Kruskal-style algorithm for molecule reduction I: Cubic NLS

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Combinatorics from singular SPDEs to kinetic equations
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Cubic NLS

Let $d \geqslant 3$, we consider the following cubic Schrödinger equation:

$$\begin{cases} (i\partial_t - \Delta_\beta)u = -\lambda^2 u|u|^2 \quad \text{over } \mathbb{R}^+ \times \mathbb{T}_L^d \\ u(0,\cdot) = u_{\text{in}} \end{cases}$$

where $L \gg 1$, $\Delta_\beta = \dfrac{1}{2\pi}\displaystyle\sum_{k=1}^{d} \beta_k \partial_k^2$ and $\widehat{u_{\text{in}}}(k) = \sqrt{\phi_{\text{in}}(k)}X_k$ with $\phi_{\text{in}} \in \mathcal{S}(\mathbb{R}^d, \mathbb{R}^+)$ and $(X_k)_{k\in\mathbb{Z}_L^d}$ are i.i.d. Gaussian random variables.

Wave Kinetic Equation

The wave kinetic equation is defined by:

$$\begin{cases} \partial_t \phi = \mathcal{K}(\phi, \phi, \phi) \quad \text{sur } \mathbb{R}^+ \times \mathbb{R}^d \\ \phi(0, \cdot) = \phi_{\text{in}} \end{cases}$$

with

$$\mathcal{K}(\phi_1, \phi_2, \phi_3)(k) = \int_{\Gamma(k)} (\phi_1(k_1)\phi_2(k_2)\phi_3(k_3) - \phi_1(k)\phi_2(k_2)\phi_3(k_3) + \phi_1(k_1)\phi_2(k)\phi_3(k_3) - \phi_1(k_1)\phi_2(k_2)\phi_3(k))\, dk_1 dk_2 dk_3$$

and

$$\Gamma(k) = \{(k_1, k_2, k_3) \in (\mathbb{R}^d)^3, k_1 - k_2 + k_3 - k = 0 \text{ and } |k_1|_\beta^2 - |k_2|_\beta^2 + |k_3|_\beta^2 - |k|_\beta^2 = 0\}.$$

Derivation of the wave kinetic equation

Theorem (Deng–Hani 2023)

For all $\phi_{in} \in \mathcal{S}(\mathbb{R}^d, \mathbb{R}^+)$, there exists $\delta > 0$ such that, for L sufficiently large satisfying the scaling law $\lambda^2 = L^{d-1}$, the cubic NLS admits a smooth solution up to time

$$T = \delta T_{\text{kin}} = \delta \frac{L^2}{2}$$

and one has

$$\lim_{L \to +\infty} \sup_{t \in [0,1]} \sup_{k \in \mathbb{Z}^d_L} \left| \mathbb{E}\left[|\widehat{u}(T_{\text{kin}} \delta t, k)|^2 \right] - \phi(\delta t, k) \right| = 0.$$

Main ideas of the proof

On rewrites the equation in Fourier space

$$\partial_t \mathbf{a} = \mathcal{C}(\mathbf{a}, \bar{\mathbf{a}}, \mathbf{a}) \quad \mathbf{a}(0) = \left(\sqrt{\phi_{\text{in}}(k)} X_k \right)_{k \in \mathbb{Z}^d_L}.$$

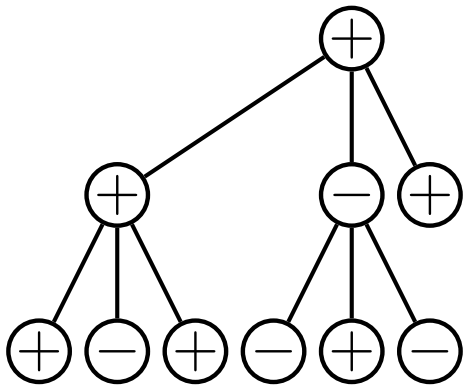
Then, the ansatz is given by

$$\mathbf{a} = \sum_{n=0}^{N} \mathbf{a}^{(n)} + \mathbf{R}_N$$

where $\mathbf{a}^{(n)}$ are oscillatory iterated integrals and $N \sim \log(L)$. The correlations $\mathbb{E}[\mathbf{a}_k(t)\overline{\mathbf{a}_k(t)}]$ produce Feynman diagrams (couples). Find their limit when $L \to \infty$ with the scaling law $\lambda^2 = L^{d-1}$.

- Regular couples associated with the wave kinetic equation.
- Irregular couples: Vanishing contribution.

Decorated trees and oscillatory integrals

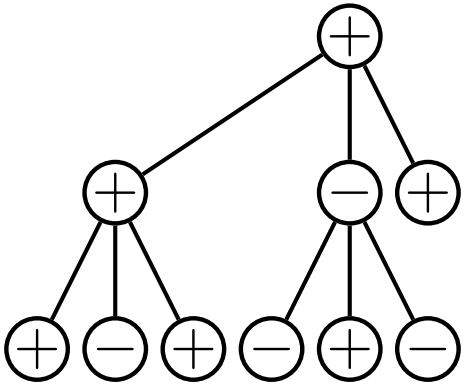


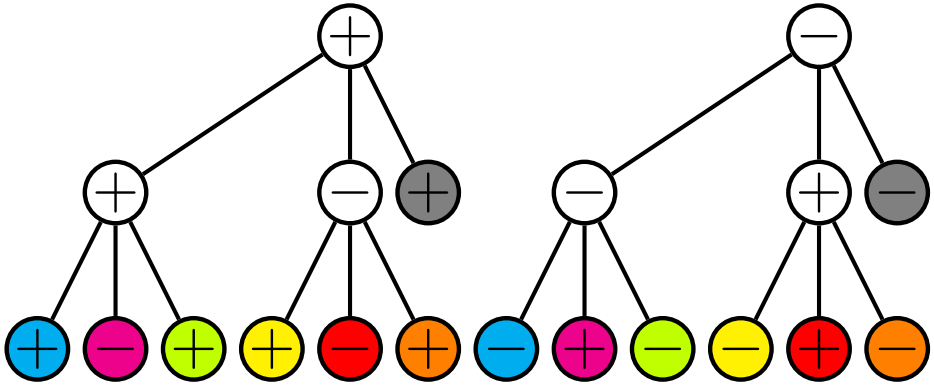
$$\int_0^t dt_1\ e^{i\pi\sigma_1\alpha_1 t_1} \times \int_0^{t_1} dt_{11}\ e^{i\pi\sigma_{11}\alpha_{11} t_{11}} \times \int_0^{t_1} dt_{12}\ e^{i\pi\sigma_{12}\alpha_{12} t_{12}}$$

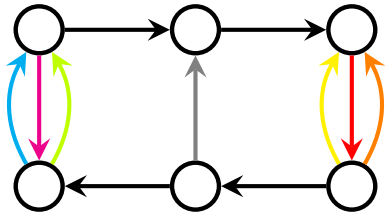
where

$$\sigma_1 = \sigma_{11} = \sigma_{13} = 1, \quad \sigma_{12} = -1, \quad \sigma_1 k_1 = \sigma_{11} k_{11} + \sigma_{12} k_{12} + \sigma_{13} k_{13},$$
$$\alpha_1 = |k_{11}|_\beta^2 - |k_{12}|_\beta^2 + |k_{13}|_\beta^2 - |k_1|_\beta^2.$$

Trees, couples and Molecules







Admissible decorations

Let $\mathbf{M}$ be a molecule and S a set of atoms. We denote by $\mathfrak{D}(\mathbf{M}, S, a, c, \Gamma, f)$ the set of decorations $(k_l)_{l \in E_{\mathbf{M}}}$ such that

$$|k_l - a_l| \leqslant 1, \quad \sum_{v : l \sim v} \sigma(v, l) k_l = c_v, \quad \left| \sum_{l : l \sim v} \sigma(v, l) |k_l|_\beta^2 - \Gamma_v \right| \leqslant \frac{1}{\delta L^2},$$

where $c_v = 0$ for v of degree 4, $\sigma(l, v)$ equals 1 if l leaves v, and -1 otherwise. Otherwise if $v \in S$, the k_l for $l \sim v$ are equal if v is non-isolated, and equal to f_v if $d(v) < 4$.

