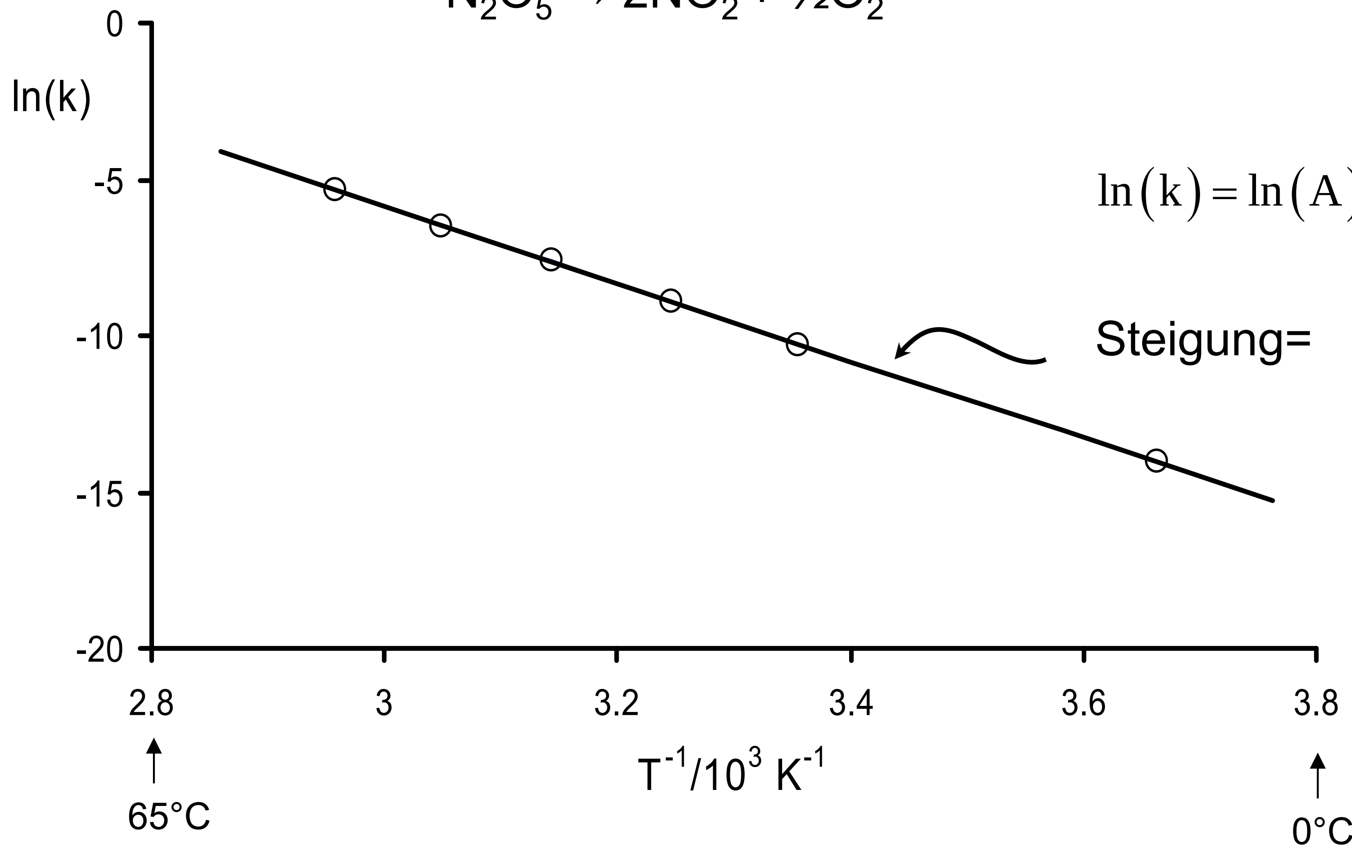
3.1) Arrhenius-Gleichung

„Arrhenius-Diagramm“

$N_2O_5 \rightarrow 2NO_2 + \frac{1}{2}O_2$



$$\ln(k) = \ln(A) - \frac{E_a}{R} \cdot \frac{1}{T}$$

Steigung= $-\frac{E_a}{R}$

[CONTRIBUTION FROM THE FIXED NITROGEN RESEARCH LABORATORY, WAR DEPARTMENT AND THE BUREAU OF SOILS, DEPARTMENT OF AGRICULTURE.]

THE THERMAL DECOMPOSITION OF GASEOUS NITROGEN PENTOXIDE. A MONOMOLECULAR REACTION.

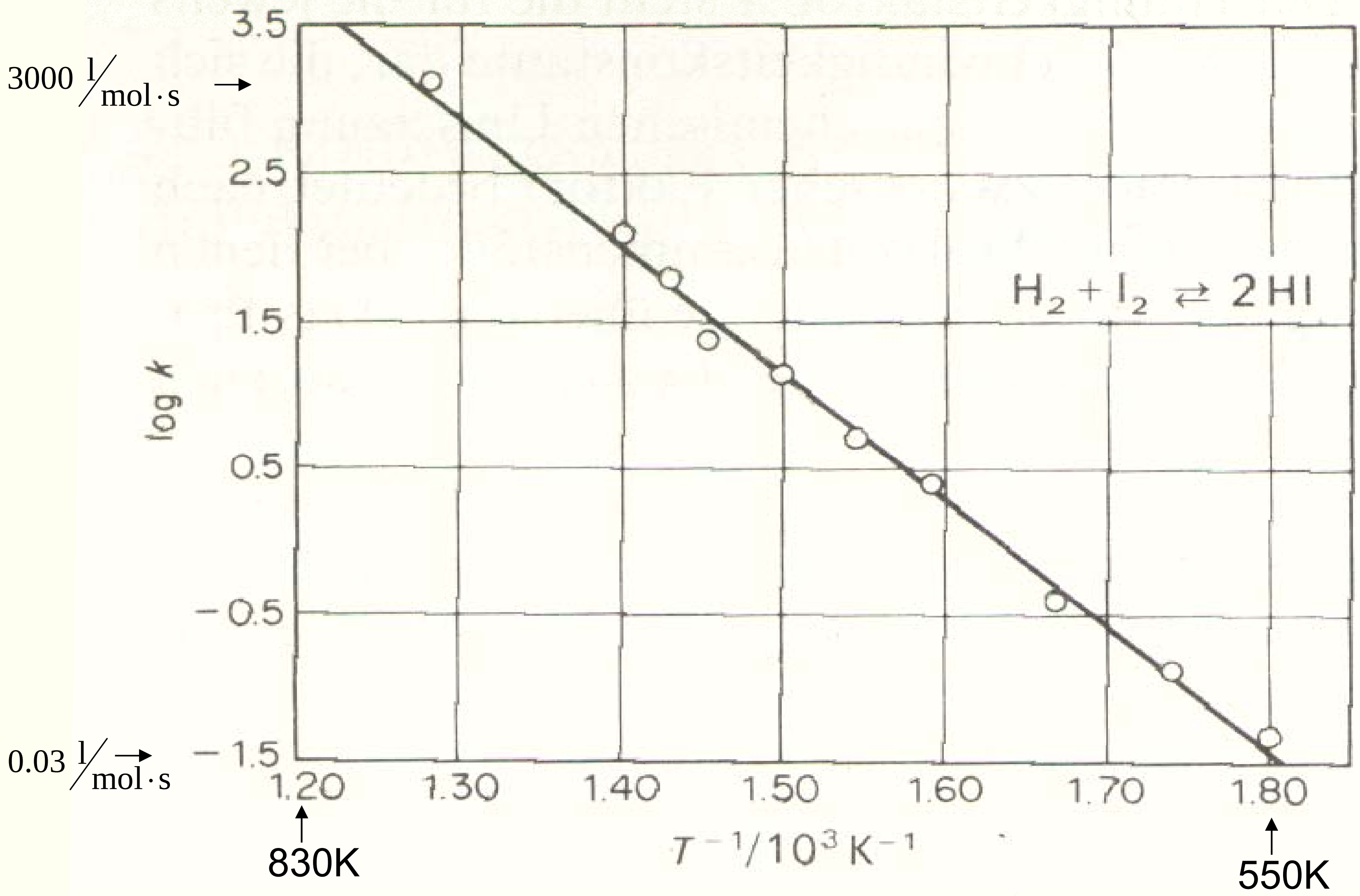
BY FARRINGTON DANIELS AND ELMER H. JOHNSTON.

Received October 9, 1920.

Reaktion 1. Ordnung

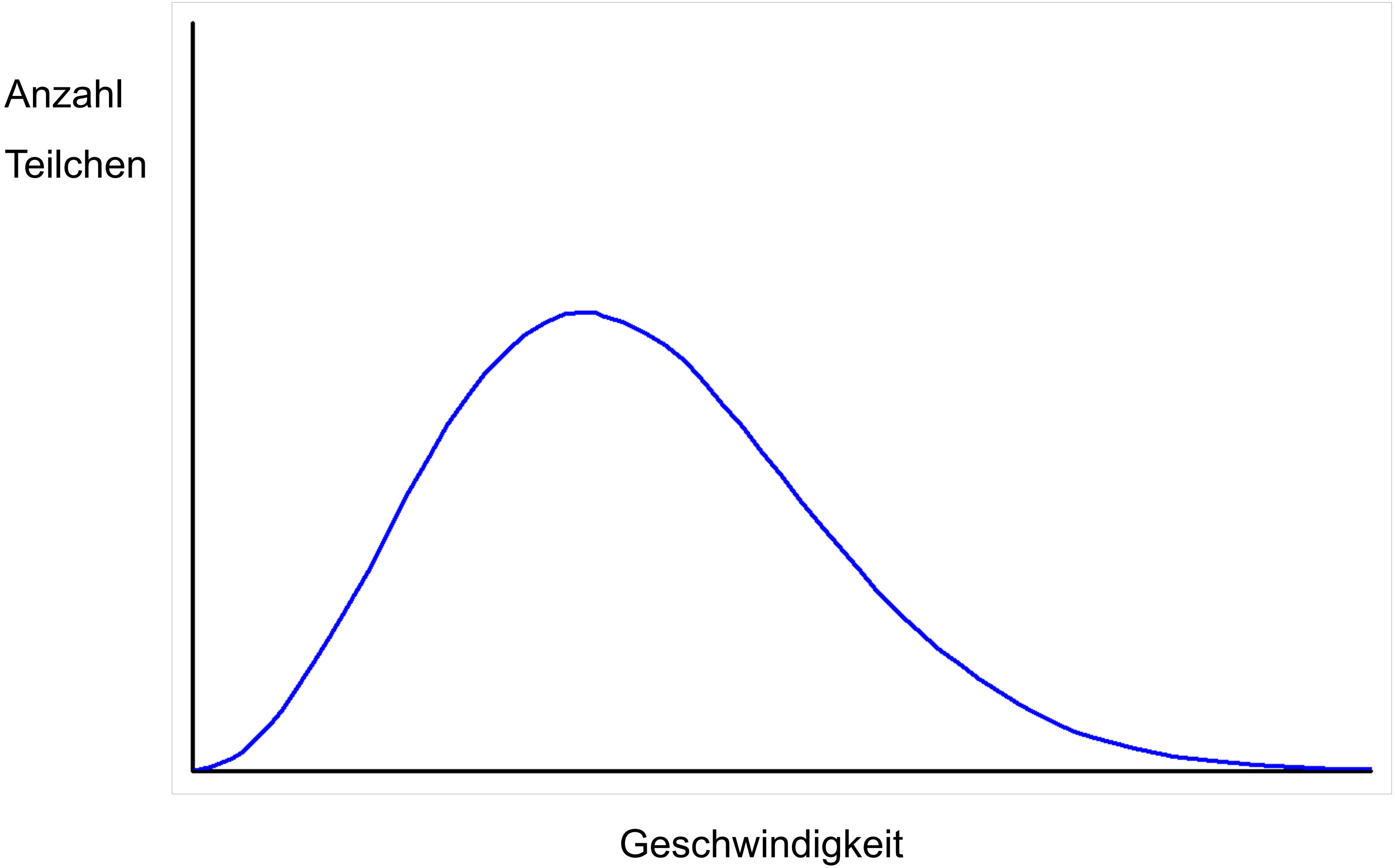
JACS, 43, 53 (1921)

