本节是对上一节的反铁磁耦合的进一步的了解.

反铁磁 Heisenberg 模型的导出

考虑两个正交的轨道, 局域在两个原子($i=1,2$)上, 设电子所处状态可以在两个轨道之间变化, 也就是在两个原子之间隧穿, 可以用以下的 hopping 哈密顿量描述该电子:

$$\mathcal{H}^t=-t\sum_s\left(\mathrm{c}_{1s}^\dagger c_{2s}+c_{2s}^\dagger \mathrm{c}_{1s}\right)$$

另外, 我们加入 on-site 的相互作用 (Hubbard 相互作用):

$$\mathcal{U}=U\sum_i n_{i\uparrow}n_{i\downarrow}$$

考虑 $U/t\gg 1$ 的强耦合区域, 此时 $\mathcal{U}$ 为零阶哈密顿量, $\mathcal{H}^t$ 则作为一阶哈密顿量.按照微扰论的思想, 先只看零阶哈密顿量, 即不考虑 hopping, 那么**基态**是具有**四重简并度**的, 两个格点上各有一个电子:

$$\{0\}=|s_1,s_2\rangle,\quad s_i=\uparrow,\downarrow,\quad i=1,2.$$

- **自旋极化态 (spin-polarized states)**: $|\uparrow,\uparrow\rangle,|\downarrow,\downarrow\rangle$
  - 这两个态同时也是三重态的两个, 还有一个三重态是 $(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle)/\sqrt{2}$; 单重态则是 $(|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle)/\sqrt{2}$
- **单占据态 (Singly occupied states)**: $|\uparrow,\downarrow\rangle,|\downarrow,\uparrow\rangle$

然后看微扰项 $\mathcal{H}^t$ 的影响. 先考虑到一阶微扰, 系统会从基态中跳出来, 会形成**双占据态(doubly occupied states)**, 两个电子在第一个点 $|\uparrow\downarrow,0\rangle$ 或者在第二个点 $|0,\uparrow\downarrow\rangle$ 上.

再进一步考虑到二阶微扰, 系统经历两次 hopping, 会跳回基态, 这将对基态能量进行修正. 设基态子空间 $\{0\}$ 对应的投影算符是 $P_0=\sum_{s_1,s_2}|s_1,s_2\rangle\langle s_1,s_2|$, 则二阶微扰理论所导出的二阶能量修正为(见 Landau 和 Lifshitz 的量子力学第六章):

$$\left\langle a\left|\mathcal{H}^{(2)}\right|b\right\rangle=-\left\langle a\left|\mathcal{H}^t\frac{1-P_0}{\mathcal{U}}\mathcal{H}^t\right|b\right\rangle=-\sum_{n\notin\{0\}}\left\langle a\left|\mathcal{H}^t\right|n\right\rangle\frac{1}{\langle n|\mathcal{U}|n\rangle}\left\langle n\left|\mathcal{H}^t\right|b\right\rangle$$

- $|a\rangle,|b\rangle\in\{0\}$ 表示基态, 共四种.
- $|n\rangle\notin\{0\}$ 表示被激发的双占据态, 一共两种.

这两种双占据态对应着上式的最后求和的两项, 实际上对每一对 $|a\rangle,|b\rangle$ 都可以用不同的**"交换路径" (exchange path)**来表示, 下面有几个例子:

- $|a\rangle, |b\rangle = |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$: 二阶能量修正是 $-2t^2/U < 0$, 两条交换路径如下, 最后都会变成 $|\downarrow,\uparrow\rangle$.
  - $|\uparrow,\downarrow\rangle \xrightarrow{\hat{H}^t} |\uparrow\downarrow, 0\rangle \xrightarrow{\hat{H}^t} |\downarrow,\uparrow\rangle$: 贡献为 $-t^2/U$
  - $|\uparrow,\downarrow\rangle \xrightarrow{\hat{H}^t} |0,\uparrow\downarrow\rangle \xrightarrow{\hat{H}^t} |\downarrow,\uparrow\rangle$: 贡献同样是 $-t^2/U$
- 对于自旋极化态 $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$, 经历一次 hopping 之后就会变成零, 因此二阶修正为零.

我们看到, 在二阶修正下, 四个基态中, 两个单占据态能量降低了,两个自旋极化态能量保持不变, 这样四重的简并度就被部分解除了, 这个**半填充两格点系统**倾向于自旋反平行排列, 这就是**反铁磁性**的特征.

实际上, 在仔细观察上面结果之后, 我们可以利用两个格点上的自旋 1/2 算符 S_1^i, S_2^i 将二阶有效哈密顿量 $\mathcal{H}^{(2)}$ 直接写出来, 是一个**各向同性反铁磁体 Heisenberg 交换**:

$$\mathcal{H}^{(2)} = J\mathbf{S}_1 \cdot \mathbf{S}_2, \quad J = \frac{4t^2}{U}$$

$$\begin{aligned}
\mathcal{H}^{(2)} &= J\mathbf{S}_1 \cdot \mathbf{S}_2 = J\left(S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z\right) \\
&= \frac{J}{2}\left(S_1^- S_2^+ + S_2^- S_1^+\right) + J S_1^z S_2^z \\
&= \frac{2t^2}{U}\left(S_1^- S_2^+ + S_2^- S_1^+\right) + \frac{4t^2}{U} S_1^z S_2^z
\end{aligned}$$

其中第二个等号利用了

$$\begin{gathered}
S_1^- S_2^+ = \left(S_1^x - iS_1^y\right)\left(S_2^x + iS_2^y\right) = S_1^x S_2^x + S_1^y S_2^y + i\left(S_1^x S_2^y - S_1^y S_2^x\right) \\
S_2^- S_1^+ = \left(S_2^x - iS_2^y\right)\left(S_1^x + iS_1^y\right) = S_1^x S_2^x + S_1^y S_2^y + i\left(S_2^x S_1^y - S_2^y S_1^x\right) \\
\Rightarrow S_1^- S_2^+ + S_2^- S_1^+ = 2\left(S_1^x S_2^x + S_1^y S_2^y\right)
\end{gathered}$$

利用这个表达式可以轻易得到:

$$\langle\uparrow,\downarrow\left|\mathcal{H}^{(2)}\right|\downarrow,\uparrow\rangle = \langle\downarrow,\uparrow\left|\mathcal{H}^{(2)}\right|\uparrow,\downarrow\rangle = \frac{2t^2}{U}$$

$$\langle\downarrow,\uparrow\left|\mathcal{H}^{(2)}\right|\downarrow,\uparrow\rangle = \langle\uparrow,\downarrow\left|\mathcal{H}^{(2)}\right|\uparrow,\downarrow\rangle = -\frac{4t^2}{U}$$

$$\langle\downarrow,\downarrow\left|\mathcal{H}^{(2)}\right|\downarrow,\downarrow\rangle = \langle\uparrow,\uparrow\left|\mathcal{H}^{(2)}\right|\uparrow,\uparrow\rangle = +\frac{4t^2}{U}$$

从后面两个式子看到, 两个单占据态的能量比两个自旋极化态的能量要低, 简并度部分解除之后单占据态才是基态.

- 以上的讨论可以推广到多格点模型, 在两个自旋通过 hopping 项耦合时, 反铁磁耦合就会被生成出来.
- 在上面的交换路径中, 双占据态是作为一种虚拟的中间态的, 因此这种交换称为**超交换 (superexchange)**.
    - 在 2.2 节中讨论的氢分子是用了变分法来描述这个效应, 变分法求出来的基态都是单占据态或者自旋极化态(也可按三重态或者单重态来分类), 不涉及双占据态和超交换的讨论, 但是结果是一样的.
    - 这一节则使用了二次量子化的方法讨论同样的效应, 我们看到了双占据态这个中间态以及超交换的这一机制.
    - 超交换和 2.1 解中的铁磁直接交换(或经验得称为 Hund 定则)是不同的, 后者是相互作用 $\mathcal{U}$ 的一阶微扰所带来的, 而前者是将 hopping 项作为微扰.

实例: 铜氧化物反铁磁体(copper-oxide antiferromagnets)

超交换耦合通常会在一些具有**未配对自旋 (unparied spins)** 的系统中出现, 其中著名的一个例子就是铜氧化物反铁磁体.

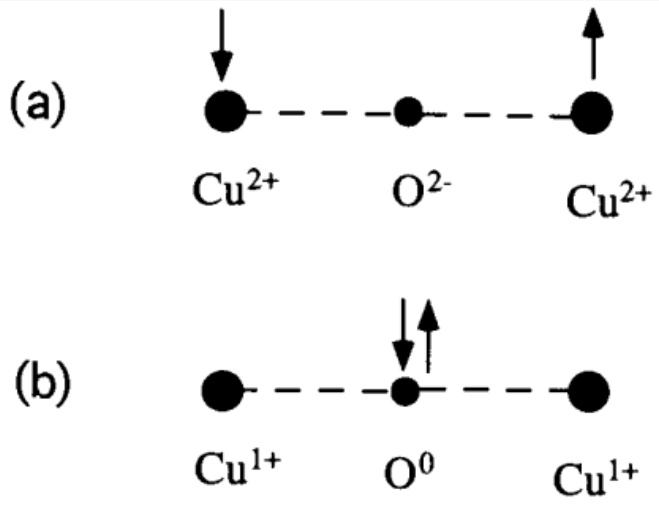


FIGURE 2.3. Superexchange in copper oxides. (a) A member of the low-energy manifold. (b) A high energy configuration in the superexchange path.

