## Real-space many-body marker for correlated $\mathbb{Z}_2$ topological insulators

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Taking the clue from the modern theory of polarization [Rev. Mod. Phys. 66, 899 (1994)], we identify an operator to distinguish between  $\mathbb{Z}_2$ -even (trivial) and  $\mathbb{Z}_2$ -odd (topological) insulators in two spatial dimensions. Its definition extends the position operator [Phys. Rev. Lett. 82, 370 (1999)], which was introduced in one-dimensional systems. We first show a few examples of noninteracting models where single-particle wave functions are defined and allow for a direct comparison with standard techniques on large system sizes. Then, we illustrate its applicability for an interacting model on a small cluster where exact diagonalizations are available. Its formulation in the Fock space allows a direct computation of expectation values over the ground-state wave function (or any approximation of it), thus, allowing us to investigate generic interacting systems, such as strongly correlated topological insulators.

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Introduction. Topological insulators represent nowadays a pillar of condensed-matter physics [1,2], defining a class of materials that are fundamentally distinct from ordinary band insulators. Their history originates in the early days of the integer quantum Hall effect where topology plays a prominent role [3,4]. Here, time-reversal symmetry is broken and different quantum states are possible, which can be distinguished by the total Chern number of occupied bands. This leads to a  $\mathbb{Z}$ classification of distinct topological states in two dimensions, different from conventional band insulators. A major step forward has been achieved when it was realized that enforcing the time-reversal symmetry the situation changes radically [5]. In this case, only two possibilities are left, thus, leading a  $\mathbb{Z}_2$ classification where trivial ( $\mathbb{Z}_2$ -even) and topological ( $\mathbb{Z}_2$ -odd) states exist. Their full characterization has been obtained in noninteracting systems where the inspection of Bloch or Wannier wave functions allows a straightforward determination of their properties [6]. For example, trivial and topological states can be distinguished by looking at the time-reversal polarization, which can be computed in terms of Wannier centers [7–9]. In addition, whenever, inversion symmetry is present, the computation is reduced to the determination of the parity of occupied states at time-reversal momenta [10].

The inclusion of electron-electron interaction, beyond simple mean-field approximations, is far from being simple and straightforward. Indeed, the analysis based upon singleparticle wave functions is lost, forcing us to deal with the many-body state in its entirety. Since the early studies on the integer quantum Hall effect, Niu and collaborators proposed an ingenious way to compute topological observables (e.g., Chern numbers) by averaging over boundary conditions suitable derivatives of the many-body wave function [11]. As originally noted in Ref. [11] and recently verified numerically [12], it turns out that the integration is actually not necessary, and the Berry curvature evaluated by computing the derivatives at fixed boundary conditions is already quantized. However, this procedure is not easily implemented since it requires the determination of the ground state for different choices of the boundary conditions [13–15], which is particularly difficult when dealing with approximate solutions of the model.

Recently, a few investigations focused on the Bernevig-Hughes-Zhang (BHZ) model [16] on the lattice, supplemented with Hubbard-like interactions, to determine their effects on the transition between trivial and topological insulators [17-19]. In one spatial dimension, density-matrix renormalization group (DMRG) can be used [19] to evaluate the local spin at the system edges, whose presence provides an indication on the topological nature of the ground state. However, this procedure is not fully satisfactory, in the view of defining a marker that can unambiguously distinguish the two band insulators. Alternatively, some approximate method can be used, as, for example, dynamical mean-field theory, to investigate either two- or three-dimensional systems [17,18]. Here, trivial and topological insulators are discriminated on the basis of the low-energy behavior of the electron selfenergy [20], which is not easily accessible within other ground-state approaches (e.g., DMRG or quantum Monte Carlo methods). Real-space Chern markers have been also introduced for noninteracting systems [21] and extended, within dynamical mean-field theory, to include the effects of electron-electron interactions [22].

