Spontaneous symmetry breaking and bifurcations in ground state fidelity for quantum lattice systems

Jian-Hui Zhao, Hong-Lei Wang, Bo Li, and Huan-Qiang Zhou

Centre for Modern Physics and Department of Physics, Chongqing University, Chongqing 400044, The People's Republic of China

Spontaneous symmetry breaking occurs in a system when its Hamiltonian possesses a certain symmetry, whereas the ground state wave functions do not preserve it. This provides such a scenario that a bifurcation, which breaks the symmetry, occurs when some control parameter crosses its critical value. It is unveiled that the ground state fidelity per lattice site exhibits such a bifurcation for quantum lattice systems undergoing quantum phase transitions. The significance of this result lies in the fact that the ground state fidelity per lattice site is universal, in the sense that it is model-independent, in contrast to (model-dependent) order parameters. This fundamental quantity may be computed by exploiting the newly-developed tensor network algorithms on infinite-size lattices. We illustrate the scheme in terms of the quantum Ising model in a transverse magnetic field and the spin 1/2 XY model in an external magnetic field on an infinite-size lattice in one spatial dimension.

Introduction. Quantum phase transitions (QPTs) [1, 2] arise from the cooperative behaviors in quantum many-body systems, in which long-range orders emerge. In the conventional Landau-Ginzburg-Wilson paradigm, the most fundamental notion is spontaneous symmetry breaking (SSB), with the symmetry-broken phase characterized by the nonzero values of a local order parameter. An SSB occurs in a system when its Hamiltonian enjoys a certain symmetry, whereas the ground state wave functions do not preserve it [3, 4]. The implication of an SSB is two-fold: first, a system has stable and degenerate ground states, each of which breaks the symmetry of the system; second, the symmetry breakdown results from random perturbations. This leads to such a scenario that a bifurcation, which breaks the symmetry, occurs, when some control parameter crosses its critical value. Conventionally, this is reflected in local order parameters.

The latest advances in our understanding of QPTs originate from the perspectives of both entanglement [5] and fidelity [6, 7, 8, 9], which are basic notions in quantum information science. In Refs. [7, 8], it has been argued that the ground state fidelity per lattice site is fundamental in the sense that it may be used to characterize QPTs, regardless of what type of internal order is present in quantum many-body states. The argument is solely based on the basic Postulate of Quantum Mechanics on quantum measurements, which implies that two non-orthogonal quantum states are not reliably distinguishable [10]. In other words, the ground state fidelity per lattice site is able to describe QPTs arising from an SSB and/or topological order [11]. This has been further confirmed in Refs. [12, 13], where topologically ordered states in the Kitaev model on the honeycomb lattice and the Kosterlitz-Thouless phase transition are investigated from the fidelity perspective, respectively. Moreover, even for systems with symmetry-breaking orders, it is advantageous to adopt the ground state fidelity per lattice site instead of using the conventional local order parameters, due to the fact that it is model-independent, although one may systematically derive local order parameters from tensor network (TN) representations of quantum many-body ground state wave functions by investigating the reduced density matrices for local areas on an infinite-size lattice [14]. However, it remains unclear whether or not it is possible for the ground state fidelity per lattice site to capture bifurcations arising from an SSB.

In this Letter, we attempt to fill in this gap. First, we demonstrate that the newly-developed TN algorithms on infinite-size lattices may produce degenerate ground states arising from an SSB, each of which results from a randomly chosen initial state subject to an imaginary time evolution. Second, it is unveiled that an SSB is reflected as a bifurcation in the ground state fidelity per lattice site for quantum lattice systems undergoing QPTs with symmetry-breaking orders [15]. The significance of this conclusion lies in the fact that, on the one hand, this establishes the connection between the fidelity approach to QPTs and the singularity theory; on the other hand, it is of practical importance since it makes possible to locate transition points without the need to compute the derivatives of the ground state fidelity per lattice site with respect to the control parameter [16]. In contrast, the von Neumann entropy, a bipartite entanglement measure, fails to distinguish degenerate symmetry-breaking ground states. We illustrate the general scheme in terms of the quantum Ising model in a transverse magnetic field and the spin 1/2 XY model in an external magnetic field. Here, it is worth emphasizing that, although the scheme is applicable to quantum lattice models in any spatial dimensions, we restrict ourselves to quantum systems on an infinite-size lattice in one spatial dimension. This is achieved by exploiting the infinite matrix product state (iMPS) algorithm initiated by Vidal [17]. The extension to quantum lattice systems in two and higher spatial dimensions, which requires to use the infinite projected entangled-pair state (iPEPS) algorithm [18], is deferred to another publication [19].