- 未配对自旋位于两个 Cu^{2+} 离子上
- 在两个铜离子之间有一个桥梁氧离子, 平均的电离态是接近于 O^{2-} 的.

先不考虑铜和氧之间的 hopping, 系统的简并基态流形为:

$$\{|0\rangle\} = \left\{\left|\mathrm{Cu}^{2+}s_1, \mathrm{O}^{2-}, \mathrm{Cu}^{2+}s_2\right\rangle, \quad s_i = \uparrow, \downarrow\right.$$

然后我们考虑铜离子和氧离子之间的 hopping 项作为微扰, 要想解除或部分解除上面四个基态的简并, 需要考虑到**四阶**的 copper-oxygen hopping, 这很容易理解, 左边铜离子上的电子到右边铜离子

需要 hop 两次, 反之同理, 一个超交换需要经历至少四次 hopping.

超交换中途的状态是能量更高的激发态, 比如说:

- $\left|\mathrm{Cu}^{1+}, \mathrm{O}^{2-}, \mathrm{Cu}^{3+} \uparrow\downarrow\right\rangle, \quad E = U_d$
  - U_d: 铜离子上两个电子的 on-site 相互作用能量
- $\left|\mathrm{Cu}^{1+}, \mathrm{O} \uparrow\downarrow, \mathrm{Cu}^{1+}\right\rangle, \quad E = 2\left(\epsilon_p - \epsilon_d\right) + U_p$, 见"上图(b)"
  - U_p: 氧离子上两个电子的 on-site 相互作用能量
  - ϵ_d: 铜离子上电子的单粒子能量
  - ϵ_p: 氧离子上电子的单粒子能量

同样, 平行自旋态(自旋极化态)的超交换是禁止的, 而单占据态就没有这个限制, 因此 hopping 项的微扰效果是部分解除了"四个基态"的简并度, 同样可以用一个 Heisenberg 哈密顿量来表示. 反铁磁耦合是由所有超交换路径之和给出的, 最终能量最低的态将主导这个系统.

2.4 Spin operator

1. 自旋 1/2 算符的定义: 在数学上, 自旋 1/2 算符是用泡利矩阵定义的双线性算符, 它的代数关系是从泡利矩阵的代数关系继承过来的, 即所谓的角动量算符对易关系

Example: Spin Algebra

我们用厄米矩阵--三个泡利矩阵来构造**双线性自旋算符(bilinear spin operators)**:

$$S^{\alpha}=\frac{1}{2}\sum_{ss'=1}^{2}a_{s}^{\dagger}\sigma_{ss'}^{\alpha}a_{s'}=\frac{1}{2}\mathbf{a}^{\dagger}\sigma^{\alpha}\mathbf{a},\quad \alpha=x,y,z$$

$$(\sigma^{x},\sigma^{y},\sigma^{z})=\left[\begin{pmatrix}0&1\\1&0\end{pmatrix},\begin{pmatrix}0&-i\\i&0\end{pmatrix},\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right]$$

三个双线性自旋算符满足角动量的代数关系, 利用前面的导出的"双线性算符之间的对易关系", 可以直接代入"泡利矩阵的对易关系"得到:

$$\left[S^{\alpha},S^{\beta}\right]=i\epsilon^{\alpha\beta\gamma}S^{\gamma}$$

2. 自旋算符所满足的恒等式及其证明: 两个自旋算符乘在一起就表征了相互作用, 因为其中出现了四个产生湮灭算符的乘积

$$\hat{\mathbf{S}}_{i}\cdot\hat{\mathbf{S}}_{j}=-\frac{1}{2}a_{i\alpha}^{\dagger}a_{j\beta}^{\dagger}a_{i\beta}a_{j\alpha}-\frac{1}{4}\hat{n}_{i}\hat{n}_{j}$$

$$\begin{aligned}\hat{\mathbf{S}}_{i}\cdot\hat{\mathbf{S}}_{j}&=\frac{a_{i\alpha}^{\dagger}\boldsymbol{\sigma}_{\alpha\beta}a_{i\beta}}{2}\cdot\frac{a_{j\gamma}^{\dagger}\boldsymbol{\sigma}_{\gamma\delta}a_{j\delta}}{2}=\frac{1}{4}a_{i\alpha}^{\dagger}a_{i\beta}a_{j\gamma}^{\dagger}a_{j\delta}\boldsymbol{\sigma}_{\alpha\beta}\cdot\boldsymbol{\sigma}_{\gamma\delta}\\&=\frac{1}{4}a_{i\alpha}^{\dagger}a_{i\beta}a_{j\gamma}^{\dagger}a_{j\delta}\left(2\delta_{\alpha\delta}\delta_{\beta\gamma}-\delta_{\alpha\beta}\delta_{\gamma\delta}\right)\\&=\frac{1}{2}a_{i\alpha}^{\dagger}a_{i\beta}a_{j\gamma}^{\dagger}a_{j\delta}\delta_{\alpha\delta}\delta_{\beta\gamma}-\frac{1}{4}a_{i\alpha}^{\dagger}a_{i\beta}a_{j\gamma}^{\dagger}a_{j\delta}\delta_{\alpha\beta}\delta_{\gamma\delta}\\&=\frac{1}{2}a_{i\alpha}^{\dagger}a_{i\beta}a_{j\beta}^{\dagger}a_{j\alpha}-\frac{1}{4}a_{i\alpha}^{\dagger}a_{i\alpha}a_{j\gamma}^{\dagger}a_{j\gamma}\\&=-\frac{1}{2}a_{i\alpha}^{\dagger}a_{j\beta}^{\dagger}a_{i\beta}a_{j\alpha}-\frac{1}{4}\hat{n}_{i}\hat{n}_{j}\end{aligned}$$

- 第二行: 利用了 Pauli 矩阵的
- 最后一行: 注意我们考虑 $i\neq j$ 的情况, 同时描述的是费米子(电子)系统, 产生湮灭算符之间有反对易关系.

3. $\mathbf{S}_i^2$ 与 $\hat{n}_i$ 的关系: 可以直接从 $\mathbf{S}_i \cdot \mathbf{S}_j$ 的计算结果得到

$$\begin{aligned}\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_i &= -\frac{1}{2} a_{i\alpha}^\dagger a_{i\beta}^\dagger a_{i\beta} a_{i\alpha} - \frac{1}{4}\hat{n}_i \hat{n}_i \\ &= -\frac{1}{2} a_{i\alpha}^\dagger \hat{n}_i a_{i\alpha} - \frac{1}{4}\hat{n}_i^2 \\ &= -\frac{1}{2} a_{i\alpha}^\dagger a_{i\alpha} \hat{n}_i + \frac{1}{2} a_{i\alpha}^\dagger a_{i\alpha} - \frac{1}{4}\hat{n}_i^2 \\ &= -\frac{3}{4}\hat{n}_i^2 + \frac{1}{2}\hat{n}_i\end{aligned}$$

   第三个等号利用了对易关系 $[\hat{n}_i, a_{i\alpha}] = -a_{i\alpha}$.

相关链接

- "泡利矩阵"

Anti-ferromagnetic ordering of Mott insulator

Experimentally, it is often found that the low-temperature phase of the Mott insulator is accompanied by the **anti-ferromagnetic ordering of the local moments**.

The origin of these magnetic correlations can be traced to a mechanism known as **superexchange** and can be understood straightforwardly within the framework of the **Hubbard model** system.

> 我们已经在"Exchange coupling"这一节中见过了不同格点单纯借由库伦相互作用的交换耦合所带来的磁性, 但这是在 Hubbard model 之外的, 这也不称为超交换(虚交换), 这是实交换.

本节是一种将 Hubbard 模型中的 hopping 项作为微扰的讨论方法，可以导出其中的反铁磁的有效哈密顿量。我们从简单的 two-site 系统谈起，然后推广到 extended system.

Two-site system

Half-filling two-site system: there are two electrons shared by two sites.

