# Variational wave functions for quantum phonons coupled to spins

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Correlated Systems with Multicomponent Local Hilbert Spaces
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UNIVERSITÀ DEGLI STUDI DI TRIESTE

F. Ferrari, R. Valenti, and FB, Phys. Rev. B **102**, 125149 (2020)

F. Ferrari, R. Valenti, and FB, work in progress

1. Motivations

2. Variational wave functions for the spin-phonon problem

3. Results
   - The one-dimensional Heisenberg model
   - The one-dimensional $J_1 - J_2$ Heisenberg model
   - The $J_1 - J_2$ Heisenberg model on the square lattice (no phonons)
   - Preliminary results with phonons

4. Conclusions

**Phonons are ubiquitous in solid-state physics**
**(Multicomponent Hilbert space)**

- Mainly considered in metals for superconducting instabilities

H. Frölich, Adv. Phys. **3**, 325 (1954)

J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957)

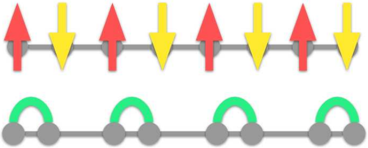
- Phonons are also relevant in Mott insulators

**The superexchange coupling $J$ is affected by lattice vibrations**

**Spin-Peierls transition in one-dimensional magnets**

J.P. Boucher and L.P. Regnault, J. Phys. I **6**, 1939 (1996)

M.C. Cross and D.S. Fisher, Phys. Rev. B **19**, 402 (1979)



**Phonons as probes to spin instabilities in two-dimensional systems**

- There is an increasing evidence for gapless spin-liquids in frustrated magnets

  Heisenberg model on the Kagome lattice

  Y. Iqbal, F. Becca, S. Sorella, and D. Poilblanc, Phys. Rev. B **87**, 060405 (2013)

  Y.-C. He, M.P. Zaletel, M. Oshikawa, and F. Pollmann, Phys. Rev. X **7**, 031020 (2017)

  $J_1 - J_2$ Heisenberg model on the square lattice

  L. Wang and A.W. Sandvik, Phys. Rev. Lett. **121**, 107202 (2018)

  F. Ferrari and F. Becca, Phys. Rev. B **102**, 014417 (2020)

  Y. Nomura, M. Imada, arXiv:2005.14142

  W.-Y. Liu, S.-S. Gong, Y.-B. Li, D. Poilblanc, W.-Q. Chen, Z.-C. Gu, arXiv:2009.01821

**Is the gapless spin liquid unstable to lattice distortions?**

**What is the pattern of lattice displacements?**

**The spin-phonon problem is generically very complicated**

- Often, an effective (purely electronic) Hamiltonian is considered (superconductivity)
- Large (infinite) Hilbert space even on small sizes

  Limitations for Exact diagonalization and DMRG calculations

  DMFT for superconductivity or polaron formation

**The adiabatic limit has been considered**

A.E. Feiguin, J.A. Riera, A. Dobry, and H.A. Ceccatto, Phys. Rev. B **56**, 14607 (1997)

D. Augier, J. Riera, and D. Poilblanc, Phys. Rev. B **61**, 6741 (2000)

F. Becca and F. Mila, Phys. Rev. Lett. **89**, 037204 (2002)

F. Becca, F. Mila, and D. Poilblanc, Phys. Rev. Lett. **91**, 067202 (2003)

**Here, we define variational wave functions**

H. Watanabe, K. Seki, and S. Yunoki, Phys. Rev. B **91**, 205135 (2015)

T. Ohgoe and M. Imada, Phys. Rev. Lett. **119**, 197001 (2017)

S. Karakuzu, L. F. Tocchio, S. Sorella, and F. Becca, Phys. Rev. B **96**, 205145 (2017)

# Quantum phonons in one dimension (the SSH model)

**Let us start softly**

- On each site there is one phonon (oscillations along the chain)
- The spin-spin super-exchange is coupled (linearly) to displacements
- For the Heisenberg model with nearest-neighbor interactions the Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^{L} \left[ J + g(a^{\dagger}_{i+1} + a_{i+1} - a^{\dagger}_{i} - a_{i}) \right] \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \omega \sum_{i=1}^{L} \left( a^{\dagger}_{i} a_{i} + \frac{1}{2} \right)$$

