Soft Hubbard Gaps in Disordered Itinerant Models with Short-Range Interaction

Hiroshi Shinaoka[1] and Masatoshi Imada[1,2]

[1]*Department of Applied Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[2]*CREST, JST, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

(Received 17 September 2008; published 6 January 2009)

We study the Anderson-Hubbard model in the Hartree-Fock approximation and the exact diagonalization under the coexistence of short-range interaction and diagonal disorder. We show that there exist unconventional soft gaps, where the single-particle (SP) density of states (DOS) A follows a scaling in energy E as $A(E) \propto \exp[-(-\gamma \log|E - E_F|)^d]$ irrespective of electron filling and long-range order. Here, d is the spatial dimension, E_F the Fermi energy and γ a nonuniversal constant. We propose a multivalley energy landscape as their origin. Possible experiments to verify the present theory are proposed.

DOI: 10.1103/PhysRevLett.102.016404 PACS numbers: 71.27.+a, 71.23.−k

Metal-insulator transitions (MIT) have been a fundamental issue in condensed matter physics for a long time. The MIT is driven either by electron correlations, for example, as Mott transitions [1], or by random potentials as Anderson transitions [2]. When the interaction causes an insulator, it opens a SP gap at the Fermi energy E_F. The Mott gap and a gap induced by an antiferromagnetic order (AF) are typical examples. On the other hand, the Anderson insulator exhibits absence of the gap with nonzero DOS at E_F, where the insulators are characterized not by the vanishing carrier number but by a singular relaxation time. This makes fundamental differences in low-energy excitations between the Anderson and Mott insulators.

In real materials, however, electron correlations and randomness inevitably coexist, which may take on aspects qualitatively different from the simple Anderson or Mott insulators [3,4]. In particular, under the influence of the interaction, Anderson insulators show qualitatively different feature. Efros and Shklovskii [5] (ES) have clarified that in the Anderson insulator with the long-range Coulomb interaction, a soft Coulomb gap opens in the SP DOS, $A(E)$ with a power-law scaling as $A(E) \propto |E - E_F|^\alpha$, $\alpha = d - 1$ near E_F. The validity of the ES theory was confirmed numerically and in experiments [6] later. In contrast, within the ES theory, short-range interactions do not generate soft gaps.

Even for short-range interaction, however, soft gaps with $\alpha \simeq 0.5$ were reported in a Hartree-Fock (HF) study in three dimensions (3D) [7]. Recent numerical studies in two dimensions also show the suppression of DOS near E_F [8,9]. These suggest the presence of an unconventional mechanism which suppresses the DOS even with short-range interaction. In contrast, a numerical study with the dynamical mean-field theory (DMFT) claimed nonzero $A(E_F)$ even in the insulating phases [10]. Several mean-field studies gave similar results [11,12]. We clearly need further studies for comprehensive understanding of the short-range case.

Since the dielectric constant diverges at the MIT, effects of the long-range part of the Coulomb interaction are restricted to low energies and the short-range part dominates electronic structures in the experimental energy scale near the MIT. Therefore, unconventional soft gaps, if they exist, may be observed near MITs in real measurements. Indeed, recent photoemission results of $SrRu_{1-x}Ti_xO_3$ [13,14] as well as a HF study with the long-range Coulomb interaction [15] indicate breakdown of the ES scaling near the MIT in 3D.

In this letter, through numerical analyses of DOS at energies lower than those of the previous studies, we show even short-range interaction drives opening of a soft gap irrespective of the electron filling, originating from a mechanism entirely different from the ES theory. We call it *soft Hubbard gap*. We show numerical evidences of the soft Hubbard gaps with the HF approximation in one and three dimensions, where DOS $A(E)$ follows an unconventional scaling in energy E as $A(E) \propto \exp[-(-\gamma \log|E - E_F|)^d]$ with γ being a nonuniversal constant. Further support by the exact diagonalization (ED) in one dimension (1D) is given. This scaling reduces to a power-law decay of $A(E)$ toward E_F for $d = 1$ and even a faster decay for $d > 1$ in contrast to the previous HF study [7]. To clarify the origin of the soft gap, we propose a phenomenological theory. The phenomenology is further numerically tested in detail against the HF results in one dimension.

