Deep Learning the Quantum Phase Transitions in Random Two-Dimensional Electron Systems

Tomoki Ohtsuki\textsuperscript{1} and Tomi Ohtsuki\textsuperscript{2}

\textsuperscript{1} NTT DATA Mathematical Systems Inc, Shinjuku-ku, Tokyo 160-0016, Japan
\textsuperscript{2} Physics Division, Sophia University, Chiyoda-ku, Tokyo 102-8554, Japan

Random electron systems show rich phases such as Anderson insulator, diffusive metal, quantum Hall and quantum anomalous Hall insulators, Weyl semimetal, as well as strong/weak topological insulators. Eigenfunctions of each matter phase have specific features, but owing to the random nature of systems, determining the matter phase from eigenfunctions is difficult. Here, we propose the deep learning algorithm to capture the features of eigenfunctions. Localization-delocalization transition, as well as disordered Chern insulator-Anderson insulator transition, is discussed.

Introduction– More than half a century has passed since the discovery of Anderson localization,\textsuperscript{1} and the random electron systems continue to attract theoretical as well as experimental interest. Symmetry classification of topological insulators\textsuperscript{2–5} based on the universality classes of random noninteracting electron systems\textsuperscript{6,7} gives rise to a fundamental question: can we distinguish the random topological insulator from Anderson insulators? Note that topological numbers are usually defined in the randomness free systems via the integration of the Berry curvature of Bloch function over the Brillouin zone, although topological numbers in random systems have recently been proposed.\textsuperscript{8–10}

Determining the phase diagram and the critical exponents requires large-scale numerical simulation combined with detailed finite size scaling analyses.\textsuperscript{11–14} This is because, owing to large fluctuations of wavefunction amplitudes, it is almost impossible to judge whether the eigenfunction obtained by diagonalizing small systems is localized or delocalized, or whether the eigenfunction is a chiral/helical edge state of a topological insulator. In fact, it often happens that eigenfunctions in the localized phase seem less localized than those in the delocalized phase [see Figs. 1(b) and 1(c) for example].

\textsuperscript{*}ootsuki.t@msi.co.jp
\textsuperscript{†}ohtsuki@sophia.ac.jp
Recently, there has been great progress on image recognition algorithms based on deep machine learning. Machine learning has recently been applied to several problems of condensed matter physics such as Ising and spin ice models and strongly correlated systems.

In this Letter, we test the image recognition algorithm to determine whether the eigenfunctions for relatively small systems are localized/delocalized, and topological/nontopological. As examples, we test two types of two-dimensional (2D) quantum phase transitions: Anderson-type localization-delocalization transition in symplectic systems, and disordered Chern insulator to Anderson insulator transition in unitary systems.

**Distinguishing Localized States from Delocalized Ones**– We start with a 2D symplectic system, which is realized in the presence of spin-orbit scattering. We use the SU(2) Hamiltonian that describes the 2D electron on a square lattice with nearest-neighbor hopping,

\[
H = \sum_{i,\sigma} \epsilon_i c_{i,\sigma}^\dagger c_{i,\sigma} - \sum_{\langle i, j \rangle, \sigma, \sigma'} R(i, j)_{\sigma, \sigma'} c_{i,\sigma}^\dagger c_{j,\sigma'},
\]

where \(c_{i,\sigma}^\dagger (c_{i,\sigma})\) denotes the creation (annihilation) operator of an electron at site \(i = (x, y)\) with spin \(\sigma\), and \(\epsilon_i\) denotes the random potential at site \(i\). We assume a box distribution with each \(\epsilon_i\) uniformly and independently distributed on the interval \([-W/2, W/2]\). The modulus of the transfer energy is taken to be the energy unit. \(R(i, j)\) is an SU(2) matrix,

\[
R(i, j) = \begin{pmatrix}
e^{i\alpha_{ij}} \cos \beta_{i,j} & e^{i\gamma_{ij}} \sin \beta_{i,j} \\
-e^{-i\gamma_{ij}} \sin \beta_{i,j} & e^{-i\alpha_{ij}} \cos \beta_{i,j}
\end{pmatrix},
\]

with \(\alpha\) and \(\gamma\) uniformly distributed in the range \([0, 2\pi]\). The probability density \(P(\beta)\) is

\[
P(\beta) = \begin{cases}
\sin(2\beta) & 0 \leq \beta \leq \pi/2, \\
0 & \text{otherwise}.
\end{cases}
\]

Examples of the eigenfunctions in delocalized [Figs. 1(a) and 1(b)] and localized phases [Figs. 1(c) and 1(d)] are shown in Fig. 1.