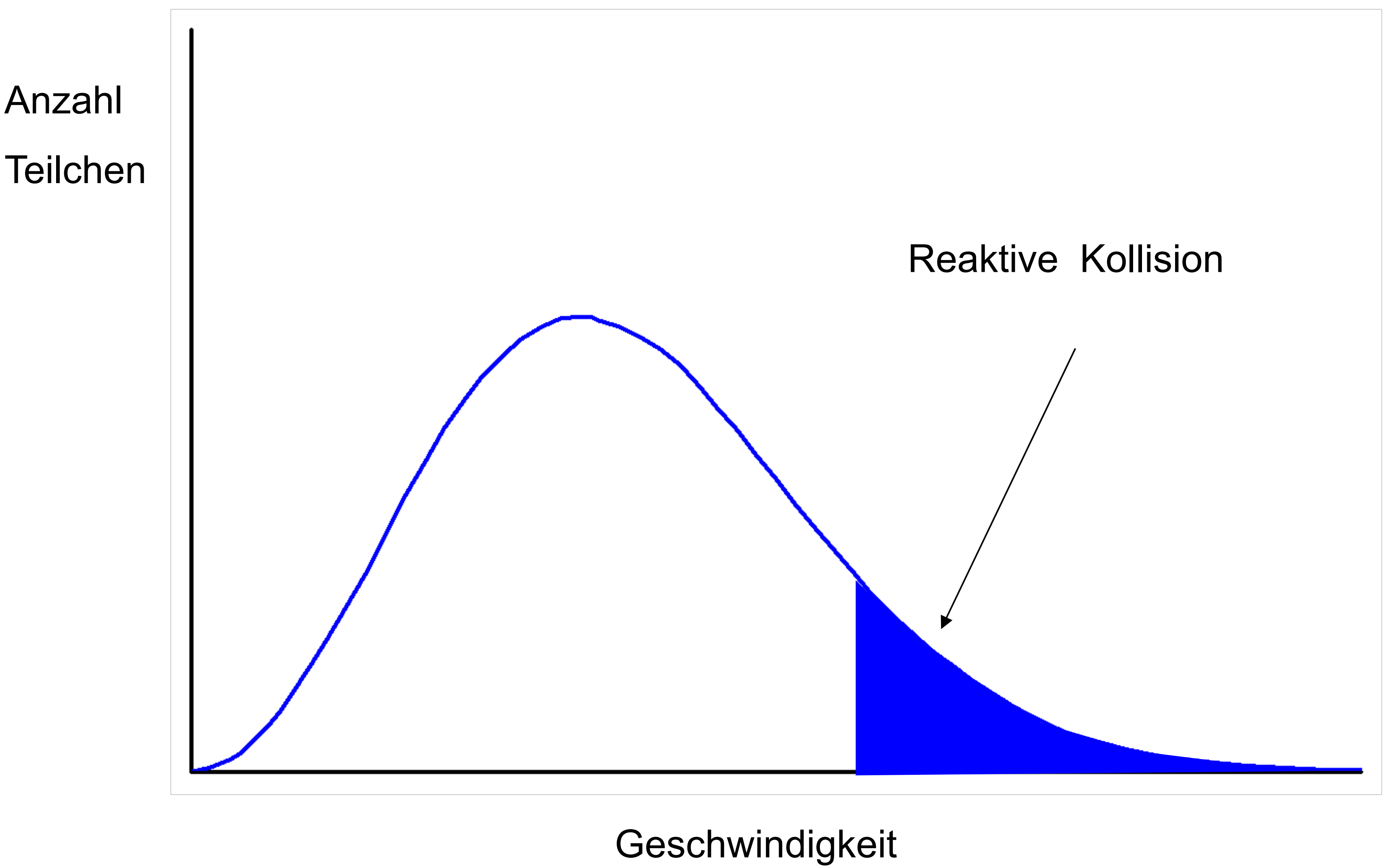
3.1) Arrhenius-Gleichung „Arrhenius-Diagramm“

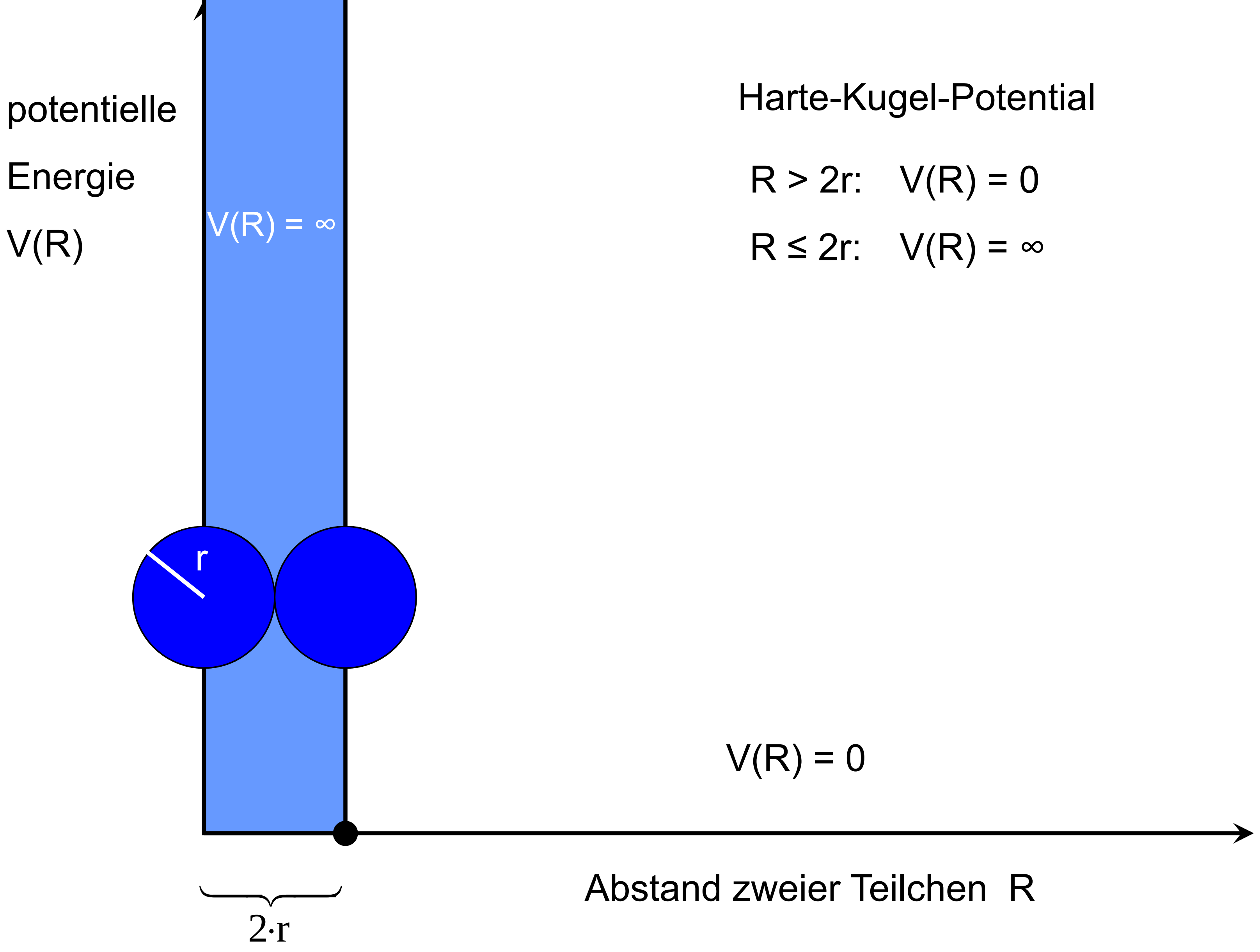


Reaktion 2. Ordnung

Quelle: Bodenstein, aus Moore/Hummel, 3. Auf.


Anzahl
Teilchen
Geschwindigkeit

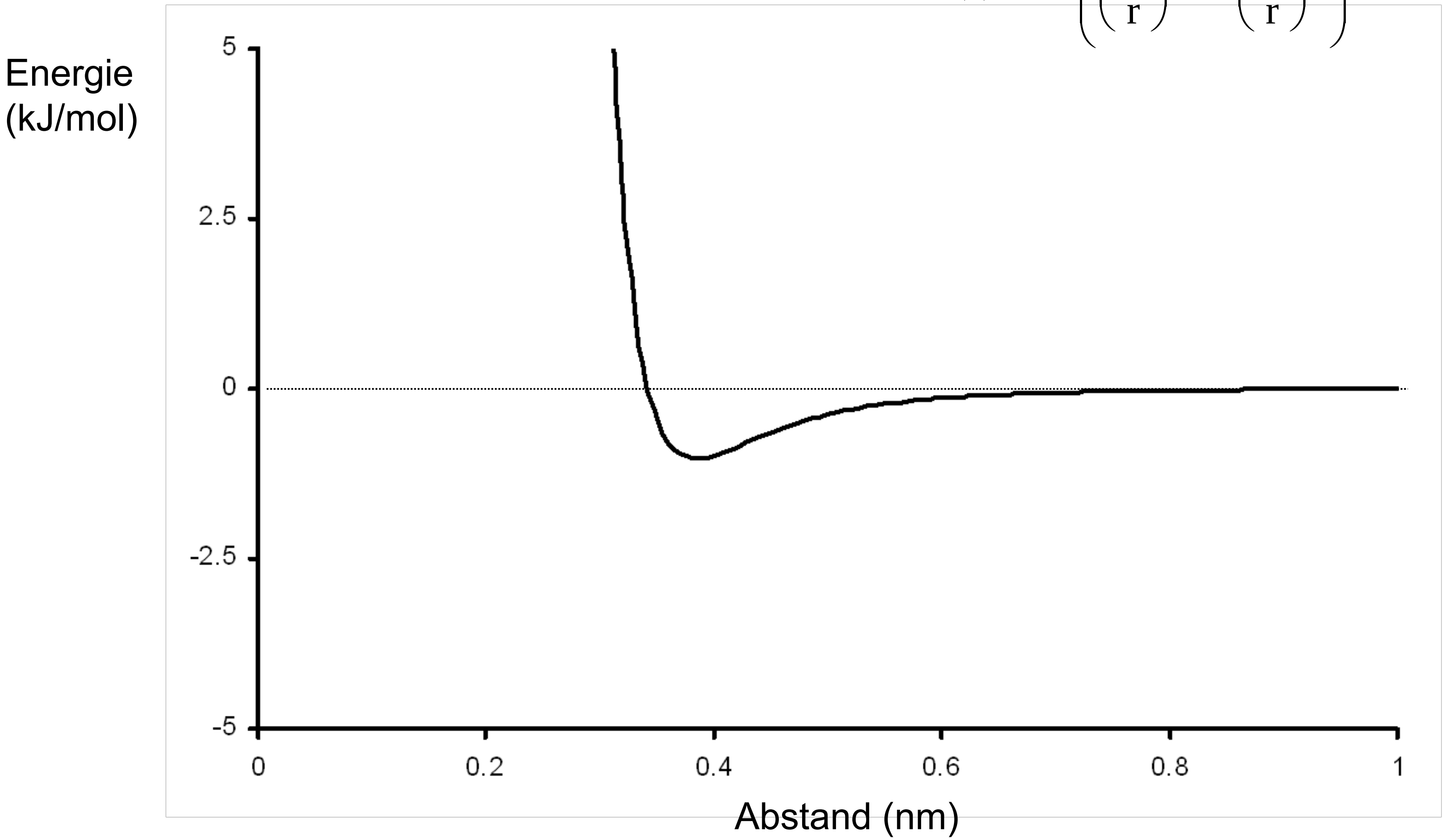

Anzahl
Teilchen
Reaktive Kollision
Geschwindigkeit



potentielle
Energie
V(R)
V(R) = ∞
Harte-Kugel-Potential
R > 2r: V(R) = 0
R ≤ 2r: V(R) = ∞
r
V(R) = 0
Abstand zweier Teilchen R
2·r