Well before these developments in the framework of topological insulators, Resta and Sorella [23] introduced a many-body operator to discriminate metals and insulators in interacting systems. Building on the modern theory of polarization [24], they focused the attention on one-dimensional models, defining

$$\hat{Z} = \exp\left(\frac{2\pi i}{M} \sum_{j=1}^{M} x_j \hat{n}_j\right),\tag{1}$$

where M is the number of sites and  $\hat{n}_j$  is the electron density operator on the jth site, whose physical coordinate is  $x_j$ . Then, the modulus of its expectation value over the (normalized) ground-state  $z=\langle\Psi_0|\hat{Z}|\Psi_0\rangle$  can be used to measure the localization length  $\lambda^2=-[M/(2\pi)]^2\ln|z|^2$ . In the thermodynamic limit, a metal is characterized by  $\lambda\to\infty$  ( $|z|\to0$ ) and an insulator by a finite  $\lambda$  ( $|z|\to1$ ). For insulators, the phase of z is related to electronic polarization (in units of the electric charge e) through the many-body Berry phase  $\gamma$  [25,26],

$$P = \frac{\gamma}{2\pi} = \frac{1}{2\pi} \text{Im ln } z. \tag{2}$$

The  $\hat{Z}$  operator is very useful to detect the Mott transition in the one-dimensional Hubbard model [27,28]. However, quite remarkably, little attention has been given to the phase (or sign, for centrosymmetric lattices) of z. In fact, two classes of interacting centrosymmetric insulators may be distinguished by having either z=1 or -1 [29]. Although in the one-dimensional noninteracting case the topological properties of the Berry phase have been already discussed in relation to the surface charge theorem [30,31], the phase of z in interacting systems has not been investigated. In addition, since then, no attempts to extend the analysis to two-dimensional systems have been pursued.

In this Letter, we perform an important step forward in this direction, defining a marker, which is inspired by Eq. (1); then, its phase can be expressed in terms of the Chern number, allowing us to discriminate between  $\mathbb{Z}_2$ -even and  $\mathbb{Z}_2$ -odd insulators. Specific examples of non-interacting lattice systems with time-reversal symmetry, such as the BHZ [16] or the Kane-Mele (KM) [5] models are provided. In addition, calculations on the interacting BHZ model (where the on-site Hubbard-U is included) are also reported for a  $3\times 3$  cluster (with 18 electrons). The present Letter will allow one to perform ground-state calculations in interacting systems and obtain a clearcut way to distinguish trivial and topological states

Settings and definitions. In the following, we will focus on two-band lattice models of spinful fermions at half-filling (i.e., with two electrons per site on average). In the BHZ model, there are two orbitals, labeled by  $\eta=\pm$ , on each site **R** of the underlying Bravais lattice; instead, in the KM model, there are two sites again labeled by  $\eta=\pm$  in the unit cell. The band structure is assumed to display a gap, leading to an insulating ground state. We will first consider Hamiltonians conserving the z projection of the total spin  $\hat{S}_z$ , which is customary in the literature [32]. In this case, the  $\mathbb{Z}_2$  invariant can be equivalently discussed in terms of the parity of the spin Chern number [33], calculated over the occupied states with spin up (or down) only [6]. The effects of symmetry-breaking perturbations are also discussed.

In order to generalize the definition of lattice position operator of Eq. (1) in finite clusters of any geometry and dimension, we have to introduce a many-body operator that commutes with lattice translations and contains the information on the average electron position. A useful definition,

which plays a central role in our treatment, is given by

$$\hat{Z}_{\sigma}(\delta \mathbf{k}) = \exp\left(i\delta \mathbf{k} \cdot \sum_{j} \mathbf{R}_{j} \hat{n}_{j,\sigma}\right),\tag{3}$$

where  $\delta \mathbf{k}$  is a yet unspecified wave vector, quantized according to the lattice geometry, and  $\hat{n}_{j,\sigma} = \sum_{\eta} \hat{n}_{j,\eta,\sigma}$  is the spin-projected electron density operator on the jth Bravais lattice site, located at  $\mathbf{R}_j$ . Whatever choice of the parameter  $\delta \mathbf{k}$ , the operator  $\hat{Z}_{\sigma}(\delta \mathbf{k})$  is a legitimate estimator of the average electron position within the cluster.

