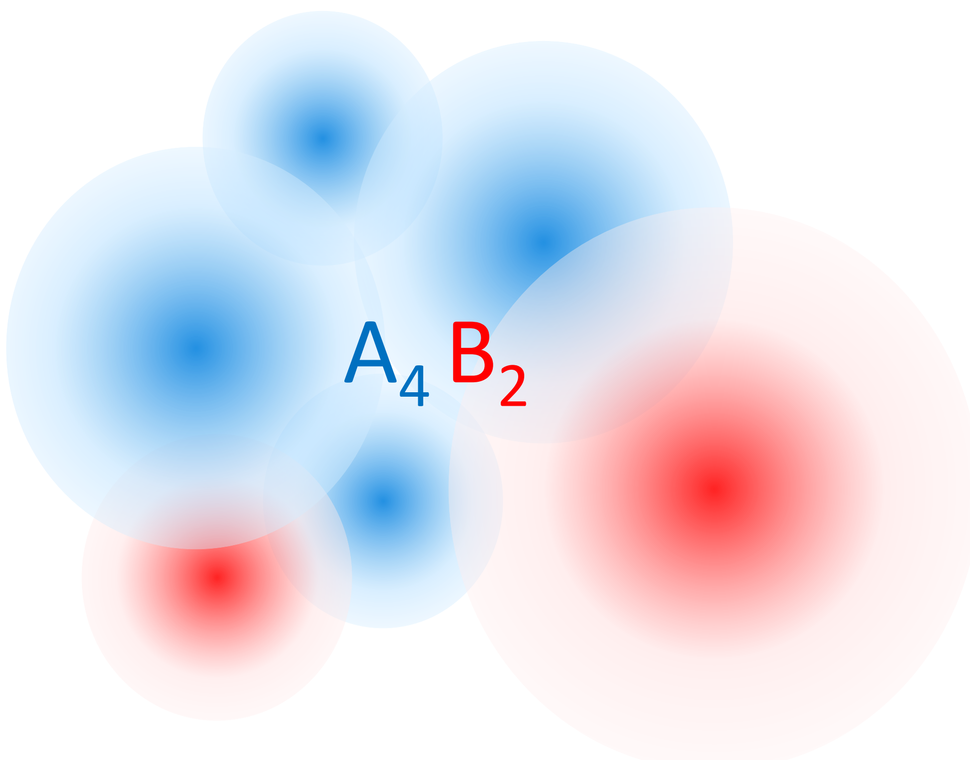
Kvantne Monte Carlo simulacije

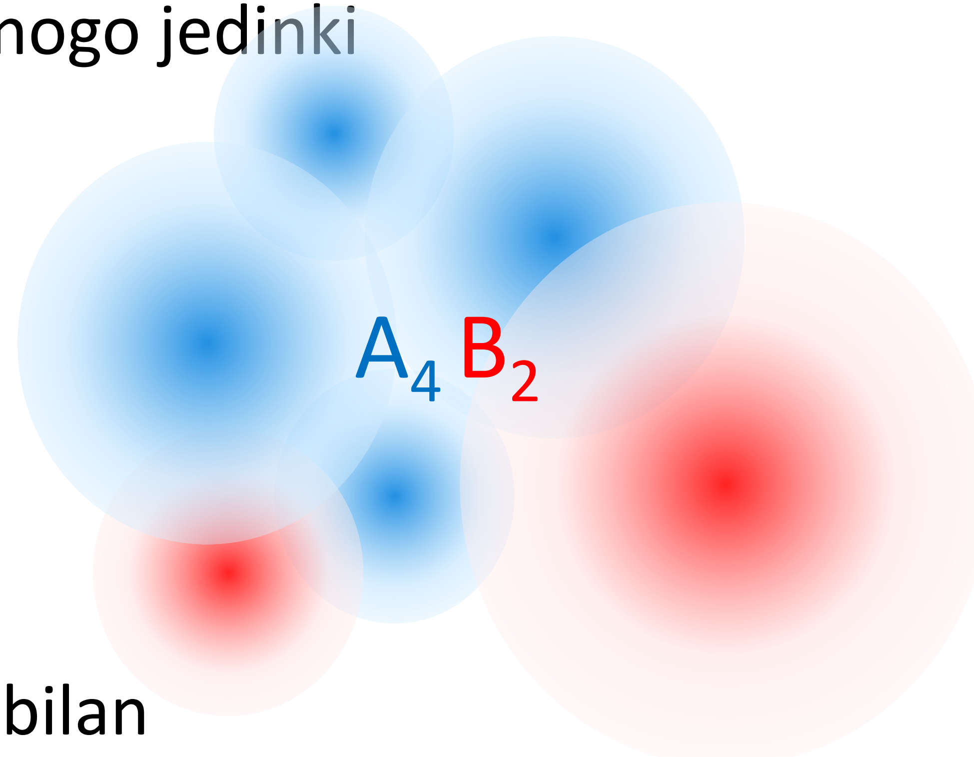
~ Petar Stipanović ~



Split, 06. 06. 2022.

≫ UVOD: Klasteri

- klasteri: agregati konačno mnogo jedinki
  - dimer A_2
  - trimer A_3
  - tetramer A_4
  - pentamer A_4B
  - …

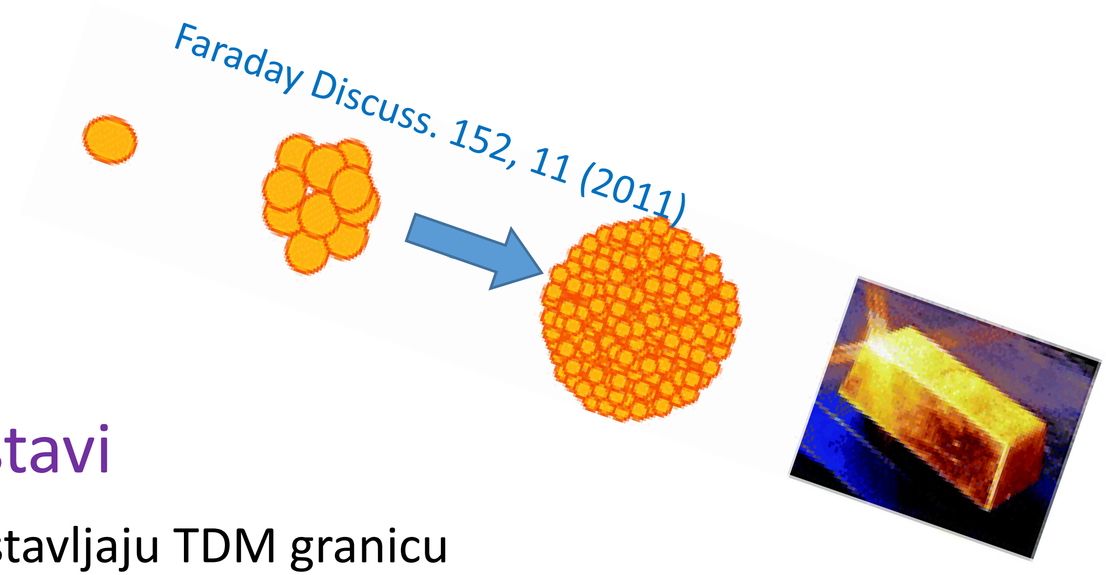


- E<0 – sustav: vezan, metastabilan
- proučavani su eksperimentalno i teorijski
- kvantni klasteri - kvantni tretman
  - tuneliranje
  - nulto gibanje
  - kvantizacija…

≫ UVOD: Klasteri

- klasteri - prijelazne forme materije

↓



- *bulk* sustavi
  - ✓ predstavljaju TDM granicu

$$N, V \to \infty$$
$$\frac{N}{V} = \text{const.}$$

- iste ih veze drže na okupu
  - van der Waalsova nama ovdje interesantna

UVOD: Klasteri

- konačan broj atoma
  - uzrok razlike
  - velik udio površinskih atoma
  - nova stanja
  - dodavanje atoma – karakteristike
  - nejednoliki prijelaz
  - magični brojevi
- klasteri se ponašaju uglavnom slično krutinama
  - iznimke:
    - He
    - H↓
    - …

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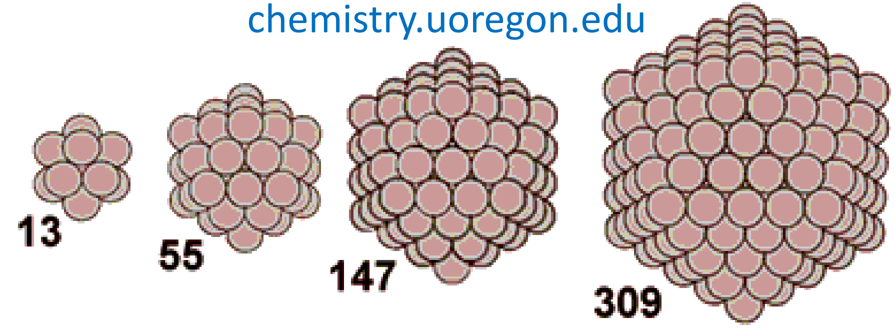
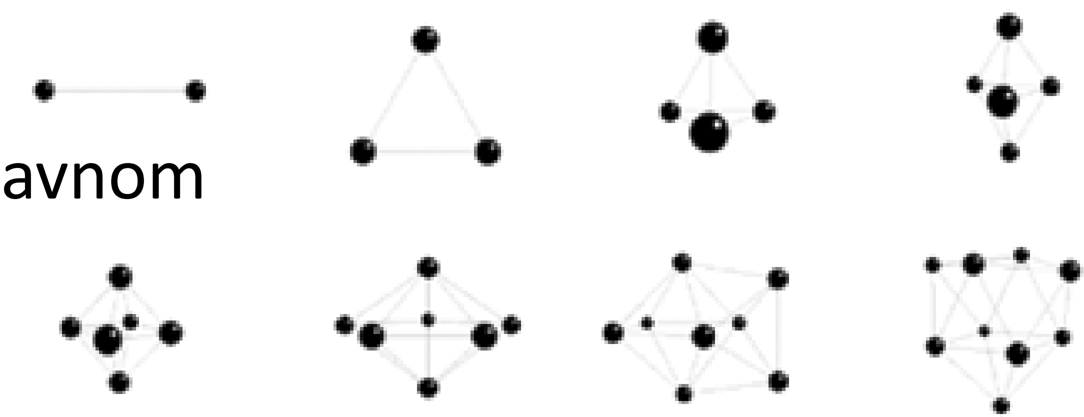
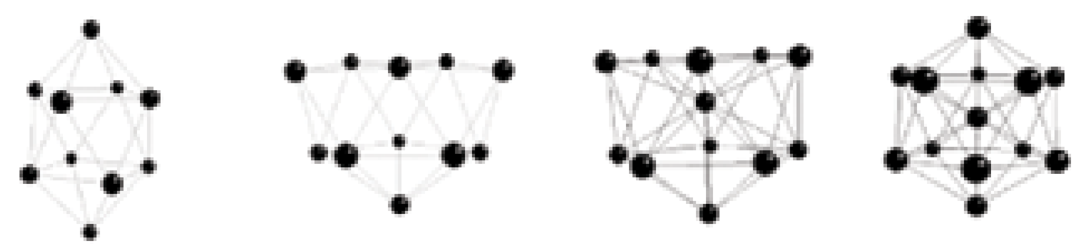


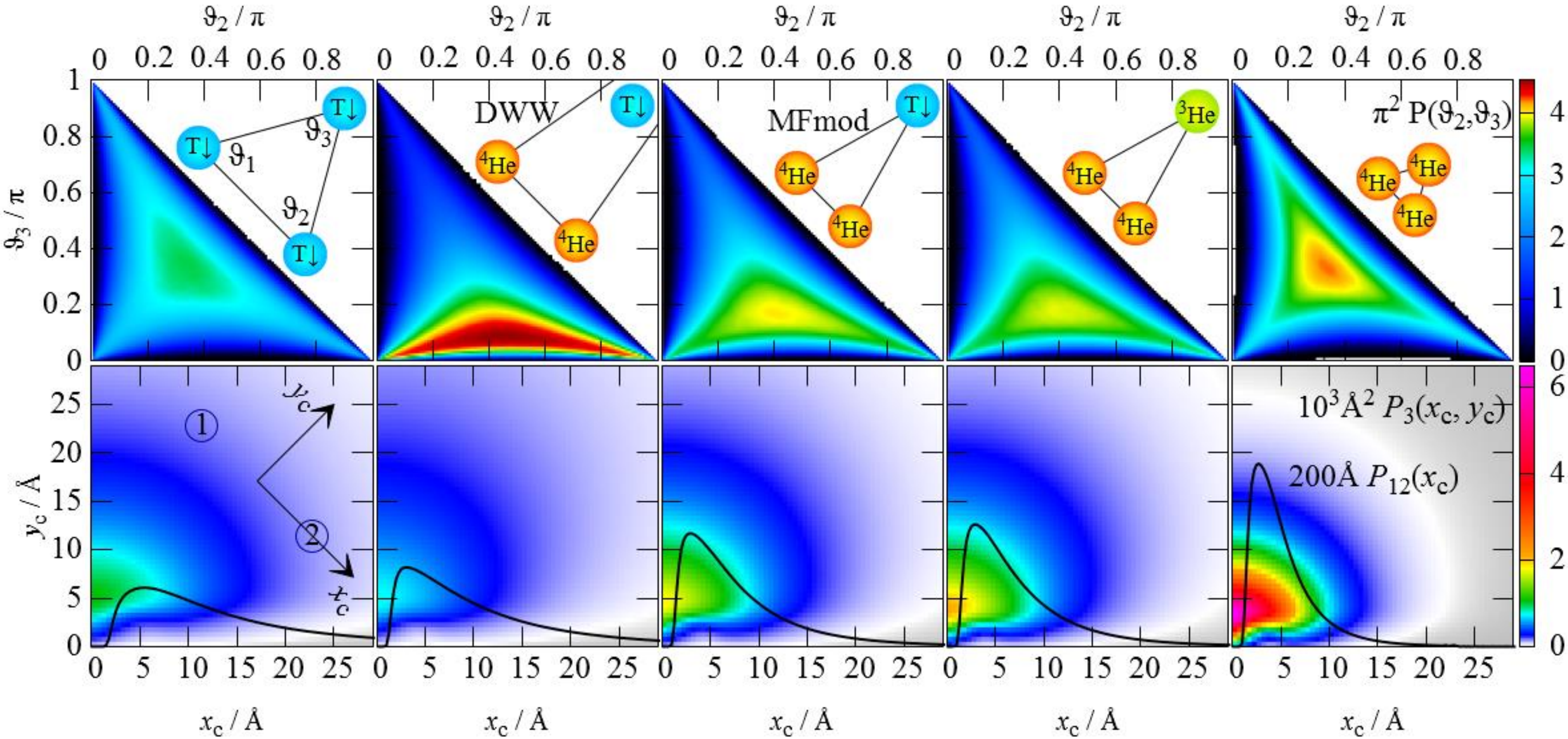


Braz. J. Phys. 36, 720 (2006)



