Deep Learning Topological Phases of Random Systems

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Classification of wave functions in random systems

- We often visualize wave functions to see what is going on in random materials.

- These wave functions in random systems show specific features → Regard $|\psi(r)|^2$ (instead of cats and dogs) as an image

- Use multilayer (four-weight layer) convolutional neural network (CNN) to classify the pattern of $|\psi(r)|^2$ and draw the phase diagram of quantum phase transition
  - 2D topological insulator (edge states)-Anderson insulator transition (exponentially localized in the bulk)
  - 2D quantum magnon Hall
  - 3D strong/weak topological insulator-ordinary insulator transition
  - 3D Weyl semimetal
Supervised training

• **Training stage**
  • Prepare thousands of eigenstates for a phase, teach the CNN that the eigenfunction belongs to this phase.
  • Minimize cross entropy, \(-\Sigma_i p_i \log p_i = -\Sigma' \log p_i\)
    • 90% for training, 10% for testing: when satisfied with the score, stop.

• **Prediction stage**
  • Diagonalize the Hamiltonian again with a set of parameters \(\{x\}\), and let the CNN judge \(|\psi(r)|^2\). Then CNN outputs probabilities: the state corresponding to parameters \(\{x\}\) belongs to a phase with probability \(p_i\) (\(i=\)Label for quantum phase such as TI, AI, metal.).

• **Tools:** Caffe, Keras+tensorflow, Keras+theano
2d topological insulator (Chern insulator)

- Haldane, PRL. 61, 2015 (‘88) for quantum Hall effect without Landau levels. Qi-Wu-Zhang model, PRB. (‘06). Disorder effect by CNN, TO JPSJ ‘16, interaction effect, CNN, Zhang-Kim PRL ‘17

- 2d topological insulator (edge states + localized bulk) $\rightarrow$ Anderson insulator (localized bulk)

$$H = \sum_x \left( (\epsilon_s + \nu_s(x))c_{x,s}^\dagger c_{x,s} + (\epsilon_p + \nu_p(x))c_{x,p}^\dagger c_{x,p} \right)$$

$$+ \sum_x \left( - \sum_{\mu=x,y} t_{s} c_{x+e_{\mu},s}^\dagger c_{x,s} - t_{p} c_{x+e_{\mu},p}^\dagger c_{x,p} \right)$$

$$+ t_{sp}(c_{x+e_x,p}^\dagger - c_{x-e_x,p}^\dagger) c_{x,s} - it_{sp}(c_{x+e_y,p}^\dagger - c_{x-e_y,p}^\dagger) c_{x,s} + \text{h.c.},$$

$|\psi(r)|^2$

(a) small $W$  (b)  (c) large $W$  (d)
Results

Probability of states near $E=0$ to be topological

Probability of states away from $E=0$ to be topological

Topological ins. Anderson ins.

Strength of randomness

energy
Application to quantum magnon Hall effect

- Effect of disorder on quantum magnon Hall in spin ice model (Xu-Ohtsuki-Shindou, PRB'16)

Holstein-Primakoff trans.

\[ H = \sum_{\langle i,j \rangle} \frac{1}{|i-j|^3} [\hat{S}_i \cdot \hat{S}_j - 3(\hat{S}_i \cdot \boldsymbol{n}_{ij})(\hat{S}_j \cdot \boldsymbol{n}_{ij})] \]

- \[ H_b \equiv H_{on} + H_{nn} + H_{nnn}, \]
- \[ H_{on} \equiv \frac{1}{2} \sum_{j \in A} \{(D+d_j)S(-b_j^\dagger b_j^\dagger - b_j b_j) + (H_Z+h_j)b_j^\dagger b_j \}
  + \frac{1}{2} \sum_{j \in B} \{(D+d_j)S(b_j^\dagger b_j^\dagger - b_j b_j) + (H_Z+h_j)b_j^\dagger b_j \}
  + H.c., \]
- \[ H_{nn} \equiv \sum_{m=1,2} \sum_{j \in A} \sum_{i=j \pm \delta_m, i \in B} \frac{JS}{4} (b_j^\dagger b_i - 2b_i^\dagger b_i - 2b_j^\dagger b_j
  + 6i(-1)^m b_j^\dagger b_i^\dagger + H.c.), \]
- \[ H_{nnn} \equiv \sum_{\alpha=A,B} \sum_{m=1,2} \sum_{j \in \alpha} \sum_{i=j \pm \epsilon_m} \frac{J'_{\alpha,m} S}{4} (-b_j^\dagger b_i - b_i^\dagger b_i - b_j^\dagger b_j
  + 3(-1)^m b_j^\dagger b_i^\dagger + H.c.), \]
FIG. 2: (color online) Energy band dispersions of magnon states as function of the wave vector $k$, calculated with open/periodic boundary condition along the $y/x$-direction. Black colored dispersions are for bulk modes, and red colored dispersions are for the chiral edge modes; those at $k<0$ are localized at $y=M>0$ and those at $k>0$ are localized at $y=0$. (a) $J_{1}^{'}S_{1}=J_{2}^{'}S_{2}=0.35$, $H_{Z}=15.8$, $D_{S}=2.2$, $J_{S}=1.0$, (b) $J_{1}^{'}S_{1}=0.35$, $J_{2}^{'}S_{2}=0.28$, $H_{Z}=15.8$, $D_{S}=2.2$, $J_{S}=1.0$.