It is useful to first prove an interesting property of the operator defined in Eq. (3). Indeed, the ground-state average of  $\hat{Z}_{\sigma}(\delta \mathbf{k})$  can be related to the overlap between the ground states of the model with and without a magnetic field piercing the two-dimensional torus. This can be easily proved by noting that the unitary operator  $\hat{Z}_{\sigma}(\delta \mathbf{k})$  implements a gauge transformation on the fermion operators,

$$\hat{Z}_{\sigma}(\delta \mathbf{k})\hat{c}_{i\,n\,\sigma}^{\dagger}\hat{Z}_{\sigma}^{\dagger}(\delta \mathbf{k}) = e^{i\delta \mathbf{k}\cdot\mathbf{R}_{j}}\hat{c}_{i\,n\,\sigma}^{\dagger},\tag{4}$$

where  $\hat{c}^{\dagger}_{j,\eta,\sigma}$  creates an electron on the Bravais site j, orbital  $\eta$ , and spin  $\sigma$ . Then, if  $|\Psi_0\rangle$  is the many-body ground state of the Hamiltonian  $\hat{\mathcal{H}}$  with periodic boundary conditions, then  $|\Psi_0(\delta \mathbf{k})\rangle = \hat{Z}_{\sigma}(\delta \mathbf{k}) |\Psi_0\rangle$  is the ground state of the Hamiltonian  $\hat{Z}_{\sigma}(\delta \mathbf{k}) \hat{\mathcal{H}} \hat{Z}_{\sigma}^{\dagger}(\delta \mathbf{k})$ . The density operators in the transformed Hamiltonian are left invariant by the gauge transformation, whereas the hopping terms of the electrons with spin  $\sigma$  acquire a phase factor which can be attributed, via the Peierls substitution, to the presence of a (pure) gauge field, i.e., the presence of an integer number of magnetic quantum fluxes piercing the torus. Note that periodic-boundary conditions are preserved by the gauge transformation due to the quantization of  $\delta \mathbf{k}$ . As a result, the ground-state average of  $\hat{Z}_{\sigma}(\delta \mathbf{k})$  without the quantum flux, equals the overlap between the ground states of the model with and without the quantum flux,

$$\langle \Psi_0 | \hat{Z}_{\sigma}(\delta \mathbf{k}) | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0(\delta \mathbf{k}) \rangle. \tag{5}$$

This relation is exact but rests upon the precise definition of the phase factor of the ground state  $|\Psi_0(\delta \mathbf{k})\rangle$ , which must be chosen according to the previous derivation.

The analysis of noninteracting centrosymmetric models in one spatial dimension provides a useful check on the method, as we show in the Supplemental Material [34].

The BHZ model. Let us focus now on the BHZ model, defined on a a square lattice with  $N=L\times L$  sites by the Hamiltonian  $\hat{\mathcal{H}}=\sum_{\sigma}\hat{\mathcal{H}}_{\sigma}$  with

$$\hat{\mathcal{H}}_{\sigma} = -\frac{t}{2} \sum_{\langle i,j \rangle, \eta} \eta \hat{c}_{i,\eta,\sigma}^{\dagger} \hat{c}_{j,\eta,\sigma} + m \sum_{i,\eta} \eta \hat{c}_{i,\eta,\sigma}^{\dagger} \hat{c}_{i,\eta,\sigma}$$
$$-\frac{\lambda}{2} \sum_{\langle i,j \rangle} e^{i\varphi_{ij}^{\sigma}} \hat{c}_{i,+,\sigma}^{\dagger} \hat{c}_{j,-,\sigma} + \text{H.c.}, \tag{6}$$

where  $\langle i, j \rangle$  are nearest-neighbor sites and the phase factor  $\varphi_{ij}^{\uparrow} = -\varphi_{ij}^{\downarrow}$  depends on the vector  $\mathbf{r}_{ij} = \mathbf{R}_j - \mathbf{R}_i$ , i.e.,  $\pm \pi/2$  for  $\mathbf{r}_{ij} = (\pm 1, 0)$ , 0 for  $\mathbf{r}_{ij} = (0, 1)$ , and  $\pi$  for  $\mathbf{r}_{ij} = (0, -1)$ .