The Anderson-Hubbard Hamiltonian is defined by

$$\mathcal{H} = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} (V_i - \mu) n_{i\sigma}, \tag{1}$$

on lattices with N_s sites and N_e electrons, where t is a hopping integral, U the on-site repulsion, $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) the creation (annihilation) operator for an electron with spin σ on the site i, $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ and μ the chemical potential. The random potential V_i is spatially uncorrelated and assumed to follow two models of the distribution $P_V(V_i)$:

the box type of width $2W$, $P_V(V_i) = 1/2W$ ($|V_i| < W$) with the average $\langle V_i \rangle = 0$, and the Gaussian type, $P_V(V_i) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-V_i^2/2\sigma^2)$ ($\sigma^2 = W^2/12$). For both the distributions, $\mu = U/2$ corresponds to half filling. We take the lattice spacing as the length unit.

We first employ the HF approximation, where the wave function is approximated by a single Slater determinant consisting of a set of orthonormal SP orbitals $\{\phi_n\}$ (n is an orbital index). The HF equation reads

$$\left\{\mathcal{H}_0 + U\sum_i (\langle n_{i\downarrow}\rangle n_{i\uparrow} + \langle n_{i\uparrow}\rangle n_{i\downarrow})\right\}\phi_n = \epsilon_n \phi_n, \quad (2)$$

where $\mathcal{H}_0$ is the one-body part of the Hamiltonian and we neglect $\langle c_{i\uparrow}^\dagger c_{i\downarrow}\rangle$. To find a site-dependent mean-field solution $\langle n_{i\sigma}\rangle$ for the HF equations, we employ the iterative scheme. One typically needs from several to several tens of initial guesses in obtaining convergent physical quantities such as AF order parameters and DOS.

Figure 1(a) shows the ground-state phase diagram at half filling in three dimensions. We identify insulating phases by extrapolation of the localization lengths ξ to the bulk limit. The localization length ξ is defined by the asymptotic behavior of SP orbitals near E_F at long distances as $\phi_n \propto \exp(-r/\xi)$, where r is the distance from the center of the orbital. We obtain the AF magnetic transition points by fitting the AF magnetic order parameter with the mean-field critical exponent, 1/2. Detailed analyses of the phase diagram will be discussed elsewhere. For $U < 6$ and with increasing W from 0, metals appear from AFI as in the 2D result [16], with further reentrant transition to insulators (AFI or PI). Naively one might expect $A(E_F) > 0$ for $W > 0$. Figure 1(b) shows DOS for typical parameters. Indeed, there are no soft gaps when U or t is zero. However, we find soft Hubbard gaps over the entire insulating phases in the case of $U > 0$ and $t > 0$ regardless of the AF magnetic order. Although a power-law scaling $A(E) \propto |E - E_F|^\alpha$ with exponents $0.5 < \alpha < 1$ looks fit in the range $|E - E_F| > 0.1$ (not shown) being consistent with the previous HF study [7], closer look for $|E - E_F| < 0.1$ fits better with $A(E) \propto \exp(-(-\gamma \log|E - E_F|)^3)$ with $\gamma > 0$ rather than the power-law scaling.