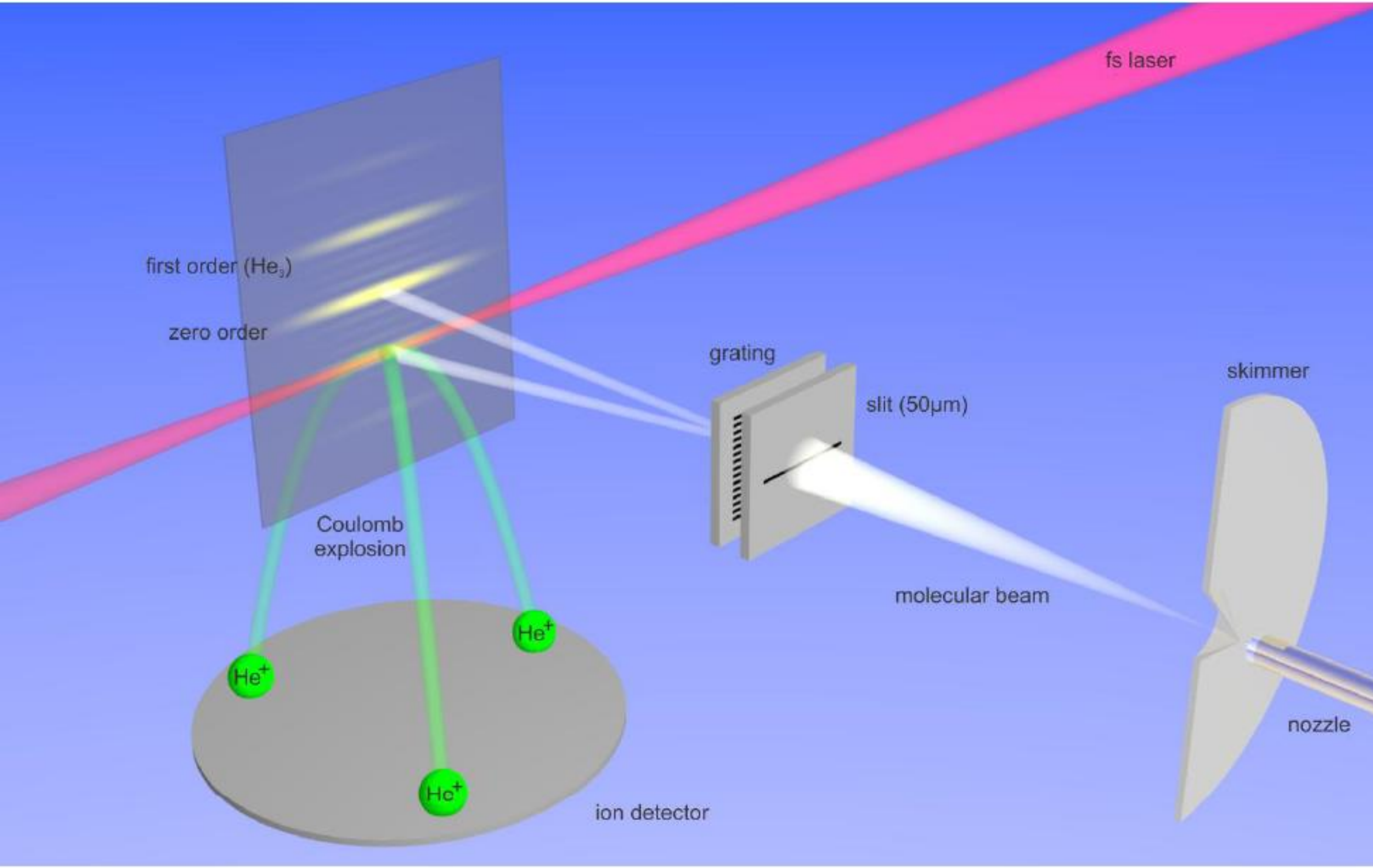
≫ Proučavani – računalnim eksperimentima

- razne distribucijske funkcije



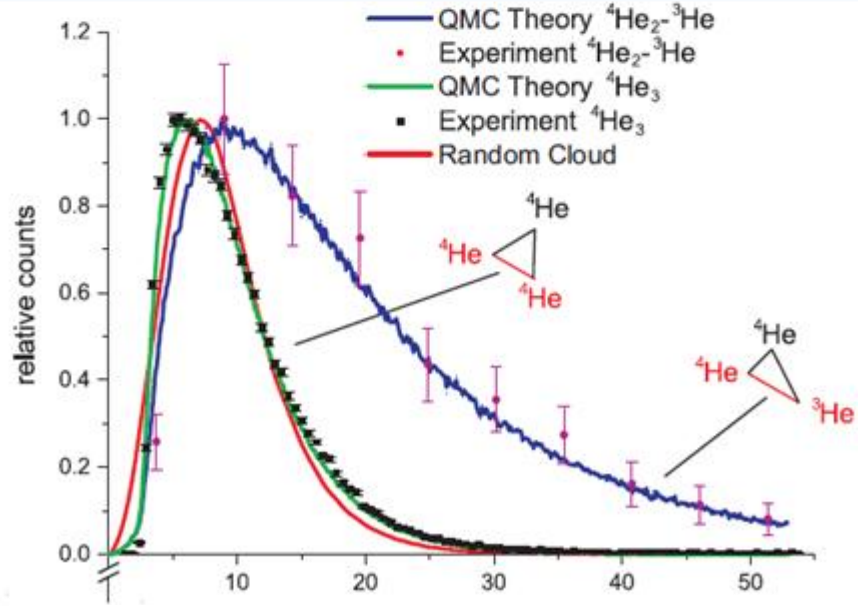
Više u: *Physical Review Letters*. **113** (2014)

≫ Proučavani - eksperimentalno

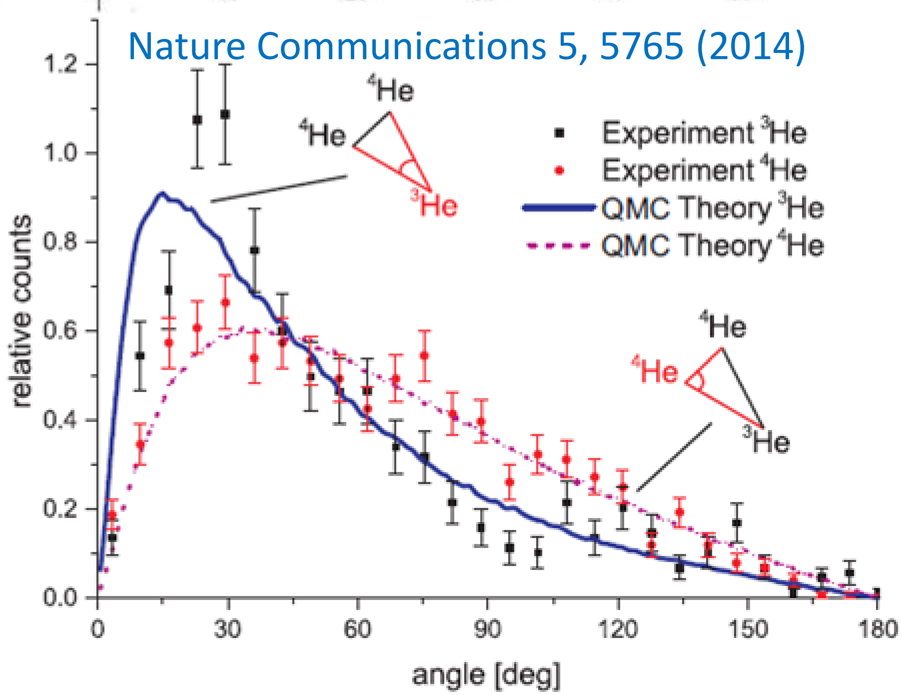


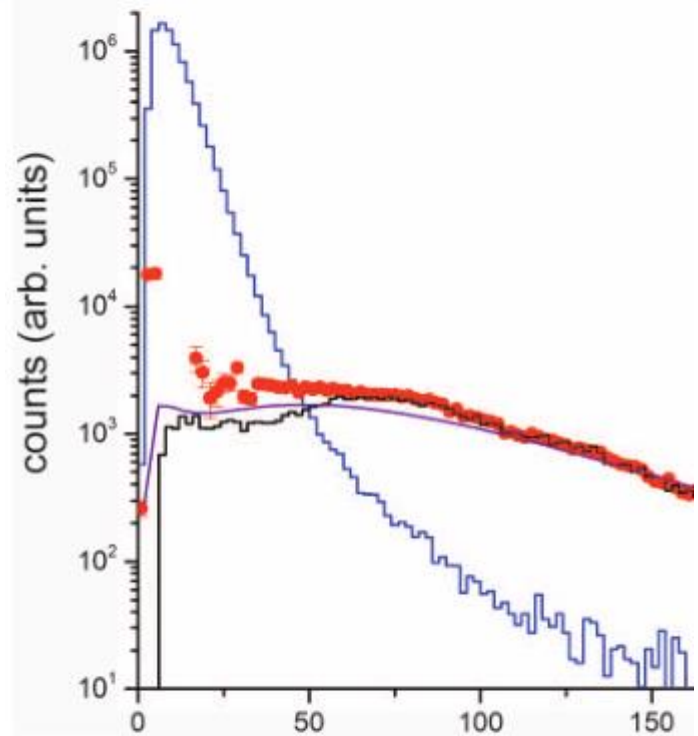
Maksim Kunitski *et al.*, Science **348**, 551 (2015)

≫ Struktura – eksperimenti



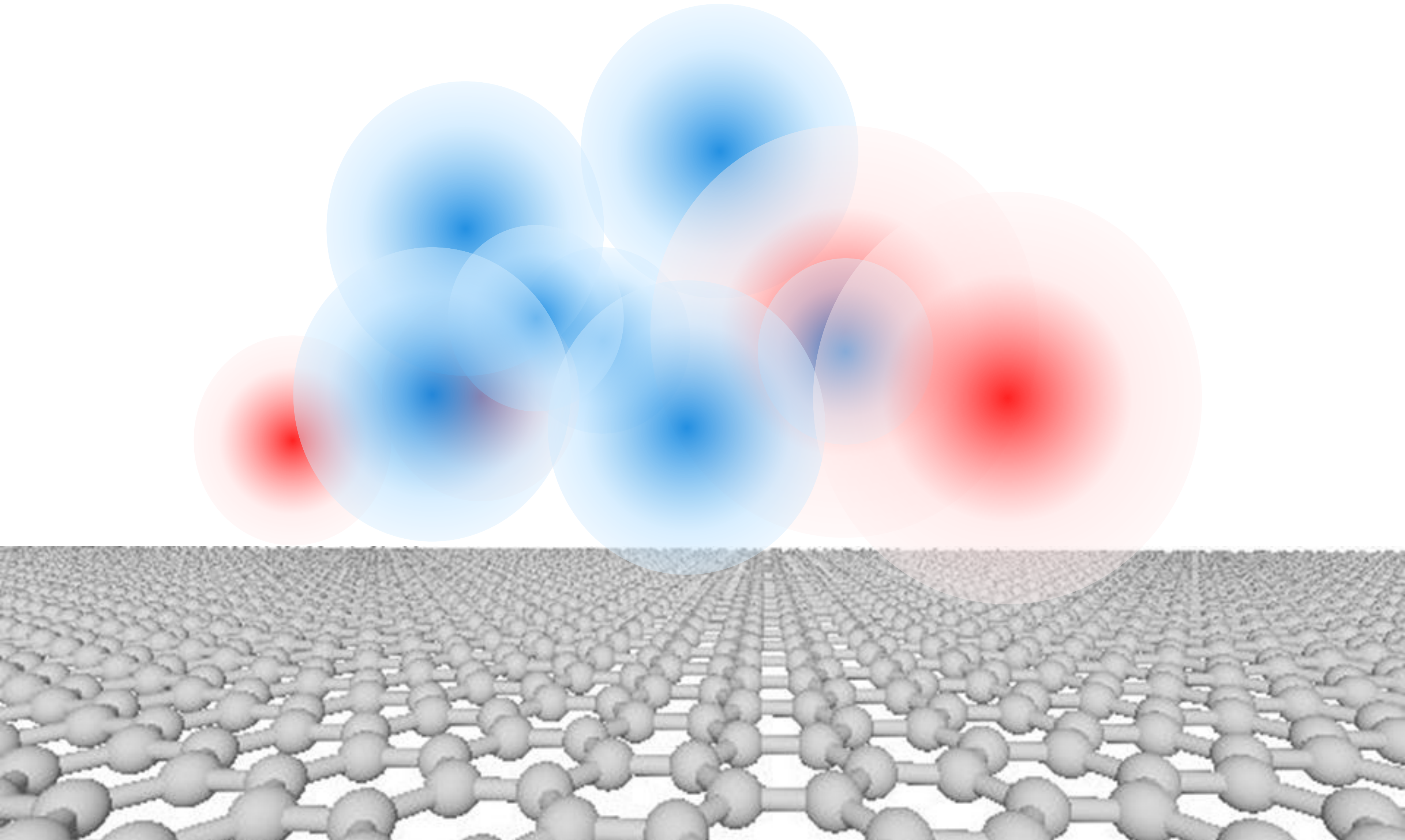
Nature Communications 5, 5765 (2014)





Maksim Kunitski *et al.*, Science **348**, 551 (2015)