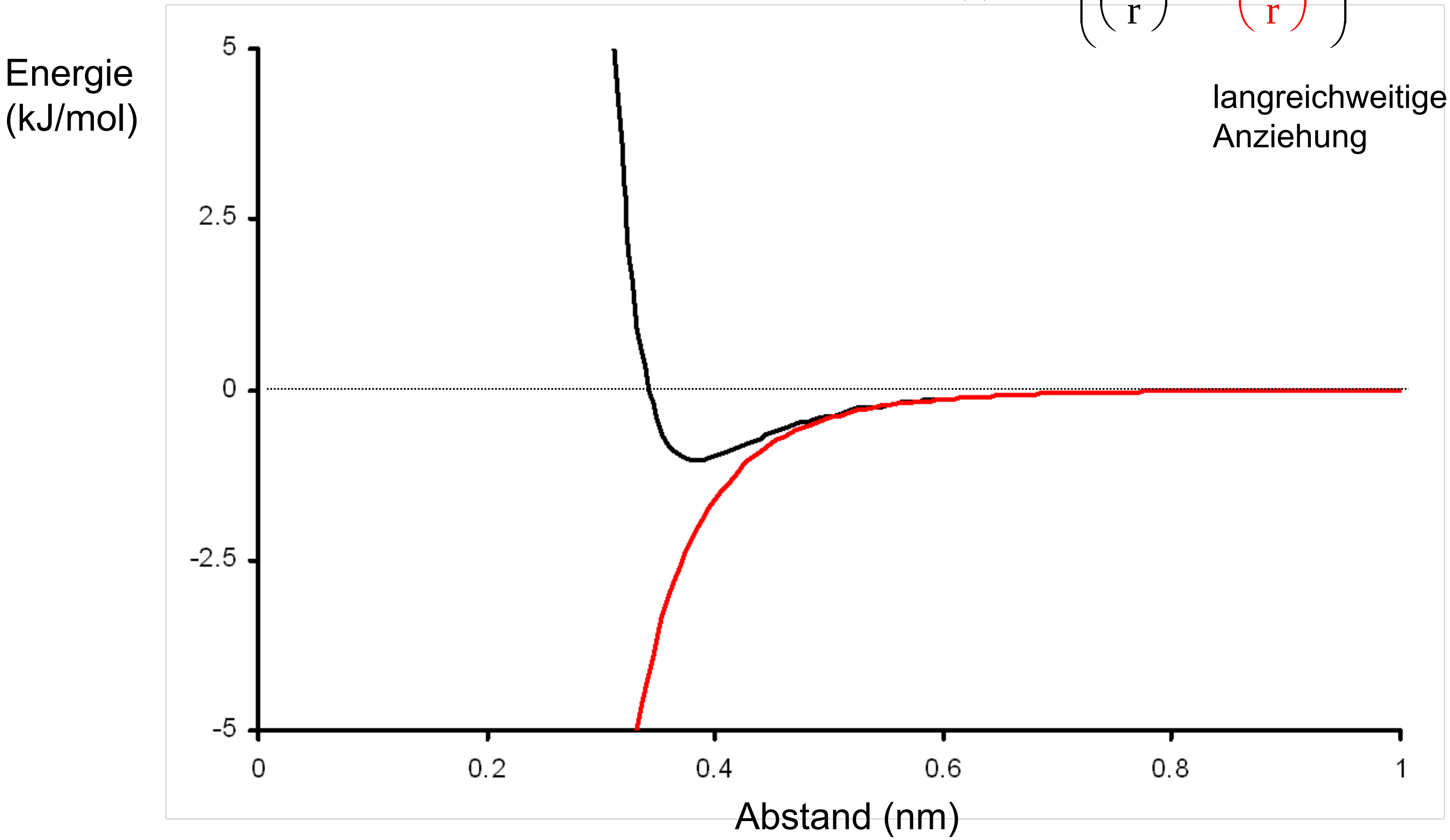
Lennard-Jones-Potential

$$V(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$



Lennard-Jones-Potential

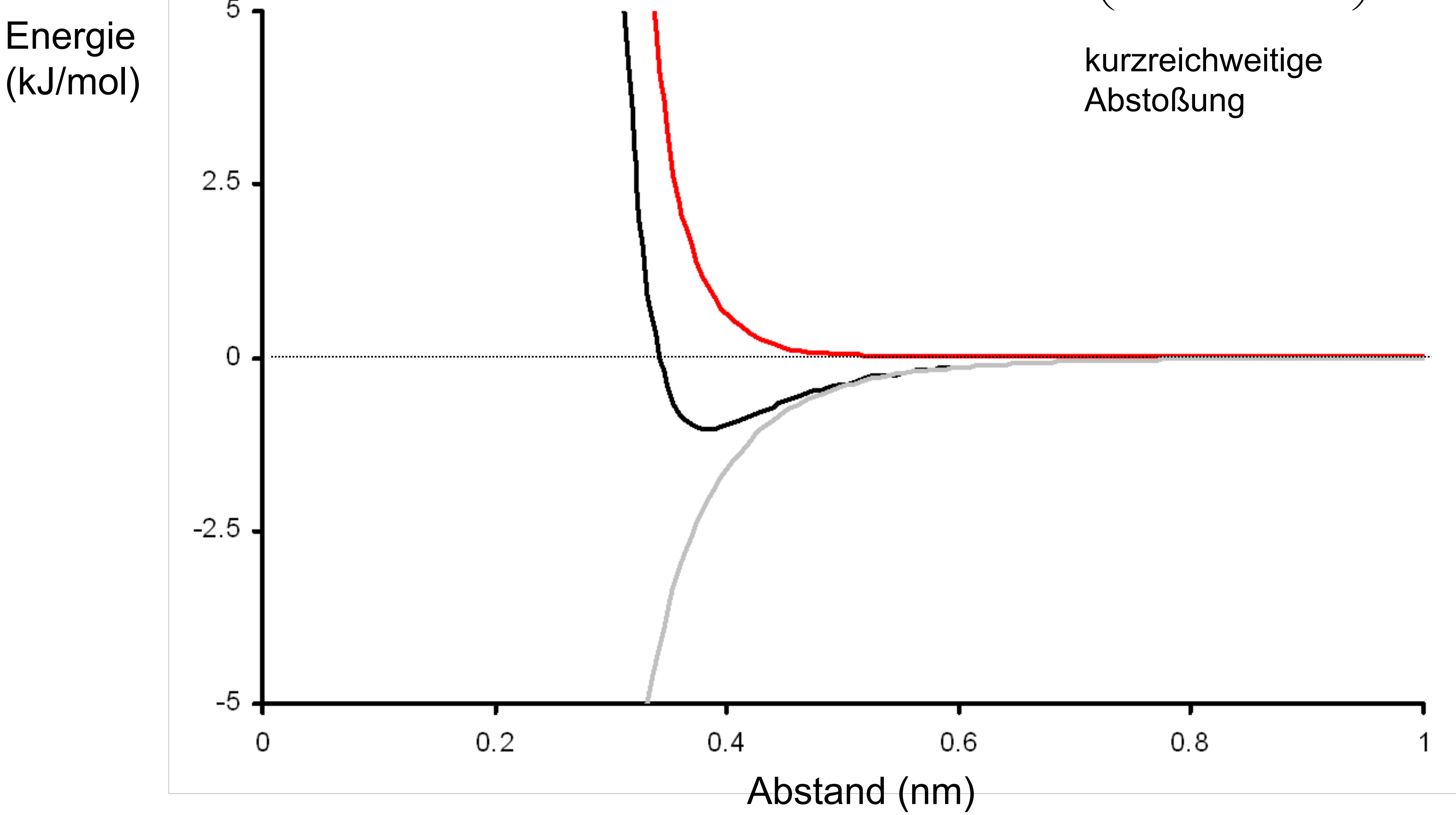
$$V(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$



Lennard-Jones-Potential

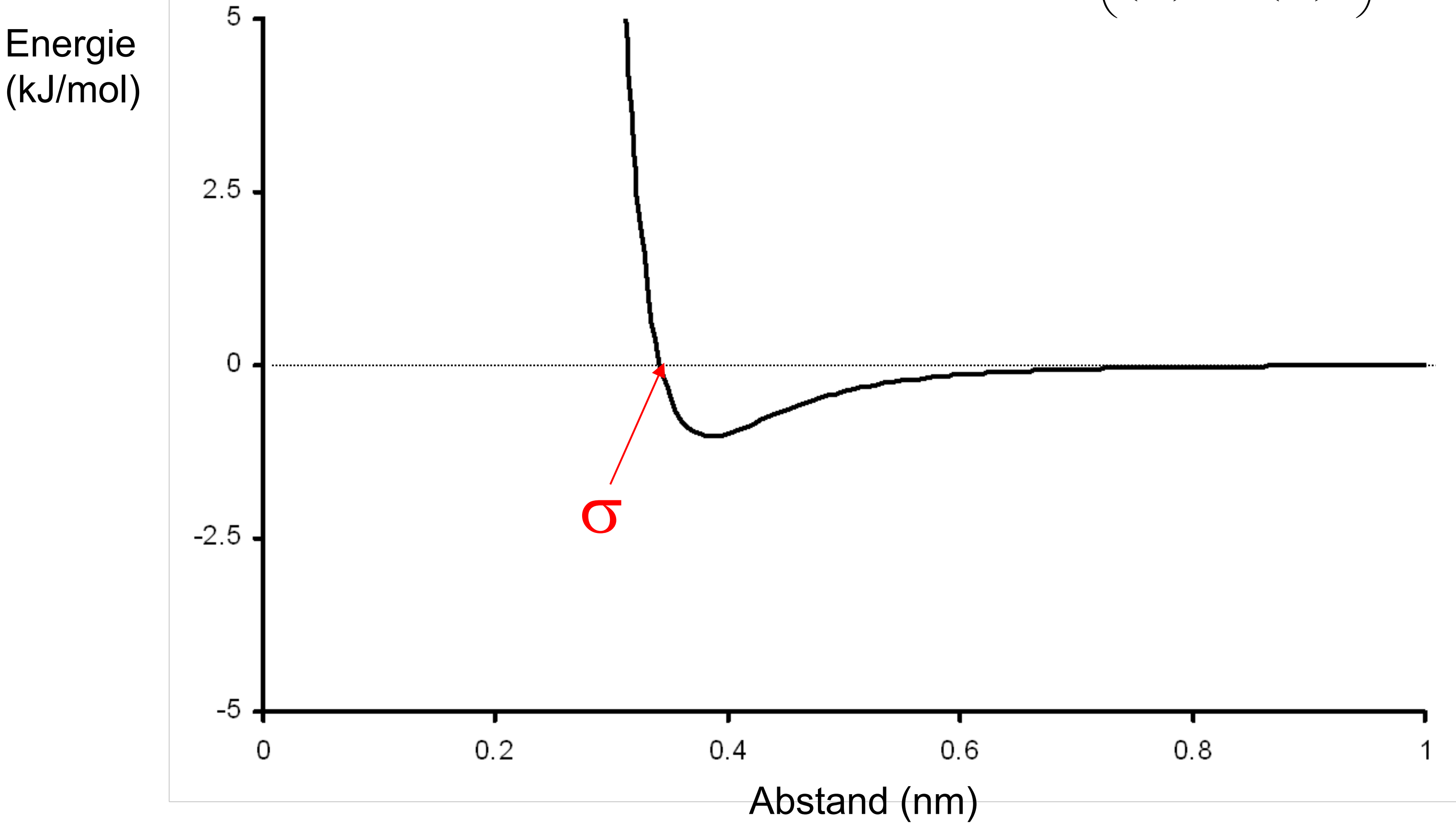
$$V(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

