

Project 13:

Stochastic Series expansion for a bond alternating Heisenberg model

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Computational Methods in Many-Body Physics Exam

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The staggered dimer

How to adapt the QMC method for changing bond strengths?

Results

Questions

The staggered dimer

Staggered Heisenberg dimer visualization:

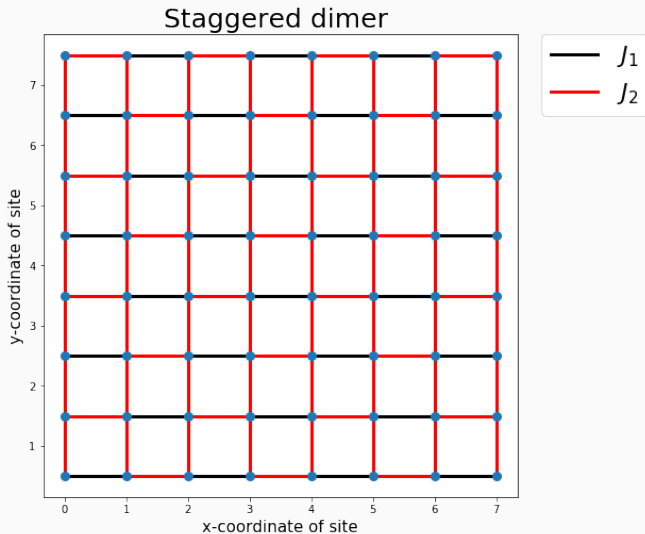


Figure 1: The staggered dimer lattice

Staggered dimer Hamiltonian I:

Hamiltonian:

We can write down the Hamiltonian of the dimerized system:

$$\hat{H} = \sum_b \left(\hat{H}_b^{\text{off-diag.}} - \hat{H}_b^{\text{diag.}} + C_0 J_b \right) \quad (1)$$

$$\hat{H}_b^{\text{off-diag.}} = \frac{J_b}{2} \left(S_{i(b)}^+ S_{j(b)}^- + S_{j(b)}^+ S_{i(b)}^- \right) \quad (2)$$

$$\hat{H}_b^{\text{diag.}} = J_b \left(S_{i(b)}^z S_{j(b)}^z - C_0 \right) \quad (3)$$

At the level of the Hamiltonian, what defines the staggered dimer, or any other configuration of bonds for that matter, is thus the set of couplings $\{J_b\}$.

Staggered dimer Hamiltonian II:

Matrix elements:

Diagonal matrix elements:	Off-diagonal elements:
$H_b^{\text{diag.}} \uparrow\uparrow \rangle = J_b(C_0 - 1/4) \uparrow\uparrow \rangle$	$H_b^{\text{off-diag.}} \uparrow\uparrow \rangle = 0$
$H_b^{\text{diag.}} \downarrow\downarrow \rangle = J_b(C_0 - 1/4) \downarrow\downarrow \rangle$	$H_b^{\text{off-diag.}} \downarrow\downarrow \rangle = 0$
$H_b^{\text{diag.}} \uparrow\downarrow \rangle = J_b(C_0 + 1/4) \uparrow\downarrow \rangle$	$H_b^{\text{off-diag.}} \downarrow\downarrow \rangle = \frac{J_b}{2} \uparrow\downarrow \rangle$
$H_b^{\text{diag.}} \downarrow\uparrow \rangle = J_b(C_0 + 1/4) \downarrow\uparrow \rangle$	$H_b^{\text{off-diag.}} \downarrow\downarrow \rangle = \frac{J_b}{2} \downarrow\uparrow \rangle$

Observation:

We can still avoid the negative weights by choosing $C_0 = 1/4$!

Staggered dimer Hamiltonian III:

Dimerized couplings:

To achieve a dimerized configuration, we can define the coupling J_b according to:

$$J_b = \begin{cases} \text{if } \text{mod}(y, 2) = 0 : & \begin{cases} J_1, & \text{if } \text{mod}(x, 2) = 0 : \\ J_2, & \text{if } \text{mod}(x, 2) \neq 0 : \end{cases} \\ \text{if } \text{mod}(y, 2) \neq 0 : & \begin{cases} J_1, & \text{if } \text{mod}(x, 2) \neq 0 : \\ J_2, & \text{if } \text{mod}(x, 2) = 0 : \end{cases} \end{cases} \quad (4)$$

We simply note the bond type when building the lattice. The bonds are then sorted such that J_2 bonds are in front of the bonds list and J_1 bonds are in the back of the list.