Here, we take  $\delta k_x = \delta k_y = \frac{2\pi}{L}$  and introduce the ratio,

$$\rho_{\sigma} = \frac{\langle \Psi_0 | \hat{Z}_{\sigma}(\delta k_x, \delta k_y) | \Psi_0 \rangle}{\langle \Psi_0 | \hat{Z}_{\sigma}(\delta k_x, 0) | \Psi_0 \rangle \langle \Psi_0 | \hat{Z}_{\sigma}(0, \delta k_y) | \Psi_0 \rangle}.$$
 (7)

Then, we can exploit Eq. (5) in order to express  $\rho_{\sigma}$  in terms of overlaps, independently of the chosen global phase of the ground states,

$$\rho_{\sigma} = \frac{\langle \Psi_0(-\delta k_x, 0) | \Psi_0(0, \delta k_y) \rangle}{\langle \Psi_0(-\delta k_x, 0) | \Psi_0 \rangle \langle \Psi_0 | \Psi_0(0, \delta k_y) \rangle}.$$
(8)

For a noninteracting model, the ground state is written as a Slater determinant of the single-particle eigenfunctions, and each overlap is written as the determinant of the matrix built out of the overlaps of the single-particle states. Expressing each single-particle eigenstate in the Bloch form, the determinant can be explicitly evaluated in the thermodynamic limit as

$$\rho_{\sigma} = \prod_{q} \frac{\langle u_{q+\delta k_{x},\sigma} | u_{q-\delta k_{y},\sigma} \rangle}{\langle u_{q+\delta k_{x},\sigma} | u_{q,\sigma} \rangle \langle u_{q} | u_{q-\delta k_{y},\sigma} \rangle} 
= \prod_{q} [1 - \delta k_{x} \delta k_{y} (\langle \partial_{q_{x}} u_{q,\sigma} | \partial_{q_{y}} u_{q,\sigma} \rangle - \langle \partial_{q_{x}} u_{q,\sigma} | u_{q,\sigma} \rangle \langle u_{q,\sigma} | \partial_{q_{y}} u_{q,\sigma} \rangle)] 
= \exp \left[ - \int_{BZ} dq_{x} dq_{y} (\langle \partial_{q_{x}} u_{q,\sigma} | \partial_{q_{y}} u_{q,\sigma} \rangle - \langle \partial_{q_{x}} u_{q,\sigma} | u_{q,\sigma} \rangle \langle u_{q,\sigma} | \partial_{q_{y}} u_{q,\sigma} \rangle) \right] 
= |\rho_{\sigma}| \exp(i\pi C_{\sigma}).$$
(9)

Therefore,  $\rho_{\sigma}$  is expressed in terms of the off-diagonal components of the metric-curvature tensor [26], and its phase is written as the integral of the Berry curvature, implying that it is just  $\pi$  times the spin Chern number of the occupied spin- $\sigma$  manifold. The results of  $\rho_{\sigma}$  as a function of the lattice size L are shown in Fig. 1 for two cases corresponding to trivial and topological insulators. For this model,  $\rho_{\sigma}$  is real on finite clusters, and its modulus tends to 1 in the thermodynamic limit. We emphasize that the sign of  $\rho_{\sigma}$  provides a clear

FIG. 1. The quantity  $\rho_{\sigma}$  for the BHZ model with  $t = \lambda = 1$  as a function of the linear lattice size  $L = \sqrt{N}$ . In the upper panel m = 0.1, corresponding to a  $\mathbb{Z}_2$  topological insulator; in the lower panel m = 3, corresponding to a trivial insulator. Note that in the BHZ model  $\rho_{\sigma}$  is real.

marker for the topological nature of the ground state since it does not depend on the cluster size.

The KM model. We now consider the Kane-Mele model, defined in the honeycomb lattice with 2N sites, which are labeled by  $\alpha=(i,\eta)$  (where i denotes the unit cell of the Bravais lattice and  $\eta$  the site in the unit cell). The Hamiltonian is given by

$$\hat{\mathcal{H}} = -t \sum_{\langle \alpha, \beta \rangle} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta} + \frac{2i}{\sqrt{3}} V_{SO} \sum_{\langle \langle \alpha, \beta \rangle \rangle} \hat{c}_{\alpha}^{\dagger} \sigma \cdot (\mathbf{d}_{\gamma, \beta} \times \mathbf{d}_{\alpha, \gamma}) \hat{c}_{\beta}$$
$$+ \sum_{\alpha} m_{\alpha} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha} + i V_{R} \sum_{\langle \alpha, \beta \rangle} \hat{c}_{\alpha}^{\dagger} \hat{\mathbf{z}} \cdot (\sigma \times \mathbf{d}_{\alpha, \beta}) \hat{c}_{\beta}, \tag{10}$$