Infinite matrix product state algorithm and spontaneous symmetry breaking. For quantum many-body systems on an infinite-size lattice in one spatial dimension, Vidal [17] has developed a variational algorithm to compute their ground state
wave functions based on their MPS representations, which is a variant of the MPS algorithm [20, 21] on a finite-size lattice in one spatial dimension. Here, we briefly recall the key ingredients of the algorithm. Assume that the Hamiltonian is translationally invariant, and consists of the nearest-neighbor interactions: $H = \sum_i h^{i,i+1}$, with $h^{i,i+1}$ being the nearest-neighbor two-body Hamiltonian density. Attached to each site is a three-indices tensor $\Gamma_{\lambda A B r}$ or $\Gamma_{B B r}$, and to each bond a diagonal (singular value) matrix $\lambda A$ or $\lambda B$, depending on the evenness and oddness of the $i$-th site and the $i$-th bond, respectively. Here, $s$ is a physical index, $s = 1, \cdots, d$, with $d$ being the dimension of the local Hilbert space, and $l$ and $r$ denote the bond indices, $l, r = 1, \cdots, \chi$, with $\chi$ being the truncation dimension. The imaginary time evolution amounts to computing $|\Psi(\tau)\rangle = \exp(-iH\tau)|\Psi(0)\rangle/\exp(-iH\tau)|\Psi(0)\rangle$. For large enough $\tau$ and a generic initial state $|\Psi(0)\rangle$, it yields a good approximation to the ground state wave function, as long as there is a gap in the spectrum of the system. Following the Suzuki-Trotter decomposition [22], the imaginary time evolution operator is reduced to a product of two-site evolution operators acting on sites $i$ and $i+1$: $U(i,i+1) = \exp(-ih^{i,i+1}\delta\tau)$, $\delta\tau \ll 1$. Notice that, a two-site gate $U(i,i+1)$ renders the state not in the form of a MPS and breaks the translational invariance. The former is performed by performing a singular value decomposition of a matrix contracted from one $\Gamma_{A B r}$, one $\Gamma_{B B r}$, one $\lambda A$ and two $\lambda B$’s, and only the $\chi$ largest singular values are retained. This yields the new tensors $\Gamma_{A B r}$, $\Gamma_{B B r}$, and $\lambda A$, which are used to update the tensors for all the sites, thus restoring the translational invariance under two site shifts. Repeating this procedure until the ground state energy converges, one may generate the systems’ ground state wave functions in the MPS representations.

Remarkably, for a system with symmetry-breaking orders, the iMPS algorithm automatically produces degenerate ground states arising from an SSB in the symmetry-broken phase, each of which breaks the symmetry of the system. Moreover, the symmetry breakdown results from the fact that an initial state has been chosen randomly. It is worth mentioning that, for quantum lattice systems in one spatial dimension, continuous symmetries cannot be spontaneously broken [23], due to strong quantum fluctuations [24]. Therefore, we shall restrict ourselves to the discussion of quantum lattice systems with a discrete symmetry group $Z_2$ [25].

Bifurcations in the ground state fidelity per lattice site. Now consider a quantum many-body system, with a discrete symmetry group $Z_2$, on an infinite-size lattice in one spatial dimension. Assume that the system undergoes a continuous QPT with $Z_2$ symmetry spontaneously broken, when a control parameter $\lambda$ varies. According to the definition [7, 8], the ground state fidelity per lattice site, $d_{\lambda_1, \lambda_2}$, is the scaling parameter, which characterizes how fast the fidelity $F_{\lambda_1, \lambda_2} \equiv |\langle \Psi(\lambda_2)|\Psi(\lambda_1)\rangle|$ between two ground states $|\Psi_{\lambda_1}\rangle$ and $|\Psi_{\lambda_2}\rangle$ goes to zero when the thermodynamic limit is approached. In fact, the ground state fidelity $F_{\lambda_1, \lambda_2}$ asymptotically scales as $F_{\lambda_1, \lambda_2} \sim d_{\lambda_1, \lambda_2}/L$, with $L$ the number of sites in a finite-size lattice. Remarkably, the ground state fidelity per lattice site is well defined in the thermodynamic limit, and satisfies the properties inherited from the fidelity $F(\lambda_1, \lambda_2)$: (i) normalization $d(\lambda, \lambda) = 1$; (ii) symmetry $d(\lambda_1, \lambda_2) = d(\lambda_2, \lambda_1)$; and (iii) range $0 \leq d(\lambda_1, \lambda_2) \leq 1$.