kurzreichweitige
Abstoßung



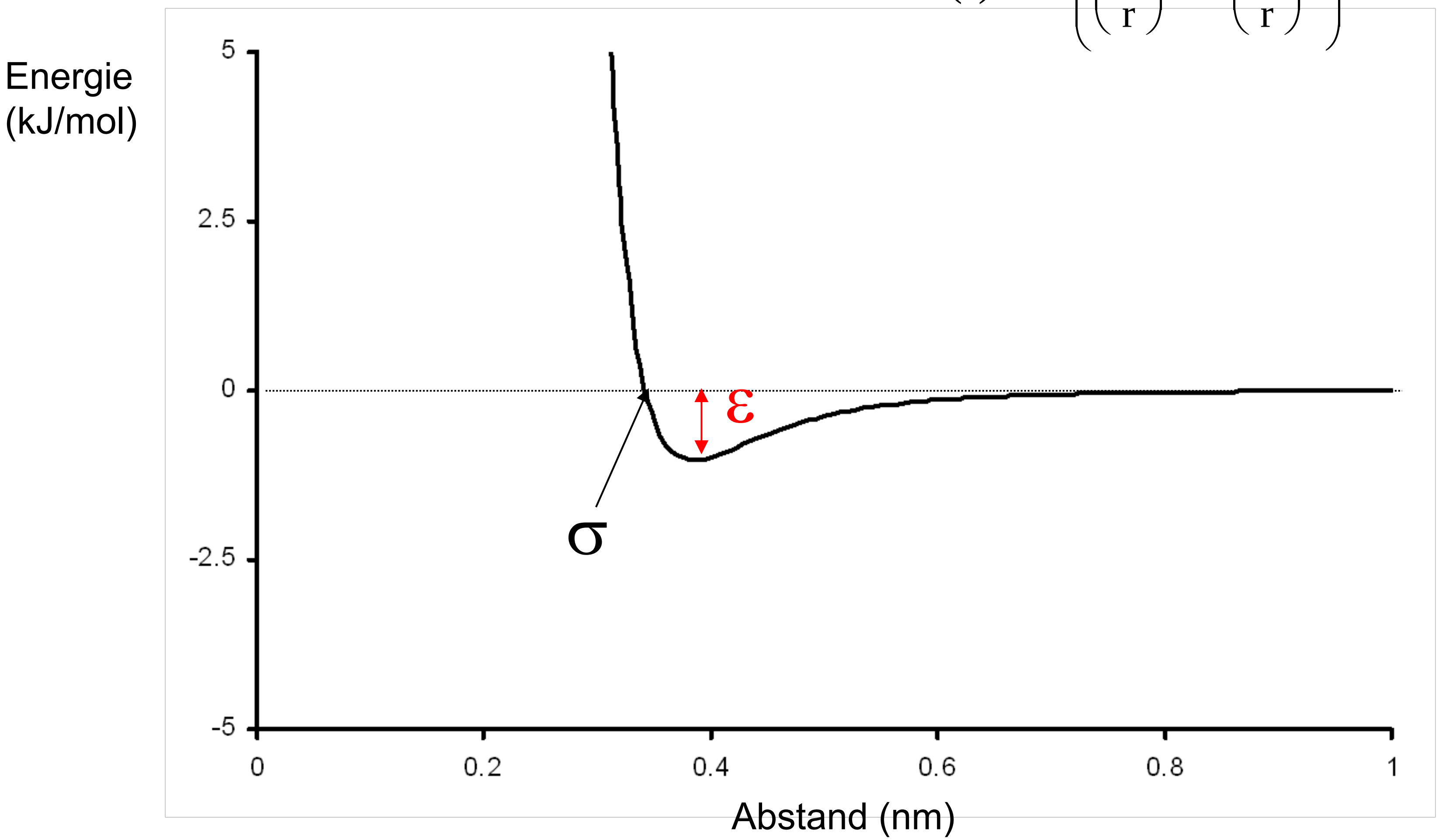
Lennard-Jones-Potential

$$V(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$



Lennard-Jones-Potential

$$V(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$



Lennard-Jones-Potential

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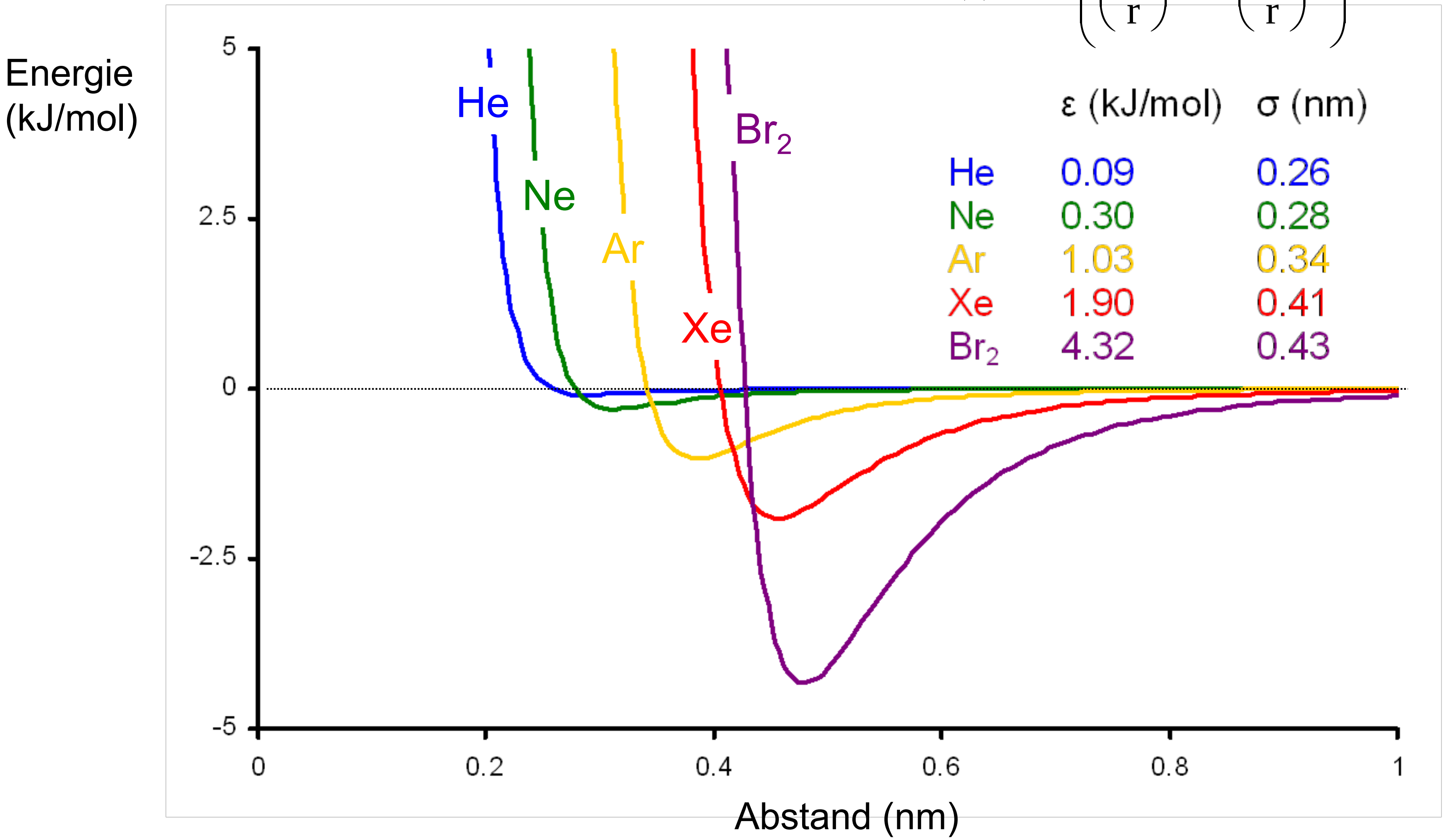
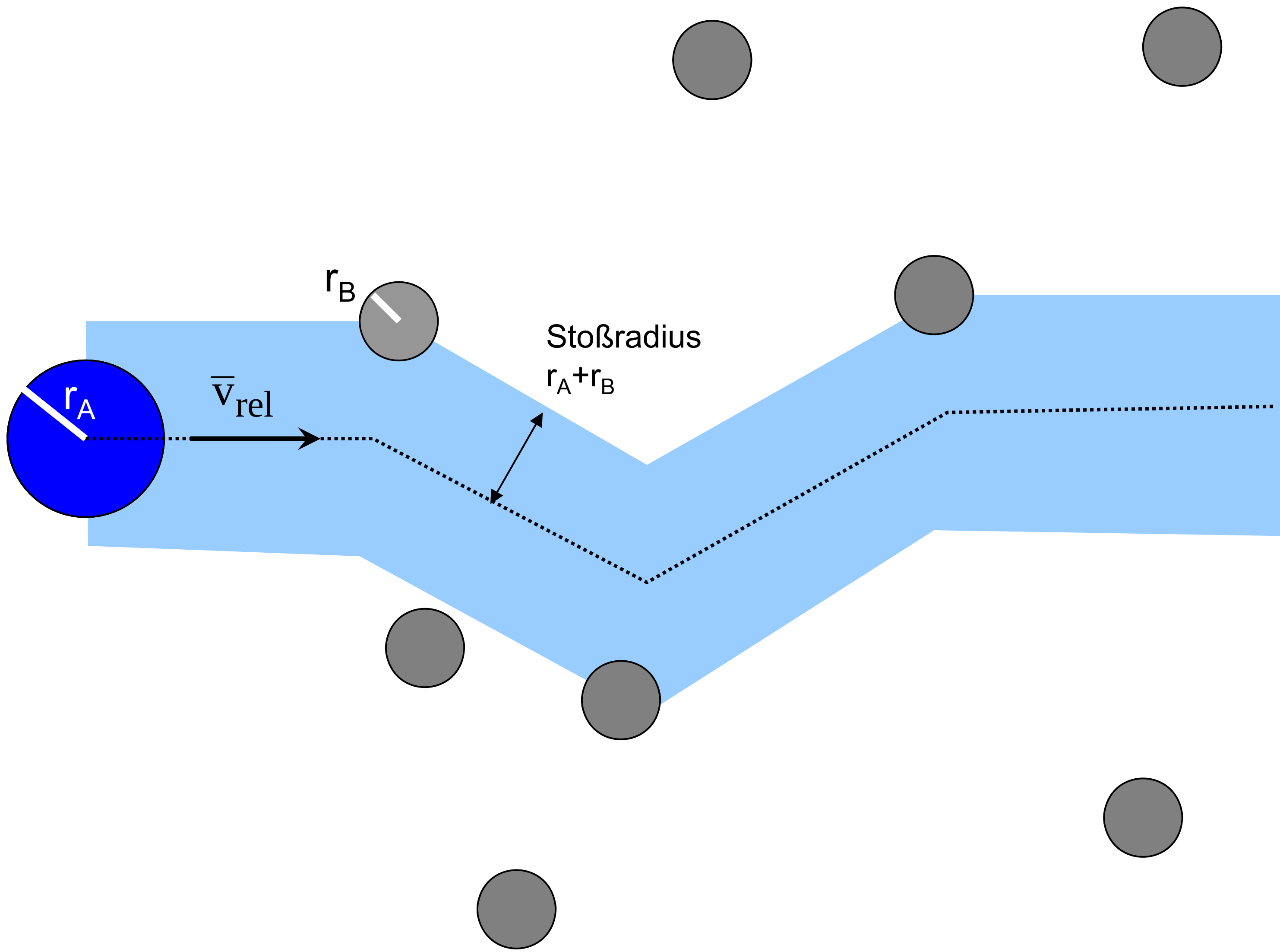
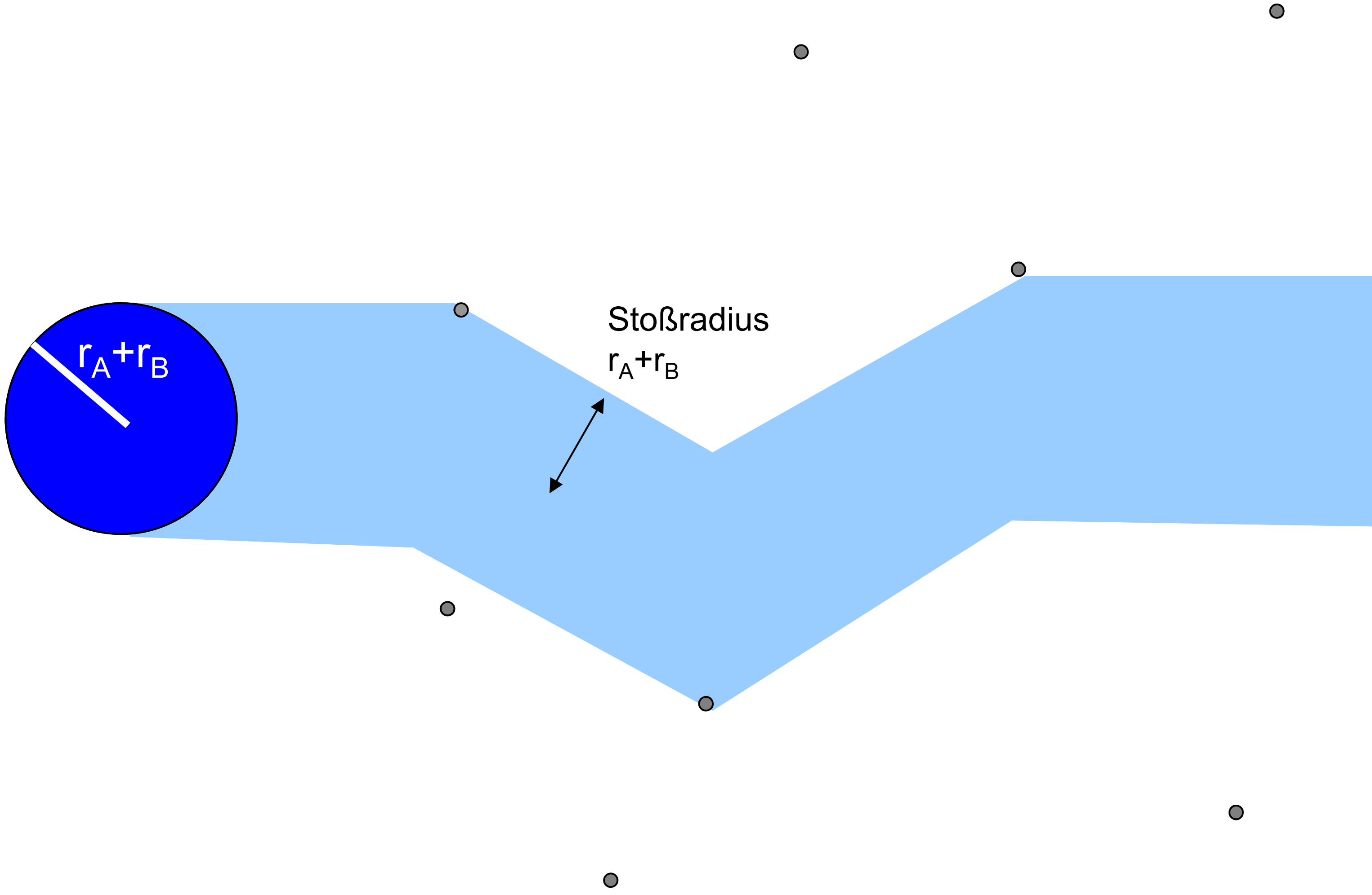