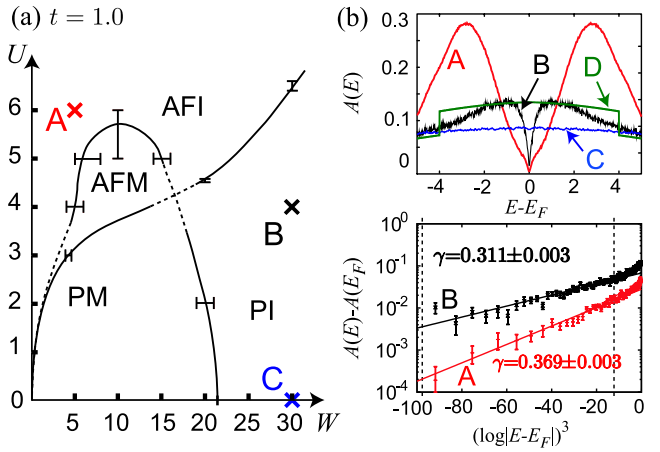

FIG. 1 (color online). (a) Ground-state phase diagram of 3D Anderson-Hubbard model at half filling for Gaussian distribution of P_V. AFI, AF insulator; AFM, AF metal; PI, paramagnetic insulator (Anderson insulator); PM, paramagnetic metal. (b) DOS with system size $8 \times 8 \times 250$: A ($t = 1$, $U = 6$, $W = 5$), B ($t = 1$, $U = 4$, $W = 30$), C ($t = 1$, $U = 0$, $W = 30$), D ($t = 0$, $U = 4$, $W = 30$). We employ Lorentz broadening with a broadening factor 1.25×10^{-3} and 6.25×10^{-4} for A and B, respectively. The broken lines denote $|E - E_F| = 10^{-2}$ and 10^{-1}. The DOS fits well with $A(E) \propto \exp(-(-\gamma \log|E - E_F|)^3)$ shown by the fitting lines for $10^{-2} < |E - E_F| < 10^{-1}$ as shown in the lower panel.

In Fig. 3(a), we further show DOS with ED in 1D. We assume a scaling function that $A(\epsilon, N_s^{-1}) = N_s^{-\beta} f(\epsilon N_s^{\beta/\alpha}) = \epsilon^\alpha g(N_s^{-\beta/\alpha}\epsilon^{-1})$ corresponding to $A(\epsilon, N_s^{-1} = 0) \propto \epsilon^\alpha$ and $A(\epsilon = 0, N_s^{-1}) \propto N_s^{-\beta}$ ($\epsilon = |E - E_F|$). As shown in Fig. 3(b), DOS well converges to this scaling function with $\alpha = 0.075$ and $\beta = 0.375$. Although a possible logarithmic scaling cannot be excluded because of the small system size, the ED results are consistent with the HF results and support a mechanism of the soft gap working beyond the mean-field level. Because the soft gap is restricted to very low energies in our 1D study, further analyses at lower energies are desired in 2D, where only a pseudogap has been found so far [8].

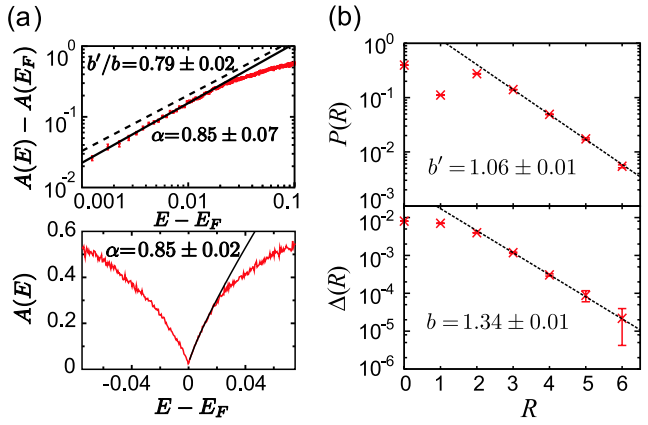

FIG. 2 (color online). (a) DOS by HF in 1D at $t = 0.3$, $U = 1.0$, $W = 2.0$, $E_F = U/2 - 1$ ($N_s = 14$). Fitting of DOS gives $\alpha = 0.85 \pm 0.07$ (solid line), which is in good agreement with the expected exponent of $b'/b = 0.79 \pm 0.02$ (broken line). (b) Numerical estimates of $P(R)$ and $\Delta(R)$. Fitting by Eqs. (4) and (6) gives $b' = 1.06 \pm 0.01$ and $b = 1.34 \pm 0.01$.

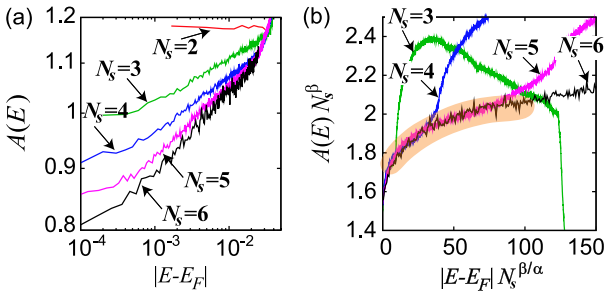

FIG. 3 (color online). (a) DOS in 1D with ED (open boundary condition): $t = 0.1$, $U = 1.0$, $W = 1.0$, $E_F = U/2$, ($N_s = 2$, 3, 4, 5, 6). We average the DOS over 3.2×10^7 realizations of disorder for $N_s = 6$. (b) Scaling plot by $A(\epsilon, N_s^{-1}) = N_s^{-\beta} f(\epsilon N_s^{\beta/\alpha})$ ($\alpha = 0.075$, $\beta = 0.375$).