There are six basis states:

- Two **spin-polarized states** $a_{1\uparrow}^{\dagger}a_{2\uparrow}^{\dagger}|\Omega\rangle, a_{1\downarrow}^{\dagger}a_{2\downarrow}^{\dagger}|\Omega\rangle$, are **zero energy eigenstates**.
  - According to Pauli principle, the hopping between site 1 and site2 is inhibited, and then double occupacy in one site is also inhibited.
  - So Hubbard Hamiltonina acts on the two states and get 0.
- Four states that satisfy $S_{\text{total}}^{z}=0$, $|s_1\rangle=a_{1\uparrow}^{\dagger}a_{2\downarrow}^{\dagger}|\Omega\rangle, |s_2\rangle=a_{2\uparrow}^{\dagger}a_{1\downarrow}^{\dagger}|\Omega\rangle, |d_1\rangle=a_{1\uparrow}^{\dagger}a_{1\downarrow}^{\dagger}|\Omega\rangle$, and $|d_2\rangle=a_{2\uparrow}^{\dagger}a_{2\downarrow}^{\dagger}|\Omega\rangle$
  - $|s_i\rangle$: **singly occupied** subspaces, with projector $\hat{P}_s=\sum_{i=1,2}|s_i\rangle\langle s_i|$
  - $|d_i\rangle$: **doubly occupied** subspaces, with projector $\hat{P}_d=\sum_{i=1,2}|d_i\rangle\langle d_i|$

So the eigenstates with non-zero energy of the two-site system are superposition of $|s_i\rangle$ and $|d_i\rangle$, all satisfy $S_{\text{total}}^{z}=0$.

- Generally: Because this is a two-site system, we can simply diagonalize the 4×4 Hamiltonian exactly to obtain ground state. However, this method doesn't work for large system.
- **Strong coupling limit** $U/t\gg 1$: the ground state will be composed predominantly of states with no double occupancy, $|s_i\rangle$.

- Perturbation theory: treats the hopping part $\hat{H}_t$ as a weak perturbation of the Hubbard interaction $\hat{H}_U$ and projects the insulating system onto a **low-energy effective spin Hamiltonian**. Here is where the magnetism originates from.
- This perturbation theory can be easily extended to extended lattice system.

Exactly diagonalization of $\hat{H}_t$

Perturbation theory of $\hat{H}_t$ (Shrieffer-Wolff transformation/Nakajima transformation)

Firstly, do a canonical transformation of the Hamiltonian

$$\hat{H} \mapsto \hat{H}' \equiv e^{-t\hat{O}}\hat{H}e^{t\hat{O}} = e^{-t[\hat{O},]}\hat{H} \equiv \hat{H} - t[\hat{O},\hat{H}] + \frac{t^2}{2!}[\hat{O},[\hat{O},\hat{H}]] + \cdots$$

where we have use "BH identity". Now we have

$$\begin{aligned}\hat{H}' &= \hat{H} - t[\hat{O},\hat{H}] + \frac{t^2}{2!}[\hat{O},[\hat{O},\hat{H}]] + \cdots \\ &= \hat{H}_t + \hat{H}_U - t\left[\hat{O},\hat{H}_t + \hat{H}_U\right] + \frac{t^2}{2!}\left[\hat{O},[\hat{O},\hat{H}]\right] + \cdots\end{aligned}$$

Choose a good $\hat{O}$ such that 1st order terms add to zero:

$$\hat{H}_t + t\left[\hat{H}_U,\hat{O}\right] = 0$$

where we can use the following ansatz:

$$t\hat{O} = \left[\hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d} - \hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s}\right]/U$$

这个 $\hat{O}$ 的形式是非常通用的, 证明主要用到下面几个性质:

$$\hat{P}_s\hat{P}_d = 0, \hat{H}_U\hat{P}_s = 0, \hat{P}_s\hat{H}_t\hat{P}_s = \hat{P}_d\hat{H}_t\hat{P}_d = 0$$

其中第二个性质表明 Hubbard interaction part $\hat{H}_U$ 是完全处于"双占据子空间"的; 第三个性质表明 hopping part $\hat{H}_t$ 是双占据子空间和单占据子空间之间的桥梁, 作用在双占据态上变成单占据态, 反之亦然.

下面给出证明. 首先代入 $\hat{O}$ 的取值, 并化简:

$$
\begin{aligned}
\hat{H}_t + t\left[\hat{H}_U, \hat{O}\right] &= \hat{H}_t + \frac{1}{U}\left[\hat{H}_U, \hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d} - \hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s}\right] \\
&= \hat{H}_t + \frac{1}{U}\begin{bmatrix} \hat{H}_U\left(\hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d} - \hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s}\right) \\ -\left(\hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d} - \hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s}\right)\hat{H}_U \end{bmatrix} \\
&= \hat{H}_t - \frac{1}{U}\left(\hat{H}_U\hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s} + \hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d}\hat{H}_U\right)
\end{aligned}
$$

然后对其四个 2×2 分块元分别证明为零:

$$
\begin{aligned}
&\hat{P}_\mathrm{s}\left(\hat{H}_t + t\left[\hat{H}_U, \hat{O}\right]\right)\hat{P}_\mathrm{s} \\
&= \hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{s} - \frac{1}{U}\left(\hat{P}_\mathrm{s}\hat{H}_U\hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s}\hat{P}_\mathrm{s} + \hat{P}_\mathrm{s}\hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d}\hat{H}_U\hat{P}_\mathrm{s}\right) \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
&\hat{P}_d\left(\hat{H}_t + t\left[\hat{H}_U, \hat{O}\right]\right)\hat{P}_d \\
&= \hat{P}_d\hat{H}_t\hat{P}_d - \frac{1}{U}\left(\hat{P}_d\hat{H}_U\hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s}\hat{P}_d + \hat{P}_d\hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d}\hat{H}_U\hat{P}_d\right) \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
&\hat{P}_d\left(\hat{H}_t + t\left[\hat{H}_U, \hat{O}\right]\right)\hat{P}_s \\
&= \hat{P}_d\hat{H}_t\hat{P}_s - \frac{1}{U}\left(\hat{P}_d\hat{H}_U\hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s}\hat{P}_s + \hat{P}_d\hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d}\hat{H}_U\hat{P}_s\right) \\
&= \hat{P}_d\hat{H}_t\hat{P}_s - \frac{1}{U}\hat{P}_d\hat{H}_U\hat{P}_\mathrm{d}\hat{H}_t \\
&= \hat{P}_d\hat{H}_t\hat{P}_s - \hat{H}_t = \hat{H}_t\hat{P}_s - \hat{H}_t = 0
\end{aligned}
$$

其中第四个等号利用了

$$
\begin{aligned}
\frac{1}{U}\hat{P}_d\hat{H}_U\hat{P}_\mathrm{d} &= \hat{P}_d\sum_{j=1,2}\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\sum_{i=1,2}|d_i\rangle\langle d_i| \\
&= \hat{P}_d\sum_{i=1,2}|d_i\rangle\langle d_i| = \hat{P}_d\hat{P}_d = 1
\end{aligned}
$$

最后的结果为零只在作用于单占据态时成立. 类似地,最后一个分量

$$
\begin{aligned}
&\hat{P}_s\left(\hat{H}_t + t\left[\hat{H}_U, \hat{O}\right]\right)\hat{P}_d \\
&= \hat{P}_s\hat{H}_t\hat{P}_d - \frac{1}{U}\left(\hat{P}_s\hat{H}_U\hat{P}_\mathrm{d}\hat{H}_t\hat{P}_\mathrm{s}\hat{P}_d + \hat{P}_s\hat{P}_\mathrm{s}\hat{H}_t\hat{P}_\mathrm{d}\hat{H}_U\hat{P}_d\right) \\
&= \hat{P}_s\hat{H}_t\hat{P}_d - \frac{1}{U}\hat{H}_t\hat{P}_\mathrm{d}\hat{H}_U\hat{P}_d \\
&= \hat{P}_s\hat{H}_t\hat{P}_d - \hat{H}_t = \hat{H}_t\hat{P}_d - \hat{H}_t = 0
\end{aligned}
$$

> 的最后一个等号也只在作用于双占据态时成立. 而这两个分量作为 4×4 矩阵 $\hat{H}_t+t\left[\hat{H}_U,\hat{O}\right]$ 的两个非对角 2×2 分块, 本来就作用于对应的单占据态分量, 双占据态分量, 故为零的条件自然满足.

all term $\sim t$ vanish and we obtain an effective Hamiltonian:

$$\hat{H}'=\hat{H}_U+\frac{t}{2}\left[\hat{H}_t,\hat{O}\right]+\mathcal{O}\left(t^3\right)$$