VMC i DMC metoda



≫ METODE: VMC

- varijacijski teorem

$$E_0 \leq \int \psi^*(\vec{R})\mathcal{H}\psi(\vec{R})\mathrm{d}\vec{R} \qquad \vec{R} = (\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_\mathrm{a}})$$

- Hamiltonijan

$$\mathcal{H} = \mathcal{T} + \mathcal{V} \equiv -D_{\vec{R}}\nabla^2_{\vec{R}} + V(\vec{R}) \qquad D_i = \hbar^2/(2m_i)$$

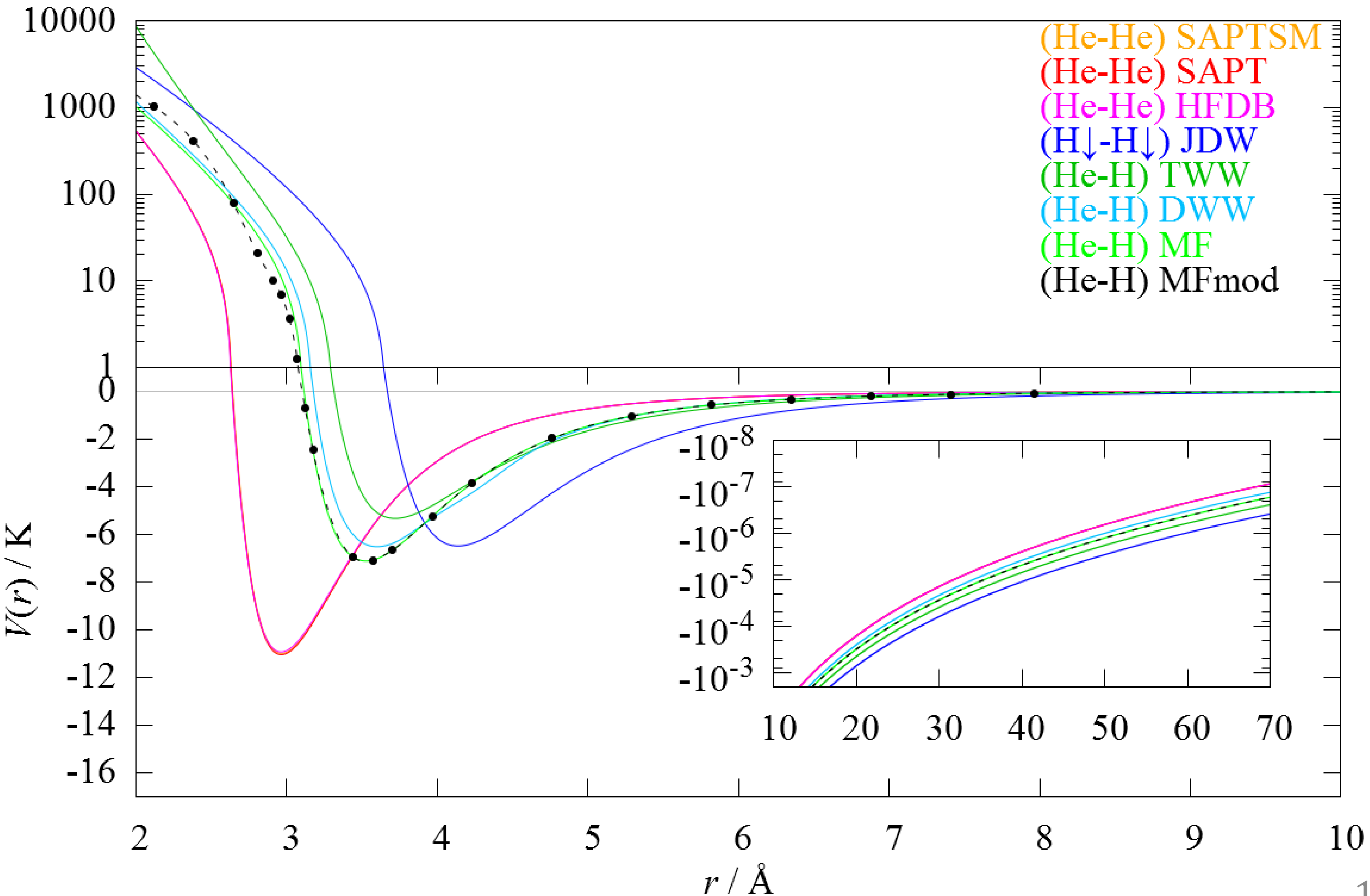
$$\equiv -\sum_{i=1}^{N_\mathrm{a}} D_i \nabla_i^2 + \sum_{i<j=1}^{N_\mathrm{a}} V_{ij}(r_{ij}) + \sum_{i=1}^{N_\mathrm{a}} V_\mathrm{p}(\vec{r}_i)$$

- prilagodba integrala za Metropolisov algoritam

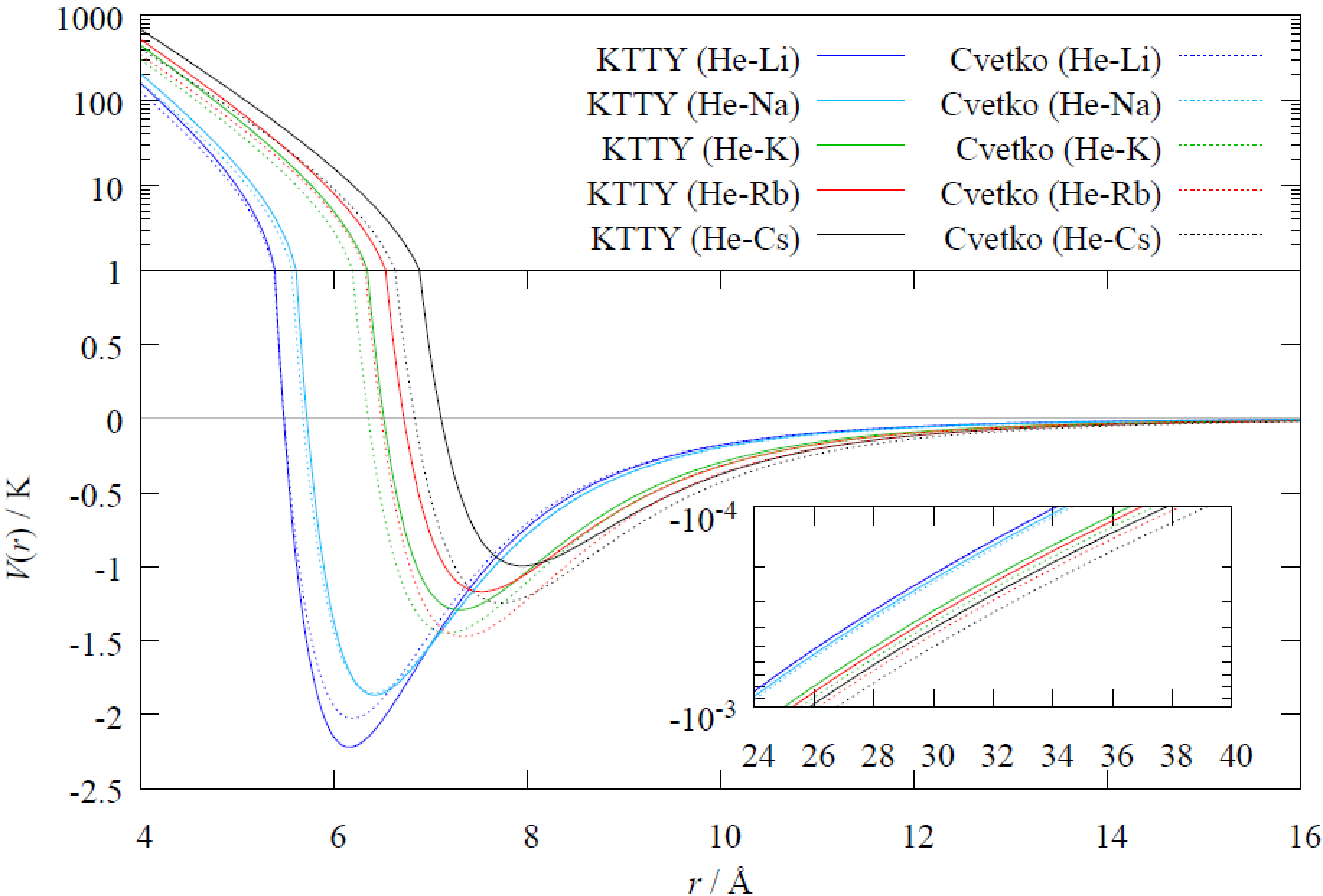
$$E_\mathrm{VMC}[\psi] = \int \psi^*(\vec{R})\mathcal{H}\psi(\vec{R})\mathrm{d}\vec{R} = \int \psi^*(\vec{R})\psi(\vec{R}) \left[\frac{\mathcal{H}\psi(\vec{R})}{\psi(\vec{R})}\right] \mathrm{d}\vec{R}$$

$$\equiv \int \psi^*(\vec{R})\psi(\vec{R}) \left[E_\mathrm{L}(\vec{R})\right] \mathrm{d}\vec{R}$$

» METODA: Potencijali



≫ METODA: Potencijali



≫ METODA: ψ u slobodnom prostoru

- probne valne funkcije

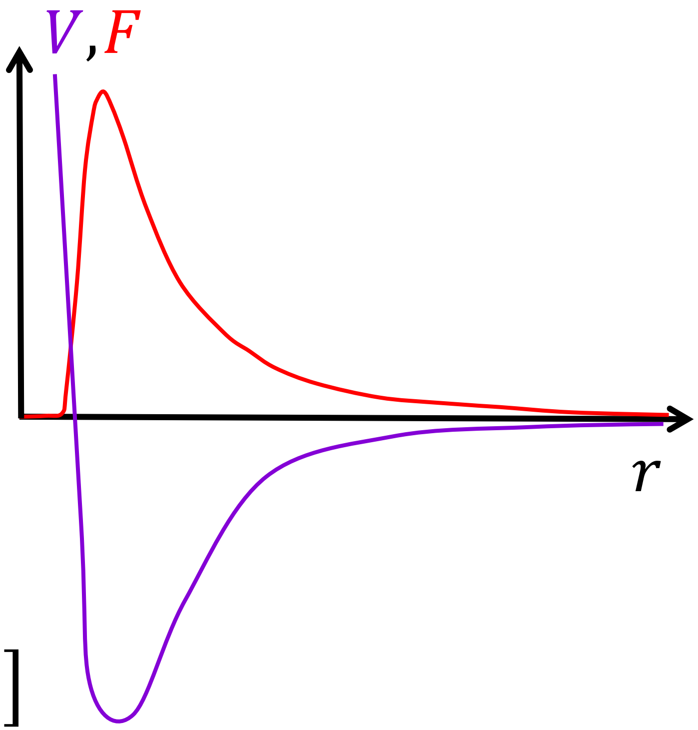
$$\psi(\vec{R}) = \prod_{i<j=1}^{N+M} F_{ij}(r_{ij})$$

- različiti oblici korelacijskih funkcija

$$F_{ij}(r_{ij}) = \exp\left[-\left(\frac{b_{ij}}{r_{ij}}\right)^5 - s_{ij}r_{ij}\right]$$

$$F_{ij}(r_{ij}) = \exp\left[-(\alpha_{ij}/r_{ij})^{\gamma_{ij}} - s_{ij}r_{ij}\right]/r_{ij}$$

$$F_{ij}(r_{ij}) = \exp[-a_{ij}\exp(-b_{ij}r_{ij}) - s_{ij}r_{ij}]$$

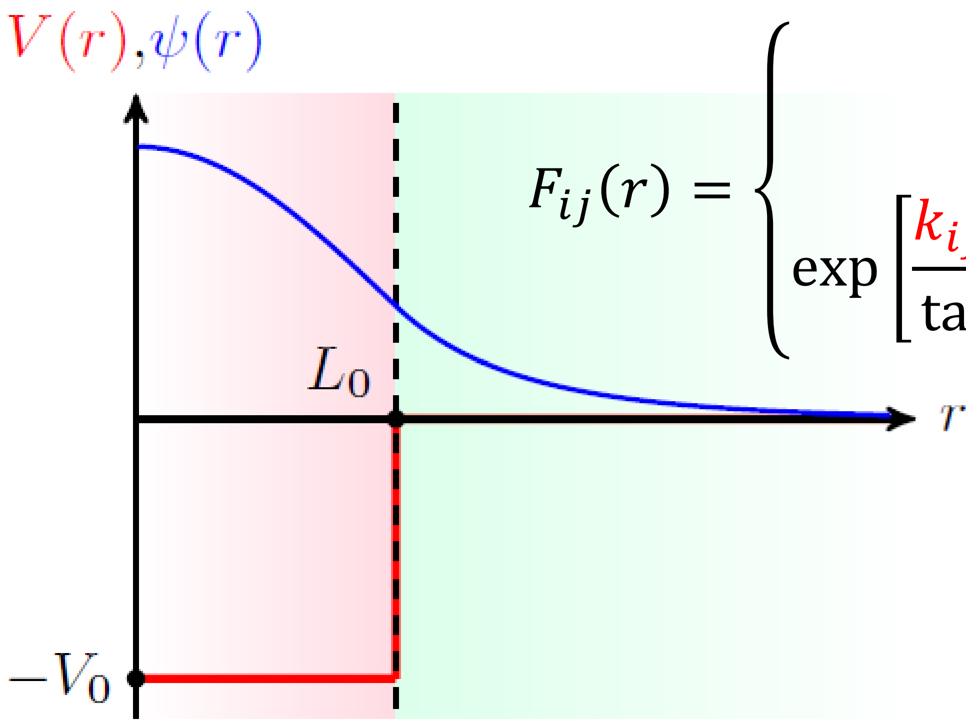


≫ METODA: ψ u slobodnom prostoru

- dvočestične korelacijske funkcije optimalne za male klastere

$$F_{ij}(r_{ij}) = \exp\left[-(\alpha_{ij}/r_{ij})^{\gamma_{ij}} - s_{ij}r_{ij}\right]/r_{ij}$$