For \(E = 0\) (band center), from the finite size scaling analyses of the quasi-1D localization length, it is known that the states are delocalized when \(W < W_{c}^{SU2}(\approx 6.20)\), while they are localized when \(W > W_{c}^{SU2}\). We impose periodic boundary conditions in \(x\)- and \(y\)-directions, and diagonalize systems of \(40 \times 40\). From the resulting 3200 eigenstates with Kramers degeneracy, we pick up the 1600th eigenstate (i.e., a state close to the band center). For simplicity, the maximum modulus of the eigenfunction is shifted to the center of the system. Changing \(W\) and the seed of the random number stream (Intel MKL MT2023), we prepare 2000 samples of states, i.e., 1000 for \(W < W_{c}^{SU2}\) and 1000 for \(W > W_{c}^{SU2}\). We then teach the machine...
whether the states belong to the localized (delocalized) phase.

For our network architecture, we consider two types of simple convolutional neural network (CNN), which output two real numbers, i.e., probabilities for each phase, given $40 \times 40$ input eigenfunction. The first one is a very simple network with two weight layers, which first convolves the input with a $5 \times 5$ filter with stride 1 to 10 channels, then applies max pooling with a kernel size of $2 \times 2$ and stride 2, and finally performs fully connected linear transformation to output the learned probabilities. The loss function can then be defined by the cross entropy of probabilities and the localized/delocalized labels. The second, rather deep one with four weight layers is a variant of LeNet\(^{28}\) included in Caffe\(^{29}\) (with the input size changed to $40 \times 40$), which utilizes rectified linear unit (ReLU) as its activation function. See Fig. 2 for illustration and detailed parameters. The network weight parameters (to be trained) are sampled from gaussian distribution, the scale of which is determined by the number of input and output dimensions,\(^{30}\) except for the first convolution layer connected to the raw input: since we are dealing with eigenfunctions, whose typical values at each lattice site are much smaller than those of gray-scale images, we have manually chosen the weight initialization scale to be 100, which worked better in practice for the two networks. As the stochastic gradient descent solver, we have used the RMSProp solver\(^{31}\) with the parameters in the Caffe MNIST example (which is contained as examples/mnist/lenet_solver_rmsprop.prototxt in the Caffe source). Before the training, we always partition the training data into 90% and 10%, and use the latter as the validation set during the training. The solver performs enough iterations so that the validation error becomes stationary. We have used a workstation: Intel Xeon E5-1620 v4, single CPU with 4 cores with GPU Quadro K420 and GPGPU TESLA K40 running on Linux CentOS 6.8.

We then test 5 sets of ensemble, each consisting of 100 eigenstates, and let the machine...
judge whether the states are localized or not. The resulting probability for eigenfunction to be delocalized, $P$, is shown in Fig. 3(a).

We then apply the results of the learning around $E = 0$ to judge whether the states around $E = 1.0, 2.0,$ and $3.0$ are delocalized. Results are shown in Fig. 3(b), in which we observe that,
with increasing $E$, that is, as we move from band center to band edge, the electron begins to be localized with a smaller strength of the disorder $W$, qualitatively consistent with the finite size scaling analysis.\textsuperscript{27} There seems to be, however, a systematic deviation of the 50\% criterion of localization-delocalization transition and the actual critical point with increasing $E$. This may be due to the appearance of bound states near the band edge, which is absent in the machine learning around $E = 0$. We have further applied the results of SU(2) model machine learning for the Ando model,\textsuperscript{32} and verified that once the machine learns the eigenfunction features in certain systems, it can be applied to other systems belonging to the same class of quantum phase transition (see Supplemental material for detail\textsuperscript{33}).