Staggered Heisenberg dimer visualization:

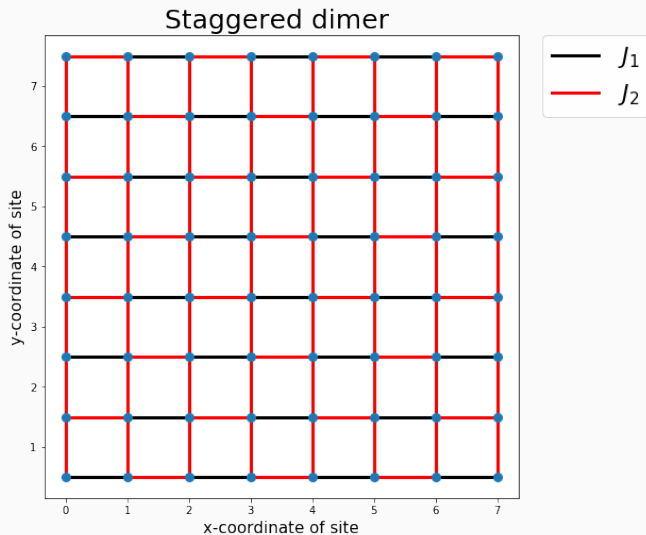


Figure 2: The staggered dimer lattice

**How to adapt the QMC method for
changing bond strengths?**

Adapting the QMC to the dimerized case I:

Off-diagonal update:

The lattice remains bipartite:

- To get a non-zero contribution, we still need an even number of off-diagonal operators in the string.
- The probability with which we flip a given loop covering is independent of J .

Conclusion: We do not have to change the off-diagonal update in the dimered case!

Adapting the QMC to the dimered case II:

Diagonal update:

Looking at the matrix elements, we see that the different bond strengths simply differ by a factor of J_b from the matrix elements for the $J = 1$ isotropic case.

For anisotropic bonding, we can thus define,

$$\beta_b^{\text{eff.}} = J_b \beta, \quad (5)$$

and then change the acceptance probabilities as:

$$P_{\text{accept}}^{\text{Insert}} = \min \left\{ \frac{\beta_b^{\text{eff}} N_b}{2(L - n)}, 1 \right\} \quad (6)$$

$$P_{\text{accept}}^{\text{Remove}} = \min \left\{ \frac{2(L - n + 1)}{\beta_b^{\text{eff}} N_b}, 1 \right\} \quad (7)$$

Adapting the QMC to the dimered case III:

Selecting a bond:

Because a strong bond in the operator string contributes a factor J_1/J_2 more than a weak bond, it doesn't make sense to sample a lot of weak bonds.

We thus change our selection probability for a given bond to :

$$P_b^{\text{sel}} = \begin{cases} \frac{J_2}{J_1 N_B(J_1) + J_2 N_B(J_2)}, & \text{if } J_b = J_2 \\ \frac{J_1}{J_1 N_B(J_1) + J_2 N_B(J_2)}, & \text{if } J_b = J_1 \end{cases} \quad (8)$$

Adapting the QMC to the dimered case IV:

Selecting a bond in practice:

Assuming that selecting a specific bond, is independent of selecting a bond of that particular bond type, we can write:

$$P_b^{\text{sel}} = \frac{P(\text{Bond type} = b)}{N_b(\text{Bond type} = b)} \quad (9)$$

With:

$$P(\text{Bond type} = b) = \begin{cases} \frac{N_B(J_2)J_2}{J_1N_B(J_1)+J_2N_B(J_2)}, & \text{if } J_b = J_2 \\ \frac{N_B(J_1)J_1}{J_1N_B(J_1)+J_2N_B(J_2)}, & \text{if } J_b = J_1 \end{cases} \quad (10)$$

In short:

I first select which type of bond to operate on according to equation 10 and then uniformly choose between all the bonds of the selected type.

Results

Energy per site for various couplings:

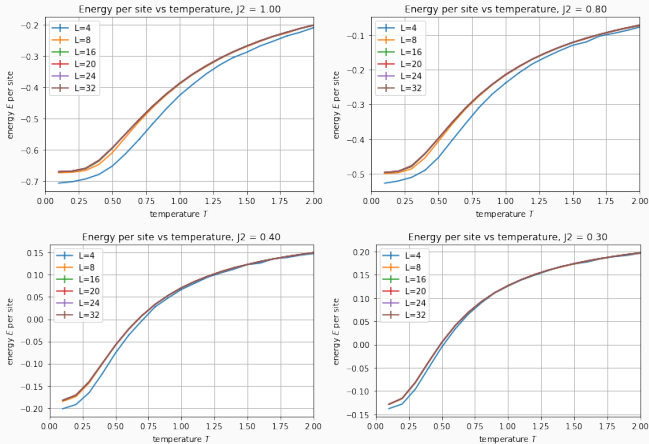


Figure 3: Energy per site for various coupling strengths and lattice sizes

Heat capacity for various couplings:

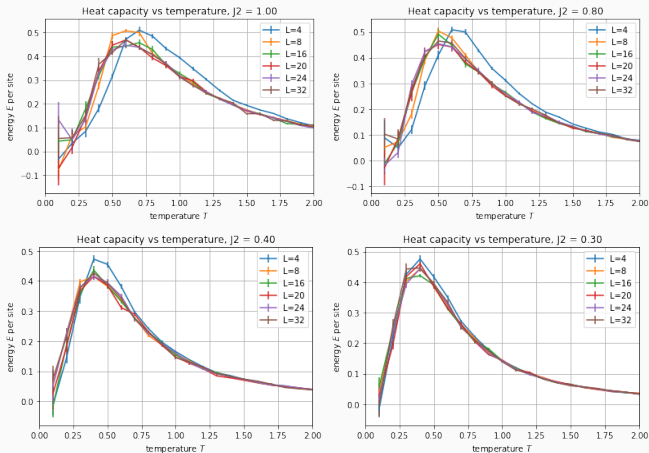


Figure 4: Heat capacity for various coupling strengths and lattice sizes

Stagnant magnetization for various couplings I:

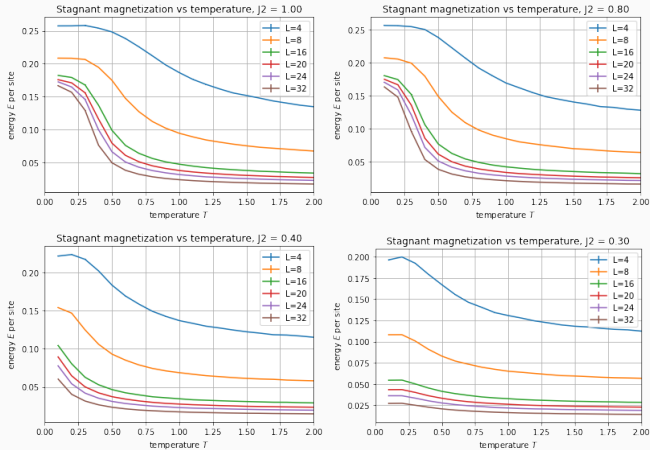


Figure 5: Stagnant magnetization for various coupling strengths and lattice sizes

Stagnant magnetization for various couplings II:

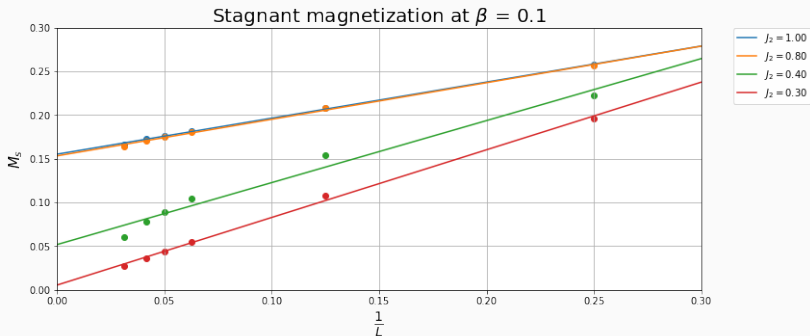


Figure 6: Stagnant magnetization vs system size for different coupling ratios

Heat capacity for various couplings II:

Summary:

- Note that for $J_1 = 0.3$ the heat capacity and energy per site becomes almost size independent
- We've also observed, that for larger coupling ratios, the stagnant magnetization disappears.

Thus we are likely observing the Neel to dimer phase transition, driven by the coupling ratio $\alpha = J_2/J_1$. **Can we probe this transition more directly?**

Generalized finite size scaling for quantum systems I:

Can we probe the $T \rightarrow 0$ properties of the phase transition?

There are essentially two ways of going about this:

- We can probe the properties of interest at sufficiently low T and then extrapolate.
 - Huge computational cost as $\langle n \rangle$ grows with decreasing T .
- Generalized finite size scaling approach
 - As we will see, this also has a similar problem, but only for larger lattices.

Generalized finite size analysis in quantum systems II:

Scaling function:

In quantum systems, the dynamics cannot be separated out of the ground state properties. The scaling function is thus:

$$f = f(\xi/L, \xi_T/L_T) \quad (11)$$

Question: Can we relate ξ_τ and L_τ to simulation parameters?

Dynamical exponent:

We can think of the quantum system as a $d + z$ classical system. Here:

$$\xi_T = \xi^z \quad (12)$$

For the dimerized 2D Heisenberg model, $z = 1$. (Sandvik lecture notes)[1]

Generalized finite size analysis in quantum systems III:

Partition function as a path integral:

Partition function:

$$Z = \text{tr} \left[e^{-\beta \hat{H}} \right] = \sum_{\lambda} \langle \lambda | e^{-\beta \hat{H}} | \lambda \rangle \quad (13)$$

As we have seen in the course (TEBD), we can think of statistical physics as taking place in imaginary time.