Now we discuss a possible origin of the soft gap. For simplicity without loss of generality, we restrict ourselves to a SP excitation for the electron side, namely, $E > E_F$. We consider the case of $r_{\rm int} \ll \xi$, where $r_{\rm int}$ is the range of the interaction in the model. For $t \neq 0$, virtual hopping of electrons generates effective interaction, which exponentially decreases with the mutual distance. This effect is not considered in the ES theory which regards electrons as classical particles. The DOS averaged over the random potential is obtained as

$$A(E) = \left\langle \int_{-\infty}^{\infty} P_V(V_1) A_1(E, V_1) dV_1 \right\rangle_{\{V_{\bar{1}}\}}, \qquad (3)$$

where the symbol $\{V_{\bar{1}}\}$ denotes a set of random potentials V_i except for V_1. Note that $A_1(E, V_1)$ is the DOS under the condition of the fixed V_1 at the site 1 and implicitly depends on $\{V_{\bar{1}}\}$. Here we decompose the average over the random potential into the part for V_1 as described by $\int P_V(V_1) dV_1$ at fixed configurations of $\{V_{\bar{1}}\}$ and the subsequent average with respect to $\{V_{\bar{1}}\}$.

We discuss V_1 dependence of $A_1(E, V_1)$ for fixed $\{V_{\bar{1}}\}$. When V_1 decreases, the ground-state occupation of the site 1 changes from 0 to 1 and then from 1 to 2 at V_{1c1} and V_{1c2}, respectively. A possible ground state $|\phi_0\rangle$ at $V_1 > V_{1c1}$ is illustrated in Fig. 4(a), where the site 1 is empty and the

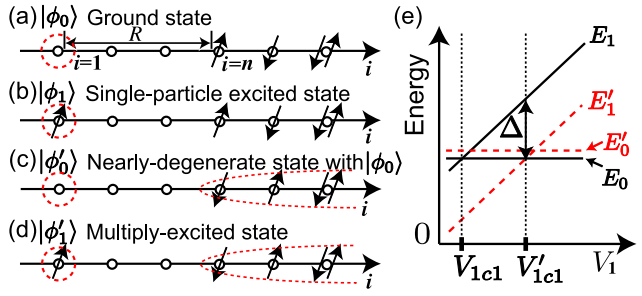

FIG. 4 (color online). Schematic illustration of (a) the ground state, (b) a SP excited state, (c) a nearly degenerate state with the ground state and (d) a multiply excited state. (e) Schematic of V_1 dependence of excitation energies.

total particle number is $N_e = N_a$ and the energy $E_0(V_1)$. Near V_{1c1} but for $V > V_{1c1}$, a SP excited state $|\phi_1\rangle$ with $N_e = N_a + 1$ and the energy $E_1(V_1)$ is defined by the electron configuration except for the site 1 is fixed to be the same as $|\phi_0\rangle$, as is illustrated in Fig. 4(b). One might think that $|\phi_1\rangle$ becomes the ground state below V_{1c1}, where $N_e = N_a + 1$. In this case, however, the SP excitation gap $E_1 - E_0$ vanishes at V_{1c1} leading to absence of a gap in the V_1-averaged DOS at the site 1. Thus the numerical evidences of the soft gaps indicate that $|\phi_1\rangle$ as a SP excited state is excluded by the electron correlation.