**Distinguishing Topological Edge States from Non-topological Ones**—We next study the topological Chern insulator to nontopological Anderson insulator transition.\textsuperscript{34–36} We use a spinless two-orbital tight-binding model on a square lattice, which consists of $s$-orbital and $p = p_x + i p_y$ orbital,\textsuperscript{37}

\begin{align*}
H &= \sum_x \left( (\epsilon_s + v_s(x)) c_{x,s}^\dagger c_{x,s} + (\epsilon_p + v_p(x)) c_{x,p}^\dagger c_{x,p} \right) \\
&\quad + \sum_x \left( -\sum_{\mu=x,y} (t_{s} c_{x+\mu,s}^\dagger c_{x,s} - t_{p} c_{x+\mu,p}^\dagger c_{x,p}) \right. \\
&\quad \left. + t_{sp} (c_{x+e_x,p}^\dagger c_{x,s} - c_{x-e_x,p}^\dagger c_{x,s}) - i t_{sp} (c_{x+e_y,p}^\dagger c_{x,s} - c_{x-e_y,p}^\dagger c_{x,s}) c_{x,s} + \text{h.c.} \right),
\end{align*}
where $\epsilon_s$, $v_s(x)$, $\epsilon_p$, and $v_p(x)$ denote atomic energy and disorder potential for the $s$- and $p$-orbitals, respectively. Both $v_s(x)$ and $v_p(x)$ are uniformly distributed within $[-W/2, W/2]$ with identical and independent probability distribution. $t_s$, $t_p$, and $t_{sp}$ are transfer integrals between neighboring $s$-orbitals, $p$-orbitals, and that between $s$- and $p$-orbitals, respectively.

In the absence of disorder, the system is a Chern insulator when the band inversion condition is satisfied: $0 < |\epsilon_s - \epsilon_p| < 4(t_s + t_p)$. We set $\epsilon_s - \epsilon_p = -2(t_s + t_p)$, $\epsilon_s = -\epsilon_p < 0$, and $t_s = t_p > 0$ so that this condition is satisfied, and set $t_{sp} = 4t_s/3$. The energy unit is set to $4t_s$. A bulk band gap appears in $|E| < E_g = 0.5$ where chiral edge states exist.

For $E = 0$, the system remains as a Chern insulator for $W < W_{c}^{CI} \approx 3.2$, while it is an Anderson insulator for $W > W_{c}^{CI}$. (Unfortunately, the estimate of $W_{c}^{CI}$ is less precise than the SU(2) model.) We impose fixed boundary conditions in the $x$- and $y$-directions, so that the edge states appear if the system is a topological insulator.

We diagonalize square systems of $40 \times 40$ sites, and from the resulting 3200 eigenstates, we pick up the 1600th eigenstate. Examples of the eigenfunctions in topological Chern [Figs. 4(a) and 4(b)] and nontopological Anderson insulators [Figs. 4(c) and 4(d)] are shown in Fig. 4. As shown in Fig. 4, it is difficult to judge whether the state is an edge state or not when $W$ is close to $W_{c}^{CI}$, see, for example, $W = 0.9W_{c}^{CI}$ [Fig. 4(b), Chern insulator phase] and $W = 1.1W_{c}^{CI}$ [Fig. 4(c), Anderson insulator phase]. In fact, learning 1000 samples for each phase gives 93% validation accuracy for four-weight-layer network compared with 98% or more as in the SU(2) model. The difficulty may be due to the fixed boundary condition where shifting the locus of the maximum of the eigenfunction amplitude is not allowed. Another reason for difficulty is that the bulk of the systems are localized in both topological and nontopological regions. To overcome these difficulties, we increased the number of samples: 27000 samples belonging to the topological phase, and 27000 to the nontopological phase.
Fig. 5. (a) Probability of eigenfunction around $E = 0$ to be judged topological edge states as a function of disorder $W$. Averages over 5 samples are taken. 50% probability is indicated as the horizontal dashed line. Since the critical disorder is less accurate, $W_c^{\text{CI}} = 3.25 \pm 0.1$ is shown as a shaded region. The dotted line is for a two-weight-layer network, while the solid one is for a four-weight-layer one. (b) Same quantity but as a function of eigenenergy $E$ inside the bulk band gap region $|E| < E_g = 0.5$. Results for $W = 1 < W_c^{\text{CI}}$ (×, solid line) and $W = 6 > W_c^{\text{CI}}$ (+, dotted line) are shown.