If additional conditions Ext of the form $k_{l_1} - k_{l_2} \in E$ with $E \subset \mathbb{Z}_L^d$ are added, we write $\mathfrak{D}(\mathbf{M}, \mathrm{Ext})$.

Rigidity Theorem

Theorem (Deng-Hani 2023)

Let $\mathbf{M}$ *a molecule with* $n \leq (\log L)^3$ *atoms and no triple bond. Then* $\mathfrak{D}(\mathbf{M})$ *is the union of at most* C^n *subsets* $\mathfrak{D}(\mathbf{M}, \mathrm{Ext})$ *and*

$$\sup \#\mathfrak{D}(\mathbf{M}, \mathrm{Ext}) \leqslant (C^+)^n \frac{1}{\delta^{(n+m)/2}} L^{(d-1)n-2\nu r}$$

with m *atoms in molecular chains I and* r *molecular chains I and II.*

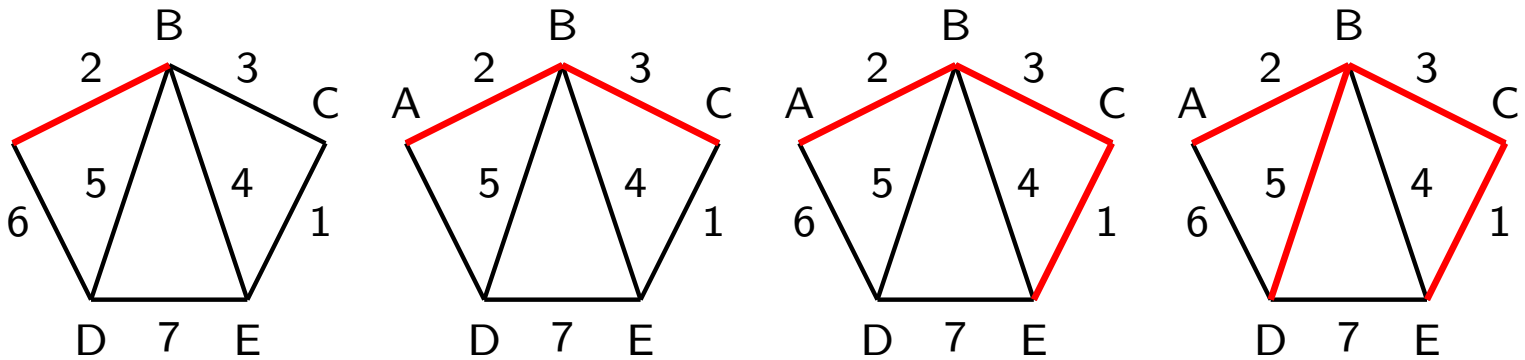
Main idea of the proof: Cutting algorithm on the molecules

$$\sup \#\mathfrak{D}(\mathbf{M}_{\mathrm{pre}}, \mathrm{Ext}_{\mathrm{pre}}) \leqslant C^+ \delta^{\Delta\kappa} L^{-(d-1)\Delta\gamma} \sup \#\mathfrak{D}(\mathbf{M}_{\mathrm{pos}}, \mathrm{Ext}_{\mathrm{pos}})$$

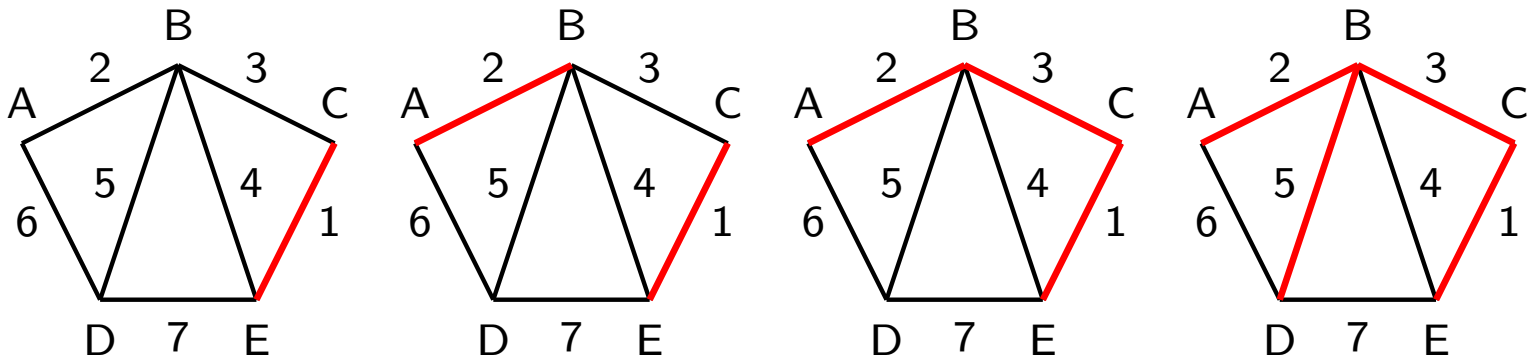
where $\mathbf{M}_{\mathrm{pre}}, \mathrm{Ext}_{\mathrm{pre}}$ (resp. $\mathbf{M}_{\mathrm{pos}}, \mathrm{Ext}_{\mathrm{pos}}$) correspond to the values of $\mathbf{M}, \mathrm{Ext}$ before (resp. after) a given step of the algorithm.

Prim versus Kruskal

Prim's Algorithm:



Kruskal's Algorithm:



Spanning trees in the literature

Spanning tree from the root:

- Dispersive equations: [Lukkarinen-Spohn; 2011], [De Suzzoni-Stingo-Touati ; 2025] .
- Boltzmann equation: [Bodineau-Gallagher-Saint-Raymond-Simonella ; 2023]. See also the algorithm **UP** in [Deng-Hani-Ma ; 2024].

Spanning trees in QFT for Hepp sectors:

- [Gallavotti-Nicolò ; 1985] and [Rivasseau ; 1991].
- Mention of Kruskal, [Rivasseau-Wang ; 2014], [Hairer-Quastel ; 2018].

Main result

Theorem (B.-Clarisse 2026)

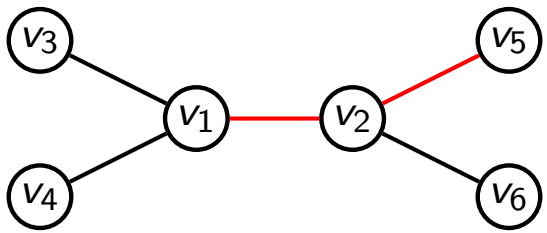
The molecule reduction algorithm introduced by Deng and Hani builds a spanning tree of a molecule associated with an irregular couple in a Kruskal manner.

Main idea of the proof:

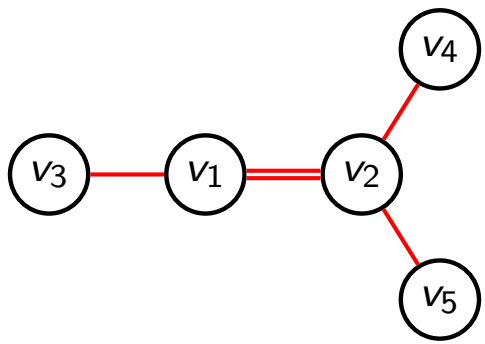
- Construction of an acyclic graph during the algorithm.
- Add a maximum of edges removed to this graph at each step.
- The new graph is still acyclic.
- The order of the steps gives edges dynamical weights.