where  $\langle \alpha, \beta \rangle$  and  $\langle \langle \alpha, \beta \rangle \rangle$  are nearest and next-nearest neighbors in the honeycomb lattice,  $\hat{c}^{\dagger}_{\alpha} = (\hat{c}^{\dagger}_{\alpha,\uparrow}, \hat{c}^{\dagger}_{\alpha,\downarrow})$ ,  $\sigma = (\sigma_x, \sigma_y, \sigma_z)$  are Pauli matrices, and  $\mathbf{d}_{\alpha,\beta}$  is a vector pointing from site  $\beta$  to  $\alpha$ , whereas  $\gamma$  denotes the common nearest neighbor of the two next-nearest-neighbor sites  $\alpha$  and  $\beta$ . The on-site (mass) term  $m_{\alpha} = \pm m$  has alternate signs on each sublattice of the honeycomb lattice.

In the absence of Rashba coupling  $(V_R = 0)$ , the total spin projection is still conserved by the Hamiltonian, and the previous analysis is readily applicable. The quantized wave vectors  $\delta \mathbf{k}$  appearing in the definition (3) must be chosen according to the quantization rules of the underlying triangular Bravais lattice. We choose  $\delta \mathbf{k}_i$  as the smallest wave vector in the direction of the *i*th primitive vector of the reciprocal lattice; in a  $L \times L$  cluster with primitive vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , we have that  $\delta \mathbf{k}_i \cdot \mathbf{a}_j = \frac{2\pi}{L} \delta_{ij}$ . As performed before, we now define

$$\rho_{\sigma} = \frac{\langle \Psi_0 | \hat{Z}_{\sigma}(\delta \mathbf{k}_1 + \delta \mathbf{k}_2) | \Psi_0 \rangle}{\langle \Psi_0 | \hat{Z}_{\sigma}(\delta \mathbf{k}_1) | \Psi_0 \rangle \langle \Psi_0 | \hat{Z}_{\sigma}(\delta \mathbf{k}_2) | \Psi_0 \rangle}.$$
 (11)

The derivation closely follows the one sketched before. Here,  $\rho_{\sigma}$  is complex on any finite sizes but becomes real for  $N \rightarrow$ 

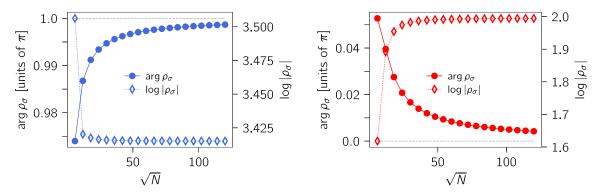


FIG. 2. Modulus (empty points) and phase (full points) of  $\rho_{\sigma} = |\rho_{\sigma}| e^{i\phi}$  in the KM model of Eq. (10) in absence of Rashba coupling  $(V_R = 0)$  as a function of the number of sites N for t = 1 and  $V_{SO} = 1/3$ . In the left panel m = 1 and the system is a  $\mathbb{Z}_2$  topological insulators, whereas in the right panel m = 2 and the system is a trivial insulator.

 $\infty$ , where its phase equals  $\pi$  times the Chern number of the band. Therefore, it represents an easily computable quantity that marks the topological transition. The numerical results for the KM model in absence of Rashba coupling are reported in Fig. 2. Even if our marker (11) is complex on any finite cluster, its phase is very close to either 0 or  $\pi$ , even on small sizes. Therefore, the identification of the topological nature of the ground state can be easily assessed.

When the Rashba coupling  $V_R$  is included, the z component of the total spin is no longer a conserved quantity. Still, we keep the same formal definition of  $\rho_\sigma$  in Eq. (11) and show that its phase remains quantized even for  $V_R > 0$ . The numerical results are reported in Fig. 3. For large N the imaginary part gets smaller and eventually tends to zero whereas the modulus  $|\rho_\sigma|$  diverges in the thermodynamic limit, however, its phase  $\phi$  can be again taken as a marker for the  $\mathbb{Z}_2$  topological transition. In fact, the convergence of the phase of  $\rho_\sigma$  to  $\pi$  (0) in the topological (trivial) phase is not affected by the presence of Rashba coupling.