FIG. 3: (color online) Two-terminal conductance as a function of energy of magnon state $E$ for several $W$ ((a) $W=1.3$ and (b) $W=2.1$), calculated for the $L \times L$ system. Solid lines with different colors denote the conductance along the $x$-direction with periodic boundary condition along the $y$-direction $G_{p}$; $L=20$ (black), $L=30$ (red), $L=40$ (blue). Broken lines with different colors denote $G_{o}-G_{p}$, where $G_{o}$ is the conductance with open boundary condition along the $y$-direction. The other parameters are the same as those given in the caption of Fig. 1 and 4 in the main text. Two direct transition points are identified as a scale-invariant point of $G_{p}$; a red colored dotted line for $E=E_{2}(W)$ and black colored dotted line for $E=E_{1}(W)$. Note that, for $E_{1}(W)<E<E_{2}(W)$, $G_{o}-G_{p}$ has a tendency to take the quantized value $(1/\hbar)$ in the thermodynamic limit.

MICROWAVE ANTENNAS EXPERIMENT

The two terminal magnon conductance calculated in the main text can be measured in a standard microwave experiment commonly used for spin wave experiments [11]. The experiment consists of two microstrip microwave antennas attached to the two-dimensional square-lattice spin ice system (Fig. 4). The two antennas are spatially separated from each other shorter than a spin coherent length, over which spin wave propagates without an energy dissipation. Note that the spin coherent length in ferromagnetic insulator such as YIG can be over millimeters, while it is at most on the order of several micrometer in ferromagnetic metals.

The role of the first antenna is for spin wave excitation and that of the second antenna is for its detection. An a.c. electric current with a frequency in the microwave regime (let us call this as 'external frequency') is introduced in the first antenna ('input signal'). The current locally excites spin wave with the same external frequency. The spin wave
Procedure

• use the training of 2D electron Chern insulator to draw a rough phase diagram
• use this rough phase diagram to determine the training regions in magnon systems
• draw the more precise phase diagram
Draw a rough phase diagram from the results of CI-AI training.

Then guess the typical regions of delocalized, topological edge and localized (AI), train CNN, draw the phase diagram.
Use the already trained CNN to draw phase diagrams with different set of parameters.

$H_z=15.8$, $D=2$, $JS=1.0$, $J'S=0.35$

$H_z=15$, $D=1.8$, $JS=0.9$, $J'S=0.4$
two-weight-layer CNN, Keras+TF, ES

four-weight-layer CNN, Keras+Theano, ES

six-weight-layer CNN, Keras+TF, ES
Comparing the methods of drawing phase diagram

• Finite size scaling (Slevin and Ohtsuki, NJP ‘14)
  • Define a nondimensional quantity $\Lambda(L, E, W, ..)$ such as conductance.
  • Plot $\Lambda(L, E, W, ..)$ as a function of $E, W$, etc. with different system sizes $L$.
  • Analyze $\Lambda(L, E, W, ..)$. Scaling invariant point is the phase boundary.
  • Precise estimate of the phase boundaries. Critical exponents.

• Machine learning method
  • Simple analysis.
    • [python train.py;] python test.py; python dataArrange.py; python plot.py
  • Wider applicability.
  • Once trained, can draw phase diagrams for different parameters.
  • Detection of states on the phase boundary.
  • Only rough estimate of the phase boundaries. Too many tuning parameters like number of hidden layers, convolution size, pooling size, bias, padding, ....
Outlook

• Several preprints have been submitted to arXiv in 2016, refereeing processes took a bit, but they are now published.

• Though still restricted to standard simplified models, machine learning methods seem to be gradually accepted among solid state physics community.
  
  • arXiv1605.01735 (Nat. Phys. ‘17) : 2D Ising model
  • arXiv1606.02318 (Science ‘17): Heisenberg model
  • arxiv1609.09087 (JPSJ ‘17): 2D Ising model, the most beautiful
  • arXiv1608.07848: 2D Hubbard model, $G(E, x, y)$
  • arXiv1609.02552: 3D Hubbard model, temperature transition
  • arXiv1611.01518: Chern insulator, bulk (PRL ‘17)
  • arXiv1609.03705 (PRB ‘17): DFT with machine learning