Good steps

Step (3S3-5G): Two degree 3 atoms v_1, v_2 are connected by a single bond. Example of edges added

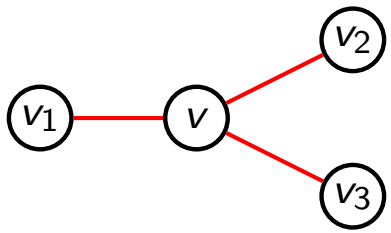


Step (3D4G): Two degree $3, 4$ atoms v_1, v_2 are connected by a double bond. Example of edges added

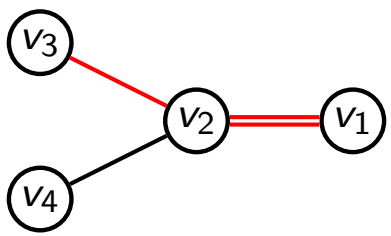


Normal steps

Step (3R-1): v is a degree-3 atom connected to three degree-4 atoms. Example of edges added



Step (2R-1): v_1 is connected to a degree-4 atom v_2 by a double bond with opposite direction. Example of edges added

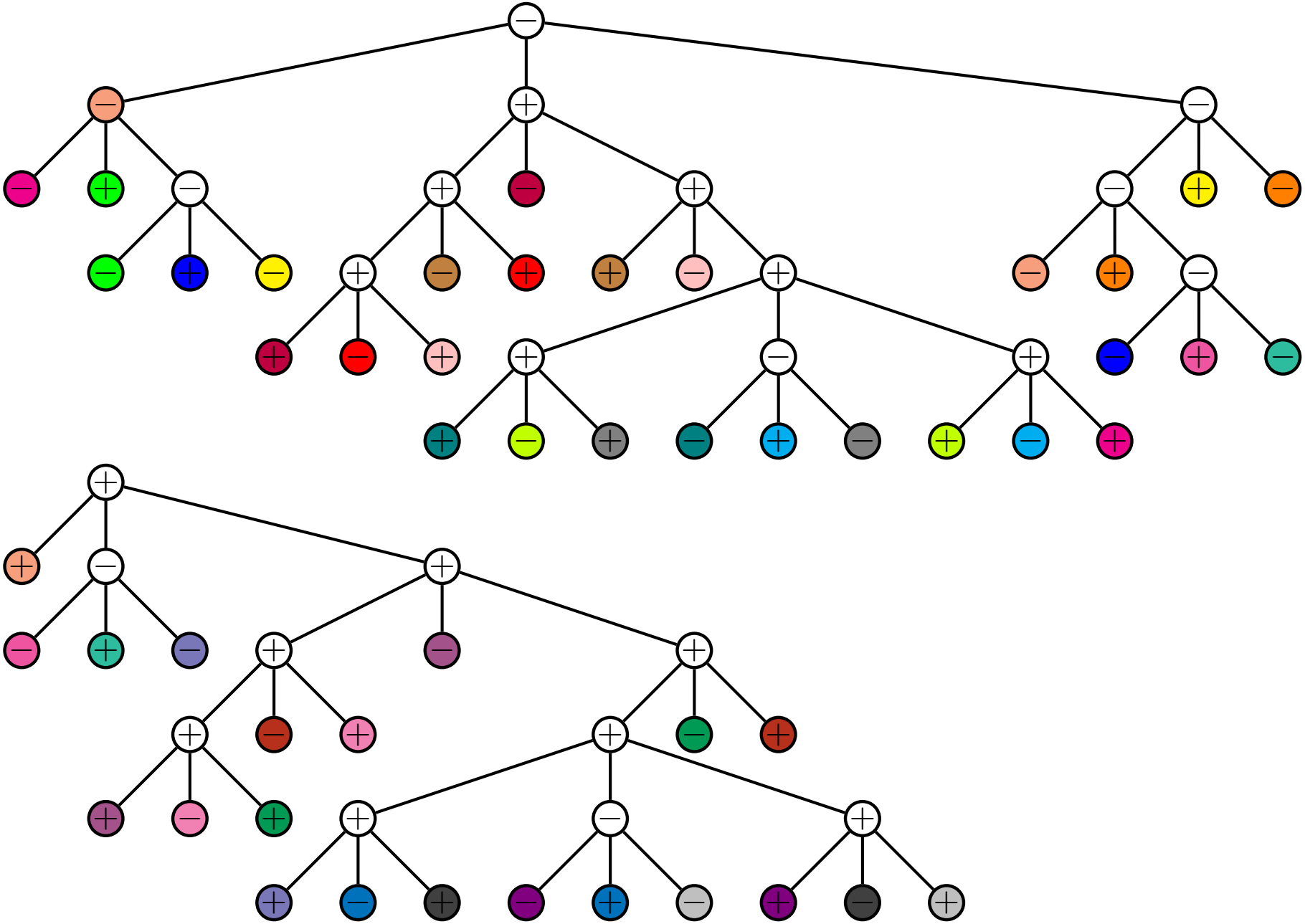


Order of the steps

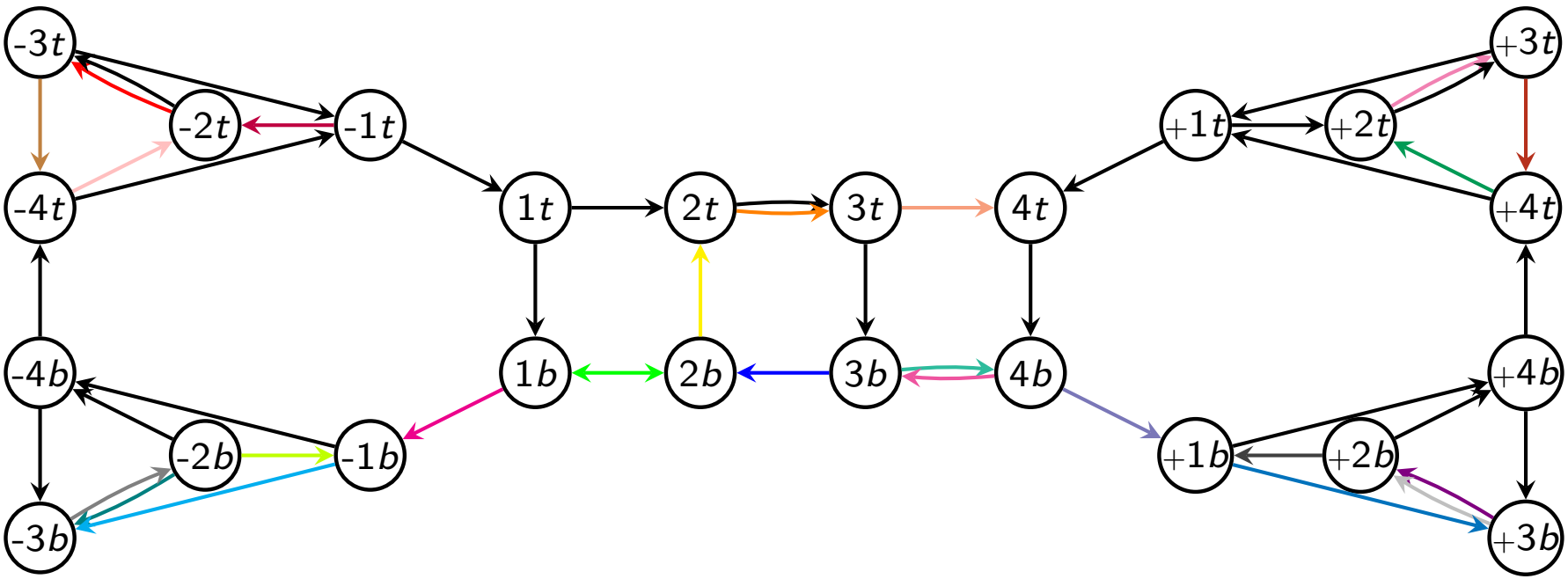
The reduction algorithm proposed by Deng and Hani contains many ordered steps that are repeated.