	ε (kJ/mol)	σ (nm)
He	0.09	0.26
Ne	0.30	0.28
Ar	1.03	0.34
Xe	1.90	0.41
Br_2	4.32	0.43



r_B
r_A
v̄_rel
Stoßradius
r_A+r_B



r_A+r_B
Stoßradius
r_A+r_B

Beispiel:

Luft (20% O_2, 80%N_2)

p= 1bar, T = 300K, v_{rel} = 630 m/s

Stoßquerschnitt 0.4 nm² $= \left(\pi \cdot r_{A\,B}{}^2\right)$

$$[O_2] = \frac{0.2}{25[\text{liter}/\text{mol}]} = 0.008\left[\frac{\text{mol}}{\text{l}}\right] = 8\left[\frac{\text{mol}}{\text{m}^3}\right]$$

$$[N_2] = \frac{0.8}{25[\text{liter}/\text{mol}]} = 0.032\left[\frac{\text{mol}}{\text{l}}\right] = 32\left[\frac{\text{mol}}{\text{m}^3}\right]$$

Stöße eines einzelnen N_2 mit O_2‘s pro Zeit:

$$z = [O_2] \cdot N_A \cdot \pi \cdot r_{AB}{}^2 \cdot |v_{rel}|$$

$$z = 8\left[\frac{\text{mol}}{\text{m}^3}\right] \cdot 6.022 \cdot 10^{23}\left[\frac{1}{\text{mol}}\right] 0.4 \cdot 10^{-18}\left[\text{m}^2\right] \cdot 630\left[\frac{\text{m}}{\text{s}}\right] = 1.2 \cdot 10^9\left[\frac{1}{\text{s}}\right]$$

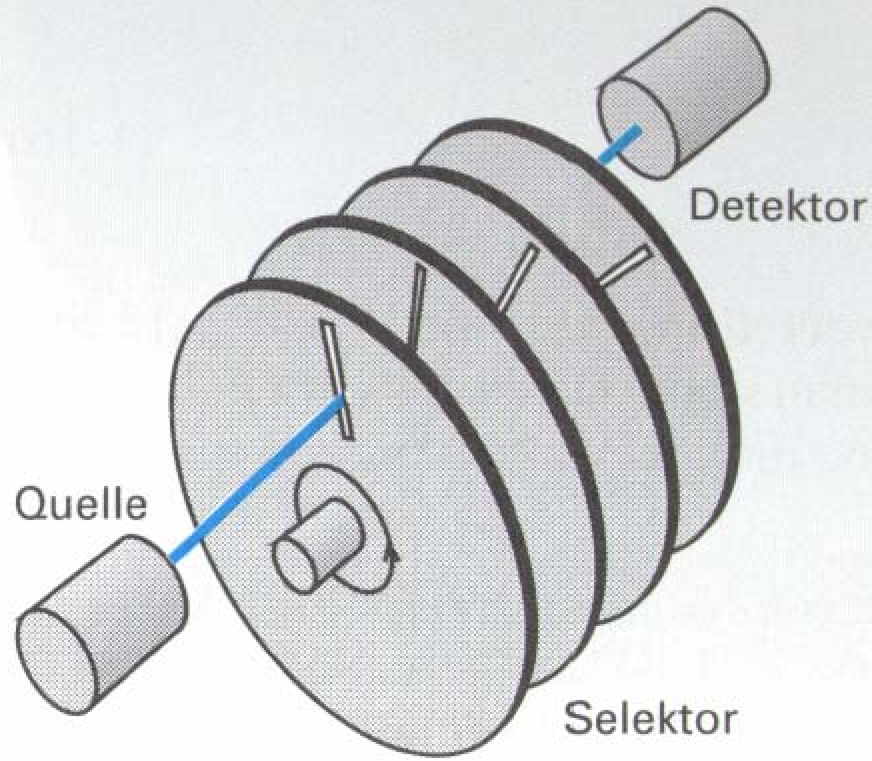
Gesamtzahl der Stöße aller N_2‘s mit allen O_2‘s (pro Volumen und Zeit)

$$\frac{Z_{AB}}{V} = z \cdot N_A [N_2]$$

$$\frac{Z_{AB}}{V} = 1.2 \cdot 10^9\left[\frac{1}{\text{s}}\right] \cdot 6.022 \cdot 10^{23}\left[\frac{1}{\text{mol}}\right] \cdot 0.032\left[\frac{\text{mol}}{\text{liter}}\right] = 2.3 \cdot 10^{31}\left[\frac{1}{\text{liter} \cdot \text{s}}\right]$$

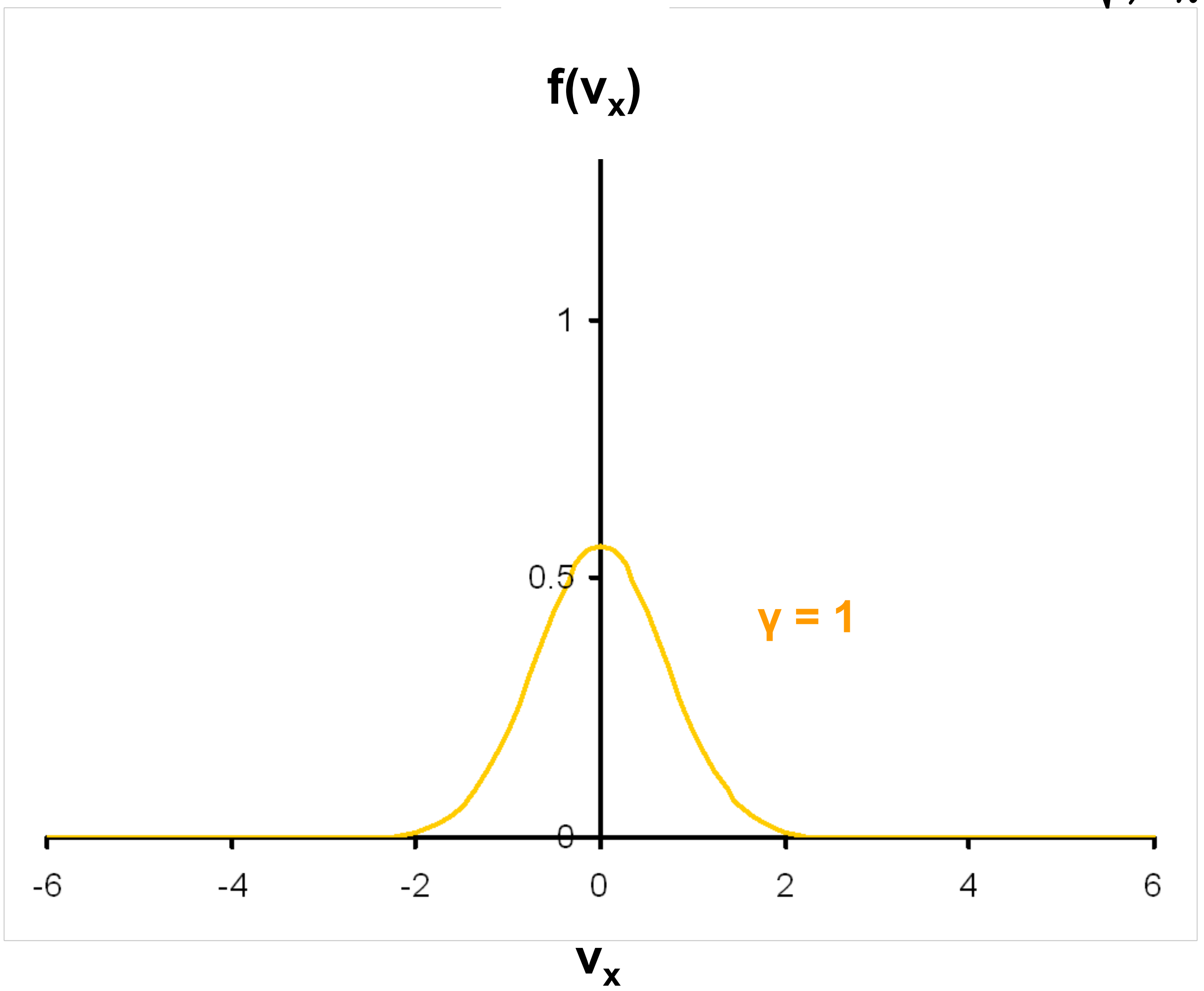
Experimentelle Bestimmung von Molekülgeschwindigkeiten