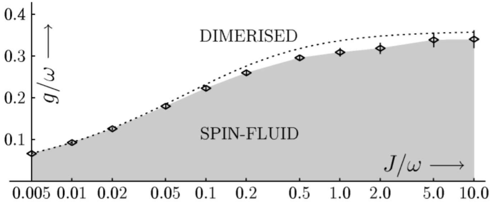
- Or equivalently , with $X_j = (a^{\dagger}_{j} + a_{j})$ and $P_j = i(a^{\dagger}_{j} - a_{j})$

$$\mathcal{H} = \sum_{i=1}^{L} [J + g(X_{i+1} - X_i)] \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{\omega}{4} \sum_{i=1}^{L} \left[ P_i^2 + X_i^2 \right]$$

- Optical phonons

# Old DMRG results for optical phonons

$$\mathcal{H} = \sum_{i=1}^{L} \left[ J + g(a^\dagger_{i+1} + a_{i+1} - a^\dagger_i - a_i) \right] \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \omega \sum_{i=1}^{L} \left( a^\dagger_i a_i + \frac{1}{2} \right)$$




- Peierls transition at finite spin-phonon couplings
- Good agreement with perturbative approaches ($J \ll \omega$)

$$J_1 \approx J + \frac{g^2}{\omega} - \frac{3g^2 J}{2\omega^2}$$

$$J_2 \approx \frac{g^2}{2\omega} + \frac{3g^2 J}{2\omega^2}$$

R.J. Bursill, R.H. McKenzie, and C.J. Hamer, Phys. Rev. Lett. **83**, 408 (1999)

G.S. Uhrig, Phys. Rev. B **57**, 14004 (1998); A. Weisse, G. Wellein, and H. Fehske, Phys. Rev. B **60**, 6566 (1999)

- Alternatively, acoustic phonons correspond to

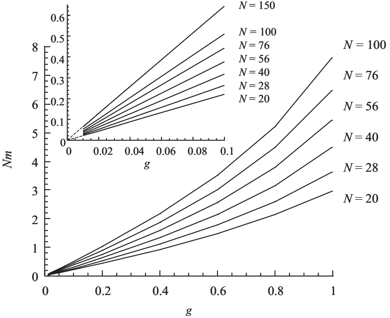
$$\mathcal{H} = \sum_{i=1}^{L} [J + g(X_{i+1} - X_i)] \, \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{\omega}{4} \sum_{i=1}^{L} \left[ P_i^2 + (X_{i+1} - X_i)^2 \right]$$

- Some evidence that the Peierls transition takes place at $g = 0$

$$m(N) = \frac{1}{N} \sum_i (-1)^{R_i} \langle X_{i+1} - X_i \rangle$$

$$m(N) = \frac{1}{Ng} F[Nm(\infty)]$$

E. Fradkin and J.E. Hirsch, Phys. Rev. B **27**, 1680 (1983)




W. Barford and R.J. Bursill, Phys. Rev. Lett. **95**, 137207 (2005)

- The full wave function for the spin-phonon problem is defined as

$$|\Psi_0\rangle = \mathcal{J}_{sp}|\Psi_s\rangle \otimes |\Psi_p\rangle$$

  - $|\Psi_s\rangle$ is the spin part (Gutzwiller projected fermions)
  - $|\Psi_p\rangle$ is the phonon part (free phonons)
  - $\mathcal{J}_{sp}$ is a Jastrow spin-phonon term

    Option 1: couple spins to the phonon numbers (bad)

    Option 2: couple spins to the phonon displacement (good)

- No truncation in the phonon Hilbert space
- "Backflow" could be implemented in the future...