In contrast to the ES theory, we assume a multivalley energy landscape, which may be characteristic to random systems. Then there exist many arbitrarily-low-energy excited states whose configurations are the same with $|\phi_0\rangle$ at the site 1 but globally different on other sites. In Fig. 4(c), we illustrate a state $|\phi_0'\rangle$ at a local minimum E_0' nearly degenerate with $|\phi_0\rangle$, whose configurations not only at the occupied site n nearest to the site 1 at the distance R but also farther sites ($> R$) are relaxed one after another. Figure 4(d) shows a SP excited state $|\phi_1'\rangle$ from $|\phi_0'\rangle$ with the energy E_1' and the site-1 occupancy identical with $|\phi_1\rangle$. Here, the two nearly-degenerate states, $|\phi_1\rangle$ and $|\phi_1'\rangle$ are separated by a barrier, where multiparticle relaxation is required to reach from one to the other. Now E_1 is given by $(V_1 - E_F) + \sum_i U_{1i} + E_0$, where U_{1i} is the interaction energy between electrons on the site 1 and those on the site i. Note that only the particles at the sites i which satisfy $R \lesssim |i - 1| \lesssim R + \xi$ interact with the site 1 with the amplitude $|U_{1i}|$ comparable to $|U_{1n}|$ because of the localized nature. On the other hand, because $E_0 \simeq E_0'$ and the configurations of $|\phi_1'\rangle$ on these sites are different from those of $|\phi_1\rangle$, E_1' is different from E_1 by typically as much as $|U_{1n}|$. Thus one can find $|\phi_1'\rangle$ with the energy E_1' lower than E_1 by as much as $|U_{1n}|$ among many nearly-degenerate states with $|\phi_1\rangle$. Now $E_1'(V_1)$ and $E_0(V_1)$ crosses at $V_1 = V_{1c1}'$ and for $V_1 < V_{1c1}'$ the ground state becomes $|\phi_1'\rangle$. Note that the excitation energy $E_1' - E_1$ is negative very near V_{1c1}' but for $V_1 > V_{1c1}'$. The state $|\phi_1'\rangle$ is not counted in DOS, because this state is not a SP excitation of $|\phi_0\rangle$, but rather a multiply excited state. Thus the energy difference $\Delta = |E_1(V_{1c1}') - E_1'(V_{1c1}')|$ is the lowest energy of SP excitations counted in A near $V_1 = V_{1c1}'$.

One might think that, as in the ES theory, it is possible to lower the energy of $|\phi_1\rangle$ from E_1 to E_1' by relaxing *local* electronic configurations only near the site n. It, however, always increases the energy of the electrons other than those on the site 1, because they have already been optimized in the ground state and the increase dominates at large R. Thus a global reconstruction is required to lower the energy.

From the above discussion, Δ scales as

$$\Delta(R) = a \exp(-bR), \qquad (4)$$

where a and b are nonuniversal positive constants. Hereafter we neglect logarithmic corrections. Under the

assumption of linear dependence of the excitation energies on V_1 as shown in Fig. 4(d), the local DOS averaged by V_1 has a gap of Δ as follows:

$$\int_{V'_{1c1}}^{\infty} P_V(V_1)A_1(E, V_1)dV_1 \propto H_s(E - E_F - \Delta), \quad (5)$$

where H_s is the Heaviside step function. The same argument applies around $V_1 = V_{1c2}$.

The distribution of R with respect to $\{V_{\bar{1}}\}$ follows

$$P(R) = a' \exp(-b'R^d), \quad (6)$$

at long distances, where a', b' are nonuniversal positive constants again. Equations (4) and (6) lead to

$$Q(\Delta) = P(R(\Delta))\left|\frac{dR}{d\Delta}\right| \propto \Delta^{-1}\exp\left(-\frac{b'}{b^d}(-\log\Delta)^d\right), \quad (7)$$

where $Q(\Delta)$ are the distribution function of Δ. Equations (5) and (7) lead to

$$A(E) \propto \int_0^{|E-E_F|} d\Delta Q(\Delta) \propto \exp\left(-\frac{b'}{b^d}(-\log|E - E_F|)^d\right), \quad (8)$$

which is consistent with the observed scaling in 1D and 3D, further also in 2D (not shown) within the HF approximation. We also confirmed that this scaling is equally valid for a discrete distribution of P_V (not shown). For $d = 1$, this leads to a power law with a nonuniversal exponent: $A(E) \propto |E - E_F|^{b'/b}$. Nonuniversal power-law distributions of energies are common in Griffith phases [17]. Equation (4) indicates that a, namely, the energy scale of the gaps vanishes as t or U vanishes. Furthermore, the exponent $\alpha = b'/b$ is expected to decrease as t becomes smaller because of the reduction of ξ. These predictions are consistent with our HF results in one dimension. However, it conflicts with a DMFT study [10] and some mean-field studies [11,12] which exhibit absence of the soft gaps. This may be because they ignore spatial correlations. The latter ignores inhomogeneity of the electronic structures. Indeed, a DMFT study with the intersite self-energy retrieves the suppression of DOS near E_F [9].