In the $Z_2$ symmetric phase, the ground state is non-degenerate, whereas in the $Z_2$ symmetry-broken phase, two degenerate ground states arise. Now let us see what this implies for the ground state fidelity per lattice site, $d_{\lambda_1, \lambda_2}$. If we choose $|\Psi_{\lambda_2}\rangle$ as a reference state, with $\lambda_2$ in the $Z_2$ symmetric phase, then the ground state fidelity per lattice site, $d_{\lambda_1, \lambda_2}$, cannot distinguish two degenerate ground states $|\Psi_{\lambda_2}\rangle$ in the $Z_2$ symmetry-broken phase. Here, $|\Psi_{\lambda_2}\rangle = P|\Psi_{\lambda_2}\rangle$, with $P$ being the operation generating the symmetry group $Z_2$. This follows from the fact that $\langle \Psi_{\lambda_2}|\Psi_{\lambda_2}\rangle = \langle \Psi_{\lambda_2}|P|\Psi_{\lambda_2}\rangle = \langle \Psi_{\lambda_2}|\Psi_{\lambda_2}\rangle$, for any large but finite size $L$. However, if we choose $|\Psi_{\lambda_2}\rangle$ as a reference state, with $\lambda_2$ in the $Z_2$ symmetry-broken phase, then $d_{\lambda_1, \lambda_2}$ is able to distinguish two degenerate ground states. Therefore, for a given truncation dimension $\chi$, a pseudo phase transition point $\lambda_2$ manifests itself as a bifurcation point [13]. An extrapolation to $\chi = \infty$ determines the critical point $\lambda_c$. Therefore, the phase transition point $\lambda_c$ manifests itself as a bifurcation point $\lambda_c$.

In contrast, the von Neumann entropy, a bipartite entanglement measure, fails to distinguish degenerate symmetry-breaking ground states. This is due to the fact that the von Neumann entropy is fully determined by the singular value matrices $\lambda A$ and $\lambda B$, whereas all the information concerning an SSB is encoded in the tensors $\Gamma_{\lambda A B r}$ and $\Gamma_{\lambda B B r}$.

Models. As an illustration, let us consider two quantum systems with the symmetry group $Z_2$. The first is the quantum Ising model in a transverse magnetic field on an infinite-size lattice in one spatial dimension. It is described by the Hamiltonian:

$$H = -\sum_{\alpha=x,y,z} S^{i\alpha} S^{i+1\alpha} + \lambda S^{i0},$$

where $S^{i\alpha} (\alpha = x, z)$ are the Pauli spin operators of the $i$-th site. The second is the spin 1/2 XYX model in an external magnetic field, with the Hamiltonian:

$$H = \sum_{\alpha=x,y,z} S^{\alpha} S^{\alpha+1} + \Delta x S^{\alpha} S^{\beta} + S^{\alpha} S^{\alpha+1} + h S^{\alpha},$$

where $S^{\alpha} (\alpha = x, y, z)$ are the Pauli spin operators of the $i$-th...
spin 1/2, $\Delta$ denotes the anisotropy in the internal spin space, and $h$ is an external magnetic field. The model possesses a $Z_2$ symmetry, generated by the operation: $S^{(i)}_x \rightarrow -S^{(i)}_x$ and $S^{(i)}_y \rightarrow -S^{(i)}_y$. Note that $\Delta_1 < 1$ and $\Delta_2 > 1$ correspond to easy-plane and easy-axis behaviors, respectively. The ordered phase in the easy-plane (easy-axis) case arises from an SSB along the $x(y)$ direction, with a non-zero order parameter, i.e., the magnetization $\langle S^{(i)}_z \rangle$ below the critical field $h_c$. Here we shall choose $\Delta_1 = 0.25$, for which it is critical at $h = h_c$, with $h_c \sim 3.210(6)$ from the quantum Monte Carlo simulation [27].