Abb. 1.14 Aufbau eines Geschwindigkeitsfilters. Die Moleküle verlassen die Quelle (Heizgerät oder kleine Öffnung in einer Wand) in Form eines Strahls und bewegen sich auf die rotierenden Scheiben zu. Nur Moleküle mit einer bestimmten Geschwindigkeit erreichen den Detektor durch alle Schlitze hindurch; diese Geschwindigkeit ist proportional zur Rotationsgeschwindigkeit der Scheiben.

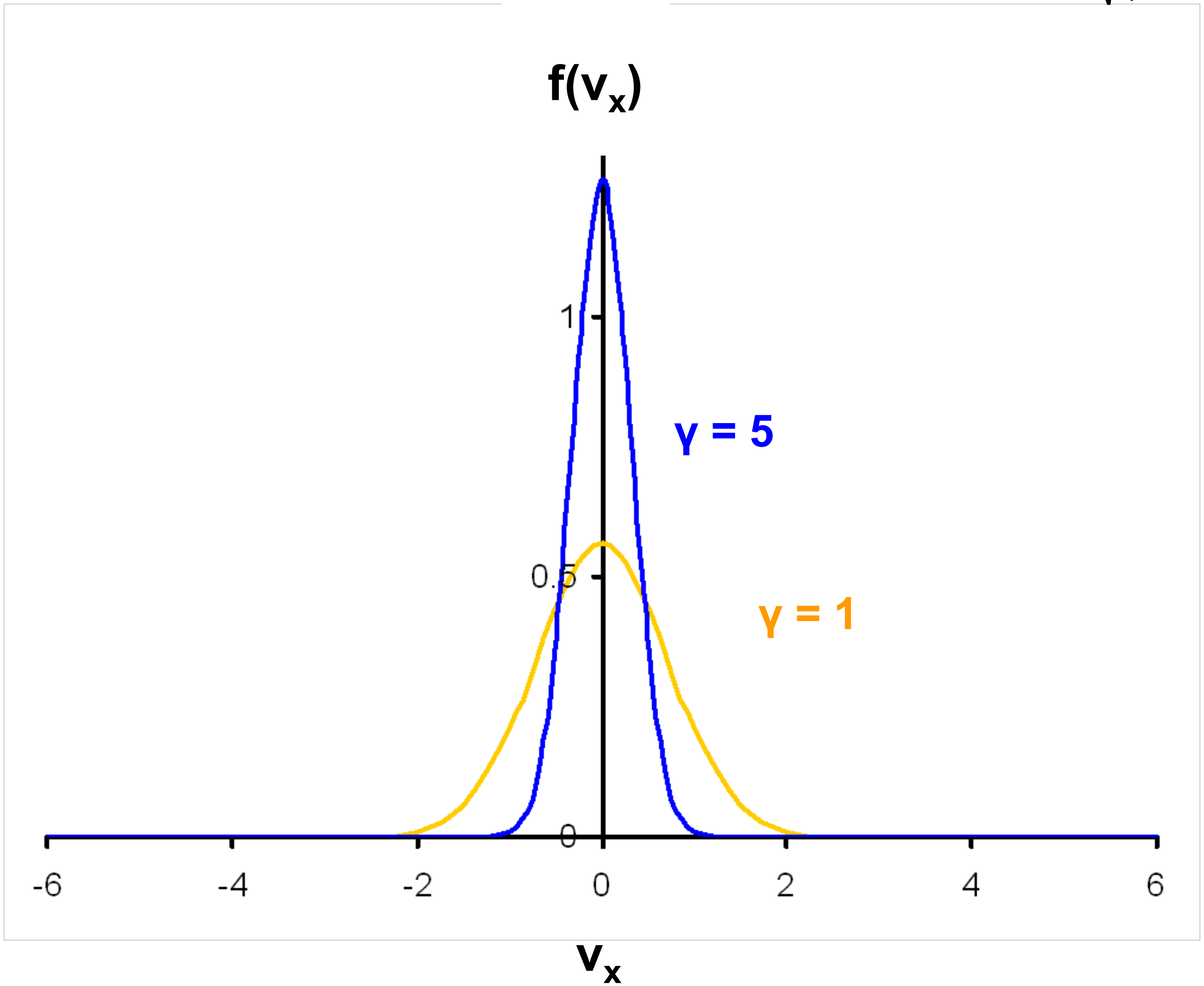


Quelle: Atkins, 3. Aufl.

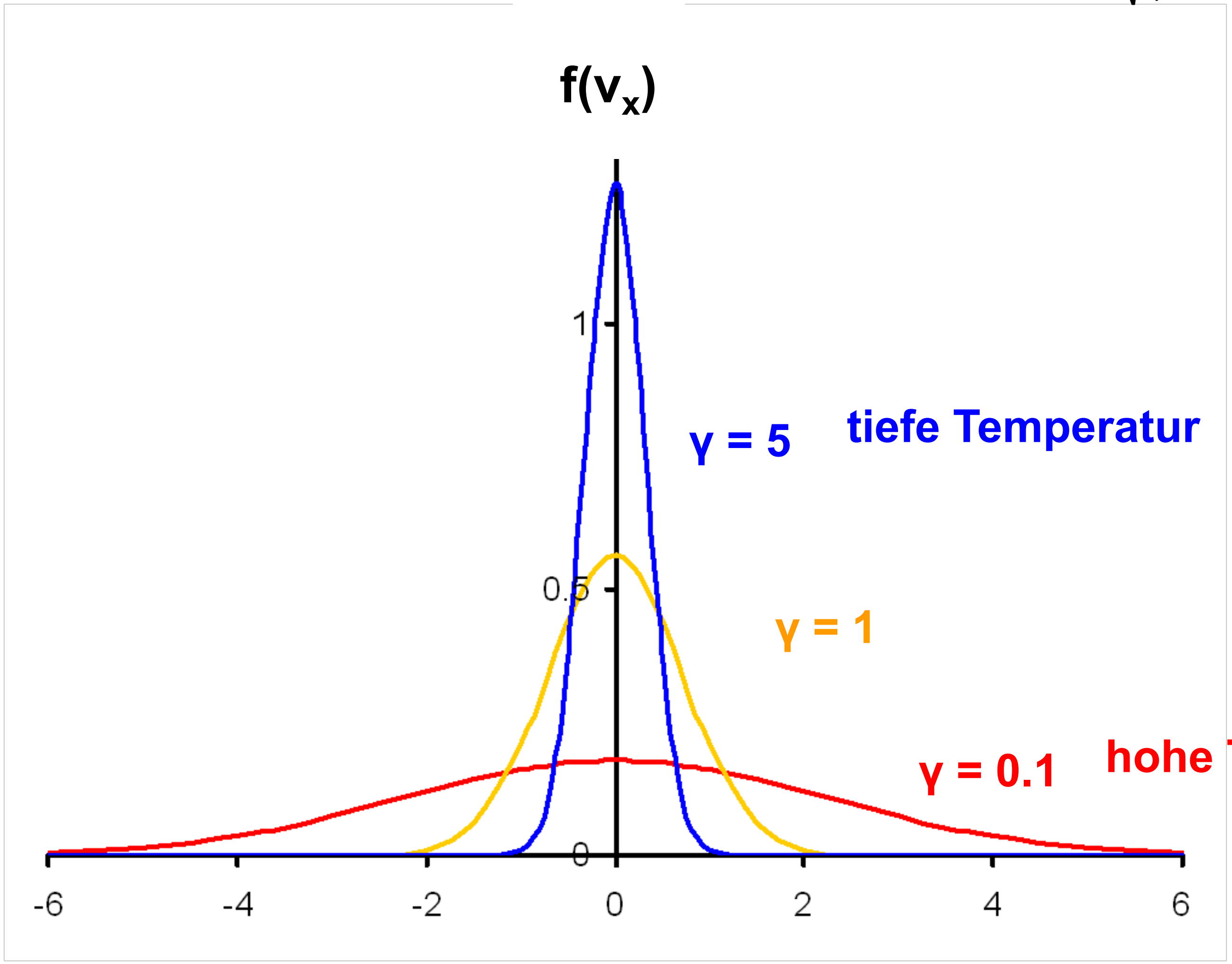
$$f(v_x) = \sqrt{\gamma / \pi} \cdot e^{-\gamma v_x{}^2}$$



