# Lieb-Thirring bounds for interacting Bose gases

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*joint work with*
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Dedicated to my 94-year-old grandmother Margit Forslund who had a stroke a few days ago.


# Outline of Talk

1. Introduction
2. Repulsion $\Rightarrow$ local exclusion principle
3. Local uncertainty principle
4. General Lieb-Thirring type inequalities
5. Applications to various interactions

# The interacting Bose gas

$N$-particle Hamiltonian with repulsive pair interaction $W(\boldsymbol{x})$:

$$\hat{H}_N = \hat{T} + \hat{V} + \hat{W} = \sum_{j=1}^{N} (-\Delta_j + V(\boldsymbol{x}_j)) + \sum_{1 \leq j < k \leq N} W(\boldsymbol{x}_j - \boldsymbol{x}_k),$$

acting on normalized $\psi \in L^2_{\mathsf{sym}}(\mathbb{R}^{dN})$. $\frac{\hbar^2}{2m} = 1$.

Total energy in the state $\psi$:

$$E[\psi] = \langle \psi, \hat{H}_N \psi \rangle = T_\psi + V_\psi + W_\psi$$

# Local particle density

The one-particle density associated to $\psi$:

$$\rho_\psi(\boldsymbol{x}) := \sum_{j=1}^{N} \int_{\mathbb{R}^{d(N-1)}} |\psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{j-1}, \boldsymbol{x}, \boldsymbol{x}_{j+1}, \ldots, \boldsymbol{x}_N)|^2 \prod_{k \neq j} d\boldsymbol{x}_k$$

Normalized $\int_{\mathbb{R}^d} \rho_\psi = N$,

$\int_Q \rho_\psi =$ expected number of particles on $Q \subseteq \mathbb{R}^d$.

**AIM:** Replace functionals of $\psi \in L^2(\mathbb{R}^{dN})$ (where $N \to \infty$) by functionals of $\rho_\psi \in L^1(\mathbb{R}^d)$

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# The dilute gas (3D)

Dilute limit $a^3\bar{\rho} \to 0$ while $N \to \infty$

Gross-Pitaevskii limit: $Na/L \sim const.$ $\Rightarrow$

$$E[\psi_0] \to \mathcal{E}_{\mathsf{GP}}[\phi_0], \qquad \rho_{\psi_0}(\boldsymbol{x}) \to |\phi_0(\boldsymbol{x})|^2,$$

$$\mathcal{E}_{\mathsf{GP}}[\phi] := \int_{\mathbb{R}^3} \left(|\nabla\phi|^2 + V|\phi|^2 + 4\pi a|\phi|^4\right) d\boldsymbol{x}, \quad \int_{\mathbb{R}^3} |\phi|^2 = N$$

'Thomas-Fermi' limit: $Na/L \to \infty$ $\Rightarrow$

$$E[\psi_0] \to \mathcal{E}_{\mathsf{TF}}[\rho_0], \qquad \rho_{\psi_0} \to \rho_0,$$

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Rigorous treatments first by Dyson 1957 (hard-sphere & $V = 0$), more recently and generally by Lieb, Yngvason, Seiringer, ...

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# Pauli repulsion and energy inequalities

Pauli exclusion: say $q \in \mathbb{N}$ particles allowed in each one-particle state of $\hat{H}_1 = -\Delta_{\mathbb{R}^d} + V(\boldsymbol{x})$

$\Rightarrow$ Lieb-Thirring inequality: (Lieb, Thirring, 1975)

$$\hat{H}_{N,\text{Pauli}} = \hat{T} + \hat{V} = \sum_{j=1}^{N} \left(-\Delta_j + V(\boldsymbol{x}_j)\right) \geq -q \sum_{k=0}^{\infty} |\lambda_k| \geq -q\, C_d \int_{\mathbb{R}^d} |V_-(\boldsymbol{x})|^{1+\frac{d}{2}}\, d\boldsymbol{x}$$