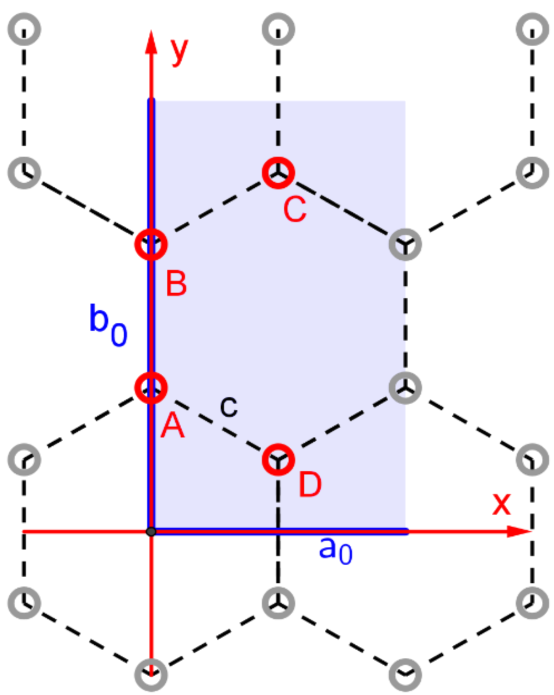
- dvočestične korelacijske funkcije za modele klastera

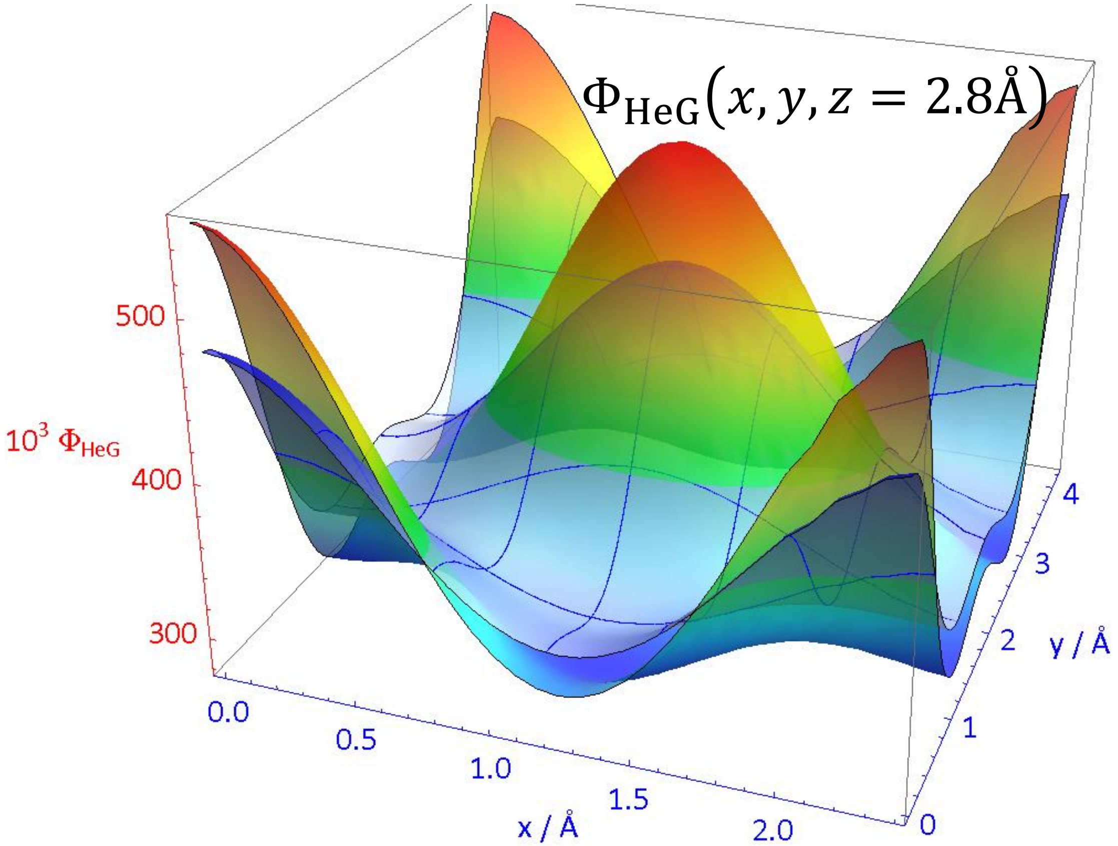


$$F_{ij}(r) = \begin{cases} \dfrac{\sin(k_{ij}r)}{r} & ;r \leq L_{ij} \\ \exp\left[\dfrac{k_{ij}(r - L_{ij})}{\tan(k_{ij}L_{ij})}\right] \cdot \dfrac{\sin(k_{ij}L_{ij})}{r} & ;r > L_{ij} \end{cases}$$

≫ METODA: ψ u ograničenom prostoru

- primjer: He_n (sličan tkućini) na grafenu
- probna valna funkcija $\psi_T(\vec{R}) = \prod_{i<j=1}^{N} F_{ij}(r_{ij}) \prod_{i=1}^{N} \Phi_i(\vec{r_i})$
- glatka $\Phi(z) = e^{-\left(\frac{a_2}{z}\right)^{a_3} - a_4 z^{a_5}}$
- korugirana $\Phi_{HeG}(x,y,z)$

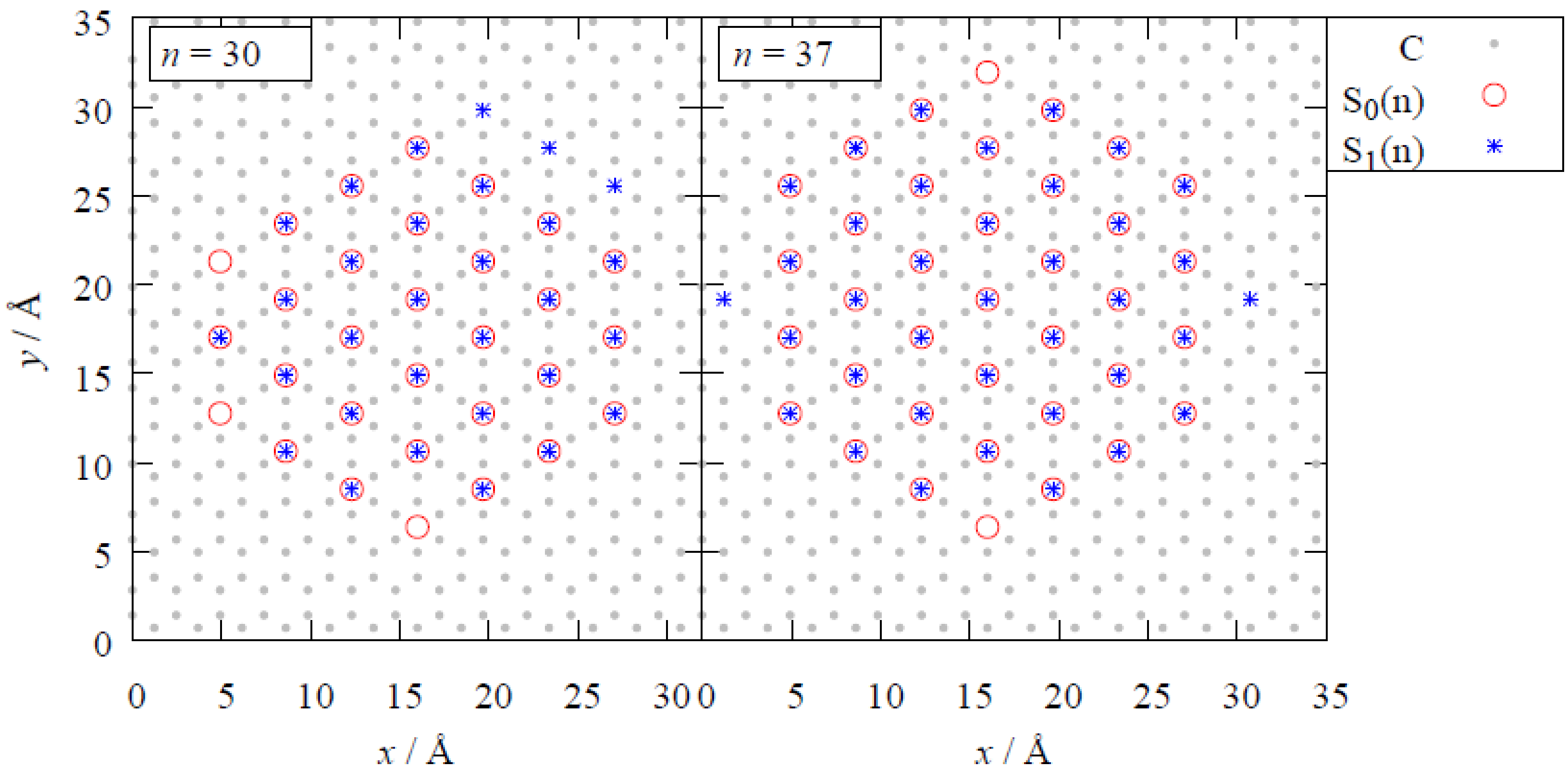




≫ METODA: ψ u ograničenom prostoru

- primjer: He_n (sličan krutini) na grafenu
- probna valna funkcija $\psi_T(\vec{R}) = \prod_{i<j=1}^{N} F_{ij}(r_{ij}) \prod_{i=1}^{N} \Phi_i(\vec{r_i})$

$$\psi_K(\vec{R}) = \psi_T(\vec{R}) \prod_{i=1}^{N} h(\vec{\rho}_{iI}) \quad ; \quad \vec{\rho}_I \in S(n)$$

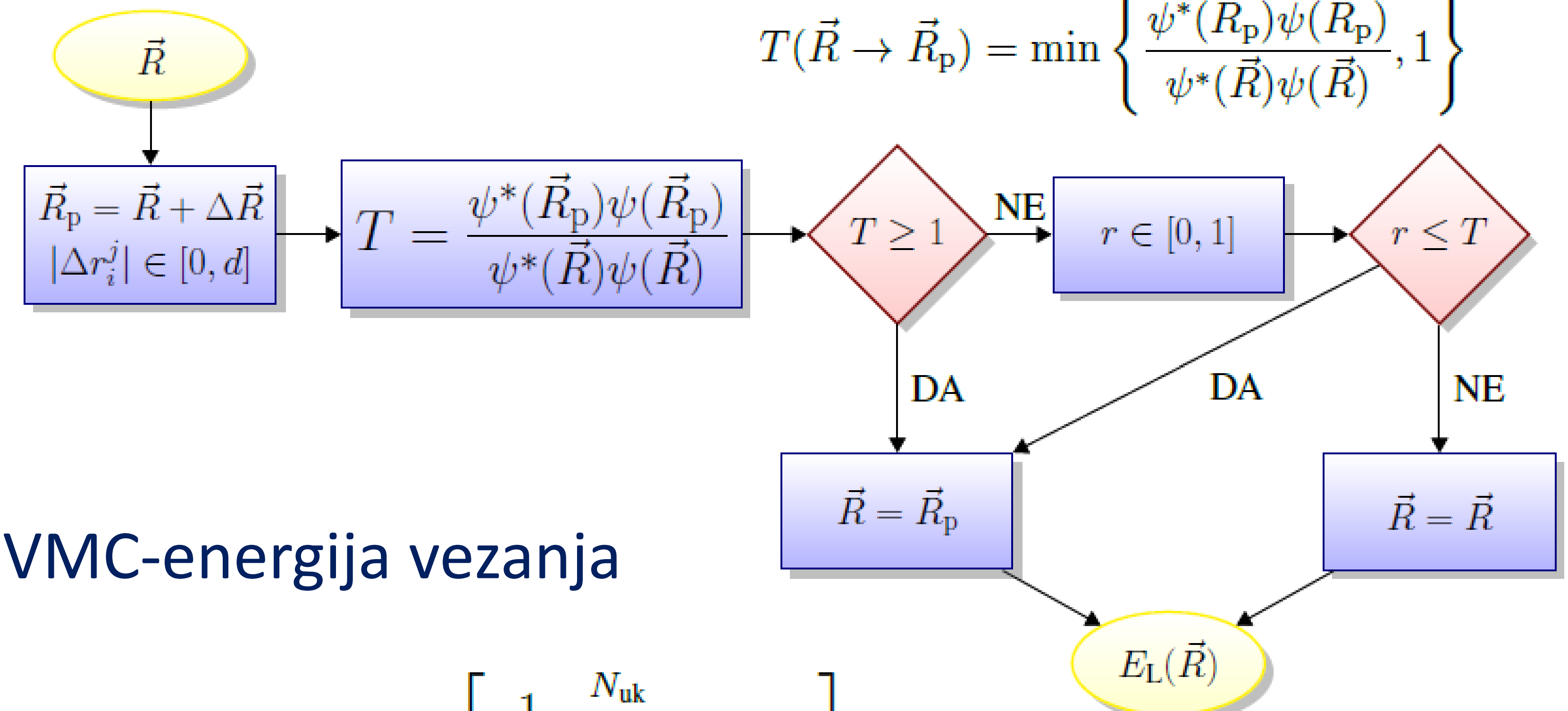


≫ METODA: VMC

- računanje lokalne energije unutar jednog koraka simulacije

$$E_L = \frac{\mathcal{H}\psi(\vec{R})}{\psi(\vec{R})}$$

$$T(\vec{R} \to \vec{R}_\mathrm{p}) = \min\left\{ \frac{\psi^*(\vec{R}_\mathrm{p})\psi(\vec{R}_\mathrm{p})}{\psi^*(\vec{R})\psi(\vec{R})}, 1 \right\}$$