- Start from an uncorrelated BCS Hamiltonian

$$\mathcal{H}_0 = \sum_{i,j,\sigma} t_{i,j} c^\dagger_{i,\sigma} c_{j,\sigma} + \sum_{i,j} \Delta_{i,j} c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + h.c.$$

$\{t_{i,j}\}$ and $\{\Delta_{i,j}\}$ define the mean-field Ansatz

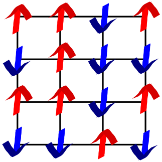
- Obtain the ground state $|\Phi_0\rangle$

- Apply the Gutzwiller projector $\mathcal{P}_G$ and the spin-spin Jastrow factor $\mathcal{J}_{ss}$

$$\boxed{|\Psi_s\rangle = \mathcal{J}_{ss} \mathcal{P}_G |\Phi_0\rangle}$$

$$\mathcal{P}_G = \prod_i (n_{i,\uparrow} - n_{i,\downarrow})^2$$

$$\mathcal{J}_{ss} = \exp\left[\frac{1}{2} \sum_{i,j} v_{ss}(i,j) S^z_i S^z_j\right]$$



- Take the coherent state for the phonon modes with momentum $k$

$$|\Psi_p\rangle = \exp(z a_k^\dagger)|0\rangle_p = \prod_j \exp(z e^{ikR_j} a_j^\dagger)|0\rangle_p$$

The real variable $z$ is a fugacity variational parameter which determines

$$\langle n_j \rangle_p = \frac{\langle \Psi_p | a_j^\dagger a_j | \Psi_p \rangle}{\langle \Psi_p | \Psi_p \rangle} = z^2$$

$$\langle X_j \rangle_p = \frac{\langle \Psi_p | (a_j^\dagger + a_j) | \Psi_p \rangle}{\langle \Psi_p | \Psi_p \rangle} = 2z \cos(kR_j)$$

- The momentum $k$ modulates the direction of sites displacements

(the Peierls instability corresponds to $k = \pi$)

- Spin-phonon coupling with densities

$$\mathcal{J}_{sp} = \mathcal{J}_n = \exp\left[\sum_{i,j} v_n(i,j) S_i^z S_j^z n_j\right]$$

Monte Carlo sampling in the Fock space with given $\{n_i\}$

$$|\Psi_p\rangle = \sum_{n_1,\ldots,n_L} \frac{z^{N_p} e^{ik\sum_j R_j n_j}}{\sqrt{n_1!\cdots n_L!}} |n_1,\ldots,n_L\rangle$$

- Spin-phonon coupling with displacements

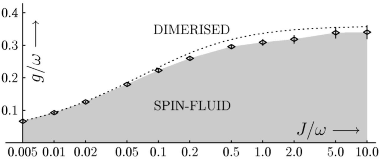
$$\mathcal{J}_{sp} = \mathcal{J}_X = \exp\left[\frac{1}{2}\sum_{i,j} v_X(i,j) S_i^z S_j^z (X_i - X_j)\right]$$

Monte Carlo sampling in the real space with given $\{X_i\}$

$$|\Psi_p\rangle = \int dX_1\cdots dX_L \left[\prod_j e^{\phi_j(X_j)}\right] |X_1,\ldots,X_L\rangle$$