$$f(v_x) = \sqrt{\gamma/\pi} \cdot e^{-\gamma v_x{}^2}$$



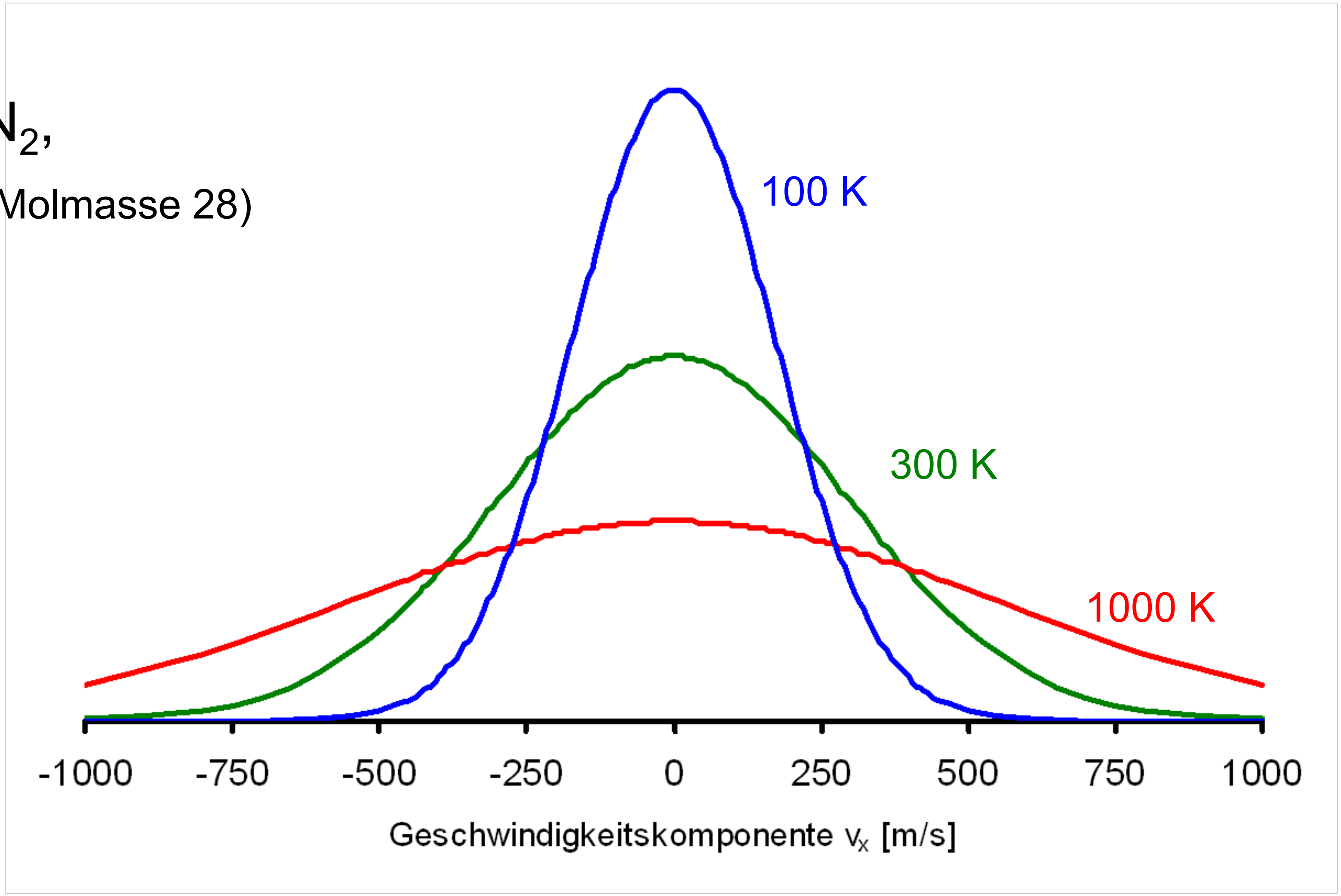
$$f(v_x) = \sqrt{\gamma/\pi} \cdot e^{-\gamma v_x^2}$$



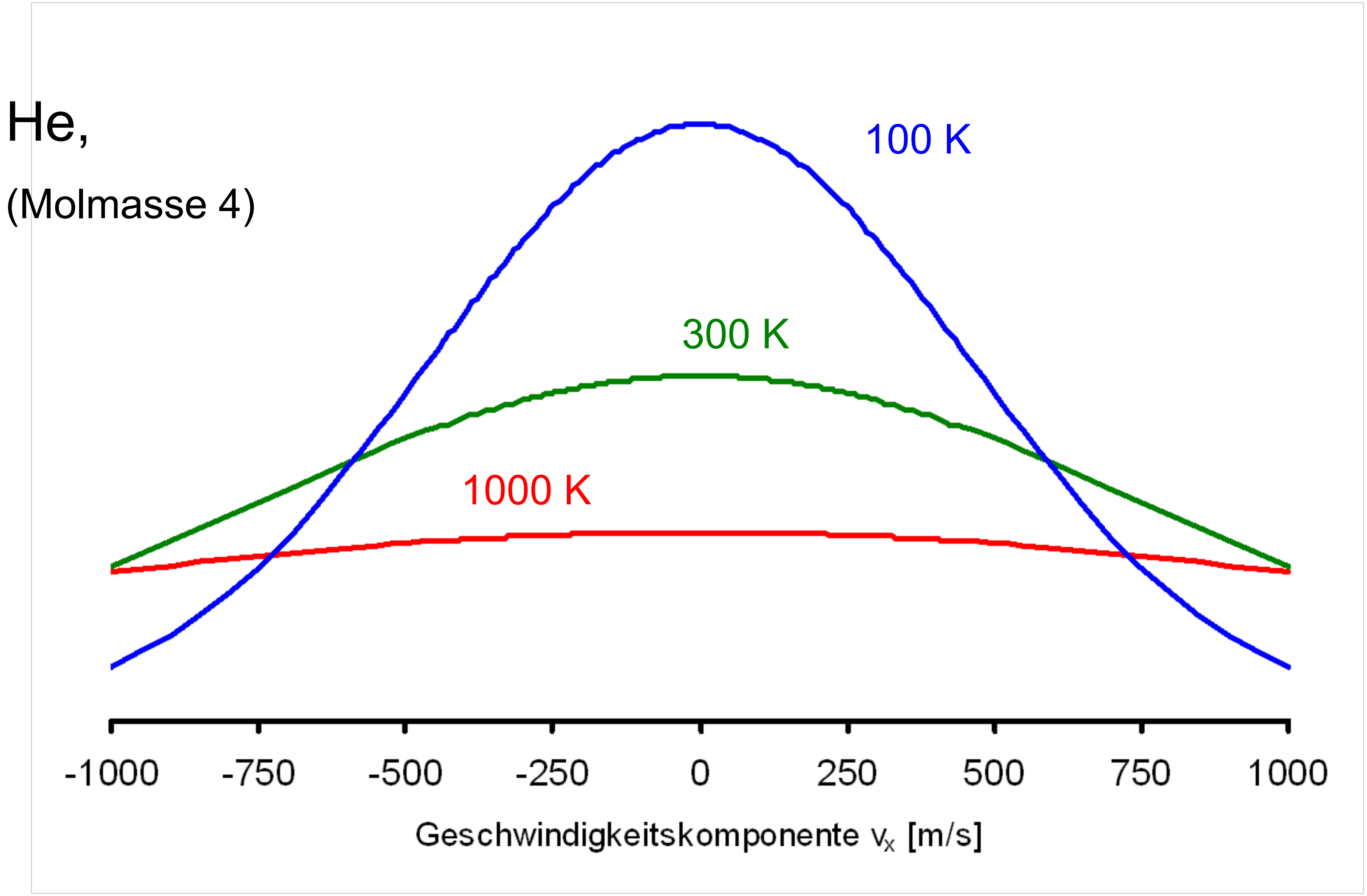
v_x

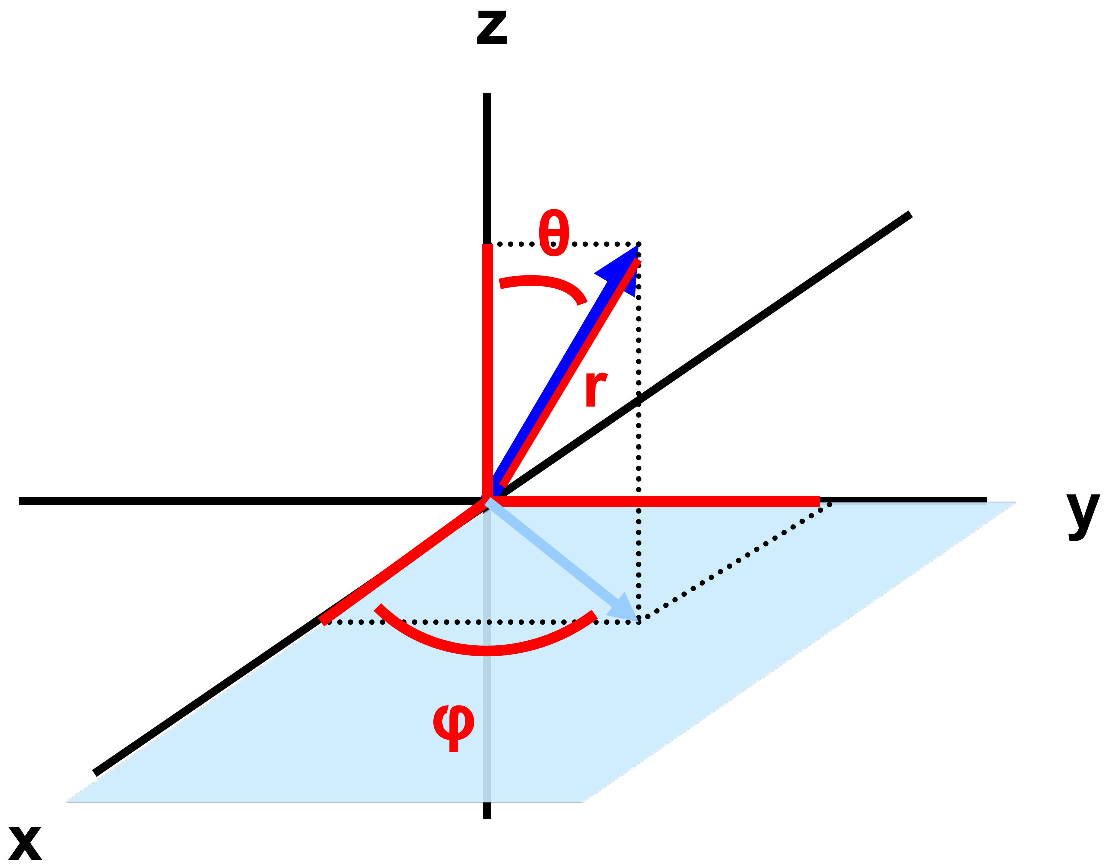
Geschwindigkeitskomponente in x- Richtung

Eindimensionale Maxwell-Boltzmann-Geschwindigkeitsverteilung



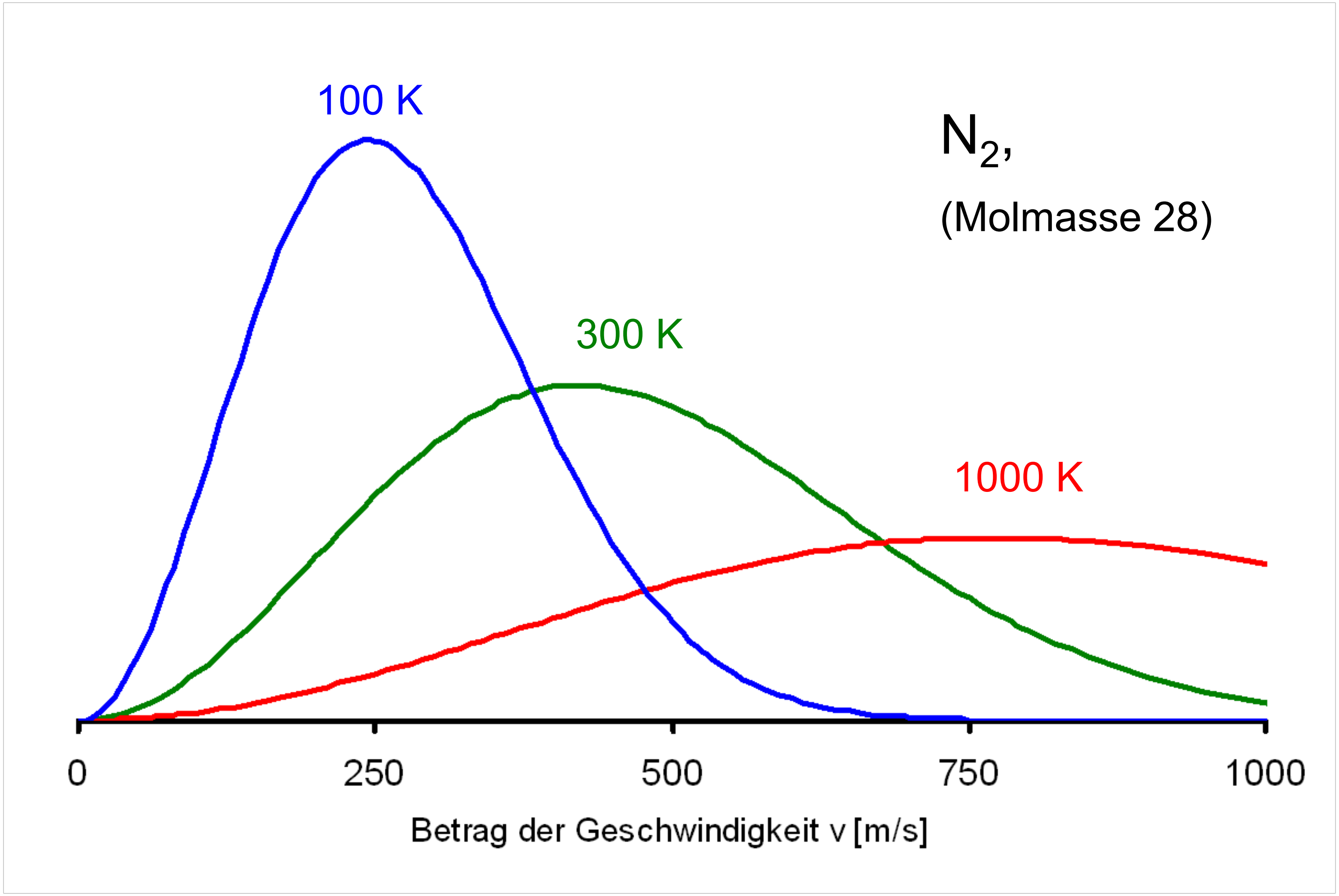
Eindimensionale Maxwell-Boltzmann-Geschwindigkeitsverteilung