Simulation results. In Fig. 1 we present the probability mass function for the quantum Ising model in a transverse magnetic field in the $Z_2$ symmetry-broken phase ($\lambda = 1/2$). Suppose a random variable $K$ follows the binomial distribution with parameters $n$ and $p$, then the probability of getting exactly $k$ successes in $n$ trials is given by the probability mass function: $Pr(K = k) = C^n_k p^k (1 - p)^{n-k}$, for $k = 0, 1, 2, \ldots, n$, where $C^n_k = n! / (k!(n-k)!)$ is the binomial coefficient. Here, by a success we mean that the order parameter $\langle S^{(i)}_z \rangle$ is positive. Our data are presented for both $n = 20$ and $n = 40$, with the truncation dimension $\chi$ to be 8. This confirms that the probability for getting the ground state with the positive order parameter $\langle S^{(i)}_z \rangle$ each simulation run is $p = 1/2$. The same pattern occurs for other choices of the truncation dimension $\chi$. Actually this is true for any model with $Z_2$ symmetry spontaneously broken. Therefore, our results demonstrate that an SSB occurs in classical simulations of quantum systems on an infinite-size lattice in the context of the iMPS algorithm.

In contrast, algorithms that simulate finite-size lattice systems are forbidden to produce degenerate symmetry-breaking ground states, since an SSB only occurs in the infinite-size (thermodynamic) limit.

In Fig. 2 we plot the ground state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, for the quantum Ising model in a transverse field. Here, the transverse magnetic field strength $\lambda$ is the control parameter. If we choose $\Psi(\lambda_3)$ as a reference state, with $\lambda_3$ in the $Z_2$ symmetry-broken phase (as shown here, $\lambda_3 = 0.9$), then $d(\lambda_1, \lambda_2)$ is able to distinguish two degenerate ground states, with a pseudo phase transition point $\lambda_4 \chi$ as a bifurcation point [28]. The critical value $\lambda_4 = 1.00015$ is determined from an extrapolation of the pseudo phase transition point $\lambda_4$ for the truncation dimension $\chi$ (see the inset in Fig. 2), which is quite close to the exact value 1. Therefore, the iMPS algorithm enables us to locate the transition point accurately from the computation of $d(\lambda_1, \lambda_2)$, with moderate computational cost. We stress that such a scaling for finite values of the truncation dimension $\chi$ has been discussed for the von Neumann entropy [29].

We have also presented $d(h_1, h_2)$ for the spin 1/2 XYX model in an external magnetic field on an infinite-size lattice in Fig. 3. Here, the external magnetic field $h$ is the control parameter. If we choose $\Psi(h_3)$ as a reference state, with $h_3$ in the $Z_2$ symmetry-broken phase (as shown here, $h_3 = 3.2$), then $d(h_1, h_2)$ is able to distinguish two degenerate ground states, with a pseudo phase transition point $h_\chi$ as a bifurcation point.

FIG. 1: (color online) The probability mass function for the quantum Ising model in a transverse magnetic field in the $Z_2$ symmetry-broken phase ($\lambda = 1/2$). If a random variable $K$ follows the binomial distribution with parameters $n$ and $p$, then the probability of getting exactly $k$ successes in $n$ trials is given by the probability mass function: $Pr(K = k) = C^n_k p^k (1 - p)^{n-k}$, for $k = 0, 1, 2, \ldots, n$, where $C^n_k = n! / (k!(n-k)!)$ is the binomial coefficient. Here, by a success we mean that the order parameter $\langle S^{(i)}_z \rangle$ is positive. Our data are presented for both $n = 20$ and $n = 40$, with $\chi = 8$. This confirms that the probability for getting the ground state with the positive order parameter $\langle S^{(i)}_z \rangle$ each simulation run is $p = 1/2$. The same pattern occurs for other choices of the truncation dimension $\chi$. Therefore, an SSB occurs in classical simulations of quantum systems on an infinite-size lattice in the context of the iMPS algorithm.