$$\phi_j(X_j) = iz\sin(kR_j)X_j - \frac{1}{4}[X_j - 2z\cos(kR_j)]^2$$

# Comparison with exact results



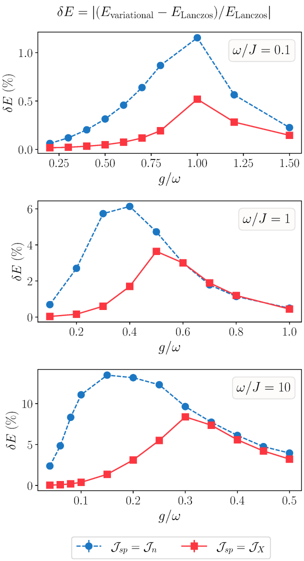

**8 sites with $n_{\max} = 5$**

**Lanczos vs VMC**

**Jastrow term with**

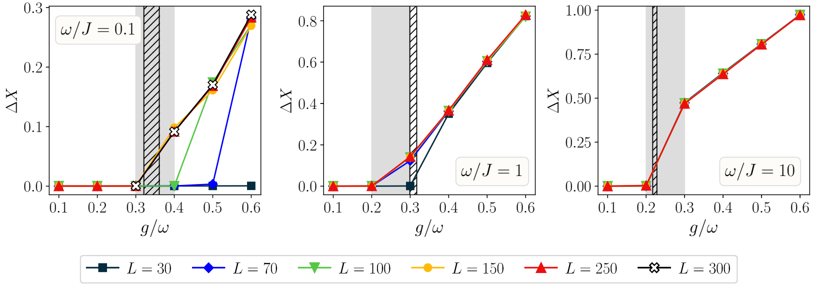
**i) occupation numbers**

**ii) displacements**



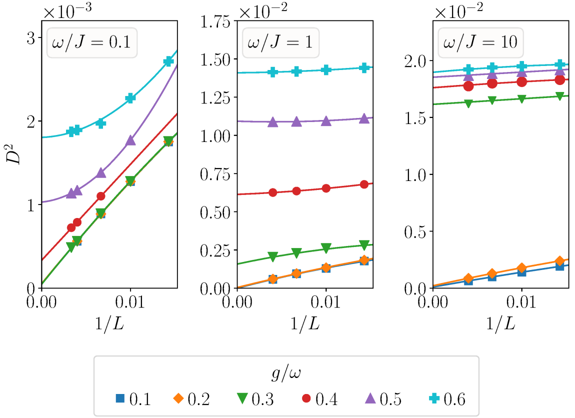
- Average phonon displacement at $k = \pi$

$$\Delta X = \left| \frac{1}{L} \sum_{j=1}^{L} e^{i\pi R_j} \langle X_j \rangle_0 \right|$$

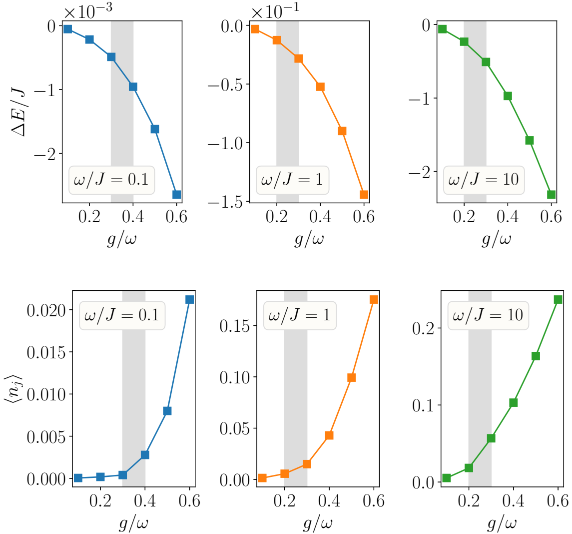


- Dimer-dimer ($z$-component) at $k = \pi$

$$D^2 = \frac{1}{L} \sum_{R=0}^{L-1} e^{i\pi R} \left( \frac{1}{L} \sum_{j=1}^{L} \langle S_j^z S_{j+1}^z S_{j+R}^z S_{j+R+1}^z \rangle_0 \right)$$

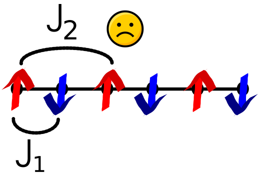


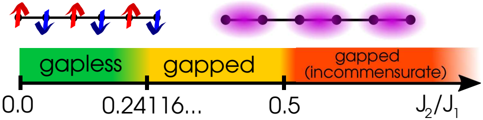
$$\Delta E = [E_{\text{var}}(g,\omega,J) - E_{\text{var}}(g=0,\omega=0,J)]/L$$