Project the Hamiltonian into **singly occupied subspace**:

$$\begin{aligned}
\hat{P}_s\hat{H}'\hat{P}_s&=\hat{P}_s\hat{H}_U\hat{P}_s+\frac{t}{2}\left[\hat{H}_t,\hat{O}\right]\\
&=\frac{1}{2U}\hat{P}_s\left[\hat{H}_t,\hat{P}_{\mathrm{s}}\hat{H}_t\hat{P}_{\mathrm{d}}-\hat{P}_{\mathrm{d}}\hat{H}_t\hat{P}_{\mathrm{s}}\right]\hat{P}_s\\
&=\frac{1}{2U}\begin{bmatrix}\hat{P}_s\hat{H}_t\left(\hat{P}_{\mathrm{s}}\hat{H}_t\hat{P}_{\mathrm{d}}-\hat{P}_{\mathrm{d}}\hat{H}_t\hat{P}_{\mathrm{s}}\right)\hat{P}_s\\-\hat{P}_s\left(\hat{P}_{\mathrm{s}}\hat{H}_t\hat{P}_{\mathrm{d}}-\hat{P}_{\mathrm{d}}\hat{H}_t\hat{P}_{\mathrm{s}}\right)\hat{H}_t\hat{P}_s\end{bmatrix}\\
&=\frac{1}{2U}\begin{bmatrix}-\hat{P}_s\hat{H}_t\hat{P}_{\mathrm{d}}\hat{H}_t\hat{P}_{\mathrm{s}}\\-\hat{P}_s\hat{H}_t\hat{P}_{\mathrm{d}}\hat{H}_t\hat{P}_s\end{bmatrix}=-\frac{1}{U}\hat{P}_s\hat{H}_t\hat{P}_{\mathrm{d}}\hat{H}_t\hat{P}_{\mathrm{s}}\\
&=-\frac{1}{U}\hat{P}_s\hat{H}_t\hat{P}_{\mathrm{d}}\hat{H}_t\hat{P}_{\mathrm{s}}=-\frac{1}{U}\hat{P}_s\hat{H}_t\hat{H}_t\hat{P}_{\mathrm{s}}=-\frac{1}{U}\hat{H}_t\hat{H}_t\hat{P}_{\mathrm{s}}
\end{aligned}$$

and then we calculate $\hat{H}_t\hat{H}_t$, always remember that it acts on **singly occupied state** because of the $\hat{P}_{\mathrm{s}}$ in front of it (we use this in 3rd, 5th and 7th equality):

$$\begin{aligned}
\hat{H}_t\hat{H}_t\hat{P}_{\mathrm{s}}&=t^2\left(a_{1\sigma}^\dagger a_{2\sigma}+a_{2\sigma}^\dagger a_{1\sigma}\right)\left(a_{1\sigma'}^\dagger a_{2\sigma'}+a_{2\sigma'}^\dagger a_{1\sigma'}\right)\hat{P}_{\mathrm{s}}\\
&=t^2\left(a_{1\sigma}^\dagger a_{2\sigma}a_{1\sigma'}^\dagger a_{2\sigma'}+a_{1\sigma}^\dagger a_{2\sigma}a_{2\sigma'}^\dagger a_{1\sigma'}+a_{2\sigma}^\dagger a_{1\sigma}a_{1\sigma'}^\dagger a_{2\sigma'}+a_{2\sigma}^\dagger a_{1\sigma}a_{2\sigma'}^\dagger a_{1\sigma'}\right)\hat{P}_{\mathrm{s}}\\
&=t^2\begin{pmatrix}-a_{1\sigma}^\dagger a_{1\sigma'}^\dagger a_{2\sigma}a_{2\sigma'}+a_{1\sigma}^\dagger\left(\delta_{\sigma\sigma'}-a_{2\sigma'}^\dagger a_{2\sigma}\right)a_{1\sigma'}\\+a_{2\sigma}^\dagger\left(\delta_{\sigma\sigma'}-a_{1\sigma'}^\dagger a_{1\sigma}\right)a_{2\sigma'}-a_{2\sigma}^\dagger a_{2\sigma'}^\dagger a_{1\sigma}a_{1\sigma'}\end{pmatrix}\hat{P}_{\mathrm{s}}\\
&=t^2\left(a_{1\sigma}^\dagger a_{1\sigma}+a_{2\sigma}^\dagger a_{2\sigma}-a_{1\sigma}^\dagger a_{2\sigma'}^\dagger a_{2\sigma}a_{1\sigma'}-a_{2\sigma}^\dagger a_{1\sigma'}^\dagger a_{1\sigma}a_{2\sigma'}\right)\hat{P}_{\mathrm{s}}\\
&=t^2\left(2+2a_{1\sigma}^\dagger a_{2\sigma'}^\dagger a_{1\sigma'}a_{2\sigma}\right)\hat{P}_{\mathrm{s}}\\
&=2t^2\left(1-2\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2-\frac{1}{2}\hat{n}_1\hat{n}_2\right)\hat{P}_{\mathrm{s}}=2t^2\left(1-2\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2-\frac{1}{2}\right)\hat{P}_{\mathrm{s}}\\
&=-4t^2\left(\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2-\frac{1}{4}\right)\hat{P}_{\mathrm{s}}
\end{aligned}$$

where we have use the identity proved before ("equ:spin_operator") in the last but second line. Finally, we obtain a low-energy effective Hamiltonian:

$$\hat{P}_s \hat{H}' \hat{P}_s = J\left(\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - \frac{1}{4}\right)\hat{P}_s, J = 4t^2/U$$

where $J = 4t^2/U > 0$ denotes the strength of the **anti-ferromagnetic exchange interaction** that couples the spins on neighboring sites.

- Conclusion: electrons subject to a strong local repulsive Coulomb interaction have a tendency to adopt an antiparallel or antiferromagnetic spin configuration between neighboring sites.
  - The final effective **anti-ferromagnetic** Hamiltonian is consistent with our choice of "projected subspace" at the beginning, i.e., the **antiparallel** singly occupied states $|s_i\rangle$.
- Why? What's the difference between parallel neighbor spins and anti-parallel neighbor spins?
  - Anti-parallel spins can take advantage of the hybridization (however small) and reduce their **kinetic energy** by hopping to a neighboring site (see Fig. 2.7).
  - Parallel spins on the other hand are restricted from participating in this **virtual process** by the Pauli principle.
- This virtual process, a mechanism that involves a two-step process,is called **superexchange**, first formulated by Anderson.

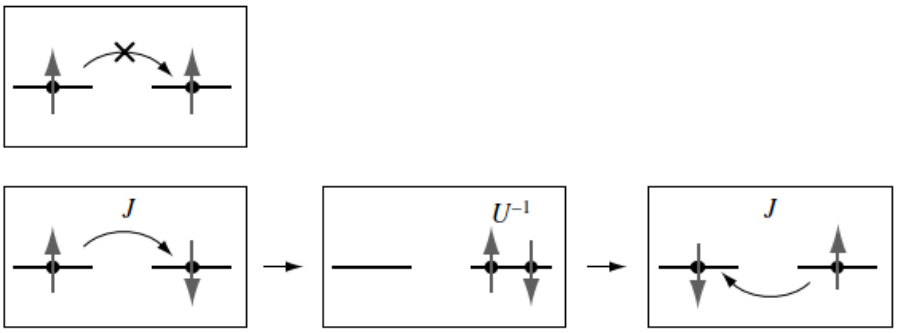


Figure 2.7 Top: hybridization of spin polarized states is forbidden by Pauli exclusion. Bottom: superexchange mechanism by which two antiparallel spins can lower their energy by a virtual process in which the upper Hubbard band is occupied.

  - 两个相邻格点上的电子杂化形成"成键态", 能量降低.

Extended lattice system

Basis states: all sites are singly occupied, and virtual exchange processes favor an antiferromagnetic arrangement of neighboring spins.

So, we can describe this **correlated magnetic insulator** by **quantum spin-(1/2) Heisenberg Hamiltonian**:

$$\hat{H} = J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n$$

- $\langle mn \rangle$: sum over neighboring spins
- $J \sim t^2/U$: positive exchange constant

In the insulating magnetic phase, while the **charge degrees of freedom** remain "quenched", **spin** fluctuations can freely propagate.

t-J Hamiltonian

- Situation: doped away from half-filling, there are vacancies appearing in the "lower Hubbard band".

For a low concentration of holes, the strong coupling Hubbard system may be described by the effective **t–J Hamiltonian**,

$$\hat{H}_{t-J} = -t \sum_{\langle mn \rangle} \hat{P}_s a^\dagger_{m\sigma} a_{n\sigma} \hat{P}_s + J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n.$$

- The vacancies can propagate through the lattice, should be described by hopping term.
- However, the passage of vacancies is frustrated by the antiferromagnetic spin correlations of the background.
  - Transport depends sensitively on the competition between the exchange energy of the spins and the kinetic energy of the holes.
  - When holes are enough, the antiferromagnetic order will be destabilized.
    - At $J = 0$ (i.e. $U = \infty$), the ground state spin configuration is known to be driven ferromagnetic by a **single** hole.

Nagaoka theorem

Let's focus on the limit case, $U = \infty$, where the interaction is very strong. This time, all 2^N states of the half-filled Hubbard model are degenerate, every site is a two-level system, with an arbitrary spin.

Nagaoka theorem: on a bipartite lattice, the ground state is ferromagnetic.

Exercise:

For a four-site “plaquette” with three electrons determine the eigenspectrum of the Hubbard system with $U = \infty$ within the manifold (a) $S^z_{\text{total}} = 3/2$, and (b) $S^z_{\text{total}} = 1/2$.

In each case, determine the total spin of the ground state.
(Hint: In (b) there are a total of 12 basis states – here it useful to arrange these states in the order in which they are generated by application of the Hamiltonian.)

- (a): three electrons are spin up, there are $C_4^3 = 4$ basis states.
- (b): two electrons are spin up, one electron is spin down, there are $C_4^2 C_2^1 = 12$ basis states.

What's the nature of SC? The mechanism of SC is believed to be rooted in the exchange of antiferromagnetic spin **fluctuations**.

Can Hubbard alone is enough to describe this phase diagram? Whether the rich phenomenology of the cuprate system is captured by the Hubbard model remains a subject of great interest and speculation.