FIG. 2: (color online) Main: The ground state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, for the quantum Ising model in a transverse field. Here, the transverse magnetic field strength $\lambda$ is the control parameter. If we choose $\Psi(\lambda_3)$ as a reference state, with $\lambda_3$ in the $Z_2$ symmetry-broken phase (as shown here, $\lambda_3 = 0.9$), then $d(\lambda_1, \lambda_2)$ is able to distinguish two degenerate ground states, with a pseudo phase transition point $\lambda_4 \chi$ as a bifurcation point [28]. The critical value $\lambda_4 = 1.00015$ is determined from an extrapolation of the pseudo phase transition point $\lambda_4 \chi$ for the truncation dimension $\chi$ (see the inset in Fig. 2), which is quite close to the exact value 1. Therefore, the iMPS algorithm enables us to locate the transition point accurately from the computation of $d(\lambda_1, \lambda_2)$, with moderate computational cost. We stress that such a scaling for finite values of the truncation dimension $\chi$ has been discussed for the von Neumann entropy [29].

In Fig. 3 we plot the ground state fidelity per lattice site, $d(h_1, h_2)$, for the spin 1/2 XYX model in an external magnetic field on an infinite-size lattice in Fig. 3. Here, the external magnetic field $h$ is the control parameter. If we choose $\Psi(h_3)$ as a reference state, with $h_3$ in the $Z_2$ symmetry-broken phase (as shown here, $h_3 = 3.2$), then $d(h_1, h_2)$ is able to distinguish two degenerate ground states, with a pseudo phase transition point $h_\chi$ as a bifurcation point.
The critical point $h_c = 3.20471$ is determined from an extrapolation of the pseudo phase transition point $h_x$ for the truncation dimension $\chi$, as seen from the inset in Fig. 3.

**Summary.** We have demonstrated that the iMPS algorithm may produce degenerate, symmetry-breaking, ground states arising from an SSB, each of which results from a randomly chosen initial state. It is shown that an SSB is reflected as a bifurcation in the ground state fidelity per lattice site for quantum lattice systems undergoing QPTs with symmetry-breaking orders. Conceptually, this establishes the connection between the fidelity approach to QPTs and the singularity theory. Practically, it is also important since it makes possible to locate transition points without the need to compute the derivatives of the ground state fidelity per lattice site with respect to the control parameter, which is usually a formidable task. We illustrated the general scheme in terms of the quantum Ising model in a transverse magnetic field and the spin 1/2 XXY model in an external magnetic field on an infinite size lattice in one spatial dimension.

Finally, we point out that we may extend our investigation to quantum lattice systems in two and higher spatial dimensions, which requires the iPEPS algorithm [18]. This is currently under active investigation [19].

**Acknowledgements.** The support from the National Natural Science Foundation of China (Grant Nos: 10774197 and 10874252) and the Natural Science Foundation of Chongqing (Grant No: CSTC, 2008BC2023) is acknowledged.