- The simplest model with spin frustration in one dimension

$$\mathcal{H} = J_1 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}$$




- Gapless phase for $J_2/J_1 < 0.241167(5)$
- Gapped (dimerized) phase for $J_2/J_1 > 0.2411674(2)$
- Incommensurate spin-spin correlations for $J_2/J_1 \gtrsim 0.5$


H. Bethe, Z. Phys. **71**, 205 (1931)

C.K. Majumdar and D.K. Ghosh, J. Math. Phys. **10**, 1388 (1969)

S. Eggert, Phys. Rev. B **54**, 9612 (1996)

A.W. Sandvik, AIP Conf. Proc. **1297**, 135 (2010)

# Low-energy singlets and triplets

- **In 1D, the transition is located by looking at the singlet-triplet crossing**

K. Okamoto and K. Nomura, Phys. Lett. A **169**, 443 (1992)

G. Castilla, S. Chakravarty, and V.J. Emery, Phys. Rev. Lett. **75**, 1823 (1995)

- In the gapless region, the lowest-energy state is a triplet
- In the gapped region, the lowest-energy state is a singlet
- A the transition, the umklapp scattering vanishes and they are degenerate

The transition can be precisely located by exact calculations on small sizes ($L \approx 20$). Here, $\alpha = J_2/J_1$

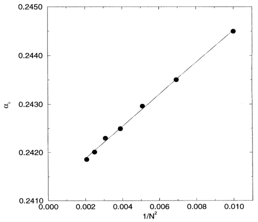



FIG. 1. $\alpha_c(N)$ vs $1/N^2$. The linear fit gives the intercept $\alpha_c = 0.2412$.

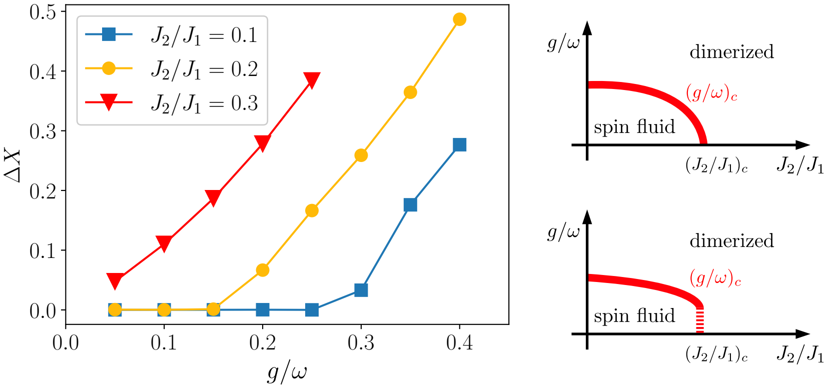
- **The best calculation gives $J_2/J_1 = 0.2411674(2)$**

A.W. Sandvik, AIP Conf. Proc. **1297**, 135 (2010)

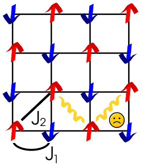
- The nearest-neighbor super-exchange is coupled to displacements

$$\mathcal{H} = \sum_{i=1}^{L} [J_1 + g(X_{i+1} - X_i)] \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_{i=1}^{L} \mathbf{S}_i \cdot \mathbf{S}_{i+2} + \frac{\omega}{4} \sum_{i=1}^{L} \left[ P_i^2 + X_i^2 \right]$$

- $\omega/J = 0.1$ and 200 sites



$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$




- Infinitely many papers with partially contradictory results


W.-J. Hu, F. Becca, A. Parola, and S. Sorella, Phys. Rev. B **88**, 060402 (2013)

S.-S. Gong *et al.*, Phys. Rev. Lett. **113**, 027201 (2014)