Quantum spin chains

- We have seen that charging effects generated by **Coulomb interaction** can lead to indirect generation of magnetic interactions, which is called **quantum magnetic correlations**.
    - In 1d, we can explain this by adding to the structureless electrons a **spin degree of freedom**.
        - Tomonaga-Luttinger liquid: governed by the coexistence of collective spin and charge excitations.
- To learn deeply about **quantum magnetic correlations**, we choose to froze the charge degree of freedom and leave the spin excitations alone.
    - In fact, such systems has been realized. Mott insulators, where interaction between the spins of localized electrons is mediated by virtual exchange processes between neighboring electrons.
- How to describe this kind of correlations?
    - We consider models of **localized quantum spins**, either in chains or in higher-dimensional quantum spin lattices.
- Contents
    - "Quantum Ferromagnet": such as the "exchange coulpings term".
    - "Quantum Antiferromagnet": such as the low-temperature phase of "the Mott insulator"

Quantum Antiferromagnet

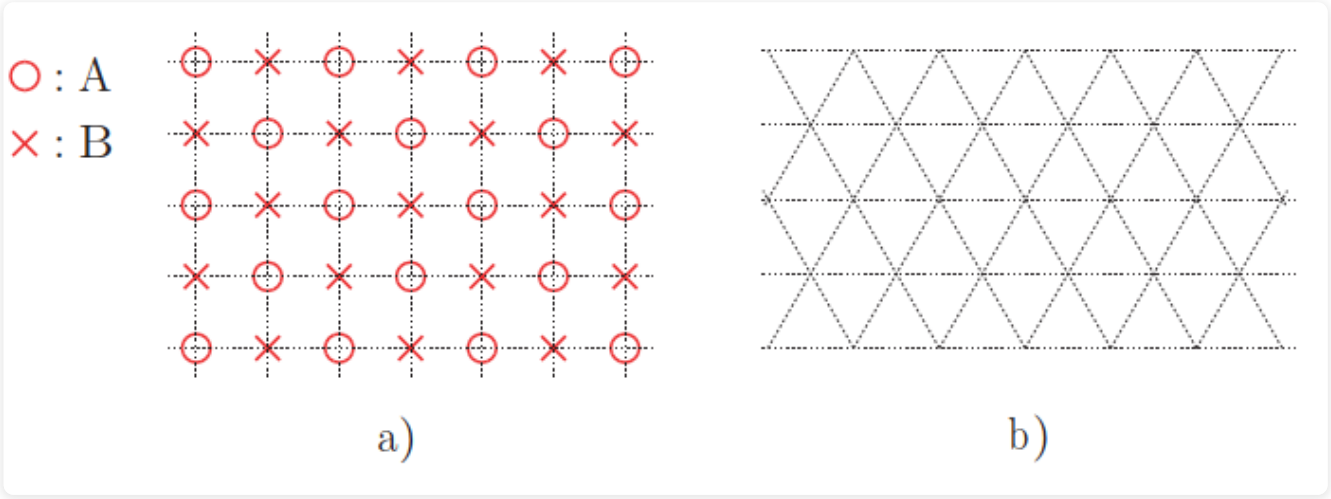
The spin S Heisenberg antiferromagnetic Hamiltonian

$$\hat{H} = J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n, \quad J > 0$$

Dependence of lattice geometry

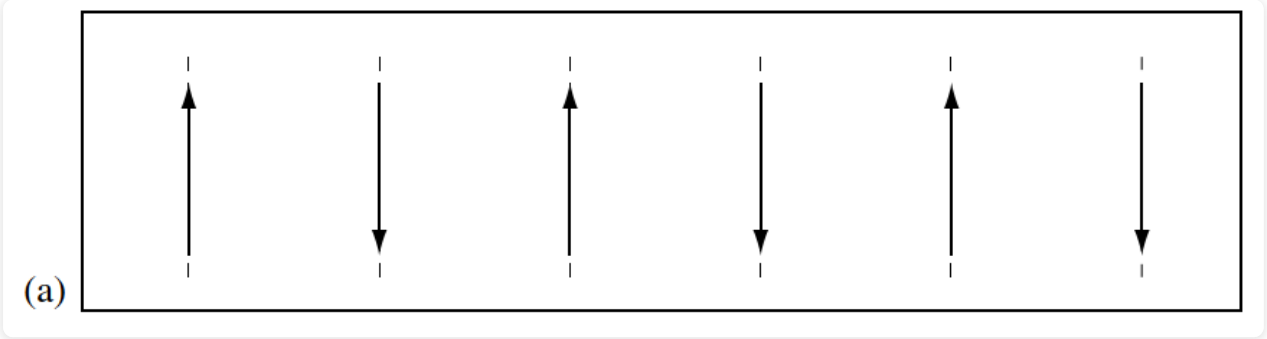
The phenomenology displayed by the antiferromagnetic Hamiltonian $\hat{H}$ depend sensitively on **the geometry of the underlying lattice**.

- Bipartite lattice: see fig a)



(a) Example of a two–dimensional bipartite lattice and (b) a non–bipartite lattice.

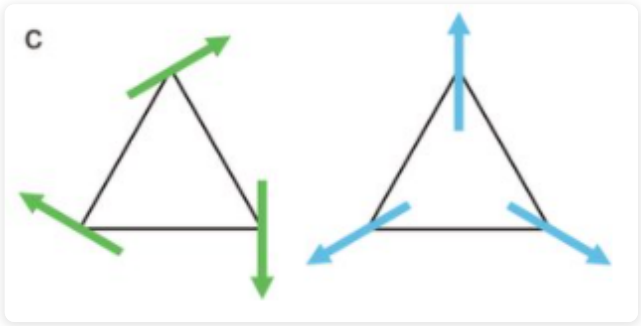
- Ground state of the Heisenberg antiferromagnet: close to **Neel state**.



Neel state configuration of the spin chain

  - Neel state: a staggered(交错的) spin configuration, where **all neighbouring spins are antiparallel**.
  - This ground state is also degenerate, i.e. a **global rotation of all spins** by the same amount does not change the energy.
  - The classical ground state — the Neel state — is now NOT an **exact eigenstate** of the quantum Hamiltonian.

        - The true ground state exhibits **zero–point fluctuations** reminiscent of the quantum harmonic oscillator or atomic chain.
        - However, when $S \gg 1$, it serves as a useful reference state from which fluctuations can be examined.
- Non-biparticle lattice: see fig b), the **triangular lattice**
    - On non–bipartite lattices such as the triangular lattice shown in Fig b), no spin arrangement can be found wherein which each and every bond can recover the full exchange energy J. 在这种晶格中, 没有办法找到一种自旋排列, 可以让每一个键结两端的自旋都是反向的.
    - Spin models of this kind are said to be **frustrated**.
    - Ground state of triangular lattice: Using only **symmetry arguments**, we can specify one of the possible ground states of a classical three site triangular lattice antiferromagnet.



One–dimensional system

$$\hat{H} = J \sum_{m} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}$$

Strategy: expand the Hamiltonian in terms of bosonic operators by Holstein-Primakoff transformation

Firstly, we do a canonical transformation which makes the Neel ground state look like a ferromagnet:

- The spins on one sublattice B, are rotated through 180° about the x-axis.
- $S_B^x \to \widetilde{S}_B^x = S_B^x, S_B^y \to \widetilde{S}_B^y = -S_B^y$, and $S_B^z \to \widetilde{S}_B^z = -S_B^z$

$$
\begin{aligned}
\hat{H} &= J \sum_m \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1} \\
&= J \sum_m \hat{S}^z_m \hat{S}^z_{m+1} + \hat{S}^x_m \hat{S}^x_{m+1} + \hat{S}^y_m \hat{S}^y_{m+1} \\
&\to J \sum_m -\hat{S}^z_m \hat{S}^z_{m+1} + \hat{S}^x_m \hat{S}^x_{m+1} - \hat{S}^y_m \hat{S}^y_{m+1} \\
&= -J \sum_m \left[\hat{S}^z_m \hat{S}^z_{m+1} - \left(\hat{S}^x_m \hat{S}^x_{m+1} - \hat{S}^y_m \hat{S}^y_{m+1} \right) \right] \\
&= -J \sum_m \left[\hat{S}^z_m \hat{S}^z_{m+1} - \frac{1}{2} \left(\hat{S}^+_m \hat{S}^+_{m+1} + \hat{S}^-_m \hat{S}^-_{m+1} \right) \right]
\end{aligned}
$$

Secondly, applying an expansion of the **Holstein-Primakoff representation**:

$$
\hat{S}^z_m = S - a^\dagger_m a_m, \hat{S}^-_m \simeq (2S)^{1/2} a^\dagger_m, \text{ and } \hat{S}^+_m \simeq (2S)^{1/2} a_m
$$

$$
\hat{H} = -NJS^2 + JS \sum_m \left[a^\dagger_m a_m + a^\dagger_{m+1} a_{m+1} + a_m a_{m+1} + a^\dagger_m a^\dagger_{m+1} \right] + \mathcal{O}\left(S^0\right)
$$