$\Leftrightarrow$ kinetic energy inequality: (cf. Thomas-Fermi)

$$T_\psi = \int_{\mathbb{R}^{dN}} \sum_{j=1}^{N} |\nabla_j \psi|^2\, dx \geq \frac{C_d'}{q^{2/d}} \int_{\mathbb{R}^d} \rho_\psi(\boldsymbol{x})^{1+\frac{2}{d}}\, d\boldsymbol{x}$$

Bosons: $q = N \to \infty$ $\Rightarrow$ trivial bounds

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# Energy inequalities for repulsive Bose gases

Replace Pauli repulsion by $W$.
Examples of new energy inequalities: (DL, Portmann, Solovej, 2014)

For hard-sphere gas, $W = W_a^{\mathsf{hs}}$ with diameter $a > 0$, in 3D:

$$T_\psi + W_\psi \ \geq \ C' \int_{\mathbb{R}^3} \min\left\{ a\rho_\psi(\boldsymbol{x})^2, \rho_\psi(\boldsymbol{x})^{5/3} \right\} d\boldsymbol{x}$$

cp. $E[\psi_0]/\mathsf{Vol} \to 4\pi a \rho^2$ as $a^3\rho \to 0$

For hard disks, $W = W_a^{\mathsf{hd}}$, $a > 0$, in 2D:

$$T_\psi + W_\psi \ \geq \ C'' \int_{\mathbb{R}^2} \frac{\rho_\psi(\boldsymbol{x})^2}{2 + \big(-\ln(a\rho_\psi(\boldsymbol{x})^{1/2}/2)\big)_+} \, d\boldsymbol{x}$$

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# Main idea: Local exclusion principle

Consider a $d$-dimensional box $Q$, and the local energy $(T+W)_\psi^Q =$

$$\sum_{j=1}^{N} \int_{\mathbb{R}^{dN}} \chi_Q(\boldsymbol{x}_j) \left( |\nabla_j \psi|^2 + \frac{1}{2} \sum_{k \neq j} W(\boldsymbol{x}_j - \boldsymbol{x}_k) |\psi|^2 \right) dx.$$

If $W \geq 0$ then

$$(T+W)_\psi^Q \geq \sum_{n=0}^{N} E_n \, p_n(Q),$$

where $E_n(|Q|; W)$ is the g.s. energy for $n$ particles on $Q$ with Neumann b.c., and $p_n(Q)$ the $n$-particle probability distribution,

$$\sum_{n=0}^{N} p_n(Q) = 1, \qquad \sum_{n=0}^{N} n \, p_n(Q) = \int_Q \rho_\psi.$$

# Local exclusion for fermions

cp. Dyson, Lenard, 1967

Let $\psi \in \bigwedge^n L^2(\mathbb{R}^d)$ be a wave function of $n$ fermions and let $Q$ be a $d$-cube. Then

$$\int_{Q^n} \sum_{j=1}^{n} |\nabla_j \psi|^2 \, dx \;\geq\; (n-1)\frac{\pi^2}{|Q|^{2/d}} \int_{Q^n} |\psi|^2 \, dx,$$

hence $e_n \geq (n-1)_+ \pi^2$, where $e_n := |Q|^{2/d} E_n$ (convenient ren.). It follows that

$$(T + W_{\text{Pauli}})_\psi^Q \geq \frac{\pi^2}{|Q|^{2/d}} \left( \int_Q \rho_\psi(\boldsymbol{x}) \, d\boldsymbol{x} - 1 \right)_+ .$$

# Local exclusion for anyons/intermediate statistics

DL, Solovej, 2011-2013

Anyons (abelian) with interchange phase $e^{\alpha\pi i} \in \mathrm{U}(1)$:

$$e_n(|Q|; n\text{-anyon interaction}) \geq (n-1)_+ C_\alpha$$

Lieb-Liniger intermediate statistics, $W_{\mathrm{LL}}(x) = \eta\delta(x)$, $\eta \geq 0$:

$$e_n(|Q|; W_{\mathrm{LL}}) \geq (n-1)_+ \xi_{\mathrm{LL}}(\eta|Q|)^2$$

**Lemma (Local exclusion principle in terms of $\rho$)**

$$(T + W_{\mathrm{A/LL}})_\psi^Q \;\geq\; \frac{e(\gamma)}{|Q|^{2/d}} \left( \int_Q \rho_\psi(\boldsymbol{x})\, d\boldsymbol{x} - 1 \right)_+,$$

