Exact diagonalization of 2D systems (simple square lattice)

Label lattice sites and bonds

- Hamiltonian construction very similar to 1D chains using site and bond maps

\[ |a(k)\rangle = |a(k_x, k_y)\rangle = \frac{1}{\sqrt{N_a}} \sum_{x=1}^{L_x} \sum_{y=1}^{L_y} e^{-i(k_x x + k_y y) T_y T_x} |a\rangle \]

\[ k_\gamma = \frac{2\pi}{L_\gamma} m_\gamma, \quad m_\gamma = 0, 1, \ldots, L_\gamma - 1, \quad \gamma = x, y \]

2D momentum states \((L_x \times L_y\) lattice)

In this case it is very difficult to construct a real-valued basis

- Use complex momentum states
- Reflection (and/or rotation) symmetries can be used for special momenta

Monday, April 19, 2010
Using reflection symmetries (LxL lattice)

There are 8 different transformations of a square
- combination of reflections and rotations
- can choose the most convenient operations

\[
\begin{pmatrix}
4 & 3 \\
1 & 2
\end{pmatrix}
\begin{pmatrix}
3 & 2 \\
4 & 1
\end{pmatrix}
\begin{pmatrix}
2 & 1 \\
3 & 4
\end{pmatrix}
\begin{pmatrix}
1 & 4 \\
2 & 3
\end{pmatrix}
\begin{pmatrix}
3 & 4 \\
2 & 1
\end{pmatrix}
\begin{pmatrix}
2 & 3 \\
1 & 4
\end{pmatrix}
\begin{pmatrix}
1 & 2 \\
4 & 3
\end{pmatrix}
\begin{pmatrix}
4 & 1 \\
3 & 2
\end{pmatrix}
\]

General form of the momentum state with other symmetries

\[
|a^{\sigma}(k, \{q\})\rangle = \frac{1}{\sqrt{N_a}} \sum_{r_x=1}^{L_x} \sum_{r_y=1}^{L_y} e^{-i(k_x x + k_y y)} T^r_x T^r_y Q |a\rangle
\]

Using three reflections; \(P_x, P_y, P_d\)

\[
Q = \begin{cases}
1, \\
(1 + p_x P_x), \\
(1 + p_y P_y), \\
(1 + p_e P_e)(1 + p_d P_d), \\
(1 + p_d P_d)(1 + p_y P_y)(1 + p_x P_x), 
\end{cases}
\quad \text{general } k
\]

\[
k = (0, k_y), (\pi, k_y) \\
k = (k_x, 0), (k_x, \pi) \\
k_x = \pm k_y \\
k = (0, 0), (\pi, \pi), \quad p_x = p_y
\]
Lanczos results for the 2D Heisenberg model

Ground state and lowest spin-S excitations on 4×4 and 6×6 lattices

A fundamental aspect of the Néel state: **Quantum-rotor excitations**

- lowest-energy excitations of finite lattices
- not captured by spin-wave theory
- correspond to global rotations of the Neel order (frozen in spin-wave theory)

Consider sublattices as two big spins

- \( S_A, S_B \sim N/2 \)
- effective interactions \( J_{AB} \sim S_A \cdot S_B / N \)
- leads to \( \Delta S = E_S - E_0 \sim S(S+1)/N \)
- \( S \) = total spin of the excitation

staggered spin correlations show signs of order in the ground state

- but larger systems required to confirm (QMC)

 Corrections to quantum-rotor energies seen for small systems

- quantum rotor energies should be good for \( S \ll N \)