

Breakdown of the Generalized Gibbs Ensemble for Current-Generating Quenches

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We establish a relation between two hallmarks of integrable systems: the relaxation towards the generalized Gibbs ensemble (GGE) and the dissipationless charge transport. We show that the former one is possible only if the so-called Mazur bound on the charge stiffness is saturated by local conserved quantities. As an example we show how a non-GGE steady state with a current can be generated in the one-dimensional model of interacting spinless fermions with a flux quench. Moreover, an extended GGE involving the quasilocal conserved quantities can be formulated for this case.

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It is commonly accepted that in generic macroscopic systems the long-time averages of local observables coincide with the results for the statistical Gibbs ensemble [1–4] and are uniquely determined by few parameters related to conserved quantities, in particular the system’s energy and particle number. Due to the presence of macroscopic number of conserved quantities such a simple scenario is not applicable to integrable systems [5–7]. However, there is a large and still growing evidence that relaxation in the latter systems is consistent with the generalized Gibbs ensemble (GGE) [8–12], where the density matrix is determined not only by the Hamiltonian H and particle number N but also by other local conserved quantities Q_i , i.e., $\rho_{\text{GGE}} \sim \exp[-\beta(H - \mu N) - \sum_i \lambda_i Q_i]$.

In this Letter we focus on the relaxation dynamics of one of the most studied integrable models: the model of interacting spinless fermions, being equivalent to the anisotropic Heisenberg (XXZ) model for which the set of Q_i has been established [13,14]. We show that ρ_{GGE} as generated only by local integrals of motion Q_i doesn’t exhaust all generic stationary states in the metallic (easy plane) regime. Instead, there are cases for which one should lift the requirement of locality of the conserved quantities and allow also for quasilocal integrals of motion [15,16]. In this Letter we call them non-GGE states, however we stress that these states can be viewed also as “extended GGE,” where the extension concerns the locality of operators. Such operators have the parity opposite to local ones Q_i . We identify one of such quasilocal quantities as the time-averaged particle current operator and we construct as well as verify it explicitly.

It has been well recognized that integrable systems in spite of interaction reveal anomalous transport properties at finite inverse temperatures $\beta = 1/T$, e.g., the dissipationless particle current. This property is manifested by a nonvanishing charge stiffness $D(\beta < \infty)$ [17–20], which in

turn is bounded from below by the local conservation laws via the Mazur bound [19,21]. The dissipationless transport and the relaxation towards GGE are probably the most prominent hallmarks of integrability, still they have been studied independently of each other so far. While it has been clear that in certain regimes the standard Mazur bound with only local Q_i does not exhaust the phenomenon of dissipationless transport and $D(\beta < \infty) > 0$ [19] we show in this Letter that GGE should be extended by taking into account quasilocal conserved quantities of different parity, in particular the time-averaged current, which saturate $D(\beta \rightarrow \infty)$ within the Mazur bound.

We study a prototype one-dimensional (1D) model of interacting particles, the tight-binding model of spinless fermions on L sites at half filling (with $N = L/2$ particles) and with periodic boundary conditions [22–25],

$$H(t) = -t_h \sum_{j=1}^L (e^{i\phi(t)} c_{j+1}^\dagger c_j + \text{H.c.}) + V \sum_{j=1}^L \tilde{n}_j \tilde{n}_{j+1}, \quad (1)$$

where $n_j = c_j^\dagger c_j$, $\tilde{n}_j = n_j - 1/2$, t_h is the hopping integral and V is the repulsive interaction on nearest neighbors. The model (1) is equivalent to the anisotropic Heisenberg (XXZ) model with the exchange interaction $2t_h$ and the anisotropy parameter $\Delta = V/2t_h$. However, we stay within the fermionic representation, where the phase $\phi(t)$ has a clear physical meaning: it represents the time-dependent magnetic flux which induces the electric field $F(t) = -\partial_t \phi(t)$. Further on we use $\hbar = k_B = 1$ and units in which $t_h = 1$. We consider here the metallic (easy-plane) regime $V < 2$ ($\Delta < 1$) where the system exhibits a ballistic particle (spin) transport at $T > 0$ [18–20,26–33].