*where for anyons $e(\gamma) = C_\alpha =$ const.*
*and for Lieb-Liniger $e(\gamma) = \xi_{\mathrm{LL}}(\gamma)^2$ concave in $\gamma = \eta|Q|$.*

# Local exclusion for pair-interacting repulsive Bose gas

Using

**Lemma ($n$-interaction in terms of pair-interaction)**

*For $W \geq 0$ one has*

$$e_n(|Q|;W) \;\geq\; \frac{n}{2} e_2(|Q|;(n-1)W) \;\geq\; \frac{1}{2}(n-1)_+ e_2(|Q|;W)$$

*where $e_2(|Q|, \lambda W)$ is monotone increasing and concave in $\lambda \geq 0$.*

one obtains

**Theorem (Local exclusion principle in terms of $\rho$)**

$$(T+W)_\psi^Q \;\geq\; \frac{1}{2} \frac{e_2(|Q|;W)}{|Q|^{2/d}} \left( \int_Q \rho_\psi(\boldsymbol{x})\, d\boldsymbol{x} - 1 \right)_+ ,$$

# Local uncertainty principle

Combine exclusion with uncertainty

**Lemma (Local uncertainty principle)**

*Let $\psi$ be an $N$-particle wave function on $\mathbb{R}^d$, and $Q$ a $d$-cube with volume $|Q|$. Then*

$$T_\psi^Q \;\geq\; c_1 \frac{\int_Q \rho_\psi^{1+2/d}\, d\boldsymbol{x}}{(\int_Q \rho_\psi\, d\boldsymbol{x})^{2/d}} - c_2 \frac{\int_Q \rho_\psi\, d\boldsymbol{x}}{|Q|^{2/d}},$$

*where the constants $c_1, c_2 > 0$ only depend on $d$.*

*Idea of proof:* $\int |\nabla \sqrt{\rho_\psi}|^2$ and Poincaré-Sobolev inequality on $Q$

# General Lieb-Thirring type inequalities

General assumptions on $W$:

**Assumption 1 (Local exclusion)**

*Given $W$, there exists a function $e(\gamma)$ with*

$$\gamma(|Q|) := \tau |Q|^{(2-\alpha)/d}, \qquad \alpha, \tau > 0,$$

*where $e(\gamma)$ is monotone increasing and concave in $\gamma$ with $e(0) = 0$, such that for any finite cube $Q$, any $N \geq 1$ and all normalized $\psi \in H^1(\mathbb{R}^{dN})$ the local energy satisfies*

$$(T+W)^Q_\psi \geq \frac{1}{2} \frac{e(\gamma(|Q|))}{|Q|^{2/d}} \left( \int_Q \rho_\psi \; - 1 \right)_+ ,$$

# General Lieb-Thirring type inequalities

General assumptions on $W$:

**Assumption 2 (Local uncertainty)**

*Given $W$, there exist $\alpha > 0$ and constants $S_1, S_2 > 0$ such that for any finite cube $Q$, any $N \geq 1$ and all normalized $\psi \in H^1(\mathbb{R}^{dN})$ we have*

$$(T+W)_\psi^Q \geq \begin{cases} S_1 \frac{\int_Q \rho_\psi^{1+2/d}}{(\int_Q \rho_\psi)^{2/d}} - S_2 \frac{\int_Q \rho_\psi}{|Q|^{2/d}}, & \text{for } 0 < \alpha \leq 2, \\ S_1 \frac{\left(\int_Q \rho_\psi^{1+\alpha/d}\right)^{2/\alpha}}{(\int_Q \rho_\psi)^{2/\alpha+2/d-1}} - S_2 \frac{\int_Q \rho_\psi}{|Q|^{2/d}}, & \text{for } \alpha > 2. \end{cases}$$

# General Lieb-Thirring type inequalities

We also need a boundedness assumption on $e(\gamma)$,

$$\underline{e}_K(\gamma) := \min\{e(\gamma), K\}, \quad K > 0,$$

(arbitrarily strong exclusion cannot be matched by uncertainty)