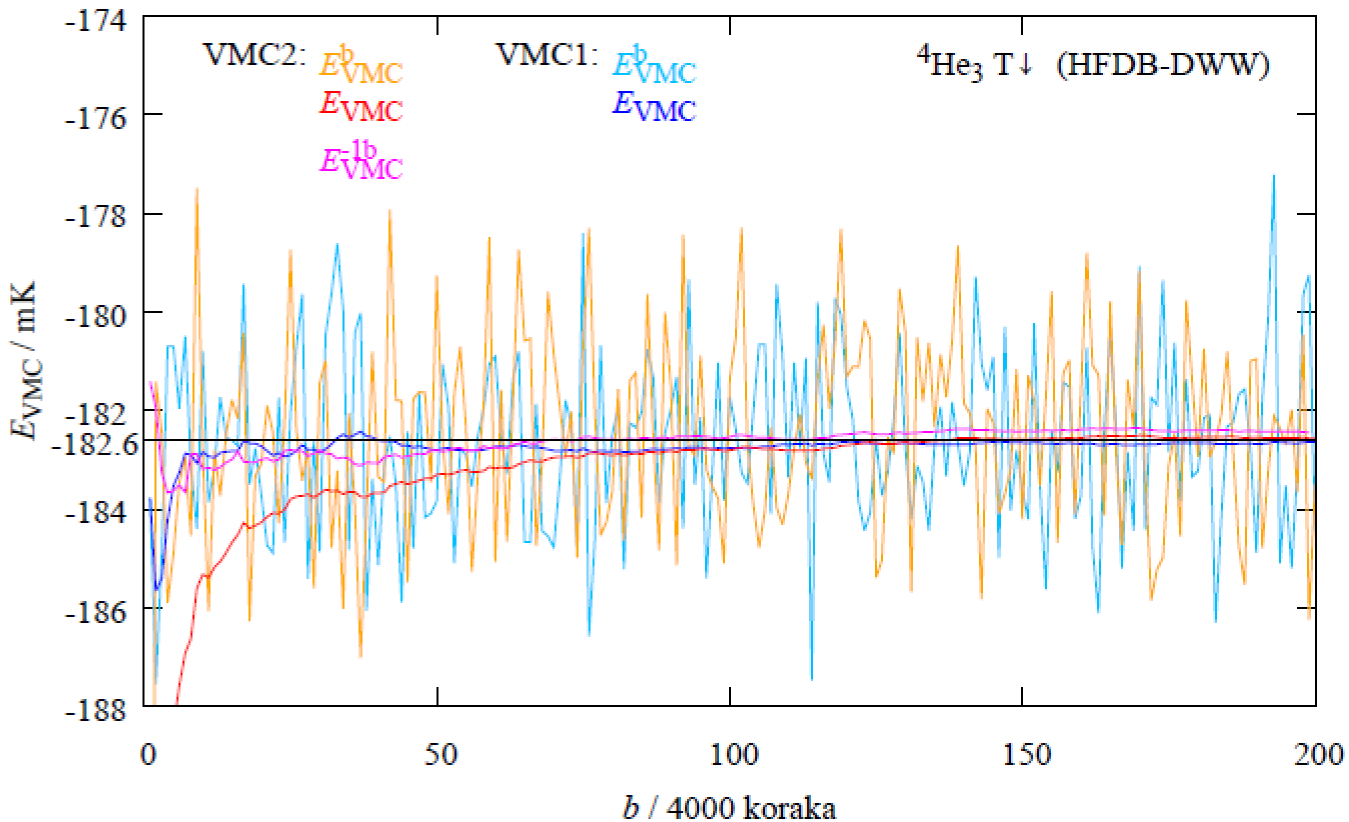
- VMC-energija vezanja

$$E_{\mathrm{VMC}}[\psi] = \lim_{N_\mathrm{uk}\to\infty}\left[\frac{1}{N_\mathrm{uk}}\sum_{i=1}^{N_\mathrm{uk}} E_\mathrm{L}(\vec{R}_i)\right]$$

≫ METODA: VMC

- procjena dobrog uzorkovanja

$$\underbrace{\boxed{k=1}\boxed{k=2}\cdots\boxed{k=N_\mathrm{k}}}_{b=1}\underbrace{\boxed{k=N_\mathrm{k}+1}\cdots}_{b=2}\cdots\underbrace{\boxed{k=(N_\mathrm{b}-1)N_\mathrm{k}+1}\cdots\boxed{k=N_\mathrm{b}N_\mathrm{k}}}_{b=N_\mathrm{b}}$$



- Optimizacija probne valne funkcije: min$\{E\}$, min$\{\sigma_E\}$

≫ METODA: DMC

- Schrödingerova jednadžba napisana u imaginarnom vremenu ($it/\hbar \to \tau$) postaje difuzijska

$$-\frac{\partial \Psi(\vec{R},\tau)}{\partial \tau} = \mathcal{H}\Psi(\vec{R},\tau)$$

- formalno rješenje $\Psi(\vec{R},\tau) = \mathrm{e}^{-\mathcal{H}\tau}\Psi(\vec{R},0)$

- razvoj po $\mathcal{H}\Upsilon_i(\vec{R}) = E_i\Upsilon_i(\vec{R})$

$$\Psi(\vec{R},0) = \sum_i c_i \Upsilon_i(\vec{R}) \qquad \Psi(\vec{R},\tau) = \sum_i c_i \mathrm{e}^{-E_i\tau}\Upsilon_i(\vec{R})$$

Problem1

- (P1) brzina konvergencije

≫ METODA: DMC

Rješenje1

- (R1) evoluciju stabiliziramo uvođenjem referentne energije

$$-\frac{\partial\Psi(\vec{R},\tau)}{\partial\tau} = (\mathcal{H} - E_{\mathrm{R}})\Psi(\vec{R},\tau)$$

$$\Psi(\vec{R},\tau) = \mathrm{e}^{-(\mathcal{H}-E_{\mathrm{R}})\tau}\Psi(\vec{R},0) = \sum_i c_i \mathrm{e}^{-(E_i-E_{\mathrm{R}})\tau}\Upsilon_i(\vec{R})$$ => (P2) ne znamo E_i

- (R2) uvodimo operator odgovoran za evoluciju $\mathcal{G} = \mathrm{e}^{-(\mathcal{H}-E_{\mathrm{R}})\tau}$

- koordinatna reprezentacija $G(\vec{R}',\vec{R},\tau) = \left\langle \vec{R}' \middle| \mathrm{e}^{-(\mathcal{H}-E_{\mathrm{R}})\tau} \middle| \vec{R} \right\rangle$

- => (P3) ne možemo istodobno simulirati cijeli $\mathcal{H}$
- Trotterov teorem za mali $\Delta\tau$

$$\mathcal{T}\mathcal{V} = \mathcal{V}\mathcal{T} \quad \Rightarrow \quad \nabla^2_{\vec{R}} V(\vec{R}) = V(\vec{R})\nabla^2_{\vec{R}}$$

≫ METODA: DMC

- (R3) aproksimacija kratkih vremenskih intervala

$$\exp\left(-\tau(\mathcal{H}-E_{\mathrm{R}})\right)=\prod_{k=1}^{N_{\mathrm{uk}}}\exp\left(-\Delta\tau(\mathcal{H}-E_{\mathrm{R}})\right)$$

- prema Trotterovom teoremu

$$\mathrm{e}^{-(\mathcal{H}-E_{\mathrm{R}})\Delta\tau}\approx\mathrm{e}^{-\mathcal{T}\Delta\tau}\mathrm{e}^{-(\mathcal{V}-E_{\mathrm{R}})\Delta\tau}\overset{\Delta\tau\to 0}{\equiv}\mathcal{G}_T\mathcal{G}_V$$

- znači: možemo odvojeno promatrati evoluciju kinetičkog i potencijalnog dijela
- popravke ovog pristupa daje Baker-Campbell-Hausdorffova (BCH) formula

$$\exp\left(\mathcal{A}\right)\exp\left(\mathcal{B}\right)=\exp\left(\mathcal{A}+\mathcal{B}+\frac{1}{2}[\mathcal{A},\mathcal{B}]+\frac{1}{12}[\mathcal{A}-\mathcal{B},[\mathcal{A},\mathcal{B}]]+\cdots\right)$$

≫ METODA: DMC

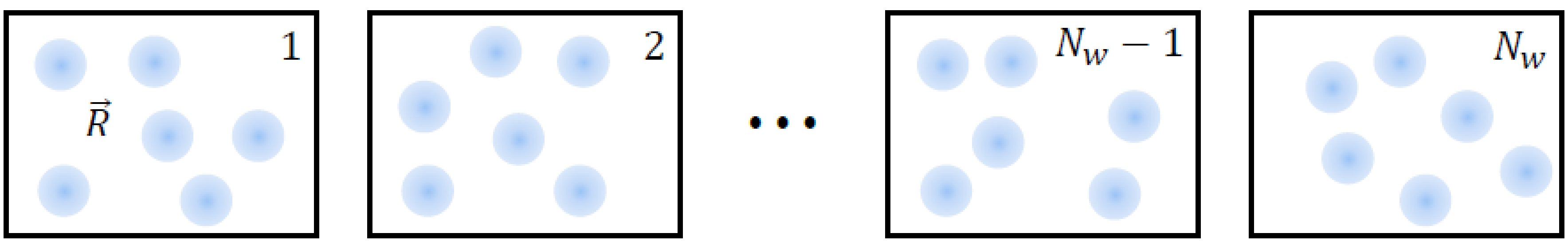
- jednadžba potencijalnog dijela (rast,pad) => nestabilnost(P4)

$$\frac{\partial G_V(\vec{R}',\vec{R},\tau)}{\partial\tau} = -\Big(V(\vec{R}) - E_\mathrm{R}\Big)\,G_V(\vec{R}',\vec{R},\tau)$$

- (R4) stabilizacija proračuna – uvođenje značajnog odabira

$$\Phi(\vec{R},\tau) = \psi(\vec{R})\cdot\Psi(\vec{R},\tau)$$

- valna funkcija u simulaciji dana je ansamblom šetača



- $\tau = \mathrm{N}\Delta\tau \to \infty$: $\quad \Phi(\vec{R},\tau) \to \psi(\vec{R})\Upsilon_0(\vec{R})$

≫ METODA: DMC

- => (P5) BCH daje

$$E'_{\mathrm{DMC}} = \frac{\langle \psi \,|\, \mathcal{H} \,|\, \Upsilon_0 \rangle}{\langle \psi \,|\, \Upsilon_0 \rangle} \overset{(2.44)}{=} E_0 + \frac{1}{2}\Delta\tau \frac{\langle \psi \,|\, [\mathcal{H}, \mathcal{V}] \,|\, \Upsilon_0 \rangle}{\langle \psi \,|\, \Upsilon_0 \rangle} + \cdots$$

- (R5) nesimetričan rastav

$$\mathcal{G}'' = \mathrm{e}^{-\frac{1}{2}\Delta\tau\mathcal{V}} \mathrm{e}^{-\frac{1}{2}\Delta\tau\mathcal{T}} \mathrm{e}^{-\frac{1}{2}\Delta\tau\mathcal{T}} \mathrm{e}^{-\frac{1}{2}\Delta\tau\mathcal{V}}$$

$$E''_{\mathrm{DMC}} = \frac{\langle \psi \,|\, \mathcal{H} \,|\, \Upsilon_0 \rangle}{\langle \psi \,|\, \Upsilon_0 \rangle} \overset{(2.50)}{=} E_0 + \frac{1}{24}\Delta\tau^2 \left[\langle \Upsilon_0 \,|\, \Delta\mathcal{H} \,|\, \Upsilon_0 \rangle - \frac{\langle \psi \,|\, \Delta\mathcal{H} \,|\, \Upsilon_0 \rangle}{\langle \psi \,|\, \Upsilon_0 \rangle} \right] + \cdots$$

≫ METODA: DMC

- (P6) DJ nakon uvođenja značajnog odabira

$$-\frac{\partial\Phi(\vec{R},\tau)}{\partial\tau} = -D_{\vec{R}}\nabla^2_{\vec{R}}\Phi(\vec{R},\tau) + D_{\vec{R}}\nabla_{\vec{R}}\cdot\left[\vec{F}(\vec{R})\Phi(\vec{R},\tau)\right] + \left[E_{\mathrm{L}}(\vec{R}) - E_{\mathrm{R}}\right]\Phi(\vec{R},\tau)$$

$$\equiv [\mathcal{A}_1 + \mathcal{A}_2 + \mathcal{A}_3]\Phi(\vec{R},\tau) \equiv \mathcal{A}\Phi(\vec{R},\tau)$$

$$\boxed{\vec{F}(\vec{R}) \equiv \nabla^2_{\vec{R}}\ln|\psi(\vec{R})|^2 = 2\frac{\nabla_{\vec{R}}\psi(\vec{R})}{\psi(\vec{R})}}$$

- (R6) djelovanje triju operatora

$$\exp(-\mathcal{A}\Delta\tau) = \exp\left(-\mathcal{A}_3\frac{\Delta\tau}{2}\right)\exp\left(-\mathcal{A}_2\frac{\Delta\tau}{2}\right)\exp(-\mathcal{A}_1\Delta\tau)$$
$$\times\exp\left(-\mathcal{A}_2\frac{\Delta\tau}{2}\right)\exp\left(-\mathcal{A}_3\frac{\Delta\tau}{2}\right) + \mathcal{O}(\Delta\tau^3)\,.$$

$$\boxed{\begin{aligned} G_1(\vec{R}',\vec{R},\tau) &= (4\pi D_{\vec{R}}\tau)^{-3N_a/2}\exp\left(-\frac{(\vec{R}-\vec{R}')^2}{4D_{\vec{R}}\tau}\right) \\ &= \prod_{i=1}^{N_a}(4\pi D_i\tau)^{-3N_a/2}\exp\left(-\frac{(\vec{r}_i-\vec{r}_i{}')^2}{4D_i\tau}\right)\end{aligned}}$$

$$\boxed{G_3(\vec{R}',\vec{R},\tau) = \exp\left(-(E_{\mathrm{L}}(\vec{R}) - E_{\mathrm{R}})\tau\right)\delta\left(\vec{R}'-\vec{R}\right)}$$

$$\boxed{G_2(\vec{R}',\vec{R},\tau) = \delta\left(\vec{R}'-\vec{R}(\tau)\right)}$$

$$\boxed{\frac{\mathrm{d}\vec{R}(\tau)}{\mathrm{d}\tau} = D\vec{F}(\vec{R}(\tau))}$$