S. Morita, R. Kaneko, and M. Imada, J. Phys. Soc. Jpn. **84**, 024720 (2015)

L. Wang *et al.*, Phys. Rev. B **94**, 075143 (2016)

D. Poilblanc and M. Mambrini, Phys. Rev. B **96**, 014414 (2017)

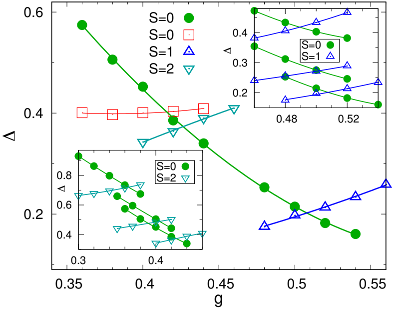
R. Haghshenas and D.N. Sheng, Phys. Rev. B **97**, 174408 (2018)

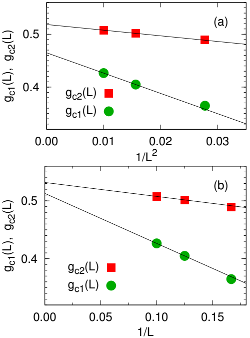
K. Choo, T. Neupert, and G. Carleo, Phys. Rev. B **100**, 125124 (2019)


- Recently, there is an emerging consensus on the phases diagram

- **In 2D, recent DMRG calculations highlighted a couple of level crossings** (on a cylinder geometry $2L \times L$ with $L = 6$, 8, and 10. Here $g = J_2/J_1$)

L. Wang and A.W. Sandvik, Phys. Rev. Lett. **121**, 107202 (2018)




- The singlet-quintuplet crossing corresponds to Néel to SL transition
- The singlet-triplet crossing corresponds to the SL to valence-bond solid

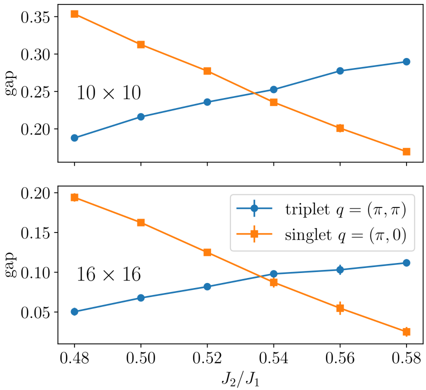
- On $6 \times 6$ for $J_2/J_1 = 0.5$:

  **Ground-state accuracy** 0.5% ($E_{ex}/J_1 = -0.50381$ vs $E_{var}/J_1 = -0.50116$)

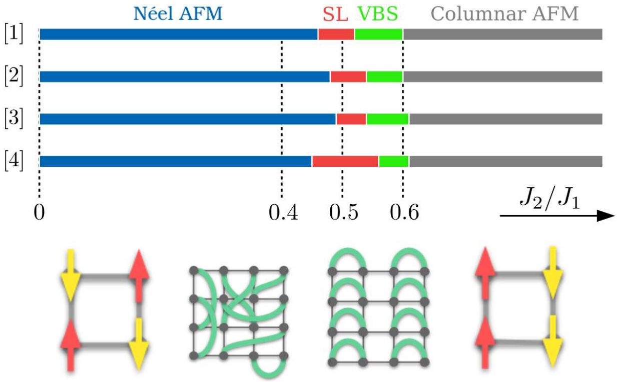
  **Triplet-state accuracy** 0.7% ($E_{ex}/J_1 = -0.49072$ vs $E_{var}/J_1 = -0.48706$)

  **Singlet-state accuracy** 1.4% ($E_{ex}/J_1 = -0.49054$ vs $E_{var}/J_1 = -0.48375$)

- On larger clusters:



# Towards a final phase diagram

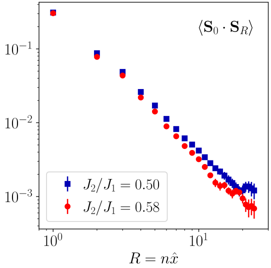



[1] L. Wang and A.W. Sandvik, Phys. Rev. Lett. **121**, 107202 (2018)