In Fig. 2(b), we show a further numerical evidence of our theory in 1D. Figure 2(b) shows $\Delta(R)$ and $P(R)$ calculated by the following procedure: First, we obtain the ground state for each realization of random potentials. We construct the lowest SP excited state by adding one electron to the lowest unoccupied orbital. Next we optimize the mean fields by the iterative scheme starting from those of the SP excited state with N_e fixed. Then Δ is obtained as the difference of these two excitation energies. We calculate R as the distance between the center of the lowest unoccupied orbital, r and those of the occupied orbitals nearest to r in the ground state. We define the center of the orbital as the site which has the maximum weight. Fitting by Eqs. (4) and (6) gives $b' = 1.06 \pm 0.01$, $b = 1.34 \pm 0.01$. Estimated exponent of $b'/b = 0.79 \pm 0.02$ is in good agreement with $\alpha = 0.85 \pm 0.07$ obtained directly from DOS. This is a numerical evidence for the validity of our theory.

Although the power-law was proposed to interpret the photoemission experiments [13,14], our HF results in 3D indicates that a different asymptotic behavior of the soft Hubbard gap emerges at lower energies, namely, <10 meV. Since recent development of photoemission spectroscopy now allows us high-resolution measurement down to 1 meV, we believe that our Letter provides incentive for such high-resolution photoemission experiments as well as for other measurement such as electrical transport measurement near the MITs.

In summary, we have found an unconventional type of soft gaps in the Anderson-Hubbard model, although only short-range interaction is present. To clarify their possible origin, we have constructed a phenomenological theory. Detailed comparisons between our theory and the non-ES soft gaps observed in experiments are left as a future challenge.

We thank B. Shklovskii for fruitful discussions. M. I. thanks Aspen Center for Physics for the hospitality. Numerical calculation was partly carried out at the Supercomputer Center, Institute for Solid State Physics, Univ. of Tokyo. This work is financially supported by MEXT under the grant numbers 16076212, 17071003 and 17064004. H. S. thanks JSPS for the financial support.

[1] N. F. Mott, Proc. Phys. Soc. London Sect. A **62**, 416 (1949).
[2] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[3] D. Belitz and T. R. Kirkpatrick, Rev. Mod. Phys. **66**, 261 (1994); N. Hanasaki *et al.*, Phys. Rev. Lett. **96**, 116403 (2006).
[4] S. V. Kravchenko *et al.*, Phys. Rev. B **51**, 7038 (1995).
[5] A. L. Efros and B. I. Shklovskii, J. Phys. C **8**, L49 (1975).
[6] B. I. Shklovskii and A. L. Efros, *Electronic Properties of Doped Semiconductors* (Springer-Verlag, Berlin, 1984).
[7] F. Fazileh *et al.*, Phys. Rev. Lett. **96**, 046410 (2006).
[8] S. Chiesa *et al.*, Phys. Rev. Lett. **101**, 086401 (2008).
[9] Y. Song *et al.*, arXiv:0808.3356v1.
[10] V. Dobrosavljević and G. Kotliar, Phys. Rev. Lett. **78**, 3943 (1997).
[11] V. Dobrosavljević, A. A. Pastor, and K. Nikolić, Europhys. Lett. **62**, 76 (2003).
[12] K. Byczuk, W. Hofstetter, and D. Vollhardt, Phys. Rev. Lett. **94**, 056404 (2005).
[13] J. Kim *et al.*, Phys. Rev. B **73**, 235109 (2006).
[14] K. Maiti, R. S. Singh, and V. R. R. Medicherla, Phys. Rev. B **76**, 165128 (2007).
[15] F. Epperlein, M. Schreiber, and T. Vojta, Phys. Rev. B **56**, 5890 (1997).
[16] D. Heidarian and N. Trivedi, Phys. Rev. Lett. **93**, 126401 (2004).
[17] R. B. Griffiths, Phys. Rev. Lett. **23**, 17 (1969).