The Mazur lower bound on $D(T > 0)$ vanishes at half filling [19,34] and it remains a challenging problem to explain why $D(T > 0)$ stays nonzero. Here, we explore the relations between the conservation laws, the origin of finite $D(T > 0)$ and the relaxation towards a non-GGE state and

show that a finite $D(T > 0)$ emerges within an extended GGE state. In our studies we use the standard particle current $J = \sum_j (ie^{i\phi(t)} c_{j+1}^\dagger c_j + \text{H.c.})$ as well a less common current with a correlated hopping to next-nearest neighbors $J' = \sum_j (ie^{2i\phi(t)} c_{j+2}^\dagger \tilde{n}_{j+1} c_j + \text{H.c.})$. The central point in our reasoning is the particle-hole (parity) transformation,

$$c_i \rightarrow (-1)^i c_i^\dagger, \quad (2)$$

which (for $\phi = 0$) does not alter the Hamiltonian $H \rightarrow H$ (at half filling) nor the local conserved quantities $Q_i \rightarrow Q_i$ [19] but reverses the currents $J \rightarrow -J$ and $J' \rightarrow -J'$, hence $J(J')$ and Q_i have different parities.

We start with numerical studies of a quantum quench which generates a non-GGE steady state. We consider a system which for $t < 0$ is either in the ground state or in the equilibrium canonical or microcanonical state [35]. In the latter case we generate a state $\rho(0) = |\Psi(0)\rangle\langle\Psi(0)|$ for the target energy $E_0 = \langle\Psi(0)|H(0)|\Psi(0)\rangle$ and with a small energy uncertainty $\delta^2 E_0 = \langle\Psi(0)|[H(0) - E_0]^2|\Psi(0)\rangle$ as discussed in Refs. [36,37]. The time evolution shown in Fig. 1 has been obtained by the Lanczos propagation method [36–38].

At $t = 0$ the magnetic flux is suddenly decreased from the initial value $\phi(0) = \phi_0 > 0$ to $\phi(t > 0) = 0$. Such a quench is equivalent to a pulse of the electric field $F(t) = \phi_0 \delta(t)$ hence it generates the particle current $\neq 0$. As shown in Fig. 1 this quench induces also $\langle J'(t) \rangle \neq 0$; however, the latter quantity increases gradually in contrast to the instantaneous generation of $\langle J(t > 0) \rangle$. Both currents reach for $t \rightarrow \infty$ finite steady values, clearly visible in Fig. 1, being the signature of dissipationless transport. Still the residual values $\langle J \rangle \neq 0$ and $\langle J' \rangle \neq 0$ cannot be explained within the GGE scenario since $\text{Tr}\{\rho_{\text{GGE}} J\} = \text{Tr}\{\rho_{\text{GGE}} J'\} = 0$ due to different symmetries under particle-hole transformation at half filling [19].

The first objective of this Letter is to establish the symmetry decomposed time-averaged density matrix

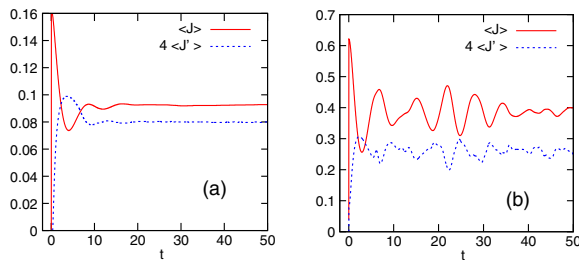


FIG. 1 (color online). Time dependence of $\langle J \rangle$ and $4\langle J' \rangle$ after quenching the flux at $t = 0$ for $L = 26$ and $V = 1$. (a) The system is initially in equilibrium microcanonical state with $\beta = 0.35$ while after the quench it has effective $\beta = 0.15$. (b) The system is in the ground state and the flux is quenched from $\phi_0 = \pi/2$ to 0.