Thirdly, doing a "Fourier transformation": $a_m = N^{-1/2} \sum_k e^{-ikm} a_k$

$$
\begin{aligned}
&\sum_m \left[a^\dagger_m a_m + a^\dagger_{m+1} a_{m+1} + a_m a_{m+1} + a^\dagger_m a^\dagger_{m+1} \right] \\
&= \frac{1}{N} \sum_{k,k'} \sum_m \left[\begin{array}{c} e^{i\left(k-k'\right)m} a^\dagger_k a_{k'} + e^{i\left(k-k'\right)(m+1)} a^\dagger_k a_{k'} \\ + e^{-i\left(k+k'\right)m} e^{-ik'} a_k a_{k'} + e^{i\left(k+k'\right)m} e^{ik'} a^\dagger_k a^\dagger_{k'} \end{array} \right] \\
&= \sum_{k,k'} \left[\begin{array}{c} \delta_{k,k'} a^\dagger_k a_{k'} + \delta_{k,k'} a^\dagger_k a_{k'} \\ + \delta_{k,-k'} e^{-ik'} a_k a_{k'} + \delta_{k,-k'} e^{ik'} a^\dagger_k a^\dagger_{k'} \end{array} \right] \\
&= \sum_k \left[a^\dagger_k a_k + a^\dagger_k a_k + e^{ik} a_k a_{-k} + e^{-ik} a^\dagger_k a^\dagger_{-k} \right] \\
&= \sum_k \left[a^\dagger_k a_k + a_{-k} a^\dagger_{-k} - 1 + e^{ik} a_k a_{-k} + e^{-ik} a^\dagger_k a^\dagger_{-k} \right] \\
&= N + \sum_k \left[a^\dagger_k a_k + a_{-k} a^\dagger_{-k} + e^{-ik} a^\dagger_k a^\dagger_{-k} + e^{ik} a_{-k} a_k \right] \\
&= N + \sum_k \begin{pmatrix} a^\dagger_k & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & e^{-ik} \\ e^{ik} & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a^\dagger_{-k} \end{pmatrix}
\end{aligned}
$$

Because the matrix kernel's determinent equals to 0, which may not be so good, we can make use of another form of the above:

$$
\begin{aligned}
&\sum_k \left[a_k^\dagger a_k + a_{-k} a_{-k}^\dagger + e^{-ik} a_k^\dagger a_{-k}^\dagger + e^{ik} a_{-k} a_k\right] \\
&= \sum_k \left[a_k^\dagger a_k + a_{-k} a_{-k}^\dagger + \frac{1}{2}\left(e^{-ik} + e^{ik}\right) a_k^\dagger a_{-k}^\dagger + \frac{1}{2}\left(e^{ik} + e^{-ik}\right) a_{-k} a_k\right] \\
&= \sum_k \left[a_k^\dagger a_k + a_{-k} a_{-k}^\dagger + \cos k a_k^\dagger a_{-k}^\dagger + \cos k a_{-k} a_k\right] \\
&= \sum_k \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}, \quad \gamma_k \equiv \cos k
\end{aligned}
$$

So after HP transformation, we obtain the following Hamiltonian:

$$
\hat{H} = -NJS(S+1) + JS \sum_k \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} + \mathcal{O}\left(S^0\right)
$$

The result above is different from ferromagnet's Fourier transformation, there are **non-particle-number-conserving terms** like $aa, a^\dagger a^\dagger$ appearing in antiferromagnet's case.

In the end, we have to do another canonical transformation to diagonalize this Hamiltonian, which preserves the commutation relations of $a, a^\dagger$. This is **Bogoliubov transformation**

$$
\begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}
$$

$$
\begin{aligned}
\begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} &= \frac{1}{\cosh^2\theta_k - \sinh^2\theta_k} \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} \\
&= \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
&\sum_k \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} \\
&= \sum_k \begin{pmatrix} \alpha_k^\dagger & \alpha_{-k} \end{pmatrix} \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
&\begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} \\
&= \begin{pmatrix} \cosh^2\theta_k + \sinh^2\theta_k + 2\gamma_k \sinh\theta_k \cosh\theta_k & \gamma_k \sinh^2\theta_k + \gamma_k \cosh^2\theta_k + 2\sinh\theta_k \cosh\theta_k \\ \gamma_k \sinh^2\theta_k + \gamma_k \cosh^2\theta_k + 2\sinh\theta_k \cosh\theta_k & \cosh^2\theta_k + \sinh^2\theta_k + 2\gamma_k \sinh\theta_k \cosh\theta_k \end{pmatrix}
\end{aligned}
$$

In order to let the off-diagonal term be zero, we can setting $\tanh 2\theta_k = -\gamma_k$,

$$
\begin{aligned}
&\gamma_k \sinh^2\theta_k + \gamma_k \cosh^2\theta_k + 2\sinh\theta_k \cosh\theta_k \\
&= \gamma_k \cosh 2\theta_k + \sinh 2\theta_k \\
&= \cosh 2\theta_k \left(\gamma_k + \tanh 2\theta_k\right) \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
&\cosh^2\theta_k + \sinh^2\theta_k + 2\gamma_k \sinh\theta_k \cosh\theta_k \\
&= \frac{\cosh 2\theta_k + 1 + \cosh 2\theta_k - 1}{2} + \gamma_k \sinh 2\theta_k \\
&= \cosh 2\theta_k - \tanh 2\theta_k \sinh 2\theta_k \\
&= \cosh 2\theta_k \left(1 - \tanh^2 2\theta_k\right) \\
&= \frac{\left(1 - \tanh^2 2\theta_k\right)}{\sqrt{1 - \tanh^2 2\theta_k}} = \sqrt{1 - \tanh^2 2\theta_k} \\
&= \sqrt{1 - \gamma_k^2} = |\sin k|
\end{aligned}
$$

So we obtain the diagonal Hamiltonian:

$$
\hat{H} = -NJS^2 + 2JS \sum_k |\sin k| \alpha_k^\dagger \alpha_k
$$

- In contrast to the ferromagnet, the spin–wave excitations of the antiferromagnet exhibit a **linear dispersion** in the limit $k \to 0$.

Experiment

Although developed in the limit of large spin $S \gg 1$, experiment shows that even for $S = 1/2$ spin chains, the **linear dispersion** is maintained.

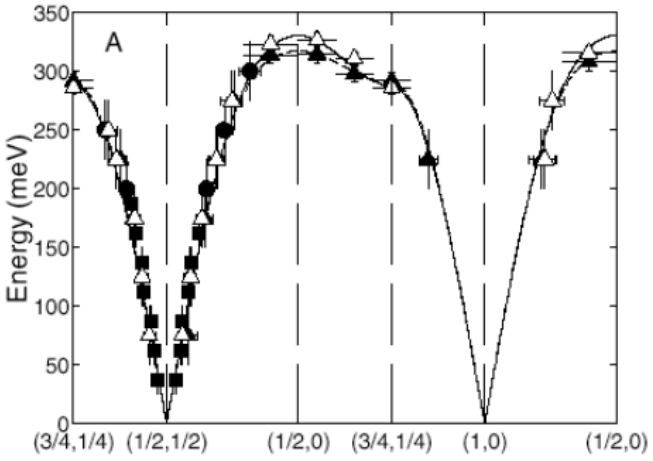


Figure 2.10: Experimentally obtained spin–wave dispersion of the high–T_c parent compound $LaCuO_4$ — a prominent spin 1/2 antiferromagnet. Figure reproduced from R. Coldea *et al.*, Phys. Rev. Lett. **86**, 5377 (2001).

More experiments reveal that:

- For chains of arbitrary half integer spin S =1/2, 3/2, 5/2, . . ., the low-energy spectrum is linear, in agreement with the results of the **harmonic approximation**.
- For chains of integer spin S = 1, 2, 3 . . ., the low-energy spectrum contains a gap, i.e. these systems do not support long-range excitations.

The above phenomenon is related with **topology**:

- As a rule, the sensitivity of a physical phenomenon to the characteristics of **a sequence of numbers** (such as half integer vs. integer) signals the presence of a mechanism of **topological origin**.
    - Specifically, the topological signature of a spin field configuration will turn out to be the number of times the classical analog of a spin (a vector on the unit sphere) will wrap around the sphere in (1 + 1)-dimensional space time.
- At the same time, the formation of a gap (observed for integer chains) represents an **interaction effect**
    - At orders beyond the harmonic approximation, spin waves begin to **interact nonlinearly** with each other, a mechanism that may (S integer) but need not (S half integer) **destroy the-wave like nature** of low-energy excitations.
    - In Section 9.3.3 we will discuss these phenomena on a deeper level.
        - Chapter 9 is devoted to a general discussion of the intriguing condensed matter phenomena generated by the conspiracy of **global (topological) structures with local interaction mechanisms**(具有局部相互作用机制的全局拓扑结构).