Step	$\Delta\chi$	$\Delta\gamma$	$\Delta\kappa$
(BR)	0	0	0
(3S3-5G)	-3	$-3+\frac{1}{6(d-1)}$	-2
(3D4G)	-3	$-3+\frac{1}{4(d-1)}$	-2
(3R-1)	-2	-2	-1
(2R-1)	-1	-1	-1

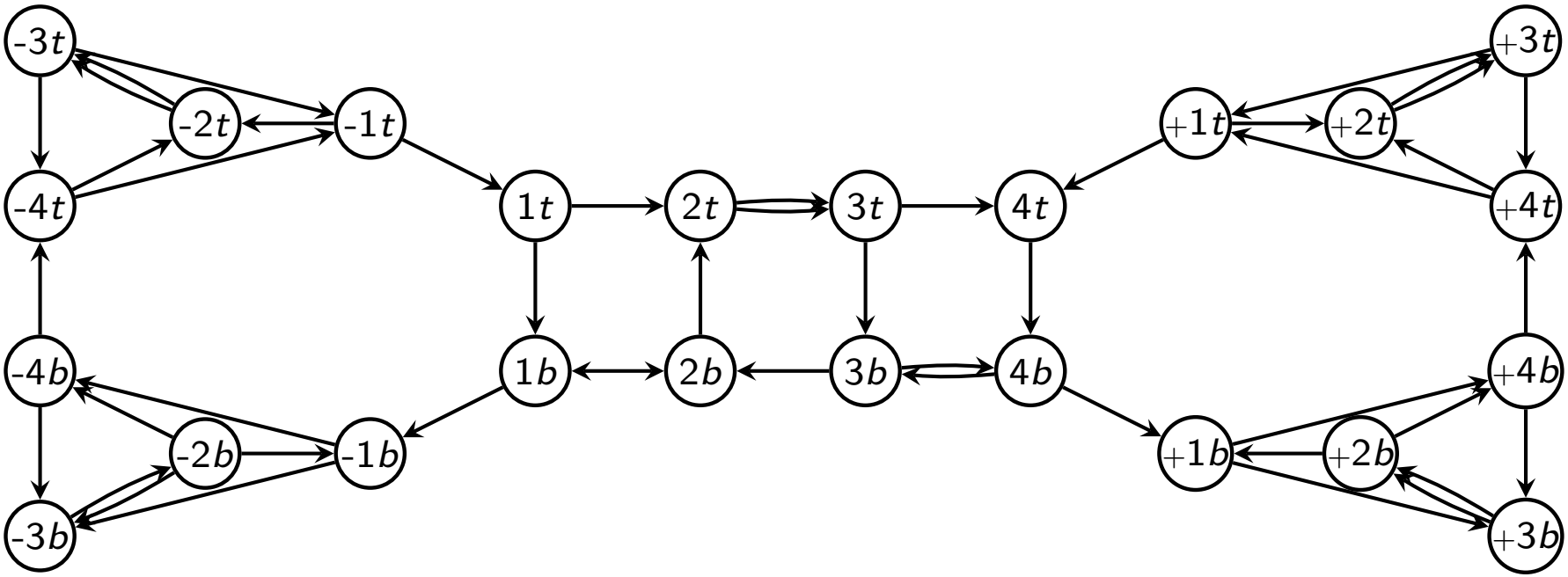
Step (BR) removes an edge which is a bridge.



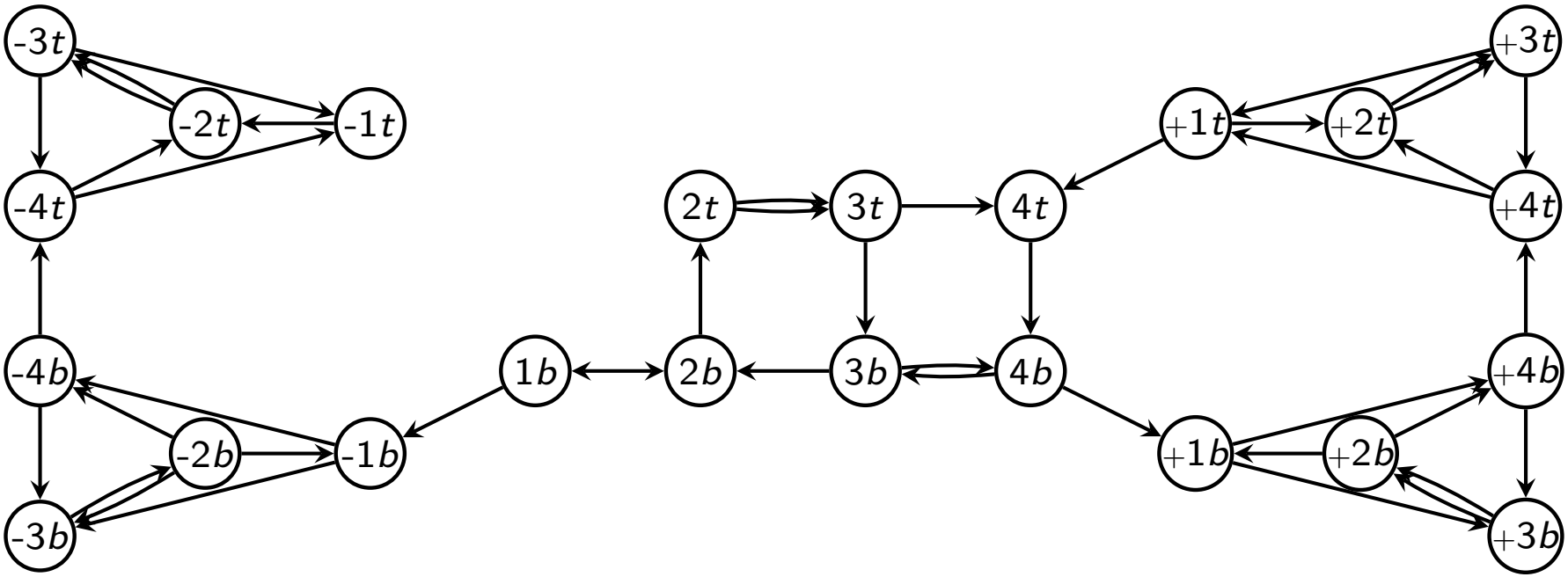
Molecule associated with the previous couple



