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Investigation of ground state and excited states of Anti-ferromagnetic Heisenberg on Honeycomb lattice using RVB wave function

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Resonating Valence Bond Wave Function

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The standard S=1/2 Heisenberg model

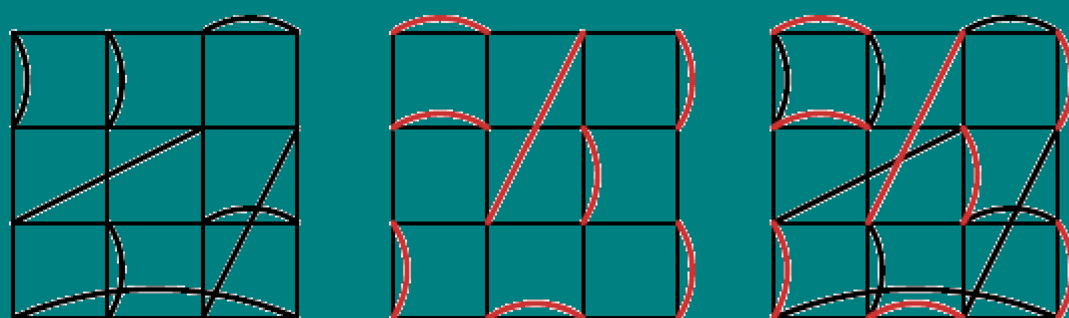
$$H = J\sum_{\langle i,j\rangle} S_i . S_j$$

The General form of a RVB wave function for N S=1/2 spins

$$|\Psi\rangle = \sum_k f_k \left|(a_1^k, b_1^k)\ldots(a_{N/2}^k, b_{N/2}^k)\right\rangle$$

$$(a,b) = \frac{1}{\sqrt{2}}(\uparrow_a\downarrow_b - \uparrow_b\downarrow_a) \qquad f_k = \prod_{i=1}^{N/2} h(a_i^k, b_i^k)$$

$$|V_k\rangle = \left|(a_1^k, b_1^k)\ldots(a_{N/2}^k, b_{N/2}^k)\right\rangle$$



$|V_k\rangle$ $\quad$ $|V_l\rangle$ $\quad$ $\langle V_k|V_l\rangle$

Resonating Valence Bond Wave Function

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The expectation value of energy is

$$E = \langle \Psi | H | \Psi \rangle = \frac{\sum_{kl} f_k f_l \langle V_k | V_l \rangle \frac{\langle V_k | H | V_l \rangle}{\langle V_k | V_l \rangle}}{\langle \Psi | \Psi \rangle}$$

The overlap between two different configurations

$$\langle V_k | V_l \rangle = 2^{N(V_k, V_l)}$$

If i,j belong to two different loops

$$\frac{\langle V_k | S_i . S_j | V_l \rangle}{\langle V_k | V_l \rangle} = 0$$

If i,j belong to the same loop

$$\frac{\langle V_k | S_i . S_j | V_l \rangle}{\langle V_k | V_l \rangle} = \pm \frac{3}{4}$$

Metropolis Algorithm

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The expectation value of energy is

$$C_{i,j} = \sum_{kl} (f_k f_l \langle V_k | V_l \rangle / \langle \Psi | \Psi \rangle) \frac{\langle V_k | S_i . S_j | V_l \rangle}{\langle V_k | V_l \rangle}$$

The weight of each term

$$P(V_k, V_l) = f_k f_l \langle V_k | V_l \rangle / \langle \Psi | \Psi \rangle$$

The fictitious energy for each pair configuration

$$E = Log(P(V_k, V_l))$$

The Metropolis acceptance probability

$$P = \min \left[\frac{h(x_{ad}, y_{ad}) h(x_{cb}, y_{cb})}{h(x_{ab}, y_{ab}) h(x_{cd}, y_{cd})} 2^{\Delta N_l}, 1 \right]$$