» METODA: DMC

- (P7) previše aproksimacija? koja su ograničenja?
- (R6) uvjeti

(U0) preklop $\Psi(\vec{R},0)$ i $\Upsilon_0(\vec{R})$ različit je od nule;
(U1) za svaki $\vec{R}$ za koji je $\Upsilon_0(\vec{R}) \neq 0$, također je i $\psi(\vec{R}) \neq 0$;
(U2) ansambl šetača je dovoljno velik kako bi se moglo uzorkovati $\Phi(\vec{R},\tau) = \psi(\vec{R})\Psi(\vec{R},\tau)$;
(U3) vremenski korak $\Delta\tau$ dovoljno je mali kako bi vrijedila dekompozicija (2.57);
(U4) vrijeme τ dovoljno je veliko da utrnu komponente pobuđenih stanja $\Psi(\vec{R},\tau) \to \Upsilon_0(\vec{R})$;

- (P8) utječe li značajni odabir na procjenu osobina sustava
- (R8)
  - miješanim estimatorima $$\left\langle \mathcal{F}(\vec{R}) \right\rangle_{\mathrm{m}} = \frac{\left\langle \psi(\vec{R}) \middle| \mathcal{F}(\vec{R}) \middle| \Upsilon_0(\vec{R}) \right\rangle}{\left\langle \psi(\vec{R}) \middle| \Upsilon_0(\vec{R}) \right\rangle}$$

    možemo odrediti srednje vrijednosti operatora koji $[\mathcal{F},\mathcal{H}] = 0$
  - čistim estimatorima ostale veličine koje su odredive iz uzorkovanih položaja

≫ METODA: DMC - algoritam

$$\left\{ \vec{R}_w \right\} \to \left\{ \vec{R}'_{i+j} = \vec{R}'_{\mathrm{p}(w)} \,\middle|\, i = \sum_{m=1}^{w-1} n_m; 1 \le j \le n_w \right\}$$

$$\left\{ \vec{R}_w \right\} \to \left\{ \left(\vec{R}^{\mathrm{m}}_w, E_{\mathrm{L}} \right) \,\middle|\, E_{\mathrm{L}} = E_{\mathrm{L}}(\vec{R}_w) \right\} \equiv S$$

DMC algoritam

⇒ Gaussov pomak: $\vec{R}^{\mathrm{m}}_a = \vec{R}^{\mathrm{m}}_w + \Delta\vec{R}$ gdje je $\Delta\vec{R}$ nasumično odabran iz $3N_{\mathrm{a}}$ Gaussove razdiobe s eksponentom $-(\Delta\vec{R})^2/(4D_{\vec{R}}\Delta\tau)$.

⇒ Računanje driftne sile: $\vec{F}_a = \vec{F}(\vec{R}^{\mathrm{m}}_a)$.

⇒ Pomoćni driftni pomak: $\vec{R}^{\mathrm{m}}_b = \vec{R}^{\mathrm{m}}_a + D_{\vec{R}} \cdot \frac{\Delta\tau}{2} \cdot \vec{F}_a$.

⇒ Računanje driftne sile: $\vec{F}_b = \vec{F}(\vec{R}^{\mathrm{m}}_b)$.

⇒ Srednji driftni pomak: $\vec{R}'_{\mathrm{p}(w)} = \vec{R}^{\mathrm{m}}_a + D_{\vec{R}} \cdot \frac{\Delta\tau}{2} \cdot \frac{\vec{F}_a + \vec{F}_b}{2}$, pohranimo u $\vec{R}^{\mathrm{m}}_b = \vec{R}'_{\mathrm{p}(w)}$.

⇒ Računanje driftne sile i lokalne nenergije: $\vec{F}' = \vec{F}(\vec{R}'_{\mathrm{p}(w)})$, $E'_{\mathrm{L}} = E_{\mathrm{L}}(\vec{R}'_{\mathrm{p}(w)})$.

⇒ Konačni driftni pomak: $\vec{R}^{\mathrm{m}}_w = \vec{R}^{\mathrm{m}}_a + D_{\vec{R}} \cdot \Delta\tau \cdot \vec{F}'$.

⇒ Određivanje statističke težine: $W\left(\vec{R}'_{\mathrm{p}(w)}\right) = \exp\left(-\left[\frac{1}{2}(E_{\mathrm{L}} + E'_{\mathrm{L}}) - E_{\mathrm{R}}\right]\Delta\tau\right)$.

⇒ Stohastička procjena broja potomaka: $n_w = \mathrm{int}\left[W\left(\vec{R}'_{\mathrm{p}(w)}\right) + ran2\right]$.

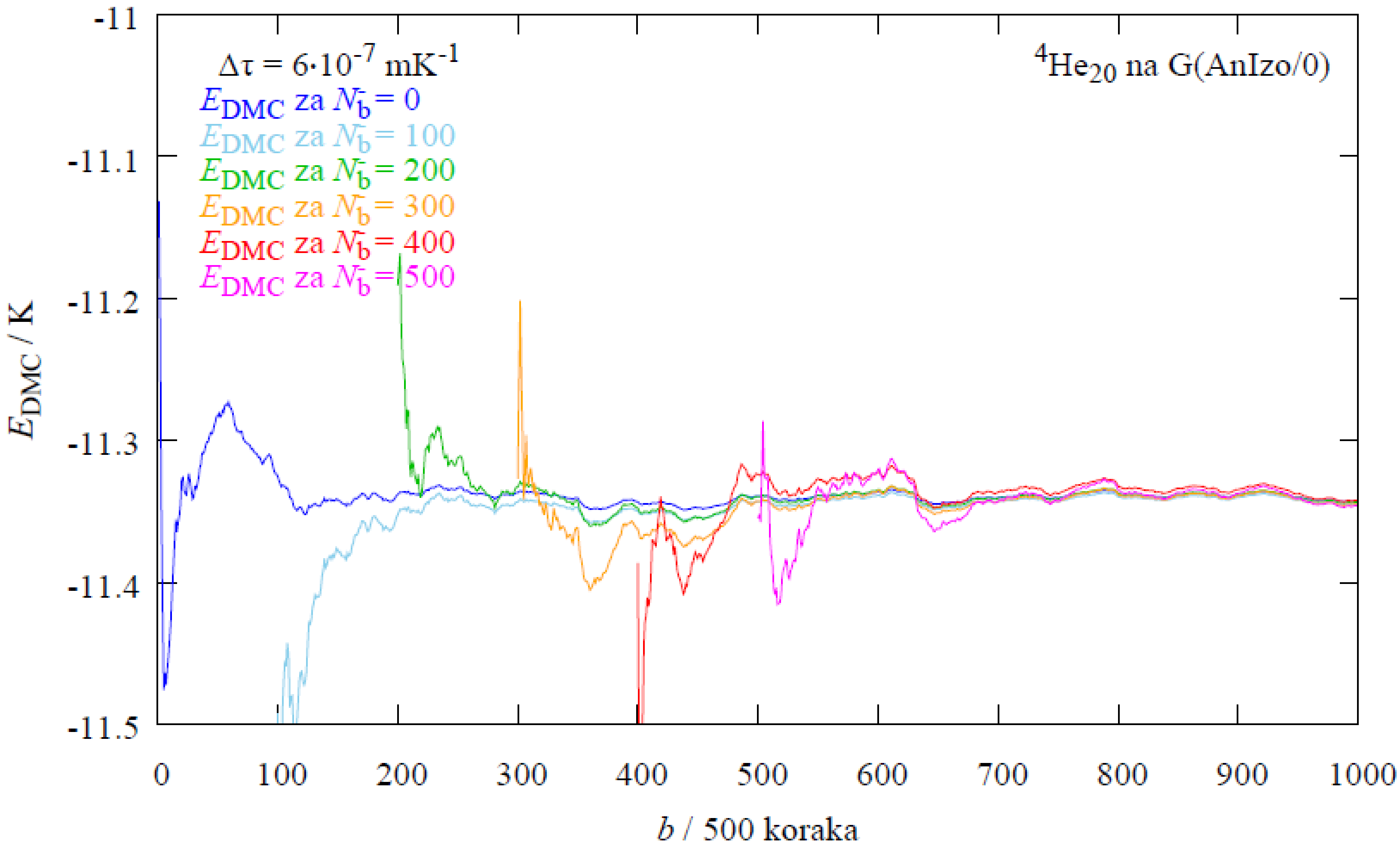
⇒ Akumulacija lokalnih energija: $\sum E_{k,w} = \sum E_{k,w} + n_w E'_{\mathrm{L}}$.

⇒ Kopiranje potomka $\vec{R}'_{\mathrm{p}(w)}$, odnosno njihovih identifikacijskih parova u novi ansambl:

$$S' = S' \cup \left\{ \left(\vec{R}^{\mathrm{m}}_{i+j}, E'_{\mathrm{L}} \right) \,\middle|\, i = \sum_{m=1}^{w-1} n_m; 1 \le j \le n_w \right\}. \tag{4.101}$$

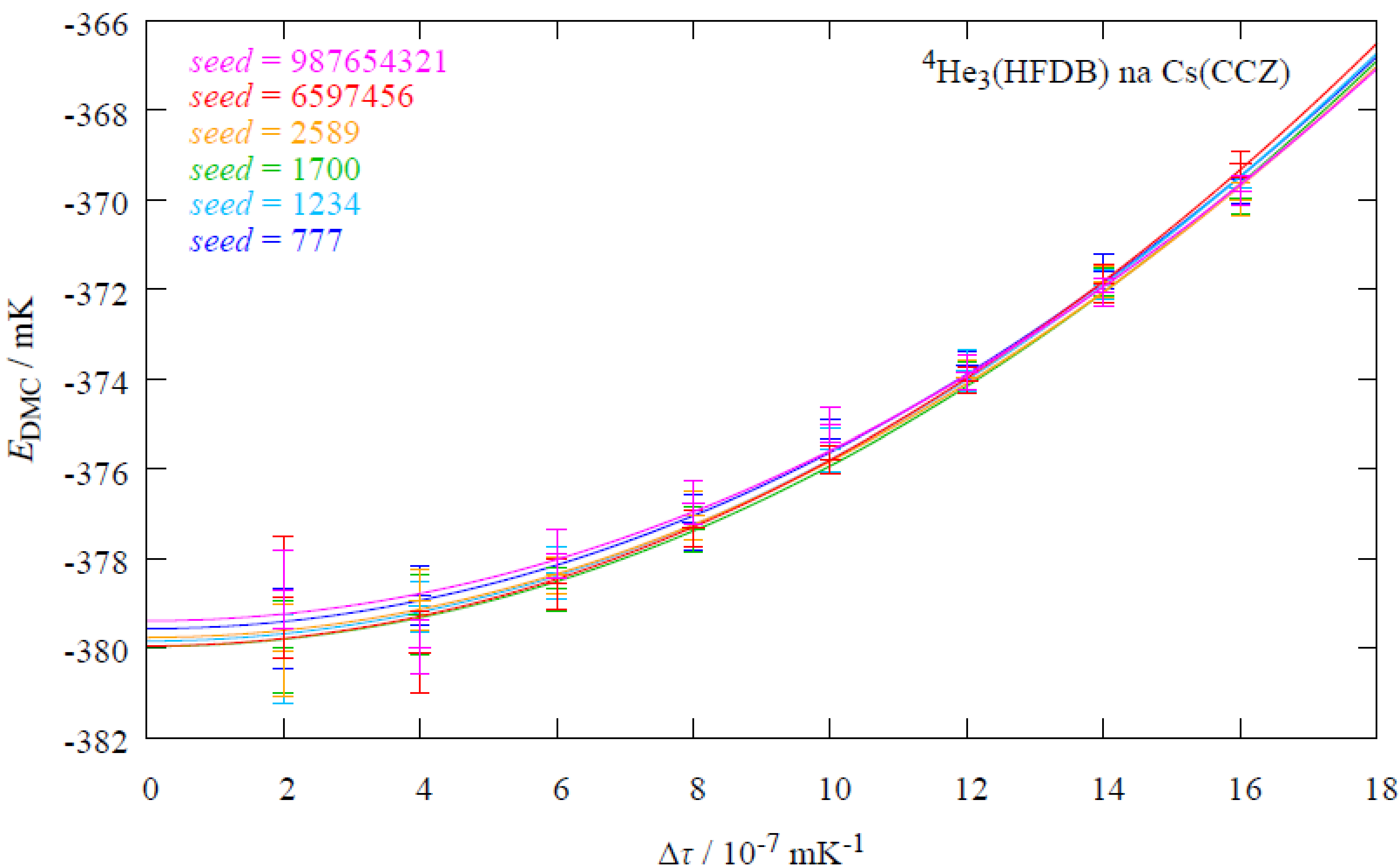
≫ METODA: DMC – uzorkovanje $E(\mathrm{b})$

$$\underbrace{\boxed{b = 1 - N_{\mathrm{b}}^{-}} \cdots \boxed{b = 0}}_{\text{odbačeno}} \underbrace{\boxed{b = 1} \cdots \boxed{b = N_{\mathrm{b}}/2}}_{E_{\mathrm{DMC1}}} \underbrace{\boxed{b = N_{\mathrm{b}}/2 + 1} \cdots \boxed{b = N_{\mathrm{b}}}}_{E_{\mathrm{DMC2}}}$$