$$\bar{\rho} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt \rho(t) = \bar{\rho}_e + \bar{\rho}_o, \quad (3)$$

where $\bar{\rho}_o$ and $\bar{\rho}_e$ are odd and even under the transformation (2), respectively. Since $\text{Tr}\{\bar{\rho} J\} = \text{Tr}\{\bar{\rho}_o J\}$ the odd component of the density matrix $\bar{\rho}_o$ is essential for the non-vanishing current $\langle J(t > 0) \rangle$, while this component is missing in ρ_{GGE} . At this stage it is instructive to recall the linear-response (LR) results

$$\langle J(t) \rangle = L \int_{-\infty}^{\infty} d\omega e^{-i\omega t} F(\omega) \sigma(\omega), \quad (4)$$

where the optical conductivity $\sigma(\omega)$ consists of the regular and the ballistic parts with the latter one determined by the charge stiffness D : $\sigma_{\text{bal}}(\omega) = 2Di/(\omega + i0^+)$. The quench of flux induces an electric field $F(\omega) = \phi_0/(2\pi)$ and the regular (dissipative) part of conductivity becomes irrelevant in the long-time regime. Then we get within the LR, i.e., for $\phi_0 \ll 1$,

$$\lim_{t \rightarrow \infty} \langle J(t) \rangle = 2LD\phi_0. \quad (5)$$

An important message following from LR, Eq. (5), is that the non-GGE component of the density matrix has to contain contributions that are linear in ϕ_0 and, therefore, can be singled out already within the first-order perturbation expansion in ϕ_0 . The unperturbed Hamiltonian $H_0 = H(t < 0)$ is given by Eq. (1) with $\phi(t)$ replaced by ϕ_0 , while the perturbation reads $H'(t) = H(t) - H_0 = (\phi_0 - \phi(t))J_0$, where $J_0 = J(t < 0)$, so that $H'(t > 0) = \phi_0 J_0$. For the sake of clarity all quantities obtained with the flux ϕ_0 will be marked with a label 0, in particular the eigenvalues E_{m0} and the eigenvectors $|m0\rangle$ of H_0 . The degeneracy of energy levels plays an important role and should not be neglected. Hence, we diagonalize the current operator in each subspace spanned by degenerate eigenstates and take the eigenvectors of J as the basis vectors of this subspace, i.e., $\langle m|J|n \rangle \propto \delta_{mn}$ if $E_m = E_n$ (within a subspace only).

We assume that the system is initially in a thermal state, i.e., $\rho_0 = \sum_m p_{m0} |m0\rangle\langle m0|$ with $p_{m0} = \exp(-\beta E_{m0}) / \sum_n \exp(-\beta E_{n0})$. Then, in the Schrödinger picture one obtains

$$\rho(t > 0) = \sum_m p_{m0} e^{-iH_0 t} U(t) |m0\rangle\langle m0| U^\dagger(t) e^{iH_0 t},$$

$$U(t > 0) = T_t \exp\left(-i \int_0^t dt' H'_I(t')\right), \quad (6)$$

where $H'_I(t')$ is the perturbation in the interaction picture. Our aim is to explicitly express $\bar{\rho}$ within the LR to the quench ϕ_0 . A straightforward calculation of Eqs. (3), (6) to first order in ϕ_0 yields

$$\bar{\rho} \approx \rho_0 + \phi_0 \sum_{E_{m0} \neq E_{n0}} \frac{P_{m0} - P_{n0}}{E_{n0} - E_{m0}} \langle m0 | J_0 | n0 \rangle |m0\rangle \langle n0|. \quad (7)$$

We should also take into account the change of current operator due to flux; hence,

$$J = J(t > 0) = J_0 - \phi_0 H_0^k, \quad (8)$$

where H_0^k is the kinetic part of H_0 , Eq. (1). Using Eqs. (7), (8), (5) one then restores the LR result for the equilibrium charge stiffness [18,39],

$$D = \frac{1}{2L} \left[-\langle H_0^k \rangle + \sum_{E_{m0} \neq E_{n0}} \frac{P_{m0} - P_{n0}}{E_{m0} - E_{n0}} |\langle m0 | J_0 | n0 \rangle|^2 \right]. \quad (9)$$