S. Liang, B. Doucut and P.W. Anderson, Phys. Rev. Let., 61, 365 (1988)

Optimization Methods

Newton Conjugate Gradient Method

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Writing the energy expectation value as

$$\langle E \rangle = \frac{\sum_p W_p E_p}{\sum_p W_p}, W_p = \prod h(x,y)^{n_{xy}}$$

The updating of the amplitude from iteration n to n+1

$$h_{n+1} = h_n - \frac{E_g'(h_n)}{E_g''(h_n)} \qquad \frac{\partial \langle E \rangle}{\partial h_a} = \left\langle \frac{n_a}{h_a} E \right\rangle - \left\langle \frac{n_a}{h_a} \right\rangle \langle E \rangle$$

Stochastic method

$$\ln(h_a^{n+1}) = \ln(h_a^n) - R\beta.sign(\frac{\partial \langle E \rangle}{\partial h_a})_n$$

arXiv: cond-mat/0605034

Ground states of RVB wave function

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In order to find ground state energy, we use VMC method.

The states can be defined variational parameters

$$a_l = \frac{h(2l+1)}{h(2l-1)} \quad \text{or} \quad h(l)$$

L is Manhatan distance. It is the number of links between point.

The different kinds of weight factors

1. Nearest neighbor RVB $\quad h(1)=1; \forall l>1, h(l)=0$

2. Power law weight factor $\quad h(1)=1; h(3)=a_1 h(1); h(5)=a_2 h(3)$

$$\forall l>5, h(l)=h(5)(l/5)^{-p}$$

3. Exponential weight factor $\quad h(1)=1; h(3)=a_1 h(1); h(5)=a_2 h(3)$

$$\forall l>5, h(l)=a_l h(5)$$

Ground states of RVB wave function

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State	-E/J	parameters
Dimmer	0.4310	h(1)=1
Power law	0.5450 0.5462	(0.13,0.22) P=2.5
Exponential	0.5438	(0.195,0.25) 0.33

The spin-spin correlation $$C(r) = (-1)^{(x+y)} \sum_i \langle S_i . S_{i+r} \rangle$$

The staggered magnetization can be determined from the tail of spin-spin correlation

$$M_s = \sqrt{\lim_{r \to L/2} \frac{C_{zigzag}(r) + C_{armchair}}{2}} = 0.26$$

$$\frac{E_{RVB}}{E_{Neel}} = \frac{0.5462}{0.3750} = 1.45$$

From Ground states to excited states

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Using the single mode approximation to evaluate the excited states energies

The excited state in SMA
$$\left|k\right\rangle = \sum_r e^{i\vec{k}.\vec{r}} \sigma_z(r)\left|\psi\right\rangle = \sum_r e^{i\vec{k}.\vec{r}} \sum_k f_k \left|V_k^r\right\rangle$$

The expectation values of the excited state energy

$$E(k) = \frac{\left\langle k\middle|H\middle|k\right\rangle}{\left\langle k\middle|k\right\rangle}$$

$$E(k) = \sum_{r,r'} \left(\sum_{k,l} P(V_k, V_l) \frac{\left\langle V_k^{\,r}\middle|H\middle|V_l^{\,r'}\right\rangle}{\left\langle k\middle|k\right\rangle}\right) e^{i\vec{k}.(\vec{r}-\vec{r}')}$$

$$E(k) = \sum_{r,r'} E(r,r') e^{i\vec{k}.(\vec{r}-\vec{r}')}$$

$$E(r,r') = E(r',r) = E(r-r')$$

From Ground states to excited states

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$$\langle V_k | V_l \rangle = \pm 2^{N(V_k, V_l)}$$

1. $$r \in l, r' \in l', i \in l'' \Rightarrow \frac{\langle V_k^r | S_i . S_j | V_l^{r'} \rangle}{\langle V_k^r | V_l^{r'} \rangle} = 0$$