**Theorem (Lieb-Thirring inequality)**

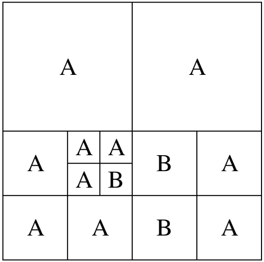
*Let $W$ satisfy Assumption 1 & 2 with an $\alpha > 0$ and $e$ replaced by $\underline{e}_K$. Then there exists an explicit constant $C_{d,\alpha,K} > 0$, such that for any $N \geq 1$ and all normalized $\psi \in H^1(\mathbb{R}^{dN})$, the total energy satisfies the bound*

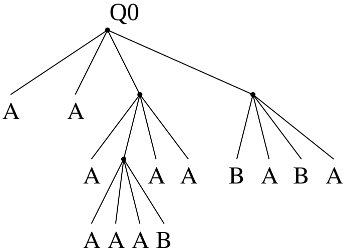
$$T_\psi + W_\psi \ \geq \ C_{d,\alpha,K} \int_{\mathbb{R}^d} \underline{e}_K \left(\gamma(2/\rho_\psi(\boldsymbol{x}))\right) \rho_\psi(\boldsymbol{x})^{1+2/d} \, d\boldsymbol{x}.$$

DL, Portmann, Solovej, 2014

# Proof uses a splitting algorithm

cp. DL, Solovej, 2011-2013




Split a cube $Q_0 \subset \mathbb{R}^d$ recursively until each sub-cube contains $\approx 2$ particles (B) or $< 2$ particles (A). Apply local uncertainty on every cube with non-constant density. Apply local exclusion on B-cubes, which also cover for A-cubes with $\sim$constant density.

# Proof cont.

The cases $0 < \alpha \leq 2$ and $\alpha \geq 2$ reverse the roles of monotonicity and concavity of $e(\gamma)$. The latter requires stronger uncertainty.

**Lemma (Combining exclusion and uncertainty)**

*Let $e(\gamma)$ be as in Assumption 1, and $\tilde{\rho} := \int_Q \rho/|Q|$. For $0 < \alpha \leq 2$,*

$$\int_Q e(\gamma(2/\rho))\rho^{1+2/d} \leq e(\gamma(2/\tilde{\rho}))\left(\int_Q \tilde{\rho}^{1+2/d} + \int_Q \rho^{1+2/d}\right),$$

*while for $\alpha \geq 2$,*

$$\int_Q e(\gamma(2/\rho))\rho^{1+2/d} \leq e(\gamma(2/\tilde{\rho}))\left(\int_Q \tilde{\rho}^{1+2/d} + \tilde{\rho}^{\frac{2-\alpha}{d}} \int_Q \rho^{1+\alpha/d}\right).$$

Plus, for A-cubes $Q_j$: $\displaystyle\sum_{j=1}^{k} \frac{|Q_j|^{-2/d} e(\gamma(|Q_j|))}{|Q_B|^{-2/d} e(\gamma(|Q_B|))} \leq \frac{1}{1 - 2^{-\min\{\alpha,2\}}}.$

# Application: Inverse-square repulsion

For $W(\boldsymbol{x}) = W_0/|\boldsymbol{x}|^2$, $W_0 \geq 0$:

$$e_2(|Q|; W) = const.(W_0) =: e,$$

so

$$T_\psi + W_\psi \geq C_{d,2,e} e \int_{\mathbb{R}^d} \rho_\psi(\boldsymbol{x})^{1+2/d} \, d\boldsymbol{x}.$$

Proceeding as in the case of fermions $\Rightarrow$

$$\hat{T} + \hat{W} + \hat{V} \geq -C' \int_{\mathbb{R}^d} |V_-|^{1+d/2} \, d\boldsymbol{x},$$

which e.g. can be applied to additional Coulomb interactions ($\Rightarrow$ nearest-neighbour $V$) to prove thermodynamic stability for charged bosons with inverse-square repulsive cores.