Cutting Molecule Algorithm

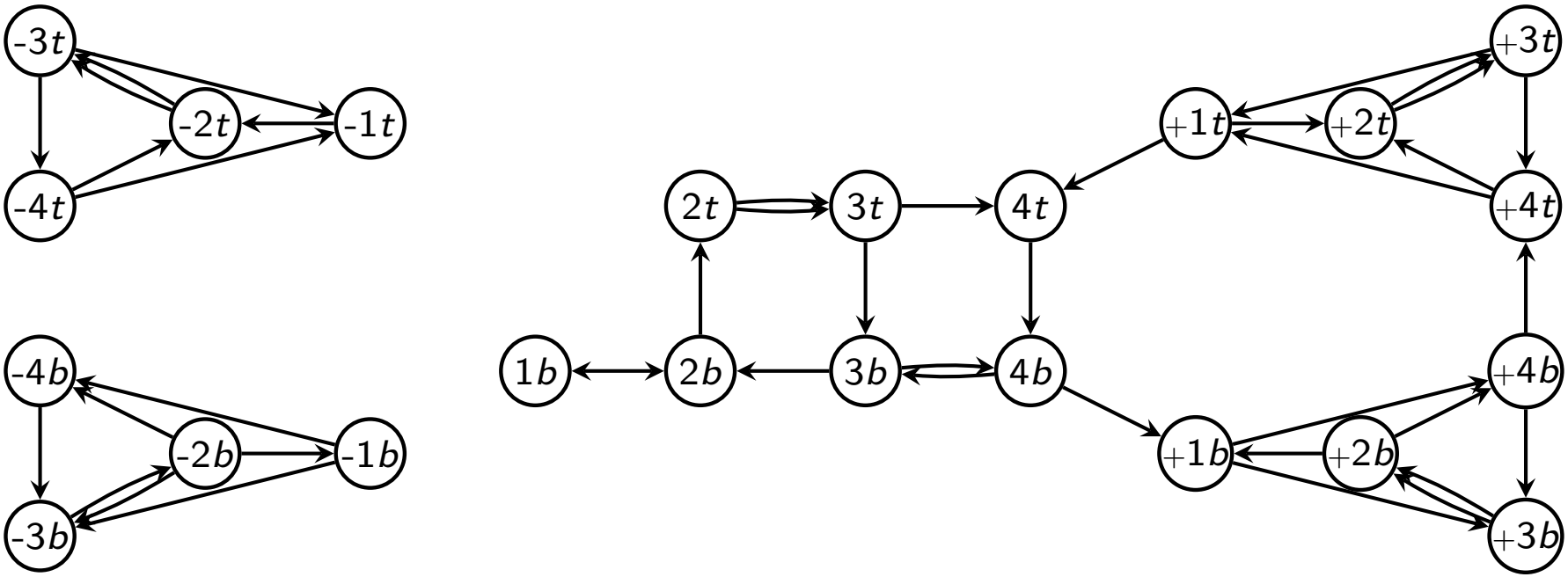


Cutting Molecule Algorithm



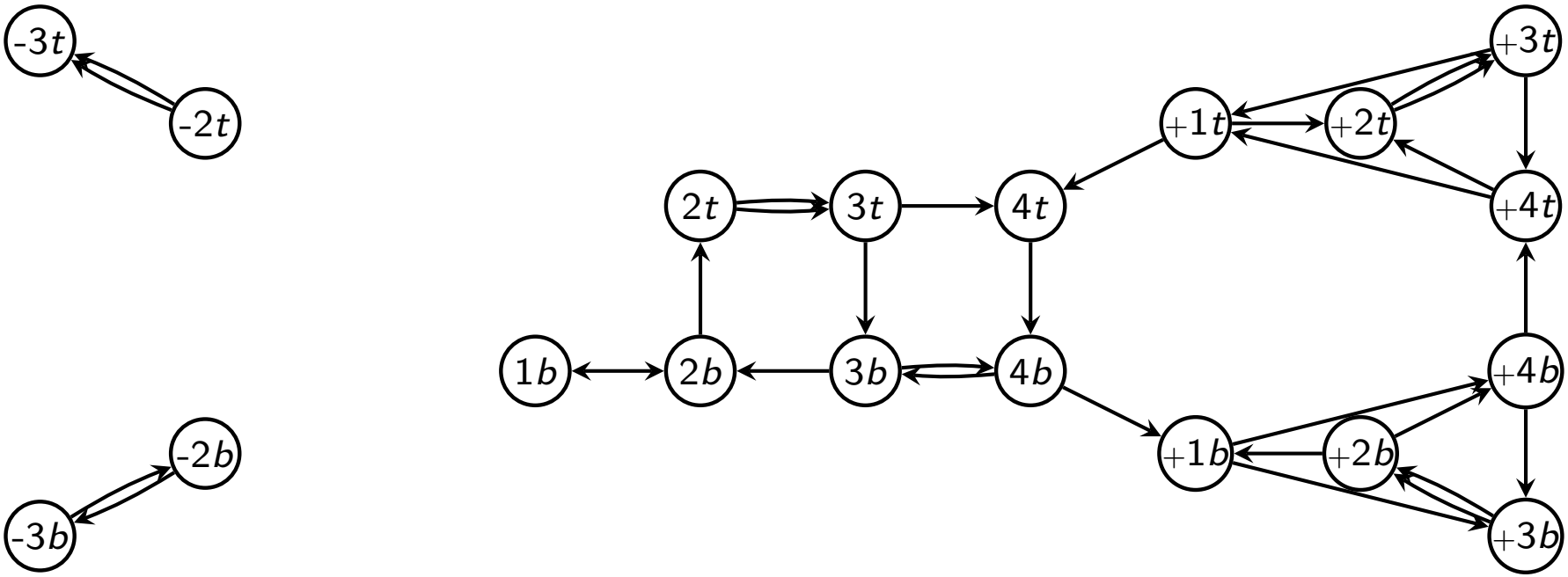
Steps: 3R1,

Cutting Molecule Algorithm



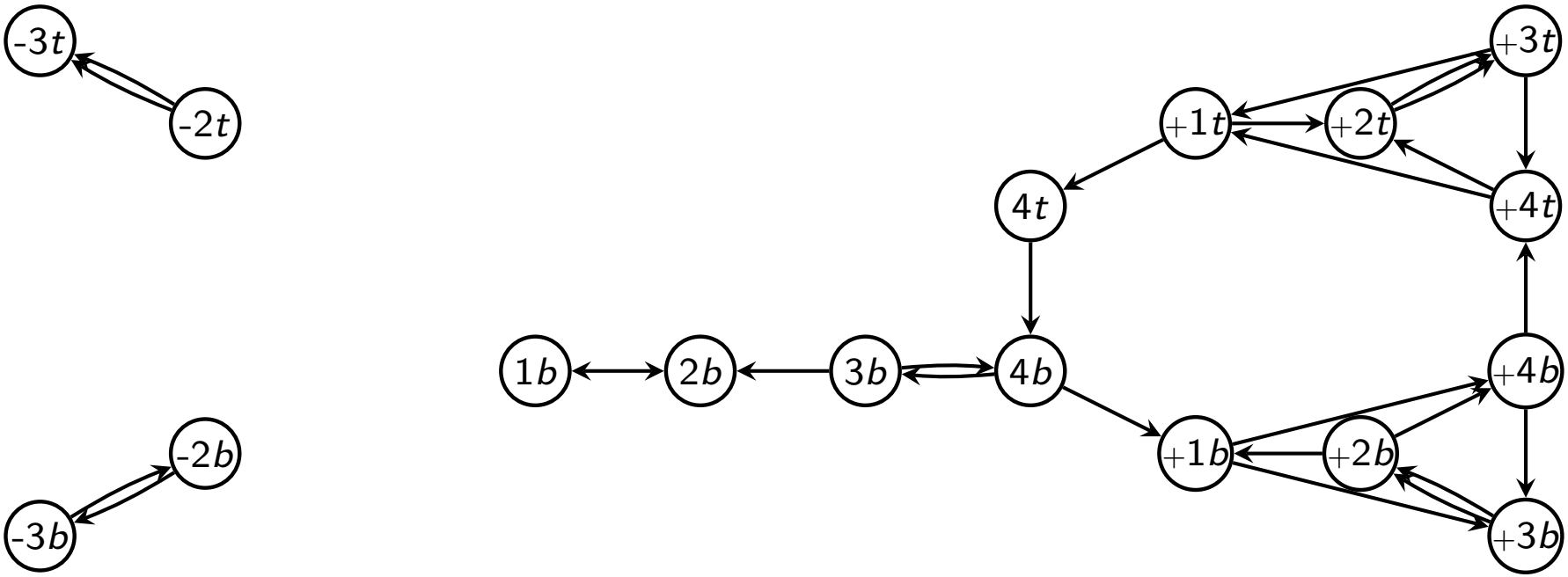
Steps: 3R1, BR, BR,

Cutting Molecule Algorithm



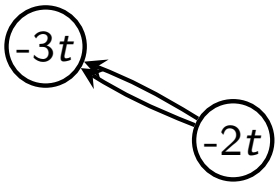
Steps: 3R1, BR, BR, 3S3-5G, 3S3-5G,

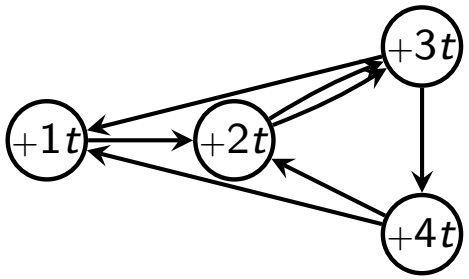
Cutting Molecule Algorithm

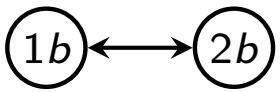


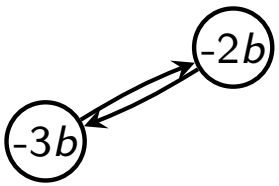
Steps: 3R1, BR, BR, 3S3-5G, 3S3-5G, 3D4G,