We can thus think of,

$$\langle \lambda | e^{-\beta \hat{H}} | \lambda \rangle, \quad (14)$$

as the Wick-rotation ($t \rightarrow -i\beta$) of:

$$\langle \lambda | e^{-iHt} | \lambda \rangle \quad (15)$$

Generalized finite size analysis in quantum systems IV:

Partition function as a path integral:

Normal path integral:

$$\langle q_b | e^{-i\hat{H}t} | q_a \rangle = \int \mathcal{D}[q(t)] e^{i \int_0^t L[q(t')] dt'} \quad (16)$$

When wick rotated we find:

$$\langle q_b | e^{-\beta \hat{H}} | q_a \rangle = \int \mathcal{D}[q(t)] e^{- \int_0^\beta L_E[q(\tau')] d\tau'} \quad (17)$$

This gives:

$$Z = \sum_{\lambda} \int \mathcal{D}[q(t)] e^{- \int_0^\beta L_E[q(\tau')] d\tau'} \quad (18)$$

For a nonzero contribution, we require: $q(\tau = 0) = q(\tau = \beta)$.

"System size" in imaginary time can be taken as β !

Generalized finite size analysis in quantum systems V:

Scaling function:

Based on the previous considerations, we are thus able to write the scaling function as:

$$f = f(\xi/L, \xi^z/\beta) \stackrel{\text{Dimerized Heisenberg}}{=} f(\xi/L, \xi/\beta) \quad (19)$$

By choosing the temperature as $\beta = L$ we are thus able to write the scaling function in terms of a single variable:

$$f = f(\xi/L) \quad (20)$$

This means that we can probe the QPT, but simulation systems at different sizes L and corresponding inverse temperatures $\beta = L$.

Probing the quantum phase transition I:

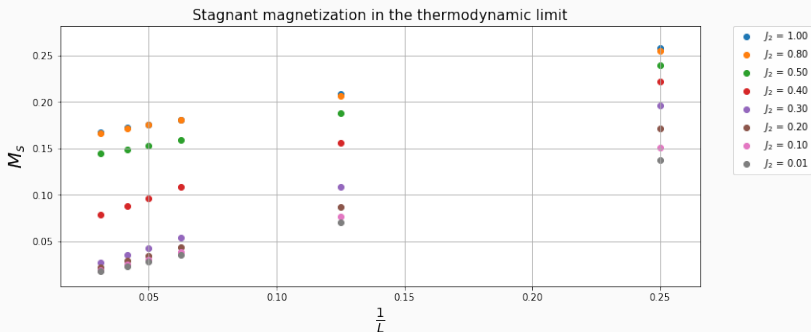


Figure 7: Stagnant magnetization in the thermodynamic limit for different couplings

Probing the quantum phase transition II:

Determining the critical coupling

As we have seen, we can use the crossing of the binder cumulant to determine the critical coupling:

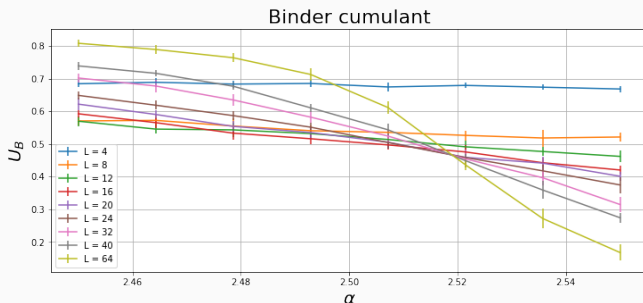


Figure 8: The binder cumulant for the staggered dimer,

$$R = \langle m^4 \rangle / \langle m^2 \rangle^2$$

Probing the quantum phase transition III:

Determining the critical coupling and estimate sub-leading corrections:

Assuming that the critical coupling can be expressed as:

$$g_c(L) = g_c(\infty) + aL^{-\omega} \quad (21)$$

We find $J_1^c = 0.40$ or $\alpha = 2.52$! This is in agreement with results in the literature [2].

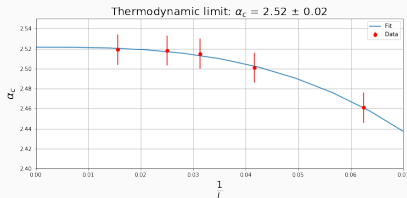


Figure 9: L-2L cuts of binder cumulants. Fit parameters:

$$a = -174, g_c(\infty) = 2.52, \omega = 2.8$$

Questions



Anders W Sandvik.

Computational studies of quantum spin systems.

In *AIP Conference Proceedings*, volume 1297, pages 135–338. AIP, 2010.



Sandro Wenzel, Leszek Bogacz, and Wolfhard Janke.

Evidence for an unconventional universality class from a two-dimensional dimerized quantum heisenberg model.

Physical review letters, 101(12):127202, 2008.

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