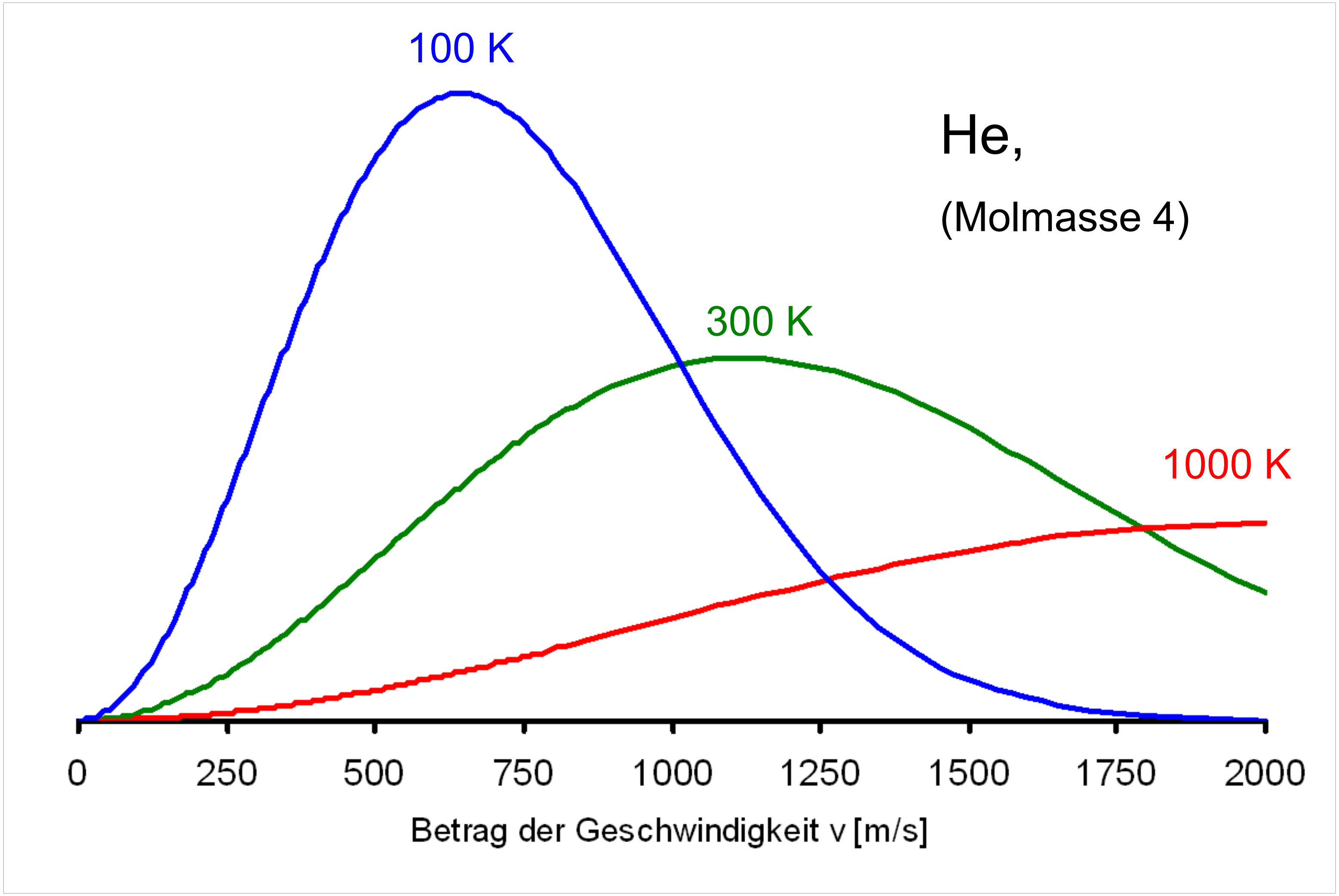


z
θ
r
y
φ
x

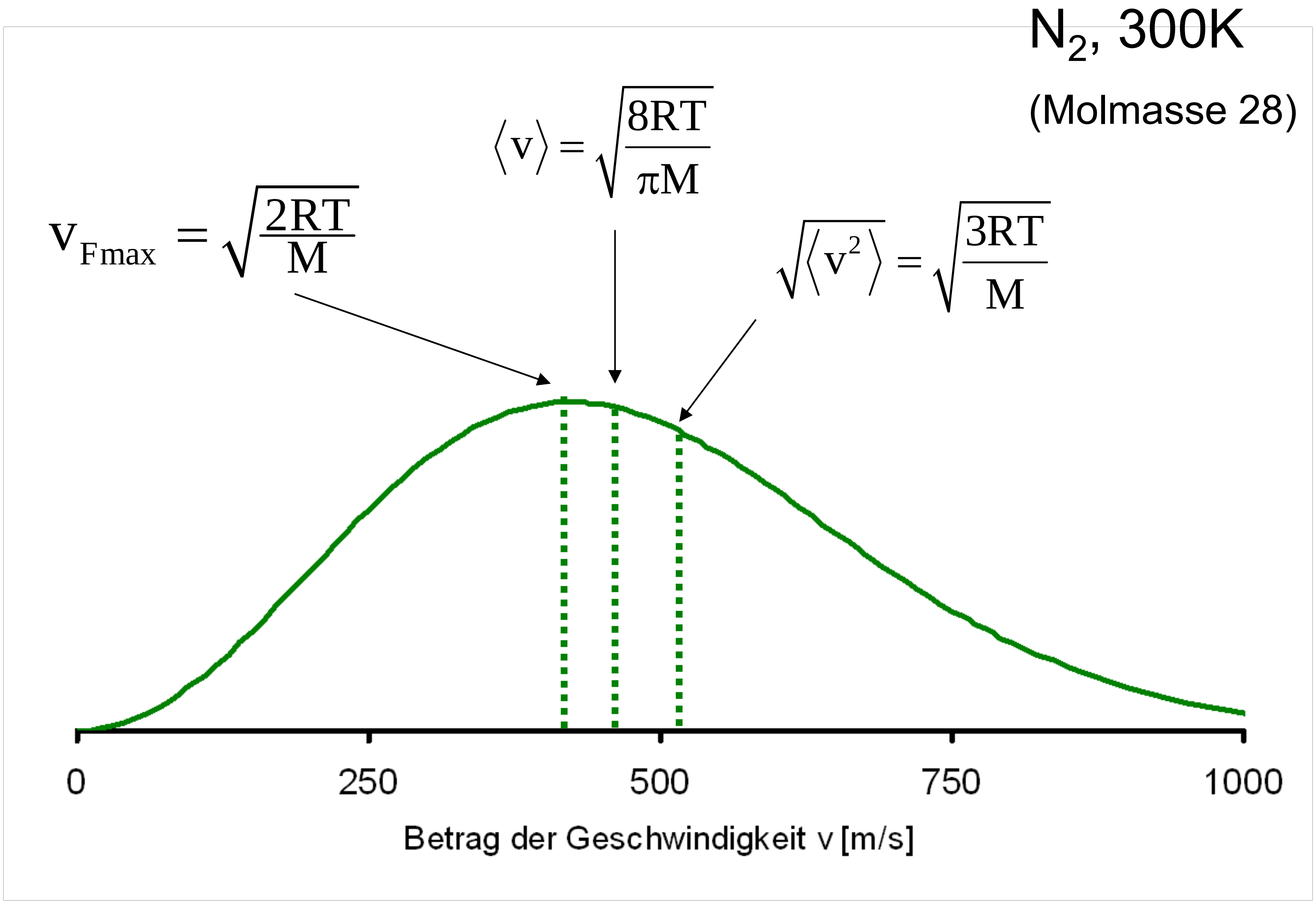
Dreidimensionale Maxwell-Boltzmann-Geschwindigkeitsverteilung



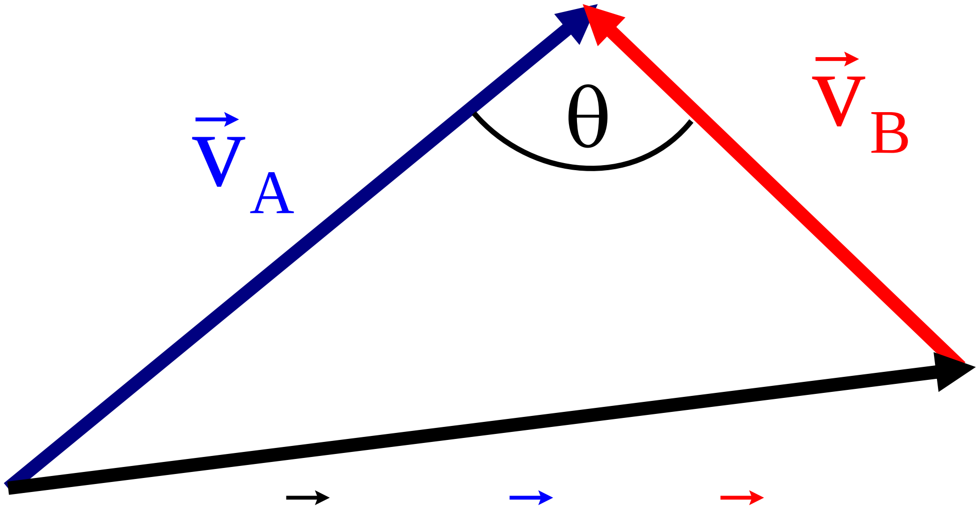
Dreidimensionale Maxwell-Boltzmann-Geschwindigkeitsverteilung



Wahrscheinlichste, Mittlere, Mittlere Quadratische Geschwindigkeit



Relativgeschwindigkeit



$$\vec{v}_R = \vec{v}_A - \vec{v}_B$$

$$\left|\vec{v}_R\right| = \sqrt{\left|\vec{v}_A\right|^2 + \left|\vec{v}_B\right|^2 - 2\left|\vec{v}_A\right| \cdot \left|\vec{v}_B\right| \cdot \cos\theta}$$