We have also increased the number of hidden units to be 32 for the first convolution layer (“conv1” in Fig. 2), 128 for the second (“conv2”), and 512 for the hidden dense connection layer (“ip1”).

In Fig. 5(a), we plot the probability of the eigenfunction to be judged topological. A new ensemble of eigenfunctions with different random number sequences has been prepared to test this method. As in the case of delocalization-localization transition, the probability fluctuates near the critical point and vanishes in the nontopological region. The validation accuracy is 90% for the case of two layers of network (dotted line), and 97% for four layers of network (solid line), which demonstrates clearly that a deeper network exhibits better performance.

We next apply the result of the deep learning around $E = 0$ to judge the states in the bulk band gap region at zero disorder, $|E| < E_g = 0.5$. We diagonalize a system for $W = 1 < W_c^{\text{CI}}$ and $W = 6 > W_c^{\text{CI}}$, take all the eigenstates with $|E| < E_g$, and let the machine judge them. Figure 5(b) shows that topological edge states other than $E = 0$ are also well distinguished from nontopological ones based on the learning around $E = 0$.

Concluding Remarks—In this paper, we focused on 2D random electron systems. We have demonstrated the validity of deep learning for distinguishing various random electron states in quantum phase transitions. For strong enough and weak enough randomness, the precision of judgement is $0.99999\cdots$, while in the critical regime, the judgement becomes less accurate. This region is related to the critical region where the characteristic length scale $\xi$ is
comparable to or longer than the system size $L$. That is, the probability $P$ for the eigenfunction to be judged delocalized/topological obeys the scaling law, $P(W, L) = f[(W - W_c)L^{1/\nu}]$, although determining the exponent $\nu$ is beyond the scope of this Letter. Since all we need to calculate are eigenfunctions with relatively small systems, the method will work for systems where the transfer matrix method is not applicable (localization problems on random\textsuperscript{38–41} and fractal lattices,\textsuperscript{42} for example).

We have used the known values of critical disorder to teach the machine. After learning the feature of eigenfunctions near the band center, the machine could capture localized/delocalized and topological/nontopological features away from the band center. We have also verified that the results of the SU(2) model learning can be applied to the Ando model.\textsuperscript{33}

In the cases of Anderson transition near the band edge in the SU(2) model [Fig. 3(b)] and that at the band center in the Ando model, the machine tends to predict the transition for a slightly smaller disorder than the estimate of finite size scaling analyses.\textsuperscript{32, 43} We have extracted the features in the middle layers to explain this tendency,\textsuperscript{33} but could not clarify how the machine judges phases. The details of judgement should be clarified in the future.

We have focused on the amplitude of eigenfunction in 2D. In higher dimensions, the same algorithm will be applicable via dimensional reduction: integration of $|\psi|^2$ over certain directions, reducing the image to two dimensions. The dimensional reduction will also work for disordered 3D strong and weak topological insulators.\textsuperscript{44} Other interesting quantities for machine learning are phase and spin texture of eigenfunctions in random electron systems. Classical waves (photon, phonon) in random media\textsuperscript{45–47} as well as disordered magnon\textsuperscript{48} are also worth machine learning.

Acknowledgments

The authors would like to thank Keith Slevin, Koji Kobayashi, and Ken-Ichiro Imura for useful discussions. This work was partly supported by JSPS KAKENHI Grant No. JP15H03700.
References

1) P. W. Anderson: Phys. Rev. 109 (1958) 1492.

2) A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig: Phys. Rev. B 78 (2008) 195125.

3) A. Kitaev: AIP Conference Proceedings 1134 (2009) 22.