Quantum ferromagnet

The **quantum Heisenberg ferromagnet**'s Hamiltonian:

$$\hat{H} = -J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n = -J \sum_m \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}, \quad J > 0$$

- $\hat{\mathbf{S}}_m$: the quantum mechanical spin operator at lattice m
  - In section 2.1, the QM spin was represented through an **electron basis**. However we can think that the spin is carried by a different object, like an atom with non-vanishing magnetic moment.
  - We don't care about the microscopic origin of the spin.
  - All we need to know:
    - the lattice operators $\hat{S}^i_m$ obey the SU(2) commutator algebra

$$\left[\hat{S}^i_m, \hat{S}^j_n\right] = i\delta_{mn}\epsilon^{ijk}\hat{S}^k_n$$

    - Total spin at each lattice site is S. So the finite-dimensional rep. of $\hat{S}^i_m$ are of dimension $2S+1$.

Global rotation symmetry

- **Ground state**: spin polarized ground state, all spins are aligned in the same direction.
  - "A" ground state: $|\Omega\rangle \equiv \otimes_m |S_m\rangle$, where $|S_m\rangle$ represents a state with maximal spin-z component: $\hat{S}^z_m |S_m\rangle = S|S_m\rangle$.

$$\begin{aligned}
\hat{H}|\Omega\rangle &= -J \sum_n \hat{\mathbf{S}}_n \cdot \hat{\mathbf{S}}_{n+1} \bigotimes_m |S_m\rangle \\
&= -J \sum_n \hat{S}^z_n \hat{S}^z_{n+1} \bigotimes_m |S_m\rangle \\
&= -J \sum_n S^2 \bigotimes_m |S_m\rangle \\
&= -NJS^2|\Omega\rangle
\end{aligned}$$

  - **Global rotation symmetry**: this system is highly degenerate, simultaneous change of the orientation of all spins doesn't change the ground state energy.

Defining **global spin operators**:

$$\hat{S}^i \equiv \sum_m \hat{S}^i_m, \quad \hat{\mathbf{S}} \equiv \sum_m \hat{\mathbf{S}}_m$$

we can use this operators to define rotated state $|\boldsymbol{\alpha}\rangle$:

$$|\boldsymbol{\alpha}\rangle \equiv e^{i(\pi/2)\boldsymbol{\alpha}\cdot\hat{\mathbf{S}}}|\Omega\rangle$$

> For example, $|(1,0,0)\rangle$
>
> Explicitly compute the state $|(1,0,0)\rangle$ Convince yourself that for general $\boldsymbol{\alpha}$, $|\boldsymbol{\alpha}\rangle$ can be interpreted as a state with rotated quantisation axis.

We can verify that the state $|\boldsymbol{\alpha}\rangle$ is degenerate with $|\Omega\rangle$, because $\hat{H}$ commute with $\hat{\boldsymbol{\alpha}}\cdot\hat{\mathbf{S}}$ actually:

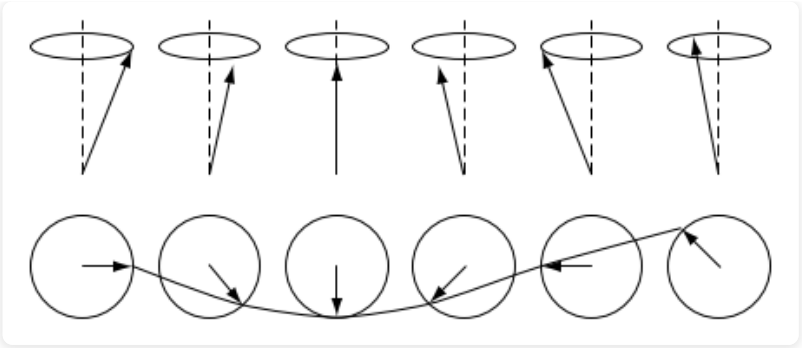
$$\begin{aligned}
\left[\boldsymbol{\alpha}\cdot\hat{\mathbf{S}}, \hat{H}\right] &= \left[\sum_m \boldsymbol{\alpha}\cdot\hat{\mathbf{S}}_m, -J\sum_n \hat{\mathbf{S}}_n\cdot\hat{\mathbf{S}}_{n+1}\right] \\
&= -J\sum_{mn}\sum_{ij}\alpha^i\left[\hat{S}^i_m, \hat{S}^j_n\hat{S}^j_{n+1}\right] \\
&= -J\sum_{mn}\sum_{ij}\alpha^i\left(\hat{S}^j_n\left[\hat{S}^i_m, \hat{S}^j_{n+1}\right] + \left[\hat{S}^i_m, \hat{S}^j_n\right]\hat{S}^j_{n+1}\right) \\
&= -J\sum_{mn}\sum_{ijk}\alpha^i\left(\hat{S}^j_n\delta_{m,n+1}i\epsilon^{ijk}\hat{S}^k_m + \delta_{mn}i\epsilon^{ijk}\hat{S}^k_m\hat{S}^j_{n+1}\right) \\
&= -J\sum_{n}\sum_{ijk}i\alpha^i\left(\epsilon^{ijk}\hat{S}^j_n\hat{S}^k_{n+1} + \epsilon^{ijk}\hat{S}^k_n\hat{S}^j_{n+1}\right) \\
&= -J\sum_{n}\sum_{ijk}i\alpha^i\left(\epsilon^{ijk}\hat{S}^j_n\hat{S}^k_{n+1} - \epsilon^{ijk}\hat{S}^j_n\hat{S}^k_{n+1}\right) \\
&= 0
\end{aligned}$$

$$\hat{H}|\boldsymbol{\alpha}\rangle = \hat{H}e^{i(\pi/2)\boldsymbol{\alpha}\cdot\hat{\mathbf{S}}}|\Omega\rangle = e^{i(\pi/2)\boldsymbol{\alpha}\cdot\hat{\mathbf{S}}}\hat{H}|\Omega\rangle = \left(-NJS^2\right)|\Omega\rangle$$

Low-lying excitations: spin-wave

Above we find a **global continuous symmetry**, so what about the corresponding **energetically low-lying excitations**?

- **Elementary excitation**: spin-wave excitation



Spin-wave excitation

- Long wavelength limit ($\lambda \to \infty$): the excitation energy vanishes.

Semi-classical approximation

- Why?
  - To explore the physics of the spin waves quantitatively, we adopt a "semiclassical" picture.
- What is semi-classical approximation?
  - Spin assumed to be large $S \gg 1$, the rotation of the spins around the ground state configuration becomes similar to the rotation of a **classical magnetic moment**.
  - Heisenberg uncertainty relation: $\Delta S^i \Delta S^j \leq \left|\left\langle \left[\hat{S}^i, \hat{S}^j\right] \right\rangle\right| = \epsilon^{ijk} \left|\left\langle \hat{S}^k \right\rangle\right|$.
    Because $|\langle \hat{S}^k \rangle| \leq S$, we obtain for the the **relative** uncertainty of $\Delta S^i / S$

    $$\frac{\Delta S^i}{S} \frac{\Delta S^j}{S} \leq \frac{S}{S^2} \overset{S \gg 1}{\longrightarrow} 0$$

    i.e. for $S \gg 1$, **quantum fluctuations** of the spin become less important.

Holstein-Primakoff transformation

- Why?
  - In the limit of large spin S(semi-classical approximation), we know that the fluctuation of spins ΔS^i is very small.
  - So it's a good idea to describe the **ordered phase** in terms of **small fluctuations** of the spins around their expectation values.
  - To make use of the fact that deviations around $|\Omega\rangle$ are small, a representation known as the **Holstein-Primakoff transformation** was introduced.
- How?

- These fluctations are conveniently represented in terms of **spin raising and lowering operators** $\hat{S}_m^{\pm} \equiv S_m^x \pm i S_m^y$

$$\left[\hat{S}_m^z, \hat{S}_n^{\pm}\right] = \pm\delta_{mn}\hat{S}_m^{\pm}, \quad \left[\hat{S}_m^+, \hat{S}_n^-\right] = 2\delta_{mn}\hat{S}_m^z$$

  Application of $\hat{S}_m^{-(+)}$ lowers (raises) the z-component of the spin at site m by one.