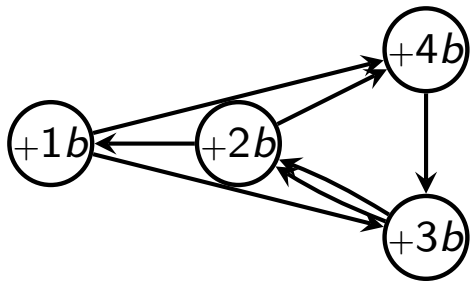
Cutting Molecule Algorithm





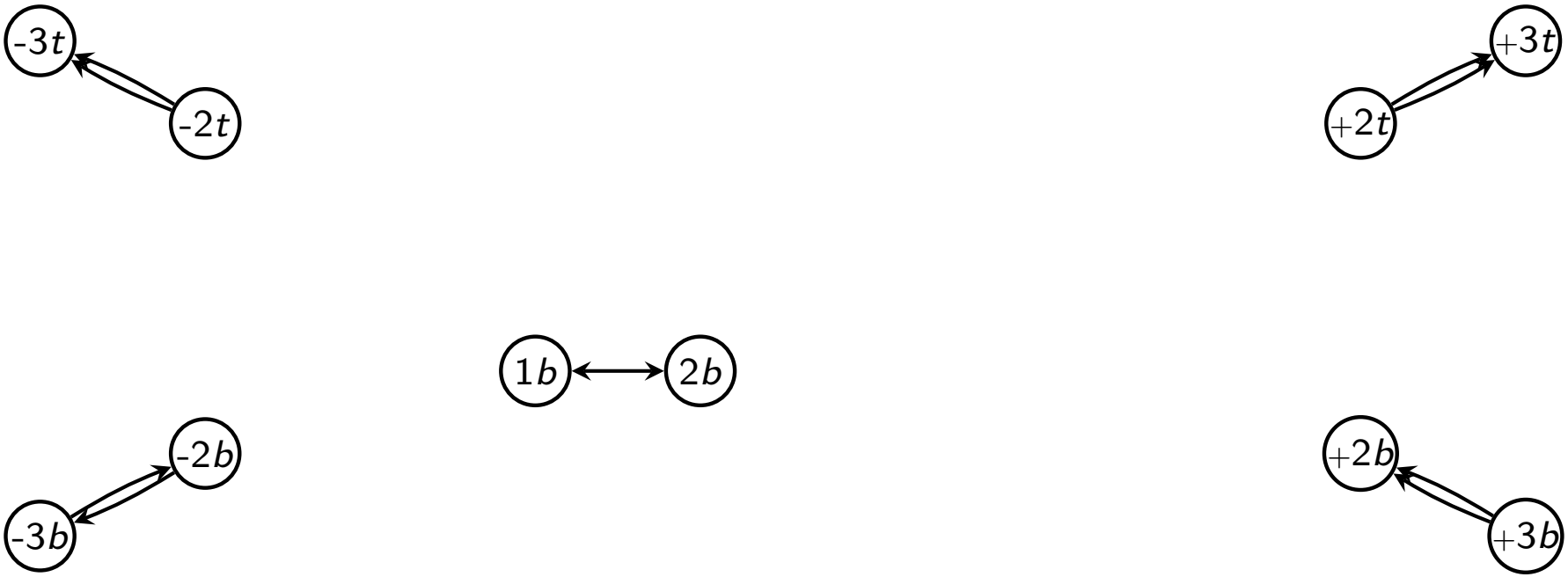






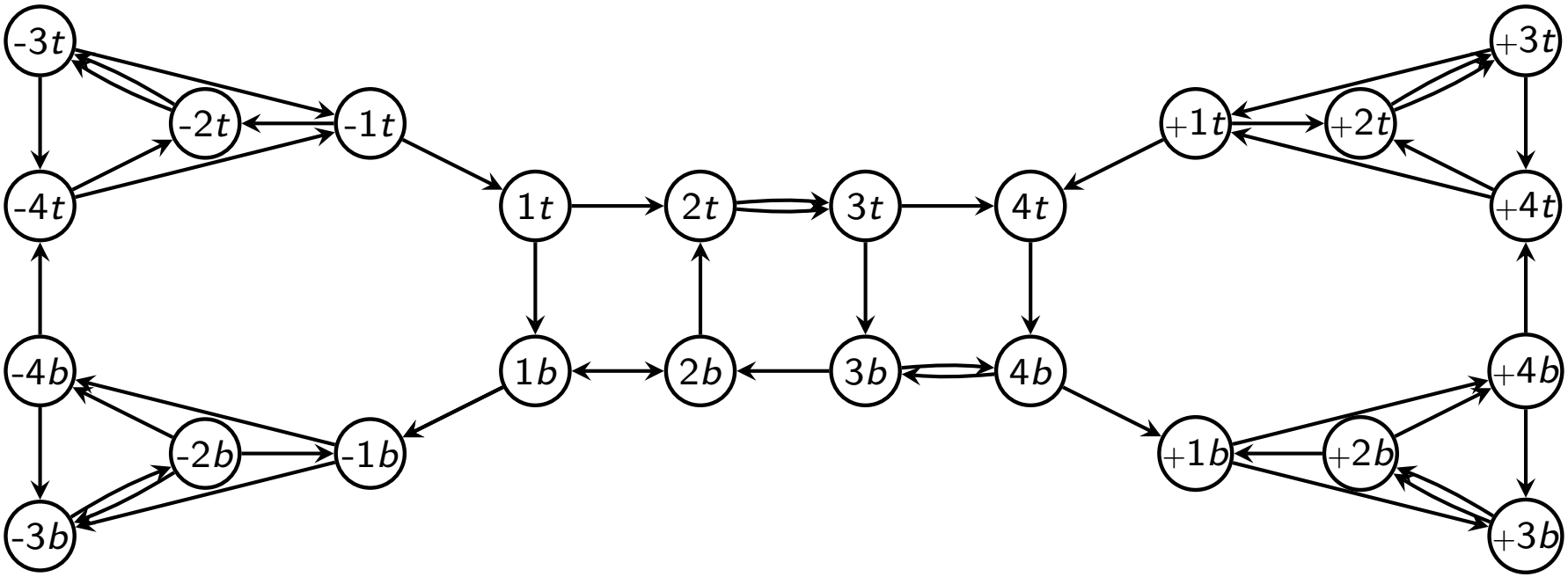
Steps: 3R1, BR, BR, 3S3-5G, 3S3-5G, 3D4G, BR, 2R-1, BR, BR, BR, BR,

Cutting Molecule Algorithm

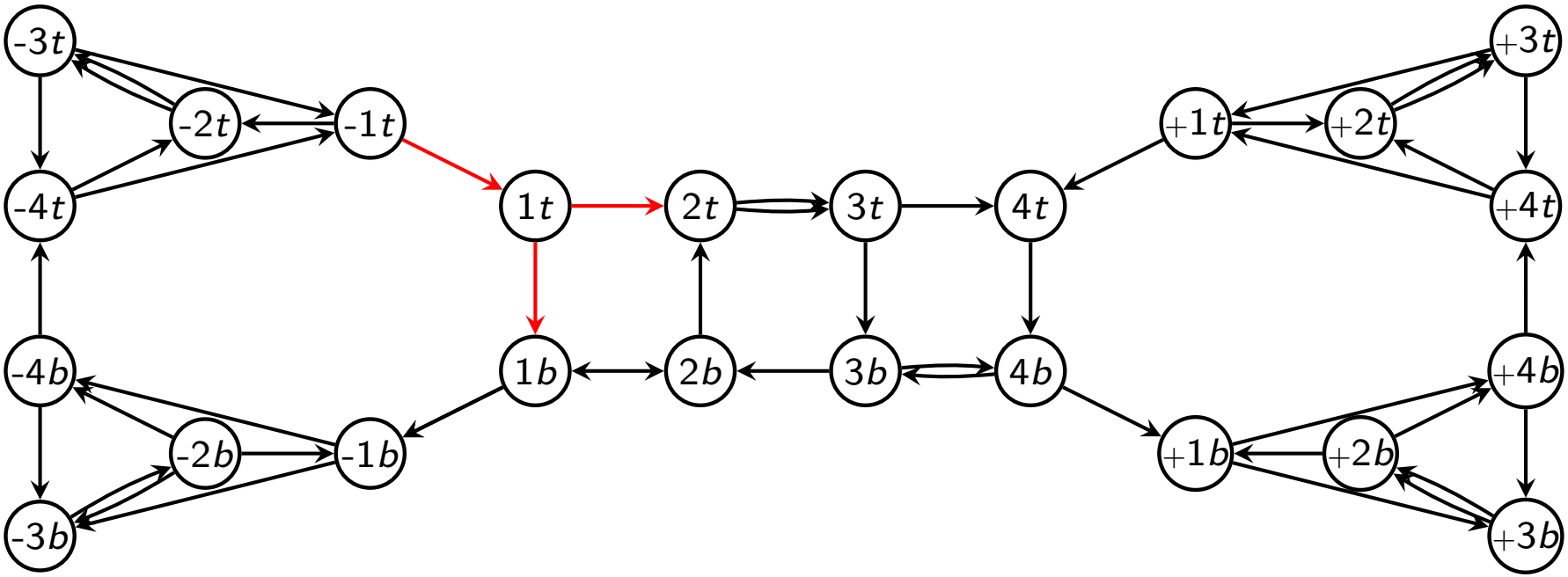


Steps: 3R1, BR, BR, 3S3-5G, 3S3-5G, 3D4G, BR, 2R-1, BR, BR, BR, BR, 3S3-5G, 3S3-5G.