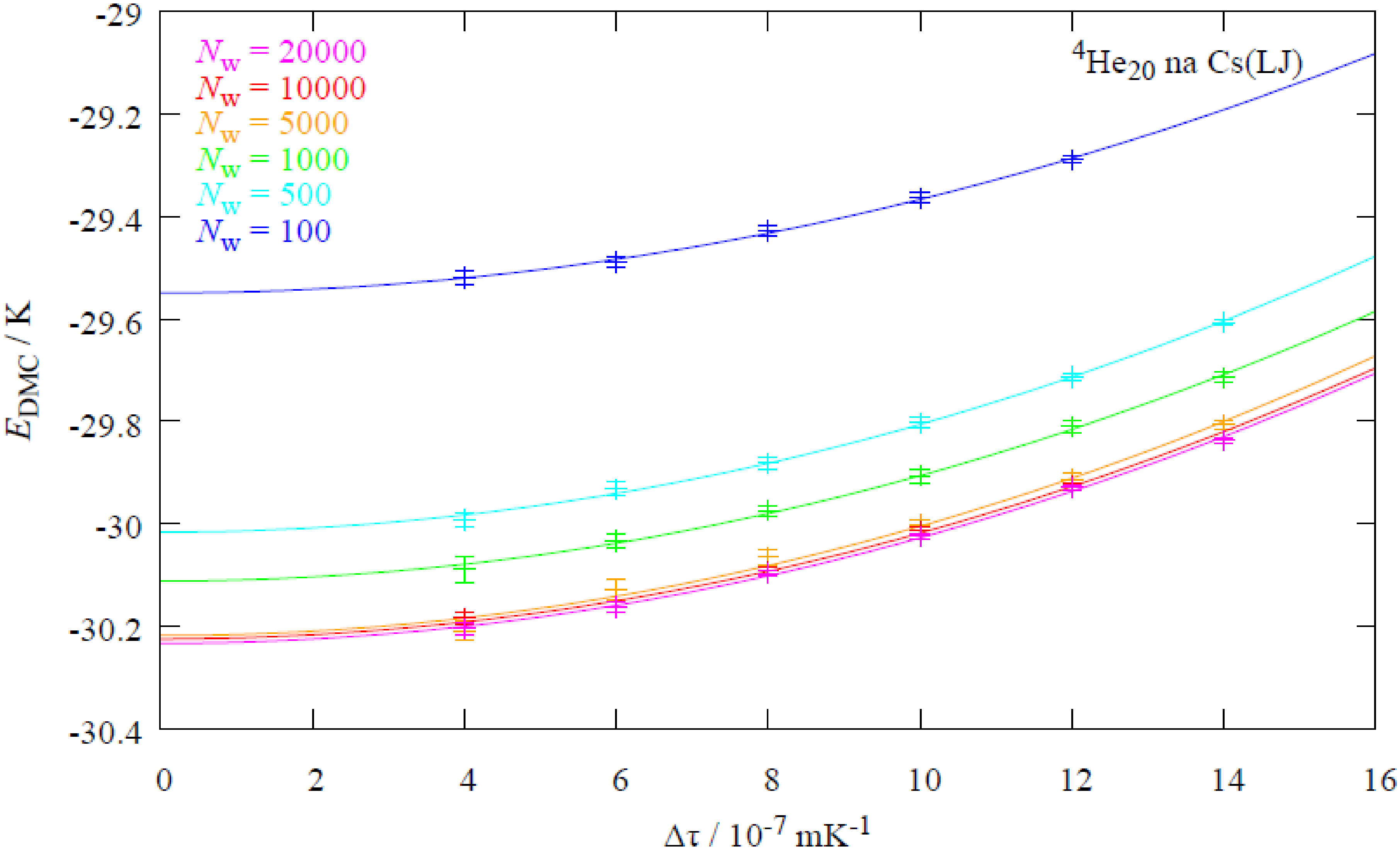


» DMC - $E(\Delta\tau)$

$$E_{\mathrm{DMC}}(\Delta\tau) = E_0(0) + a_{\mathrm{E}}\Delta\tau^2$$

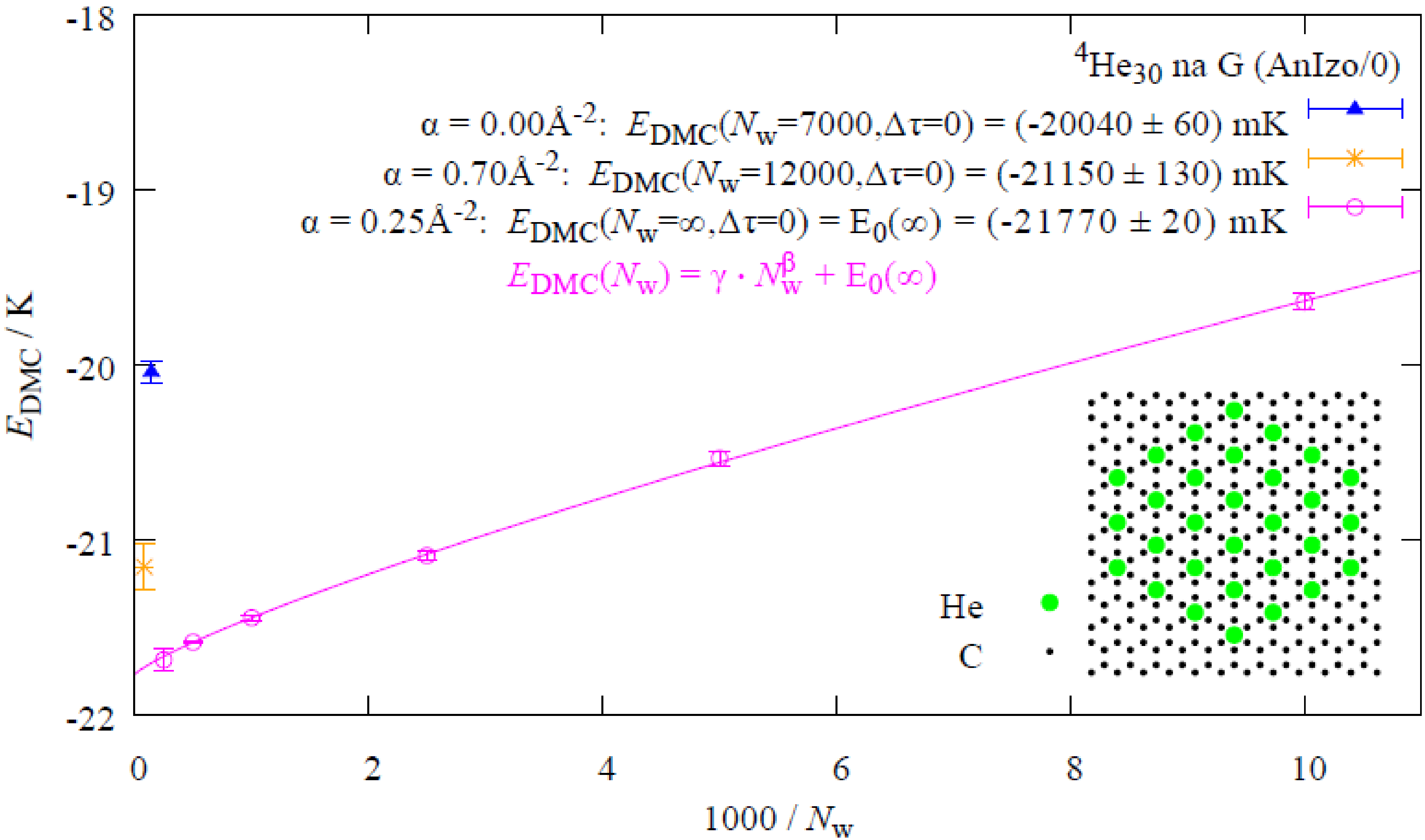


≫ DMC - $E(N_w)$



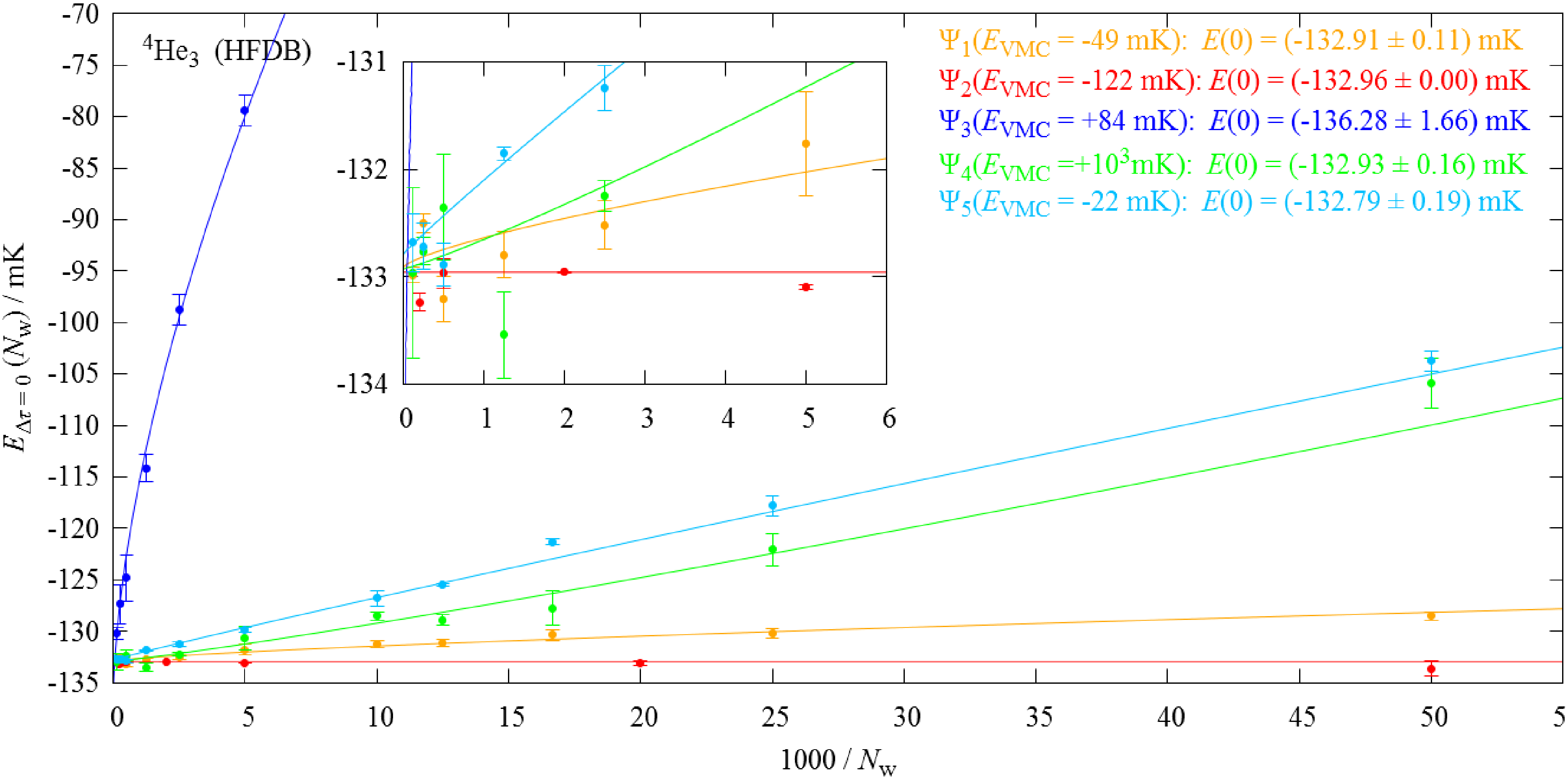
N_w = 20000
N_w = 10000
N_w = 5000
N_w = 1000
N_w = 500
N_w = 100
$^4He_{20}$ na Cs(LJ)
E_{DMC} / K
-29
-29.2
-29.4
-29.6
-29.8
-30
-30.2
-30.4
0
2
4
6
8
10
12
14
16
$\Delta\tau$ / 10^{-7} mK^{-1}

≫ DMC - $E(N_w)$



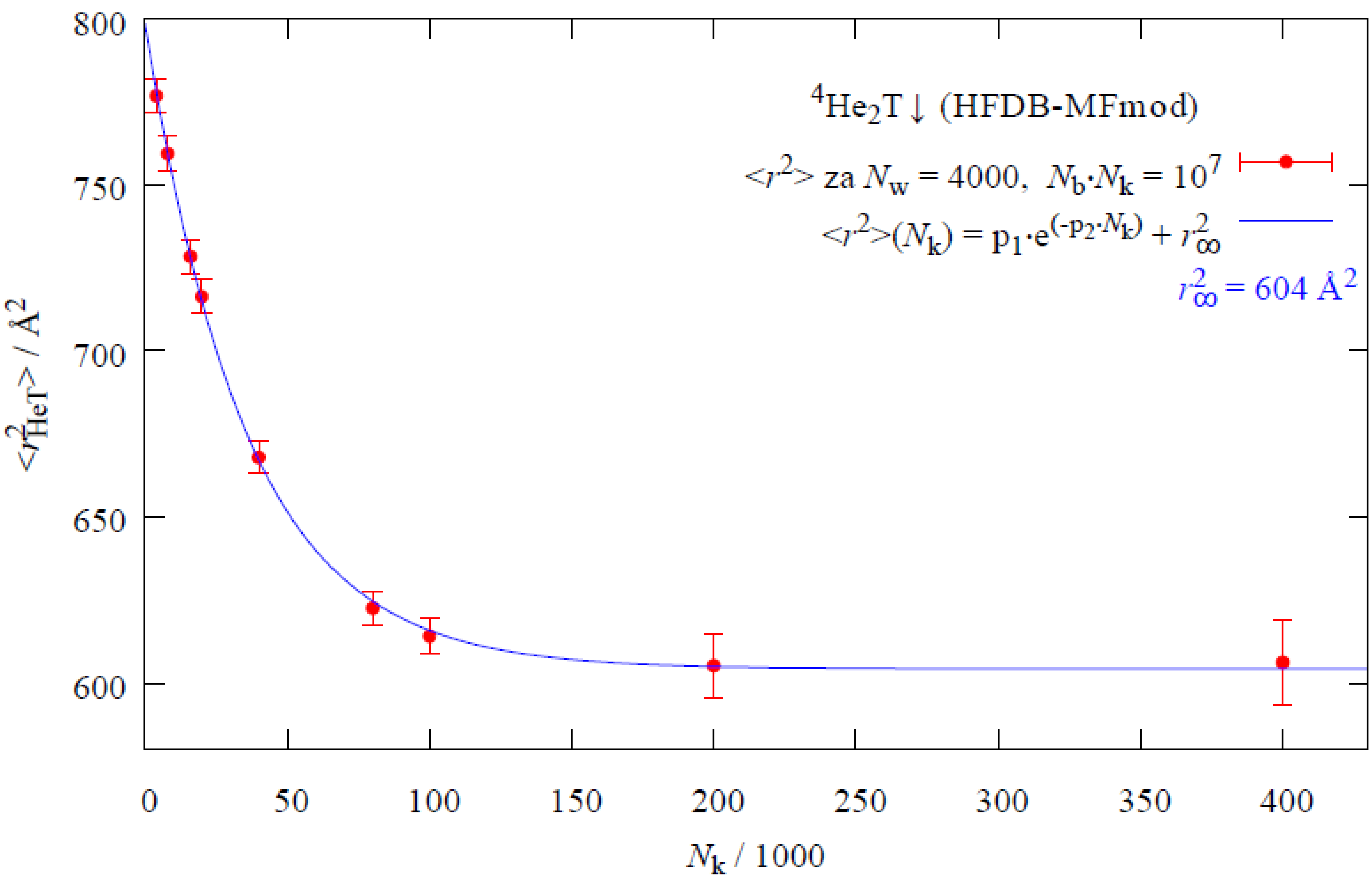
$^4He_{30}$ na G (AnIzo/0)
$\alpha = 0.00 Å^{-2}$: $E_{DMC}(N_w=7000, \Delta\tau=0) = (-20040 \pm 60)$ mK
$\alpha = 0.70 Å^{-2}$: $E_{DMC}(N_w=12000, \Delta\tau=0) = (-21150 \pm 130)$ mK
$\alpha = 0.25 Å^{-2}$: $E_{DMC}(N_w=\infty, \Delta\tau=0) = E_0(\infty) = (-21770 \pm 20)$ mK
$E_{DMC}(N_w) = \gamma \cdot N_w^{\beta} + E_0(\infty)$
He
C
E_{DMC} / K
1000 / N_w
-18
-19
-20
-21
-22
0
2
4
6
8
10