- **Holstein-Primakoff transformation**: the spin operators $\hat{S}^{\pm}, \hat{S}^z$ are specified in terms of bosonic creation and annihilation operators $a^\dagger$ and a

$$\hat{S}_m^- = a_m^\dagger \left(2S - a_m^\dagger a_m\right)^{1/2}, \quad \hat{S}_m^+ = \left(2S - a_m^\dagger a_m\right)^{1/2} a_m, \quad \hat{S}_m^z = S - a_m^\dagger a_m$$

  - Verify the "above commutation relation"

When $S \gg 1$, we can do Taylor expansion of HP transformation:

$$\hat{S}_m^z = S - a_m^\dagger a_m, \hat{S}_m^- \simeq (2S)^{1/2} a_m^\dagger, \text{ and } \hat{S}_m^+ \simeq (2S)^{1/2} a_m$$

one-dimensional Heisenberg Hamiltonian takes the form

$$\begin{aligned}
\hat{H} &= -J \sum_m \left\{ \hat{S}_m^z \hat{S}_{m+1}^z + \frac{1}{2}\left(\hat{S}_m^+ \hat{S}_{m+1}^- + \hat{S}_m^- \hat{S}_{m+1}^+\right)\right\} \\
&= -JNS^2 + JS \sum_m \left\{ a_m^\dagger a_m + a_{m+1}^\dagger a_{m+1} - \left(a_m^\dagger a_{m+1} + \text{ h.c. }\right)\right\} + \mathcal{O}\left(S^0\right) \\
&= -JNS^2 + JS \sum_m \left(a_{m+1}^\dagger - a_m^\dagger\right)\left(a_{m+1} - a_m\right) + \mathcal{O}\left(S^0\right)
\end{aligned}$$

Bilinear in Bose operators, the approximate Hamiltonian can be diagonalised by Fourier transformation:

- Firstly, we have to introduce **finite length** and **periodic boundary conditions** to do diagonalization $\hat{S}_{m+N}^z = \hat{S}_m^z, a_{m+N} = a_m$.
- Change to Fourier basis from Wannier basis (see "equ:2.24")

$$a_k = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{ikm} a_m, \quad a_m = \frac{1}{\sqrt{N}} \sum_{k}^{\text{B.Z.}} e^{-ikm} a_k, \quad \left[a_k, a_{k'}^\dagger\right] = \delta_{kk'}$$

  - Here, k is dimensionless, $k = 2\pi n/N$, whose unit is $1/a$.

- The Hamiltonian of the **one dimensional lattice system**

$$
\begin{aligned}
&\sum_m \left(a_{m+1}^\dagger - a_m^\dagger\right)\left(a_{m+1} - a_m\right) \\
&= \frac{1}{N}\sum_m \left(\sum_k^{\text{B.Z.}} \left(e^{ik(m+1)} - e^{ikm}\right) a_k^\dagger\right)\left(\sum_{k'}^{\text{B.Z.}} \left(e^{-ik'(m+1)} - e^{-ik'm}\right) a_{k'}\right) \\
&= \frac{1}{N}\sum_m \sum_{kk'}^{\text{B.Z.}} \left(e^{ik(m+1)} - e^{ikm}\right)\left(e^{-ik'(m+1)} - e^{-ik'm}\right) a_k^\dagger a_{k'} \\
&= \sum_{kk'}^{\text{B.Z.}} \frac{1}{N}\sum_m \left(e^{i\left(k-k'\right)m} e^{i\left(k-k'\right)} + e^{i\left(k-k'\right)m} - e^{i\left(k-k'\right)m} e^{-ik'} - e^{i\left(k-k'\right)m} e^{ik}\right) a_k^\dagger a_{k'} \\
&= \sum_{kk'}^{\text{B.Z.}} \delta_{k,k'}\left(e^{i\left(k-k'\right)} + 1 - e^{-ik'} - e^{ik}\right) a_k^\dagger a_{k'} \\
&= \sum_k^{\text{B.Z.}} \left(1 + 1 - e^{-ik} - e^{ik}\right) a_k^\dagger a_k = \sum_k^{\text{B.Z.}} 2\left(1 - \cos k\right) a_k^\dagger a_k
\end{aligned}
$$

- In the fourth equator, we use "equ:possion_summation".

Finally, we obtain the low energy Hamiltonian and dispersion relation of the spin excitations:

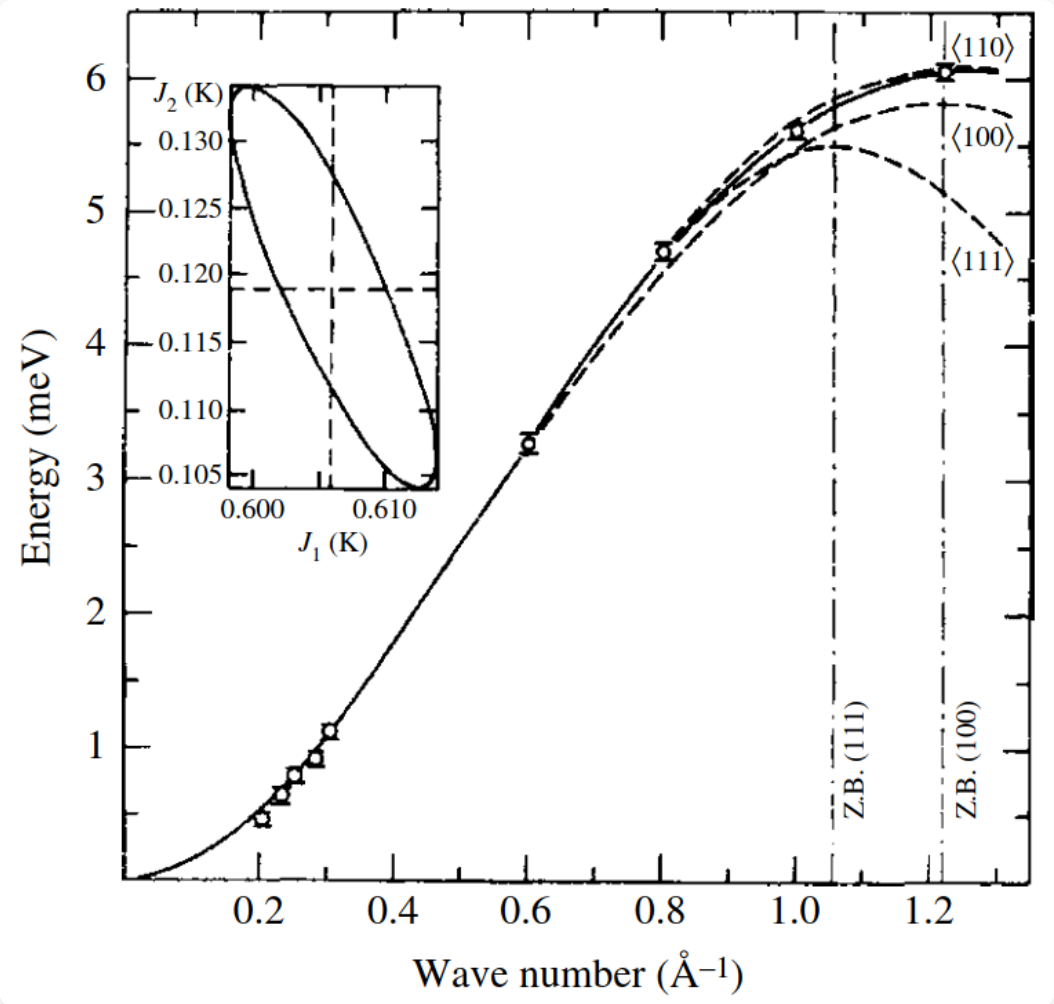
$$
\begin{aligned}
\hat{H} &= -JNS^2 + \sum_k^{\text{B.Z.}} \omega_k a_k^\dagger a_k + \mathcal{O}\left(S^0\right) \\
\omega_k &= 2JS(1 - \cos k) = 4JS\sin^2(k/2)
\end{aligned}
$$

Magnon

The elementary spin-wave excitations of the ferromagnet are called **magnons**.

- Every magnon with momentum k carries energy ω_k.
- In the long wavelength limit $k \to 0$, $\omega_k \to JSk^2$, the energy of the elementary excitation vanishes.
- Taking into account terms at higher order in the parameter $1/S$, one finds interactions between the magnons.

The comparison of theoretical predictions and experiment measurements of magon's dispersion relation:



- Experiment measurements: Spin-wave spectrum of europium oxide(氧化铕) as measured by **inelastic neutron scattering** at a reference temperature of 5.5K.
  - L. Passell, O. W. Dietrich, and J. Als-Nielser, Neutron scattering from the Heisenberg ferromagnets EuO and EuS I: the exchange interaction, Phys. Rev. B 14 (1976), 4897–907.
- At low values of momenta q, the dispersion is quadratic, in agreement with the low-energy theory.

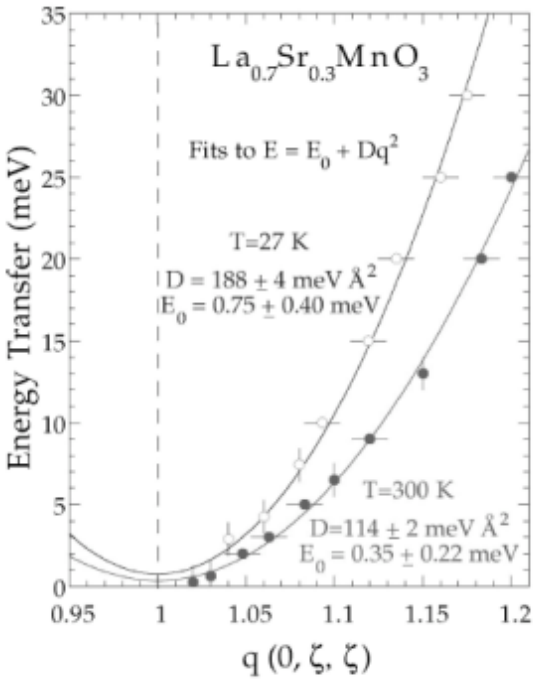


Figure 2.8: Measurements of the spin-wave dispersion relations for the ferromagnet $La_{0.7}Sr_{0.3}MnO_3$.