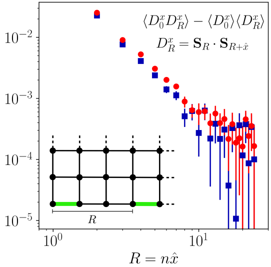
[2] F. Ferrari, F. Becca, Phys. Rev. B **102**, 014417 (2020)

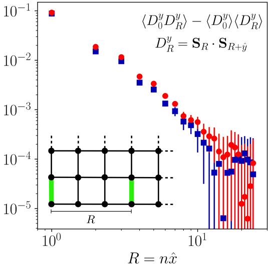
[3] Y. Nomura and M. Imada, arXiv:2005.14142

[4] W.-Y. Liu, S.-S. Gong, Y.-B. Li, D. Poilblanc, W.-Q. Chen, Z.-C. Gu, arXiv:2009.01821




- Power-law spin-spin correlations
- Power-law (?) dimer-dimer correlations
- Not much difference between $J_2/J_1 = 0.5$ and $0.58$



- On each site there is two phonons (oscillations in the plane)
- The nearest-neighbor super-exchange is coupled to longitudinal displacements
- For the $J_1 - J_2$ Heisenberg model the Hamiltonian is taken as:

$$\mathcal{H} = \sum_i \{[J_1 + g(X_{i+x} - X_i)]\,\mathbf{S}_i \cdot \mathbf{S}_{i+x} + [J_1 + g(Y_{i+y} - Y_i)]\,\mathbf{S}_i \cdot \mathbf{S}_{i+y}\}$$

$$+J_2 \sum_i [\mathbf{S}_i \cdot \mathbf{S}_{i+x+y} + \mathbf{S}_i \cdot \mathbf{S}_{i+x-y}] + \frac{\omega}{4} \sum_i \left[P_{X,i}^2 + P_{Y,i}^2 + X_i^2 + Y_i^2\right]$$

- The variational wave function generalizes the one-dimensional case:

$$|\Psi_p\rangle = \prod_j \exp(z_a e^{ik_a R_j} a_j^\dagger) \exp(z_b e^{ik_b R_j} b_j^\dagger) |0\rangle_p$$

Two fugacities $z_a$ and $z_b$ and two momenta $k_a$ and $k_b$

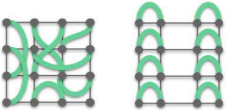
- $\omega/J = 1$ and $16 \times 16$ sites

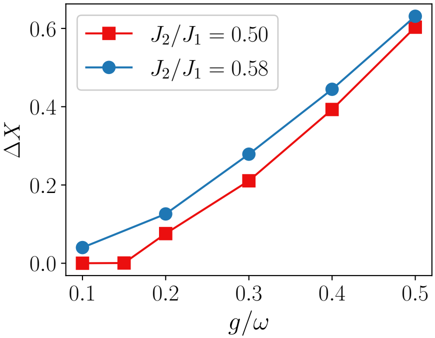
$k_a = (\pi, 0)$

$k_b = (0, 0)$

$z_a = 0$ $\quad$ $z_a \neq 0$

$z_b = 0$ $\quad$ $z_b = 0$






- A promising difference is seen...
- ...but a size scaling is needed

# Conclusions

- Qualitatively correct wave functions in the 1D Heisenberg model

  Calculations done for optical phonons

  What about acoustic phonons?

- Frustrated $J_1 - J_2$ model in 1D: dimerization for $J_2/J_1 < 0.5$

  What about $J_2/J_1 > 0.5$? Tetramerization?

  F. Becca, F. Mila, and D. Poilblanc, Phys. Rev. B **91**, 067202 (2003)

- Most interestingly: what happens in 2D?

  Phonons as probes to spin liquids and valence-bond solids

  Also important for magnetically ordered phases

  E.g., orthorhombic transition on the square lattice with $Q = (\pi, 0)$ magnetic order

  F. Becca and F. Mila, Phys. Rev. Lett. **89**, 037204 (2002)

  What about other lattices? E.g., the triangular one for $120^\circ$ magnetic order?