≫ DMC - $E(N_w, \Psi)$

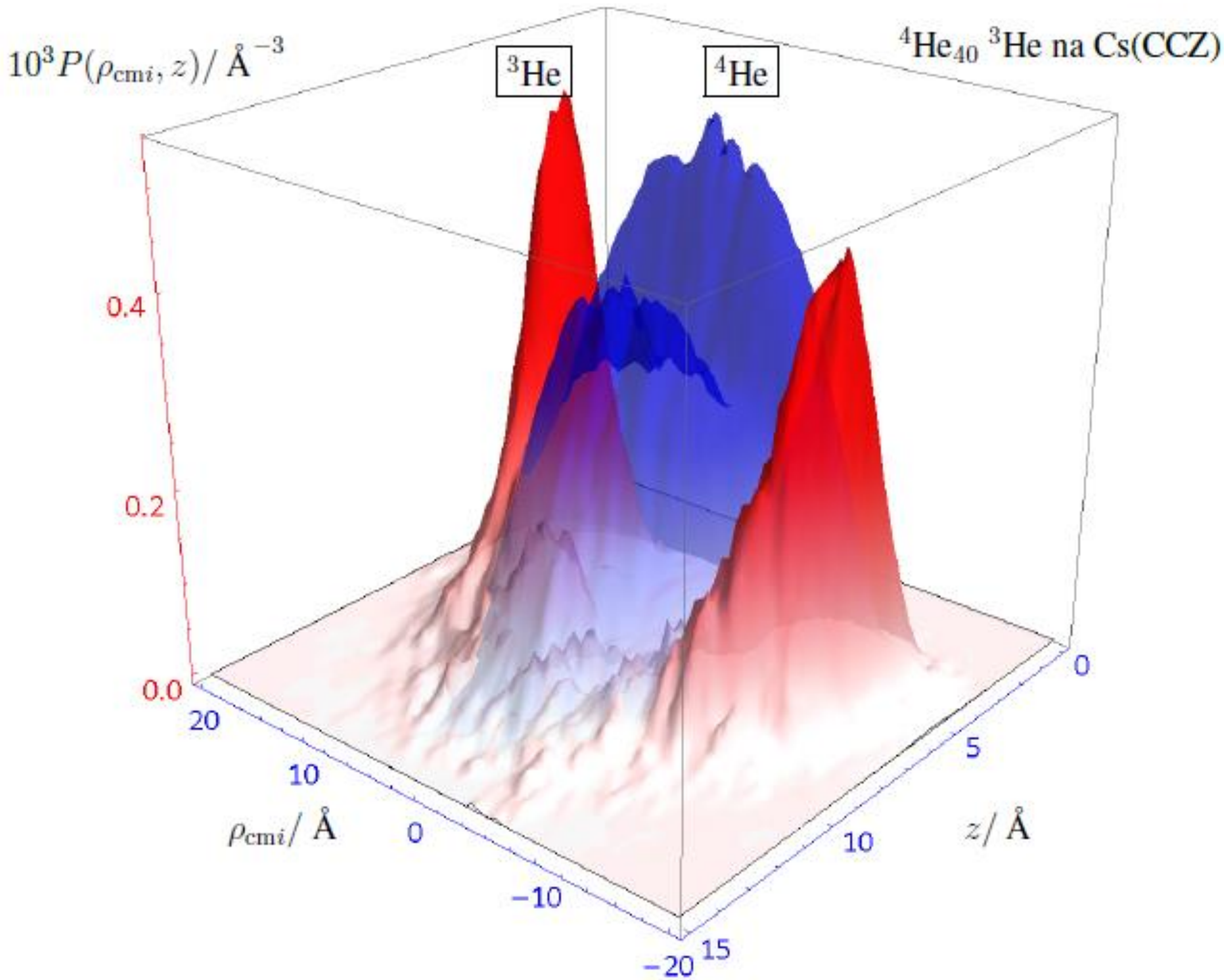


$^4He_3$ (HFDB)
$\Psi_1(E_{VMC} = -49$ mK$)$: $E(0) = (-132.91 \pm 0.11)$ mK
$\Psi_2(E_{VMC} = -122$ mK$)$: $E(0) = (-132.96 \pm 0.00)$ mK
$\Psi_3(E_{VMC} = +84$ mK$)$: $E(0) = (-136.28 \pm 1.66)$ mK
$\Psi_4(E_{VMC} = +10^3$mK$)$: $E(0) = (-132.93 \pm 0.16)$ mK
$\Psi_5(E_{VMC} = -22$ mK$)$: $E(0) = (-132.79 \pm 0.19)$ mK
$E_{\Delta\tau=0}(N_w)$ / mK
1000 / N_w

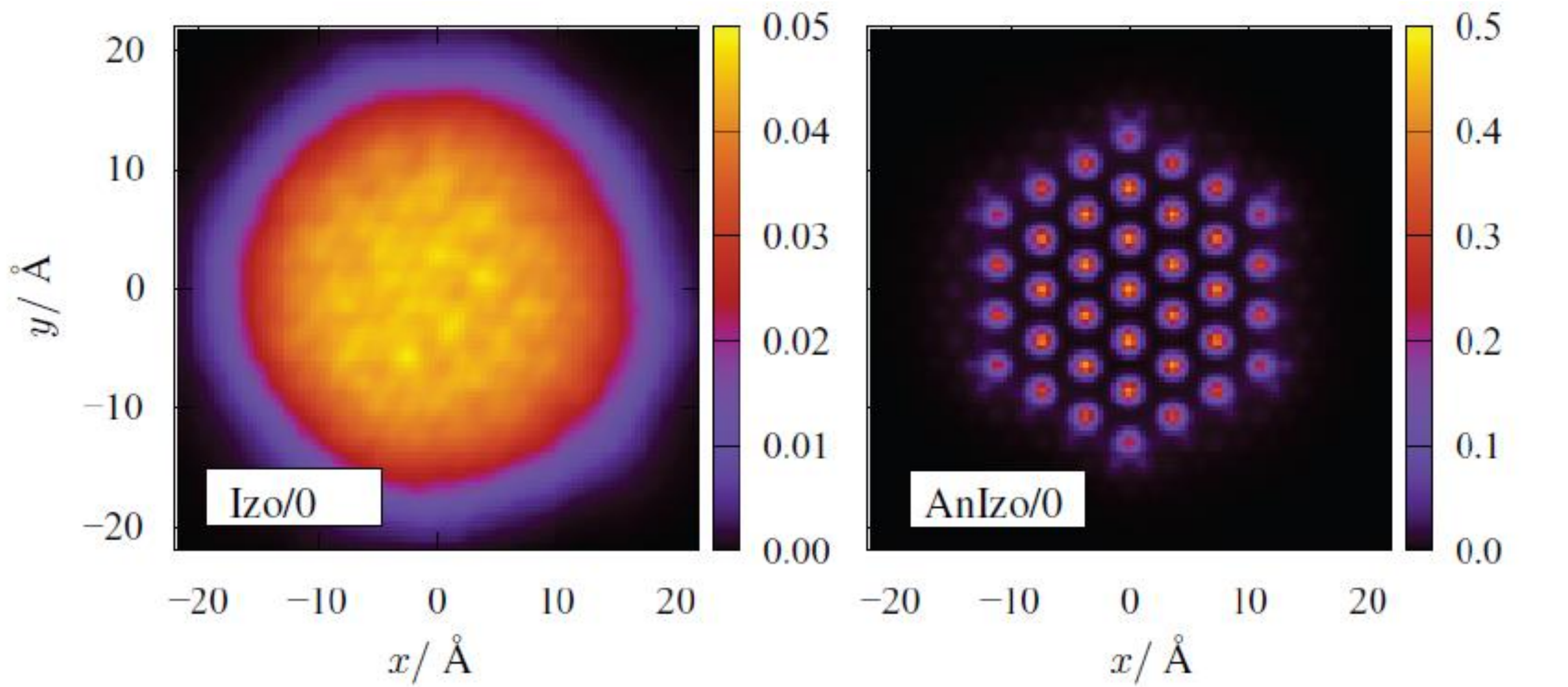
≫ DMC – čisti estimatori



≫ DMC - razdiobe



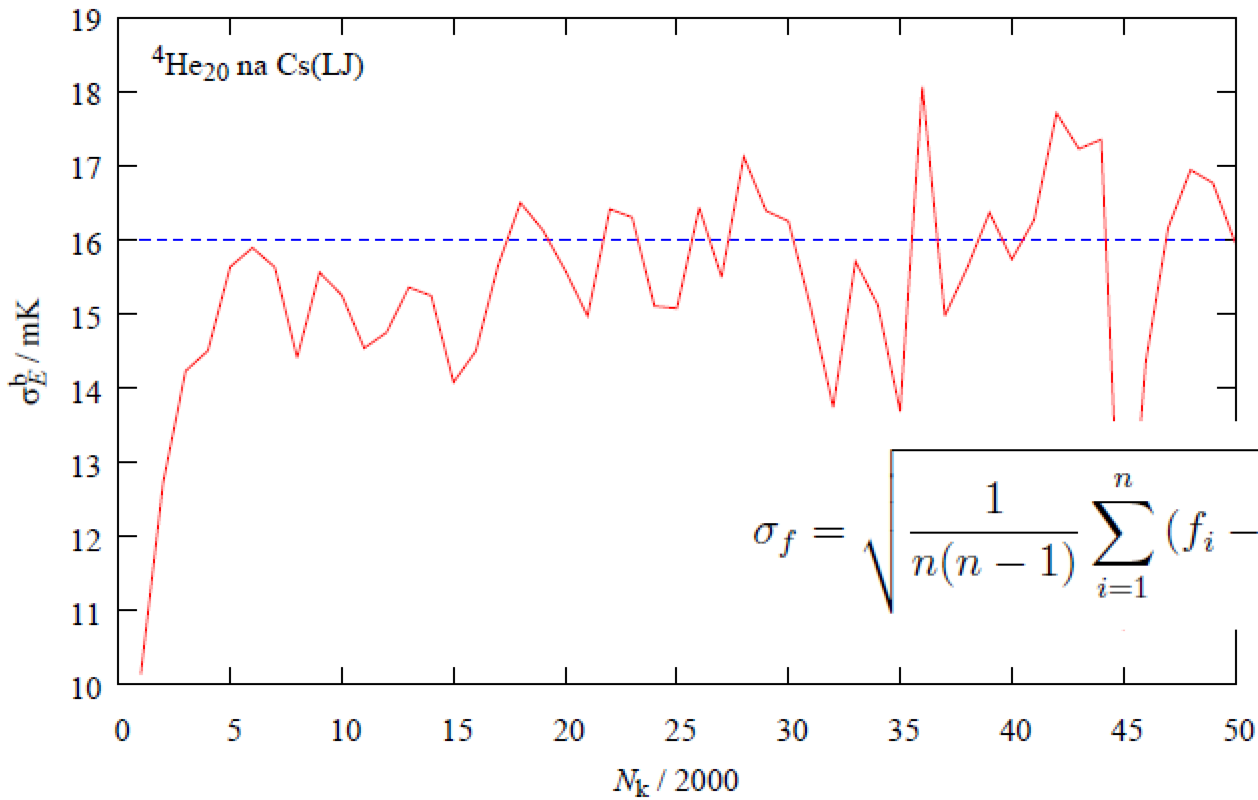
≫ DMC - struktura



DMC - devijacije

$$\underbrace{\boxed{f_1 \equiv f(k=1)}\,\boxed{f_2}\cdots\cdots\boxed{f_{N_\mathrm{k}}}}\;\underbrace{\boxed{f_{N_\mathrm{k}+1}}\cdots\cdots\boxed{f_{2N_\mathrm{k}}}}\cdots\underbrace{\boxed{f_{(N_\mathrm{b}-1)N_\mathrm{k}+1}}\cdots\boxed{f_{N_\mathrm{b}N_\mathrm{k}}}}$$

$$f(b=1) \equiv f_1^\mathrm{b} = \sum_{i=1}^{N_\mathrm{k}} f_i/N_\mathrm{k} \qquad f_2^\mathrm{b} = \sum_{i=N_\mathrm{k}+1}^{2N_\mathrm{k}} f_i/N_\mathrm{k} \qquad f_{N_\mathrm{b}}^\mathrm{b} = \sum_{i=(N_\mathrm{b}-1)N_\mathrm{k}+1}^{N_\mathrm{b}N_\mathrm{k}} f_i/N_\mathrm{k}$$



$$\sigma_f = \sqrt{\frac{1}{n(n-1)}\sum_{i=1}^{n}\left(f_i - \langle f\rangle\right)^2} = \sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{n-1}}$$

» Z12

Unutar mape VMC_H priloženo je rješenje primjera 4.1 i 4.4. Prilagodite ga da rješava problem osnovnog stanja kvantnog harmonijskog oscilatora.

Priložite:

- izvod lokalne energije za odabranu probnu valnu funkciju
- prikaz ovisnosti energije o varijacijskom parametru
- prikaz ovisnosti energije po blokovima za optimalni parametar
- prikaz ovisnosti greške najniže energije o veličini bloka
- konačnu vrijednost srednje energije i njenu devijaciju ispišite na prethodnome grafu.