{c}_{l'\sigma} + \hat{c}_{l'\sigma}^{\dagger} \hat{c}_{l\sigma} \right] + U \sum_{l} \hat{n}_{l\uparrow} \hat{n}_{l\downarrow}.$$
(L129)

$$\hat{n}_{l\sigma} = n_{\sigma} + (\hat{n}_{l\sigma} - n_{\sigma}).$$
(L130)

$$\hat{\mathcal{H}} \approx \sum_{\substack{\langle ll' \rangle \\ \sigma}} -\mathfrak{t} \left[\hat{c}_{l\sigma}^{\dagger} \hat{c}_{l'\sigma} + \hat{c}_{l'\sigma}^{\dagger} \hat{c}_{l\sigma} \right] + U \sum_{l} \hat{n}_{l\uparrow} n_{\downarrow} + n_{\uparrow} \hat{n}_{l\downarrow} - n_{\uparrow} n_{\downarrow}.$$
(L131)

$$\sum_{\vec{k}\vec{\delta}\sigma} -\mathfrak{t}\hat{c}_{\vec{k}\sigma}^{\dagger}\hat{c}_{\vec{k}\sigma}\cos\vec{\delta}\cdot\vec{k} + U\sum_{\vec{k}}\hat{n}_{\vec{k}\uparrow}n_{\downarrow} + n_{\uparrow}\hat{n}_{\vec{k}\downarrow} - n_{\uparrow}n_{\downarrow}.$$
 (L132)

$$Nn_{\uparrow} = Na \int_{-k_{F\uparrow}}^{k_{F\uparrow}} \frac{dk}{2\pi}$$
(L133)

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Hubbard Model

$$\Rightarrow \pi n_{\uparrow} = a k_{F\uparrow}. \tag{L134}$$

$$\mathcal{E}_0 = \frac{N}{\pi} \left[-2\mathfrak{t}\right] \left[\sin \pi n_{\uparrow} + \sin \pi n_{\downarrow}\right] + NU n_{\uparrow} n_{\downarrow}. \tag{L135}$$

$$\mathcal{E}_0 = \frac{-4\mathfrak{t}N}{\pi}\sin\pi n_{\uparrow} + NUn_{\uparrow}\left(1 - n_{\uparrow}\right). \tag{L136}$$

$$\frac{U}{t} > \frac{16}{\pi},\tag{L137}$$

An Unsolved Problem...



Figure 9: Six representative phase diagrams of the two-dimensional Hubbard model