Equation (7) does not yet accomplish our aim of decomposing $\bar{\rho}$ into odd and even parts with respect to (2) after the quench $\phi(t > 0) = 0$. We achieve this by using again the first-order perturbation theory for $H_0 = H - \phi_0 J$ and $J_0 = J + \phi_0 H^k$, where now H, H^k , and J are the operators after the quench, i.e., at $\phi = 0$. Substituting

$$\begin{aligned} E_{n0} &= E_n - \phi_0 \langle n | J | n \rangle, \\ |n0\rangle &= |n\rangle - \phi_0 \sum_{m: E_m \neq E_n} \frac{\langle m | J | n \rangle}{E_n - E_m} |m\rangle \end{aligned} \quad (10)$$

into Eq. (7), and assuming that there is no particle current in the initial thermal state, we finally obtain

$$\bar{\rho} = \sum_n p_n |n\rangle \langle n | (1 + \beta \phi_0 \bar{J}), \quad (11)$$

where \bar{J} is the time-averaged steady-current operator,

$$\bar{J} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt e^{iHt} J e^{-iHt} = \sum_n \langle n | J | n \rangle |n\rangle \langle n|. \quad (12)$$

The LR results [Eq. (5)] are immediately restored; however, this time with the alternative form of the charge stiffness but equivalent for $\beta < \infty$ and in the thermodynamic limit [19]

$$D = \frac{\beta}{2L} \sum_n p_n \langle n | J | n \rangle^2. \quad (13)$$

By definition \bar{J} is an integral of motion $[H, \bar{J}] = 0$. It is important to note that $\text{Tr} \bar{J}^2 / \mathcal{N} \propto L$, where $\mathcal{N} = \text{Tr} 1$ is the dimension of the Hilbert space, already implies that \bar{J} is a quasilocal quantity. Since at $\beta \rightarrow 0$,

$$\frac{1}{\mathcal{N}} \text{Tr} \bar{J}^2 = 2L \tilde{D}, \quad \text{where } \tilde{D} = \lim_{\beta \rightarrow 0} D(\beta) / \beta, \quad (14)$$

the quasilocal character of \bar{J} is consistent with the well-established fact that the charge stiffness is an intensive quantity.

We now turn to the question of whether $\bar{\rho}$ is compatible with ρ_{GGE} and the answer is clearly negative. A necessary and a sufficient condition for such compatibility, to leading order in the quench ϕ_0 , would be a decomposition in terms of local conserved Q_i ,

$$\bar{J} = \sum_i \alpha_i Q_i, \quad (15)$$

holding for some set of α_i . Assuming that $\text{Tr}\{Q_i Q_j\} \propto \delta_{ij}$ we can employ the inequality

$$\text{Tr}\{(\bar{J} - \sum_i \alpha_i Q_i)^2\} \geq 0, \quad (16)$$

which holds for any α_i and becomes an equality only for the GGE state with $\alpha_i = \alpha_i$. Now we can follow original steps by Mazur [21]. We minimize the lhs of Eq. (16) with respect to α_i ,

$$\alpha_i = \frac{\text{Tr}\{\bar{J} Q_i\}}{\text{Tr}\{Q_i^2\}} = \frac{\text{Tr}\{J Q_i\}}{\text{Tr}\{Q_i^2\}}, \quad (17)$$

and substitute this result in (16) to obtain the Mazur inequality for $\beta \rightarrow 0$,

$$\text{Tr}\{\bar{J}^2\} \geq \sum_i \frac{\text{Tr}\{J Q_i\}^2}{\text{Tr}\{Q_i^2\}}, \quad (18)$$

which is the Mazur bound on charge stiffness at $T \rightarrow \infty$ [see Eq. (14)]. Since this inequality turns into equality for GGE states, so should the Mazur bound. In other words relaxation towards GGE is possible provided the Mazur bound saturates the charge stiffness. This relation holds for an arbitrary filling N/L . In particular for $N/L = 1/2$ one finds $\text{Tr}(Q_i J) = 0$ due to the symmetry (2); hence, the rhs of (18) vanishes, and our quenched dynamics does *not* relax to GGE.