Spanning Tree

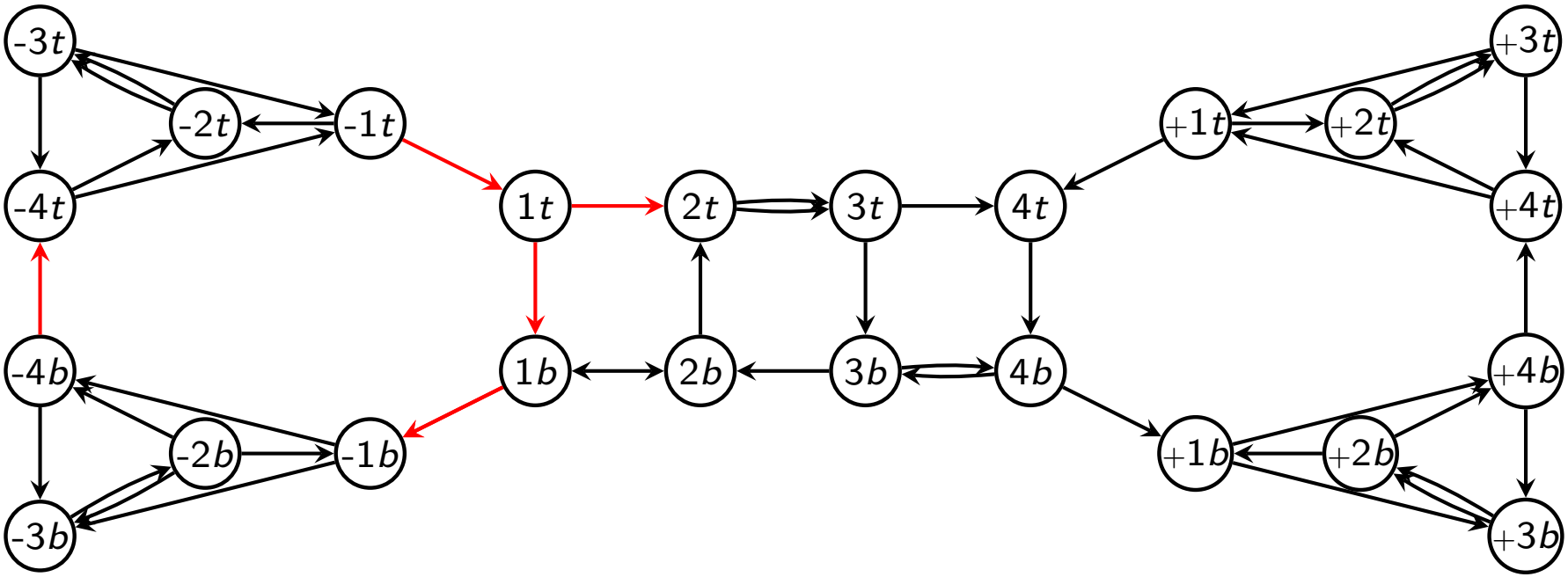


Spanning Tree



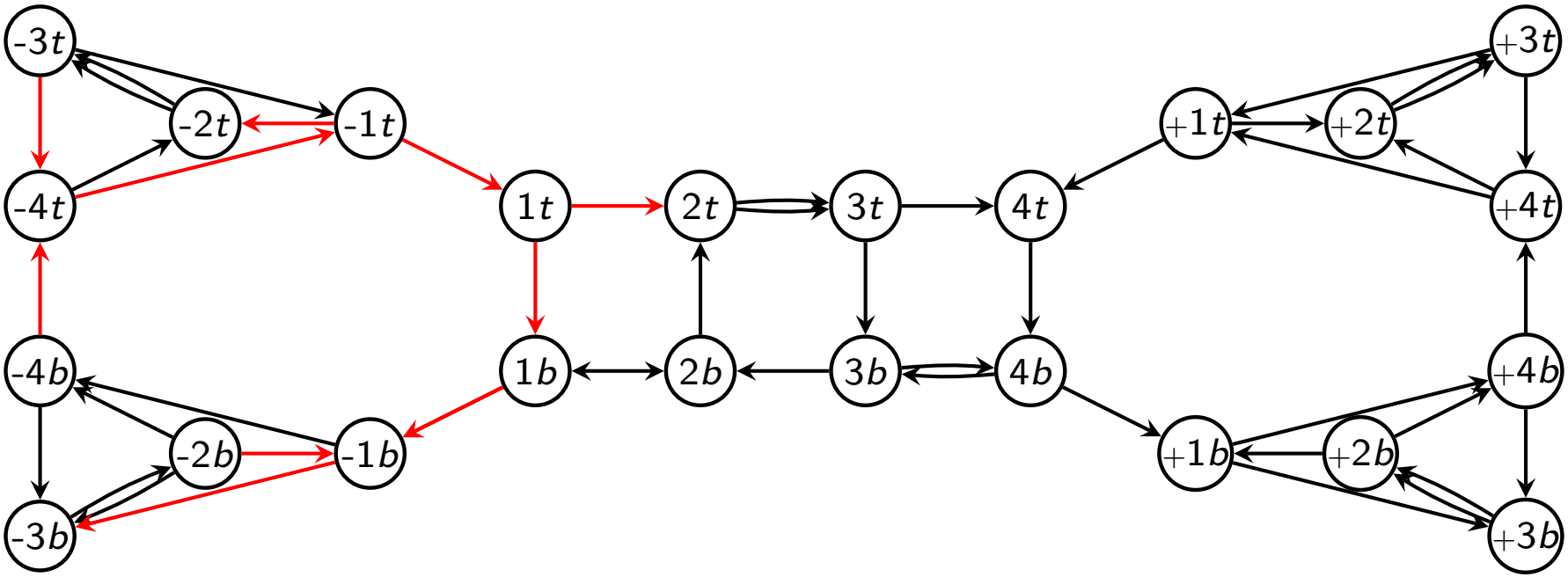
Steps: 3R1,

Spanning Tree



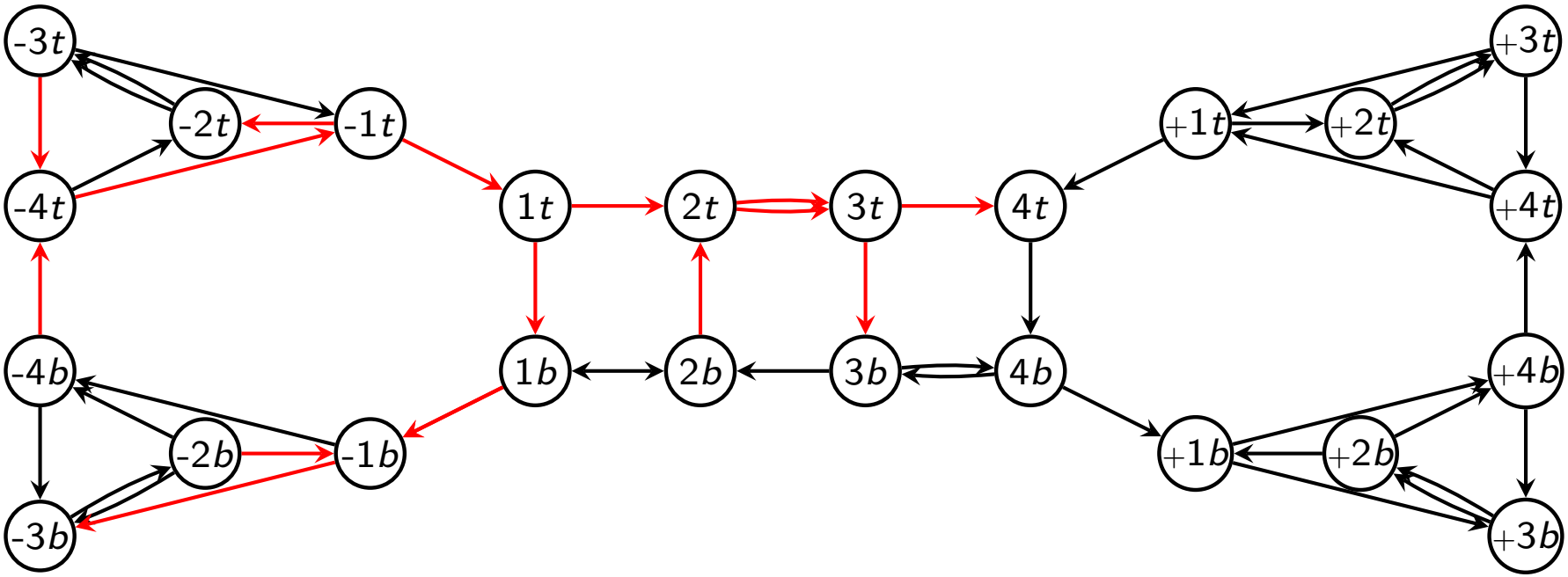
Steps: 3R1, BR, BR,

Spanning Tree



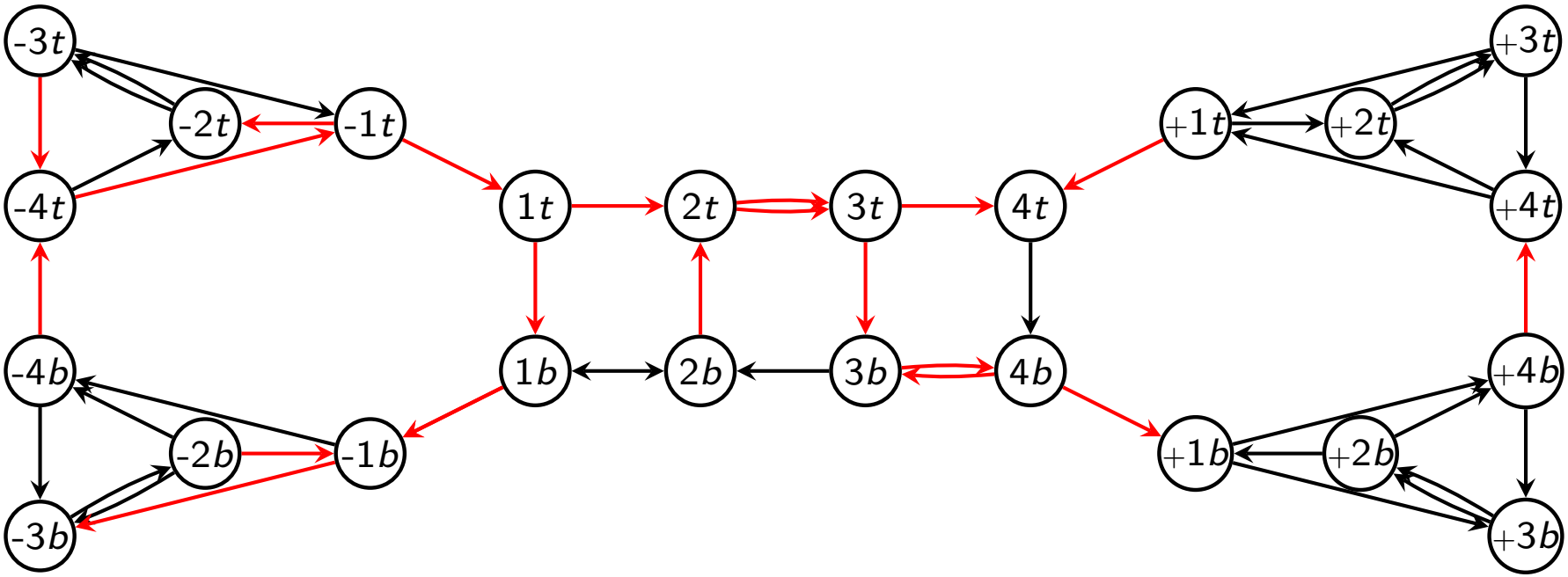
Steps: 3R1, BR, BR, 3S3-5G, 3S3-5G,

Spanning Tree



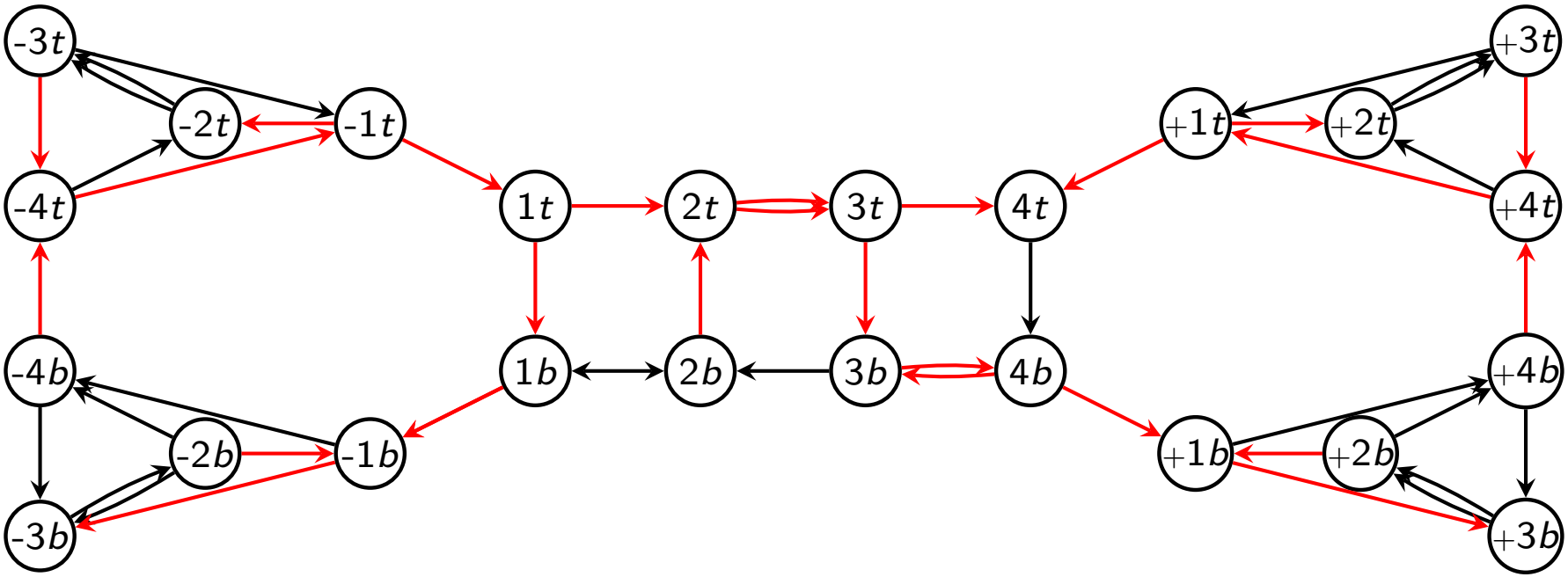
Steps: 3R1, BR, BR, 3S3-5G, 3S3-5G, 3D4G,

Spanning Tree



Steps: 3R1, BR, BR, 3S3-5G, 3S3-5G, 3D4G, BR, 2R-1, BR, BR, BR, BR,

Spanning Tree



Steps: 3R1, BR, BR, 3S3-5G, 3S3-5G, 3D4G, BR, 2R-1, BR, BR, BR, BR, 3S3-5G, 3S3-5G.

Perspectives

- New interpretation of [Erdös-Salmhofer-Yau ; 08].
- Same type of algorithms for the long time derivation of the Boltzmann equation [Deng-Hani-Ma ; 2024].
- Applications to other (dispersive) models for deriving kinetic equations.
- Use of this algorithm for getting fluctuations.
- Connection with BPHZ renormalisation and critical SPDEs.