4) M. Z. Hasan and C. L. Kane: Reviews of Modern Physics 82 (2010) 3045.

5) X.-L. Qi and S.-C. Zhang: Rev. Mod. Phys. 83 (2011) 1057.

6) M. R. Zirnbauer: Journal of Mathematical Physics 37 (1996) 4986.

7) A. Altland and M. R. Zirnbauer: Phys. Rev. B 55 (1997) 1142.

8) B. Sbierski and P. W. Brouwer: Physical Review B 89 (2014) 155311.

9) H. Katsura and T. Koma: J. Math. Phys. 57 (2016) 021903.

10) H. Katsura and T. Koma: arXiv:1611.01928 (2016).

11) A. Rodriguez, L. J. Vasquez, K. Slevin, and R. A. Romer: Phys. Rev. Lett. 105 (2010) 046403.

12) A. Rodriguez, L. J. Vasquez, K. Slevin, and R. A. Romer: Phys. Rev. B 84 (2011) 134209.

13) K. Slevin and T. Ohtsuki: New Journal of Physics 16 (2014) 015012.

14) L. Ujfalusi and I. Varga: Physical Review B 91 (2015) 184206.

15) T. Obuchi, H. Koma, and M. Yasuda: Journal of the Physical Society of Japan 85 (2016) 114803.

16) Y. LeCun, Y. Bengio, and G. Hinton: Nature 521 (2015) 436.

17) D. Silver et al.: Nature 529 (2016) 484.

18) J. Carrasquilla and R. G. Melko: arXiv:1605.01735 (2016).

19) A. Tanaka and A. Tomiya: arXiv:1609.09087 (2016).

20) G. Carleo and M. Troyer: arXiv:1606.02318 (2016).

21) P. Broecker, J. Carrasquilla, R. G. Melko, and S. Trebst: arXiv:1608.07848 (2016).

22) K. Ch’ng, J. Carrasquilla, R. G. Mello, and E. Khatami: arXiv:1609.02552 (2016).

23) L. Li, T. E. Baker, S. R. White, and K. Burke: arXiv:1609.03705 (2016).

24) E. P. van Nieuwenburg, Y.-H. Liu, and S. D. Huber: arXiv:1610.02048 (2016).

25) L. Huang and L. Wang: arXiv:1610.02746 (2016).
26) Y. Asada, K. Slevin, and T. Ohtsuki: Phys. Rev. Lett. 89 (2002) 256601.
27) Y. Asada, K. Slevin, and T. Ohtsuki: Physical Review B 70 (2004) 035115.
28) Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner: Proceedings of the IEEE 86 (1998) 2278.
29) Y. Jia, E. Shelhamer, J. Donahue, S. Karayev, J. Long, R. Girshick, S. Guadarrama, and T. Darrell: arXiv:1408.5093 (2014).
30) X. Glorot and Y. Bengio: Aistats 9 (2010) 249.
31) T. Tieleman and G. Hinton: COURSERA: Neural Networks for Machine Learning 4 (2012) Lecture 6.5.
32) T. Ando: Phys. Rev. B 40 (1989) 5325.
33) Results for Ando model and intermediate feature maps are provided online as Supplemental material.
34) J. P. Dahlhaus, J. M. Edge, J. Tworzydło, and C. W. J. Beenakker: Phys. Rev. B 84 (2011) 115133.
35) S. Liu, T. Ohtsuki, and R. Shindou: Phys. Rev. Lett. 116 (2016) 066401.
36) C.-Z. Chang, W. Zhao, J. Li, J. K. Jain, C. Liu, J. S. Moodera, and M. H. W. Chan: Phys. Rev. Lett. 117 (2016) 126802.
37) X.-L. Qi, T. L. Hughes, and S.-C. Zhang: Phys. Rev. B 78 (2008) 195424.
38) Y. Avishai and J. M. Luck: Phys. Rev. B 45 (1992) 1074.
39) R. Berkovits and Y. Avishai: Phys. Rev. B 53 (1996) R16125.
40) A. Kaneko and T. Ohtsuki: Journal of the Physical Society of Japan 68 (1999) 1488.
41) L. Ujfalusi and I. Varga: Phys. Rev. B 90 (2014) 174203.
42) Y. Asada, K. Slevin, and T. Ohtsuki: Phys. Rev. B 73 (2006) 041102.
43) U. Fastenrath, G. Adams, R. Bundschuh, T. Hermes, B. Raab, I. Schlosser, T. Wehner, and T. Wichmann: Physica A 172 (1991) 302.
44) K. Kobayashi, T. Ohtsuki, and K.-I. Imura: Physical Review Letters 110 (2013) 236803.
45) P. Sheng: Introduction to wave scattering, localization, and mesoscopic phenomena (Academic Press, San Diego, 1995).
46) C. M. Aegerter, M. Störzer, and G. Maret: Europhys. Lett. 75 (2006) 562.
47) S. Faez, A. Strybulevych, J. H. Page, A. Lagendijk, and B. A. van Tiggelen: Phys. Rev. Lett. 103 (2009) 155703.
48) B. Xu, T. Ohtsuki, and R. Shindou: arXiv:1606.02839 (2016).