As has been shown in Refs. [15,16], another set of nonlocal, but quasilocal conserved, Hermitian operators $\{Q(\varphi)\}$ exists for a dense set of commensurate interactions $\Delta = \cos(\pi l/m)$, with l, m integers, densely covering the range $|V| < 2$. They are all odd under (2), $Q(\varphi) \rightarrow -Q(\varphi)$. Quasilocality implies linear extensivity $\text{Tr}\{Q(\varphi)^2\} / \mathcal{N} \propto L$, similarly as for the local conserved operators Q_i , while $\text{Tr}\{J Q(\varphi)\} / (L\mathcal{N}) = \text{const}$, making them suitable for implementing the Mazur bound. For $\Delta = \cos(\pi/m)$ for which $T \rightarrow \infty$ limit of the Bethe ansatz result [26] is available it has been shown [16] to agree precisely with the Mazur bound, so one may conjecture that the latter is now indeed saturated. Hence our argument (15)–(18) can be used to argue that the complete time-averaged current can be expressed in terms of an integral,

$$\bar{J} = \int_{\mathcal{D}_m} d^2\varphi f(\varphi) Q(\varphi), \quad (19)$$

where $f(\varphi) = c_m/|\sin\varphi|^4$ for a suitable constant c_m and \mathcal{D}_m is a vertical strip in the complex plane with $|\operatorname{Re}\varphi - \pi/2| < \pi/(2m)$. We refer to [40] for a detailed derivation of Eq. (19) and the function $f(\varphi)$. After straightforward calculation, again using the notation and machinery of [16], one arrives at the explicit matrix-product expression for $\bar{J} = -i(J_+ - J_+^\dagger)$ in terms of local operators,

$$J_+ = \sum_j \sum_{r \geq 2} J_j^{(r)}, \quad (20)$$

with

$$J_1^{(r)} = \sum_{s_2, \dots, s_{r-1}}^{\{0, z, \pm\}} g_{s_2, \dots, s_{r-1}} (B^{s_2} \cdots B^{s_{r-1}})_{11} \sigma_1^- \sigma_2^{s_2} \cdots \sigma_{r-1}^{s_{r-1}} \sigma_r^+,$$

$$g_{s_2, \dots, s_{r-1}} := \sum_{j=0}^{\mathcal{N}_+ \{s_i\}} \binom{\mathcal{N}_+ \{s_i\}}{j} I_{j+\frac{1}{2} \mathcal{N}_z \{s_i\}}, \quad (21)$$

where $\mathcal{N}_s \{s_i\}$ denotes the number of indices in the set $\{s_i\}$ having a value s . Here $I_k := \int_{\mathcal{D}_m} d^2\varphi f(\varphi) (\cot\varphi)^{2k}$ are elementary integrals which can be evaluated as

$$I_k = -\frac{2\pi}{m(2k+1)(\sin\pi/m)^{2k+2}} \sum_{j=0}^{2k+1} \binom{2k+1}{j} (-1)^j$$

$$\times (\cos\pi/m)^{2k+1-j} \{ \operatorname{sinc}[\pi(j+1)/m] - \operatorname{sinc}[\pi(j-1)/m] \},$$

and $I_{k+1/2} = 0$ for k integer. The coefficient of Eq. (21) $(B^{s_2} \cdots B^{s_{r-1}})_{11}$ is the (1,1) component of a product of $(m-1) \times (m-1)$ matrices B^s , related to a modified Lax operator [16],

$$B_{j,k}^0 = \cos(\pi jl/m) \delta_{j,k}, \quad B_{j,k}^- = -\sin(\pi jl/m) \delta_{j,k},$$

$$B_{j,k}^+ = \sin(\pi kl/m) \delta_{j+1,k}, \quad B_{j,k}^+ = -\sin(\pi jl/m) \delta_{j,k+1}. \quad (22)$$

Pauli matrices σ_j^z are related to fermion operators via Jordan-Wigner transformation $c_j = (\prod_{i=1}^{j-1} \sigma_i^z) \sigma_j^-$. The result (21) is derived in the limit $L \rightarrow \infty$ and is valid up to corrections of order $\mathcal{O}(1/L)$ for a finite periodic ring. Explicitly, \bar{J} to all terms up to order four ($r \leq 4$) reads

$$\bar{J} = \tilde{D}(8J + 2VJ') + \sum_j (ikc_{j+3}^\dagger c_j + ik'c_{j+3}^\dagger c_{j+2}^\dagger c_{j+1} c_j$$

$$+ ik''c_{j+3}^\dagger \tilde{n}_{j+2} \tilde{n}_{j+1} c_j + \text{H.c.}) + \dots \quad (23)$$