[1] S. Sachdev, Quantum Phase Transitions, Cambridge University Press, 1999, Cambridge.
[2] X.-G. Wen, Quantum Field Theory of Many-Body Systems, Oxford University Press, 2004, Oxford.
[3] P.W. Anderson, Basic Notions of Condensed Matter Physics, Addison-Wesley: The Advanced Book Program, 1997, Reading, Mass.
[4] S. Coleman, An Introduction to Spontaneous Symmetry Breakdown and Gauge Fields, Laws of Hadronic Matter, Ed. A. Zichichi, Academic, 1975, New York.
[5] See, e.g., L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. 80, 517 (2008) and references therein.
[6] P. Zanardi and N. Paunković, Phys. Rev. E 74, 031123 (2006).
[7] H.-Q. Zhou and J.F. Barjaktarević, J. Phys. A: Math. Theor. 41, 412001 (2008); H.-Q. Zhou, J.-H. Zhao, and B. Li, J. Phys. A: Math. Theor. 41, 492002 (2008); H.-Q. Zhou, arXiv:0704.2945.
[8] H.-Q. Zhou, R. Orús, and G. Vidal, Phys. Rev. Lett. 100, 080602 (2008).
[9] P. Zanardi, M. Cozzini, and P. Giorda, J. Stat. Mech. L02002, (2007); N. Oelkers and J. Links, Phys. Rev. B 75, 115119 (2007); M. Cozzini, R. Ionicioiu, and P. Zanardi, Phys. Rev. B 76, 104420 (2007); L. Campos Venuti and P. Zanardi, Phys. Rev. Lett. 99, 095701 (2007); W.-L. You, Y.-W. Li, and S.-J. Gu, Phys. Rev. E 76, 022101 (2007); S. J. Gu et al., Phys. Rev. B 77, 245109 (2008); M. F. Yang, Phys. Rev. B 76, 180403(R) (2007); Y. C. Tzeng and M. F. Yang, Phys. Rev. A 77, 012311 (2008); J. O. Fjærestad, J. Stat. Mech. P07011 (2008).
[10] M.A. Nielsen and I.L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, 2000, Cambridge).
[11] This is even valid for thermal phase transitions if we extend the fidelity notion from pure states to mixed states to accomodate thermal fluctuations (see the first reference in [7]). In fact, the logarithmic function of the fidelity per lattice site for two thermal mixed states corresponding to different temperatures reduces to nothing but the free energy, if other non-thermal control parameters are kept fixed. This implies that the singularities in the fidelity per lattice site coincide with those in the free energy, thus showing the equivalence between the fidelity approach and the conventional one to thermal phase transitions.
[12] J.-H. Zhao and H.-Q. Zhou, arXiv:0803.0814.
[13] H.-L. Wang, J.-H. Zhao, B. Li, and H.-Q. Zhou, arXiv:0902.1670.
[14] H.-Q. Zhou, arXiv:0803.0585.
[15] Bifurcation theory studies and classifies phenomena characterized by a sudden change in behaviors arising from a small variation in a control parameter. For a review, see, J.D. Crawford, Rev. Mod. Phys. 63, 991 (1991). See also J. Araki et al., Proc. R. Soc. Lond. A345, 413 (1975) for a discussion about the spontaneously broken symmetry and the cusp catastrophe.
[16] Numerically, it is a formidable task to compute the derivatives of the ground state fidelity per lattice site with respect to the control parameter, due to stringent accuracy requirements.
[17] G. Vidal, Phys. Rev. Lett. 99, 070201 (2007).
[18] J. Jordan et al., Phys. Rev. Lett. 101, 250602 (2008).
[19] B. Li et al., in preparation.
[20] G. Vidal, Phys. Rev. Lett. 93, 040502 (2004).
[21] G. Vidal, Phys. Rev. Lett. 91, 147902 (2003).
[22] M. Suzuki, Phys. Lett. A146, 319 (1990).
[23] N. D. Mermin and H. Wegner, Phys. Rev. Lett. 17, 1133 (1966).
[24] However, the finiteness of the truncation dimension $\chi$ in
the iMPS algorithm automatically leads to infinite degenerate ground states, each of which breaks the continuous symmetry. This results in the so-called pseudo continuous SSB \[13\], for quantum lattice systems with a continuous symmetry group, e.g., \( U(1) \). In addition, the extent to which the symmetry is spontaneously broken may be quantified by introducing a pseudo-order parameter that must be scaled down to zero, in order to be consistent with the Mermin-Wegner theorem.

[25] The extension of our discussion to quantum lattice systems with other discrete groups, e.g., \( Z_N \), is straightforward.

[26] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. 60, 407 (1961); P. Pfeuty, Ann. Phys. 57, 79 (1970).

[27] J. Kurmann et al., Physica A112, 235 (1982); D. V. Dmitriev et al., J. Exp. Th. Phys. 95, 538 (2002); T. Roscilde, et al., Phys. Rev. Lett. 93, 167203 (2004).

[28] We emphasize that it is difficult, if not impossible, to figure out the bifurcation in the ground state fidelity per lattice site for the quantum Ising model in a transverse field from the exact solution of the model [26]. In fact, the Jordan-Wigner transformation, used to solve the model, changes the boundary conditions. Therefore, it affects the ground state fidelity per lattice site for finite-size systems, but not in the infinite-size (thermodynamic) limit.

[29] L. Tagliacozzo, Thiago. R. de Oliveira, S. Iblisdir, and J. I. Latorre, Phys. Rev. B78, 024410 (2008).