2. $$r, i \in l; r', j \in l' \Rightarrow \frac{\langle V_k^r | S_i . S_j | V_l^{r'} \rangle}{\langle V_k^r | V_l^{r'} \rangle} = \pm \frac{1}{4}$$

3. $$r, r' \in l; i, j \in l' \Rightarrow \frac{\langle V_k^r | S_i . S_j | V_l^{r'} \rangle}{\langle V_k^r | V_l^{r'} \rangle} = \pm \frac{3}{4}$$

4. $$r, r', i, j \in l \Rightarrow \frac{\langle V_k^r | S_i . S_j | V_l^{r'} \rangle}{\langle V_k^r | V_l^{r'} \rangle} = \pm \frac{3}{4}, \pm \frac{1}{4}$$

From Ground states to excited states

Comparison with the analytical spin wave calculation

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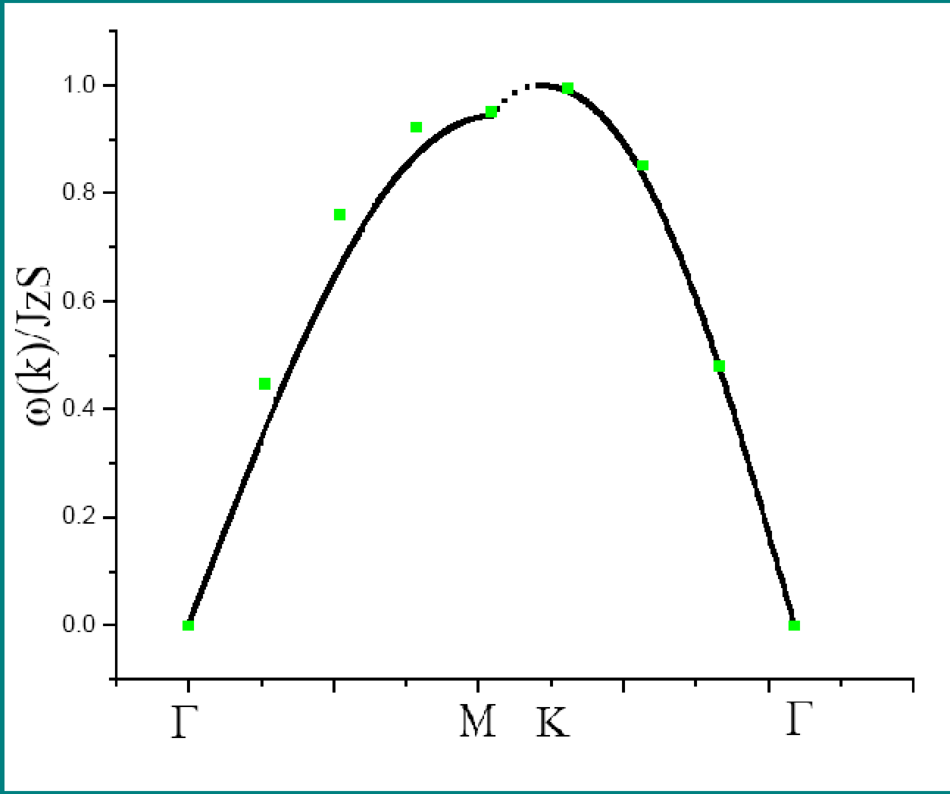
$$\omega(k) = JzS\sqrt{1-\gamma^{k}} \qquad \gamma^{k} = \frac{1}{z}\sum_{\delta} e^{i\vec{k}.\vec{r}}$$



Spin wave calculation is presented by solid line.
Points indicate numerical calculations

Conclusion

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1. The long range RVB states gives a good description of the ground state for nearest neighbor AF Heisenberg model on honeycomb lattice.

2. A fraction of classical Neel order survive in spite of the strong quantum fluctuation

3. Single mode triplet excitations above our optimized RVB states compare well with spin wave theory

Thank for your attention