For example, for $V = 1$, ($\Delta = \cos(\pi/3)$), one has explicitly

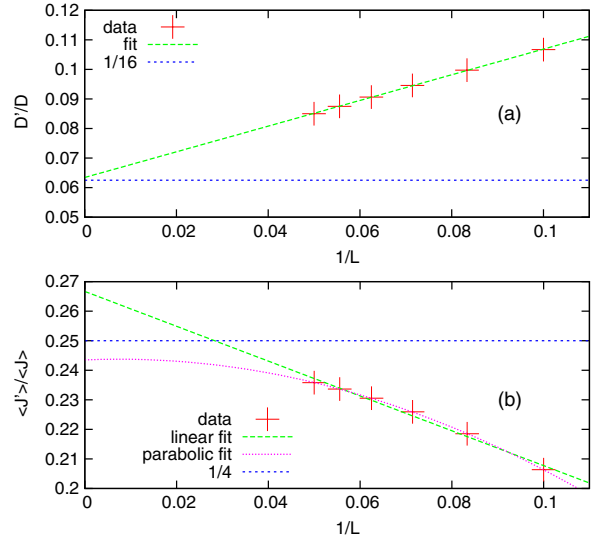


FIG. 2 (color online). a) D'/D vs $1/L$, where D' is the stiffness related with J' . b) $\langle J \rangle / \langle J' \rangle$ obtained for $\bar{\rho}$, Eq. (11), for $\beta \rightarrow 0$. Horizontal lines show analytical results. Exact diagonalization has been carried out for $V = 1$ with $\phi = \pi/L$ and $2\pi/L$ for even and odd N , respectively.

$$\tilde{D} = \frac{1}{8} - \frac{3\sqrt{3}}{32\pi}, \quad \kappa = \frac{1}{4} - \frac{9\sqrt{3}}{16\pi}, \quad \kappa' = \frac{9\sqrt{3}}{8\pi} - 1, \quad (24)$$

while $\kappa'' = \tilde{D}V^2/16$ in general.

The above analytical results are nicely corroborated by exact numerical simulations in finite systems shown in Fig. 2. From Eq. (23) one finds that the ratio of two currents should be given as $\operatorname{Tr}\{\bar{\rho}J'\}/\operatorname{Tr}\{\bar{\rho}J\} = V/4$ as confirmed in Fig. 2(b). Here, the tiny deviations from $1/4$ are presumably due to oversimplified (linear or parabolic) fitting functions. Furthermore, one can define the stiffness with respect to current J' as $D' = \langle \beta \bar{J}'^2 \rangle / (2L)$. Formula (23) immediately implies that $\bar{J}' = (V/4)\bar{J}$, and so the two stiffnesses should have a simple ratio $D'/D = (V/4)^2$ [see Fig. 2(a)].

In conclusion, we have proposed a class of global quantum quench dynamics of integrable spin chains for which the state at asymptotic times does not relax to GGE. We argue that, at least for weak quenches where linear response theory is applicable, the validity of GGE ensemble is in one-to-one correspondence with the saturation of the Mazur bound expressed in terms of strictly local conserved operators. However, if one extends the GGE ensemble by including the quasilocal conserved operators from the opposite parity sector—having linearly extensive Hilbert-Schmidt norm—then the latter can be used to describe exactly the steady state density operator after the quench. Our theory has been demonstrated in the one-dimensional model of interacting spinless fermions (XXZ spin model) within the metallic regime.

It should be noted that our results are expected to have further implications on other relevant quantities of integrable systems besides the charge stiffness. The flux-quench-induced steady current $\langle \bar{J} \rangle = 2 \sum_k \sin(k) \langle \bar{n}_k \rangle \neq 0$ is reflected into the fermion momentum-distribution function $\langle \bar{n}_k \rangle$, which also does not comply to the standard GGE. The latter quantity is the one typically measured in cold-atom experiments [41,42] and most frequently studied in connection with the GGE concept [5,8,10]. The inclusion of the quasilocal conserved quantity \bar{J} fully fixes the steady state $\langle \bar{n}_k \rangle$ within our quench protocol via extended GGE form Eq. (11). It is still tempting to construct and consider further (presumably conserved) quantities from the same polarity sector, which would fix this and related quantities for an arbitrary quench.

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