The interacting BHZ model. Here, we add the Hubbard-U interaction between electrons with the same orbital  $\eta$  in the BHZ model of Eq. (6), namely,  $\mathcal{H}_{int} = U \sum_{j,\eta} \hat{n}_{j,\eta,\uparrow} \hat{n}_{j,\eta,\downarrow}$  [19]. The ground state can no longer be written in terms of a single Slater determinant, and many-body methods are necessary to evaluate expectation values as that in

Eq. (7). Here, we perform exact diagonalizations on a  $3 \times 3$  cluster with 18 electrons to give a proof of concept for the applicability of the many-body marker that we introduced. In Fig. 4, we report the results for U=1 and 2 (with  $\lambda=1$ ) by varying the on-site term m, the noninteracting case being also reported for comparison. The ground state is topological for small values of m, and the transition to the trivial insulator is marked by an abrupt jump from negative to positive values of  $\rho_{\sigma}$ . Note that the presence of the Hubbard-U interaction shifts the transition point from m=2 at U=0 to m=2.75(5) at U=2, indicating that the electron-electron repulsion favors the topological phase.

Conclusions. To summarize, we have examined the role of the spin-projected position operator  $\hat{Z}_{\sigma}(\delta \mathbf{k})$  in the topological transition of lattice models, proving that it allows us to define a robust marker, whose phase clearly identifies the occurrence of a change in the topological properties of the ground-state wave function. The  $\hat{Z}_{\sigma}(\delta \mathbf{k})$  operator is particularly suited for wave-function-based approaches (e.g., quantum Monte Carlo, Lanczos, and density-matrix renormalization group), where the topological nature can be extracted even in small clusters. Other markers, have been introduced and employed in previous works [21,22]. However, being based on a single-particle picture (e.g., by the use of Wannier orbitals), these markers can be exploited in dynamical mean-field theory in-

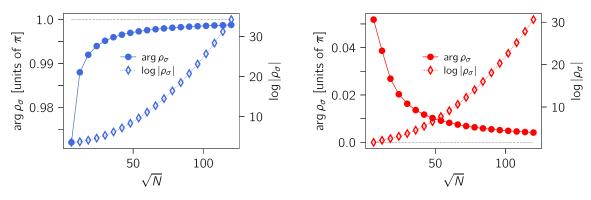


FIG. 3. The same as in Fig. 2 with a finite Rashba coupling  $V_R = 0.1$ .

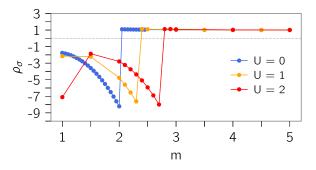


FIG. 4. The many-body  $\mathbb{Z}_2$  marker  $\rho_{\sigma}$  for the interacting BHZ model with  $t = \lambda = 1$  in the  $3 \times 3$  cluster with 18 electrons as obtained by exact diagonalization. The results are shown for U = 1 and 2, as a function of the on-site term m. The case with U = 0 (on the same cluster) is also reported for comparison. As in Fig. 1,  $\rho_{\sigma}$  is real.

vestigations, but their application to fully many-body states is not possible. Our  $\mathbb{Z}_2$  marker bears some resemblance with the many-body invariant for Chern insulators discussed in Ref. [35]; however, whereas the latter one needs calculations with different boundary conditions, our maker is defined by a *single* many-body computation. Most importantly, the definition of  $\rho_{\sigma}$ , can be exploited to study interaction-induced topological transitions in strongly correlated electron models. The very same definition can be applied even if the total spin projection  $S_z$  is not conserved, e.g., in the presence of the Rashba coupling in the Hamiltonian. Finally, the position operator could be useful also in experimental setups on quantum gases trapped in optical lattices in which high-resolution imaging is now possible [36], allowing a direct evaluation of operators, such as  $\hat{Z}_{\sigma}(\delta \mathbf{k})$ .

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