# Application: Lieb-Liniger model

Interaction: $W_{\mathrm{LL}}(x) = \eta\delta(x)$, $\eta \geq 0$

Proposition:

$$e_2(|Q|; W_{\mathrm{LL}}) \geq \xi_{\mathrm{LL}}(\eta|Q|)^2 =: e(\gamma),$$

bounded and concave with $\gamma = \eta|Q|^{(2-\alpha)/d}$, $\alpha = 1$.

Theorem/Corollary:

$$(T + W_{\mathrm{LL}})_\psi \;\geq\; C_{\mathrm{LL}} \int_{\mathbb{R}} \xi_{\mathrm{LL}}(2\eta/\rho_\psi(x))^2 \, \rho_\psi(x)^3 \, dx,$$

$C_{\mathrm{LL}} = C_{1,1,\pi^2} \gtrsim 10^{-5}$ (far from optimal).

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$C_{\mathrm{LL}} = C_{1,1,\pi^2} \gtrsim 10^{-5}$ (far from optimal).

# Application: Hard sphere interaction

Hard sphere: $W_a^{\mathsf{hs}}(\boldsymbol{x}) = \begin{cases} +\infty, & |\boldsymbol{x}| \le a, \\ 0, & |\boldsymbol{x}| > a. \end{cases}$

Proposition: (proof uses Dyson's Lemma)

$$e_2(|Q|; W_a^{\mathsf{hs}}) \ge \frac{2}{\sqrt{3}} \frac{a}{|Q|^{1/3}} =: e(\gamma),$$

i.e. linear in $\gamma = a|Q|^{(2-\alpha)/d}$, $\alpha = 3$. Use $\underline{e}_{K=\pi^2}(\gamma)$.

Theorem/Corollary:

$$(T + W_a^{\mathsf{hs}})_\psi \;\ge\; C_{\mathsf{hs}} \int_{\mathbb{R}^3} \min\left\{ \frac{2^{2/3}}{\sqrt{3}} a \rho_\psi(\boldsymbol{x})^2, \pi^2 \rho_\psi(\boldsymbol{x})^{5/3} \right\} d\boldsymbol{x},$$

$C_{\mathsf{hs}} = C_{3,3,\pi^2} \gtrsim 10^{-6}$.

# Application: Power-law interaction in 3D

Interaction $W_\beta(\boldsymbol{x}) = W_0|\boldsymbol{x}|^{-\beta}$ in $d = 3$.
For $\beta > 3$ it has finite scattering length

$$a_\beta = \Lambda_\beta \left(\frac{W_0}{2}\right)^{1/(\beta-2)}, \quad \text{where } \Lambda_\beta := \frac{\Gamma\left(\frac{\beta-3}{\beta-2}\right)}{\Gamma\left(\frac{\beta-1}{\beta-2}\right)} \left(\frac{2}{\beta-2}\right)^{2/(\beta-2)}$$

Theorem/Corollary: For $\beta > 3$ we have

$$(T + W_\beta)_\psi \;\geq\; C_{\mathsf{hs}} \int_{\mathbb{R}^3} \min\left\{\zeta \Lambda_\beta^{-1} a_\beta \rho_\psi(\boldsymbol{x})^2, \pi^2 \rho_\psi(\boldsymbol{x})^{5/3}\right\} d\boldsymbol{x},$$

$\zeta > 0.137$ a constant.
For $\beta \to \infty$ with $W_0 = a^{\beta-2}$ this reduces to the hard-sphere case.
For $\beta \to 3$ it reduces to a simple bound involving $\Lambda_\beta^{-1} a_\beta \to W_0/2$.

# Counterexamples

Bounds of the form obtained for $W_{\beta>3}$ cannot hold for sufficiently regular potentials:

**Proposition (Locally integrable potentials)**

*Let $W \in L^p_{\mathrm{loc}}(\mathbb{R}^3)$ for some $p \geq 3/2$ and scattering length $a_W > 0$ (possibly infinite). If there exists a constant $C \geq 0$ such that the inequality*

$$(T+W)_\psi \geq C \int_{\mathbb{R}^3} \min\{a_W \rho_\psi(\boldsymbol{x})^2, \rho_\psi(\boldsymbol{x})^{5/3}\}\, d\boldsymbol{x}$$

*holds for all $\psi \in H^1(\mathbb{R}^{3N})$ and $N \geq 1$, then $C = 0$.*

# Counterexamples

For $0 < a < R$ and $W_0 > 0$ let us define

$$W_{a,R}(\boldsymbol{x}) = \begin{cases} +\infty, & |\boldsymbol{x}| \le a, \\ W_0, & a < |\boldsymbol{x}| \le R, \\ 0, & |\boldsymbol{x}| > R, \end{cases}$$

a modified hard-sphere interaction with scattering length $a_W > a$.