49) A. MacKinnon and B. Kramer: ZEITSCHRIFT FUR PHYSIK B-CONDENSED MATTER 53 (1983) 1.
Supplemental Material for “Deep Learning the Quantum Phase Transitions in Random Two-Dimensional Electron Systems”

Application of SU(2) learning to Ando model—To further confirm the validity of machine learning demonstrated in the main text, we have applied the results of the SU(2) model learning to another model that describes the constant strength of spin-orbit coupling, i.e., Ando model\textsuperscript{32}(Fig. 6). In this model, $\alpha$ in Eq.(2) in the main text is set to 0, $\gamma$ is 0 for $x$-direction transfer and $\pi/2$ for $y$-direction. We set the strength of the spin-orbit coupling $\beta = \pi/6$ to compare with the previous results,\textsuperscript{32,43} $W_{c}^{\text{Ando}} \approx 5.75$. The solid line shows that the features of localization-delocalization transition learned from a model (SU(2)) can be applied to a different model (Ando), though the probability of delocalization starts to decrease with increasing $W$ slightly earlier than expected. This might be due to the corrections to scaling, which is present in Ando model but negligible in SU(2) model.

We have also set $\beta = 0$ (no spin-orbit coupling, i.e., the Anderson model, which belongs to the orthogonal class), where all the states are expected to be localized, which is actually the case of machine judgement (red +). The machine judgement is, however, too good in small disorder region $W < 5$ where the localization length becomes greater than 100 lattice cites,\textsuperscript{49} larger than the system size 40. This may be due to the standing wave like structure of eigenfunctions in this region, where the peak values are fluctuating due to disorder, from which the eigenfunctions might have been judged to be localized.

Fig. 6. Probability of eigenfunction of the Ando model to be judged delocalized as a function of disorder $W$ based on SU(2) machine learning. Averages over 5 samples are taken. $W_{c}^{\text{Ando}} \approx 5.75$ is indicated as a vertical dashed line. Results for orthogonal class (red +) are also shown.
Features in the intermediate layers—Here we show examples of features in the intermediate layers for localization-delocalization transition (Fig. 7) and topological-nontopological transition (Fig. 8).

Fig. 7. Features in the intermediate layers for states in the SU(2) model. The top two panels show the modulus squared of eigenfunctions. Results of the 1st and the 2nd convolutions are shown in the 2nd and the 3rd rows, followed by the features of the final full connection. The left column shows how a state in a delocalized region is judged to be delocalized with probability 0.9429..., while the right one shows how a state in the localized region is judged to be localized with delocalization probability 0.0708...
Fig. 8. Features in the intermediate layers for states in a Chern insulator. The top, the 2nd, the 3rd and the 4th rows mean the same as in the previous figure. The left column shows how a state in a topological insulator phase is judged to be a topological edge state with probability 0.8288..., while the right one shows how a state in the Anderson insulator phase is judged to be a topological edge state with probability 0.1221...