## Proposition (Skew potentials)

*Let $W = W_{a,R}$. Assume that for some constant $C \ge 0$,*

$$(T + W)_\psi \ge C \int_{\mathbb{R}^3} \min\{a_W \rho_\psi(\boldsymbol{x})^2, \rho_\psi(\boldsymbol{x})^{5/3}\}\, d\boldsymbol{x}$$

*holds for all $\psi \in H^1(\mathbb{R}^{3N})$ and $N \ge 1$. We allow $C$ to depend on $a_W > 0$ but not on the details of $W$ (i.e. $a$, $W_0$, and range $R$). Then $C = 0$.*

# Application: Hard disk interaction

Hard disk: $W_a^{\mathsf{hd}}(\boldsymbol{x}) = \begin{cases} +\infty, & |\boldsymbol{x}| \leq a, \\ 0, & |\boldsymbol{x}| > a. \end{cases}$

Proposition: (proof uses Dyson's Lemma in 2D)

$$e_2(|Q|; W_a^{\mathsf{hd}}) \geq \frac{2}{2 + \left(-\ln\left(2^{-1/2}\gamma\right)\right)_+} =: e(\gamma),$$

bounded and concave in $\gamma = a|Q|^{(2-\alpha)/d}$, $\alpha = 3$.

Theorem/Corollary:

$$(T + W_a^{\mathsf{hd}})_\psi \;\geq\; C_{\mathsf{hd}} \int_{\mathbb{R}^2} \frac{2\rho_\psi(\boldsymbol{x})^2}{2 + \left(-\ln(a\rho_\psi(\boldsymbol{x})^{1/2}/2)\right)_+}\, d\boldsymbol{x},$$

$C_{\mathsf{hd}} = C_{2,3,1} \gtrsim 10^{-10}$.

# Application: Power-law interaction in 2D

Interaction $W_\beta(\boldsymbol{x}) = W_0|\boldsymbol{x}|^{-\beta}$ in $d = 2$.
For $\beta > 2$ it has finite scattering length

$$a_\beta = \Xi_\beta \left(\frac{W_0}{2}\right)^{1/(\beta-2)}, \quad \text{where } \Xi_\beta := \left(\frac{2}{\beta-2}\right)^{2/(\beta-2)}$$

Theorem/Corollary: For $\beta > 2$ we have

$$(T + W_\beta)_\psi \;\geq\; C_{\mathsf{hd}} \int_{\mathbb{R}^2} \frac{\rho_\psi(\boldsymbol{x})^2}{\zeta_2 + \left(-\ln\left(2^{-1}\Xi_\beta^{-1} a_\beta \rho_\psi(\boldsymbol{x})^{1/2}\right)\right)_+} \, d\boldsymbol{x},$$

$\zeta_2 > 2.24$ a constant.
For $\beta \to \infty$ with $W_0 = a^{\beta-2}$ this reduces to the hard-disk case.
For $\beta \to 2$ and $W_0$ sufficiently large it reduces to the Lieb-Thirring inequality.

# Application: Relativistic bosons

Relativistic bosons with Coulomb repulsion:

$$\left\langle \psi, \left( \sum_{j=1}^{N} \sqrt{-\Delta_j} + \sum_{j<k} \frac{1}{|\boldsymbol{x}_j - \boldsymbol{x}_k|} \right) \psi \right\rangle \geq C \int_{\mathbb{R}^d} \rho_\psi(\boldsymbol{x})^{1+1/d} \, d\boldsymbol{x},$$

for $d \geq 2$.

Use fractional Poincaré-Sobolev inequalities for local uncertainty and an elementary bound for exclusion.

# References

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