Quantum Monte Carlo simulation of superfluid helium confined inside pre-plated nanoporous materials

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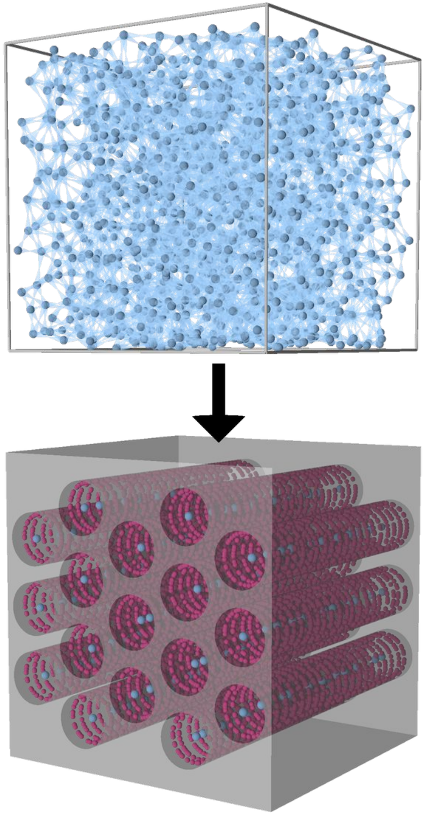
DMR-1809027
DMR-1808440
OAC-1827314

motivation

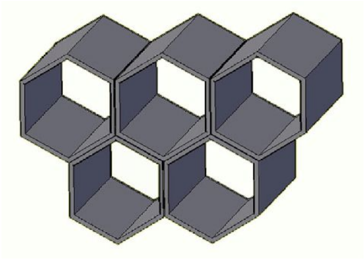
- observation of superfluid helium confined to one spatial dimension
    - long range order?
- tunability of confining potential
    - structural effects?
    - reach TLL regime?
    - experimental considerations?

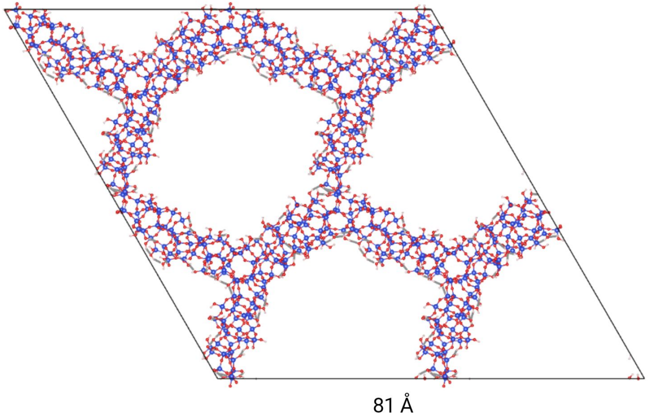


Doblin *et al.* (2016) 10.1063/1.4973468
Duc *et al.* (2015) 10.1126/sciadv.1400222
Vekhov and Hollock (2012) 10.1103/PhysRevLett.109.045303
Nyéki *et al.* (2013) 10.1103/PhysRevLett.111.215303
Tota *et al.* (2007) 10.1103/PhysRevLett.99.255301
Del Maestro *et al.* (2011) 10.1103/PhysRevLett.106.105303
Markić *et al.* (2018) 10.1103/PhysRevB.97.014513
Bertaina *et al.* (2016) 10.1103/PhysRevLett.116.135302
Astrakharchik and Boronat (2014) 10.1103/PhysRevB.90.235439

reaching the one dimensional limit

- begin with mesoporous silica
  - MCM-41





Doblin *et al.* (2016) 10.1063/1.4973468
Ugliengo *et al.* (2008) 10.1002/adma.200801489

reaching the one dimensional limit

- begin with mesoporous silica
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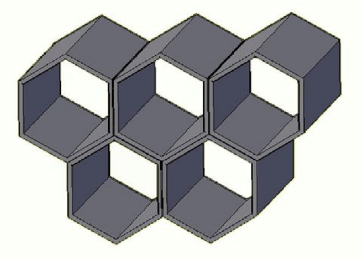
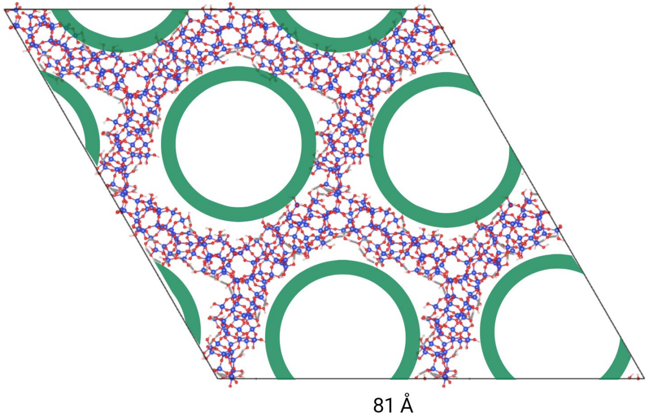
- preplate with rare gas
  - neon and argon





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reaching the one dimensional limit

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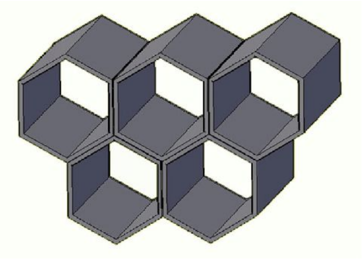

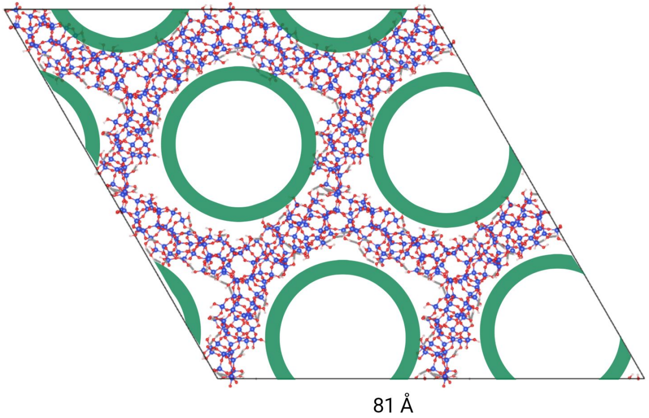

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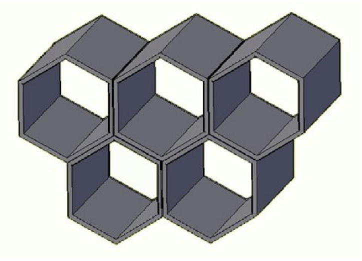
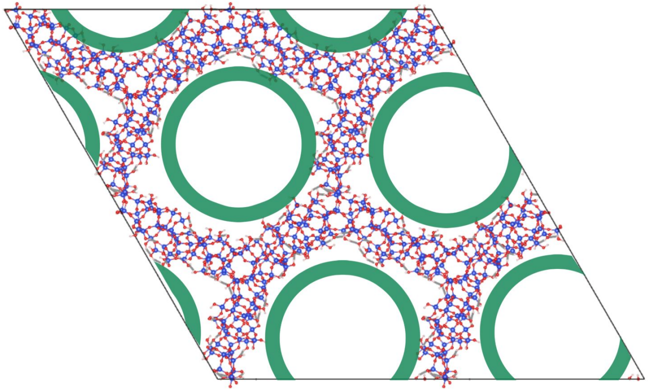
QMC simulation

→ effect of confining media





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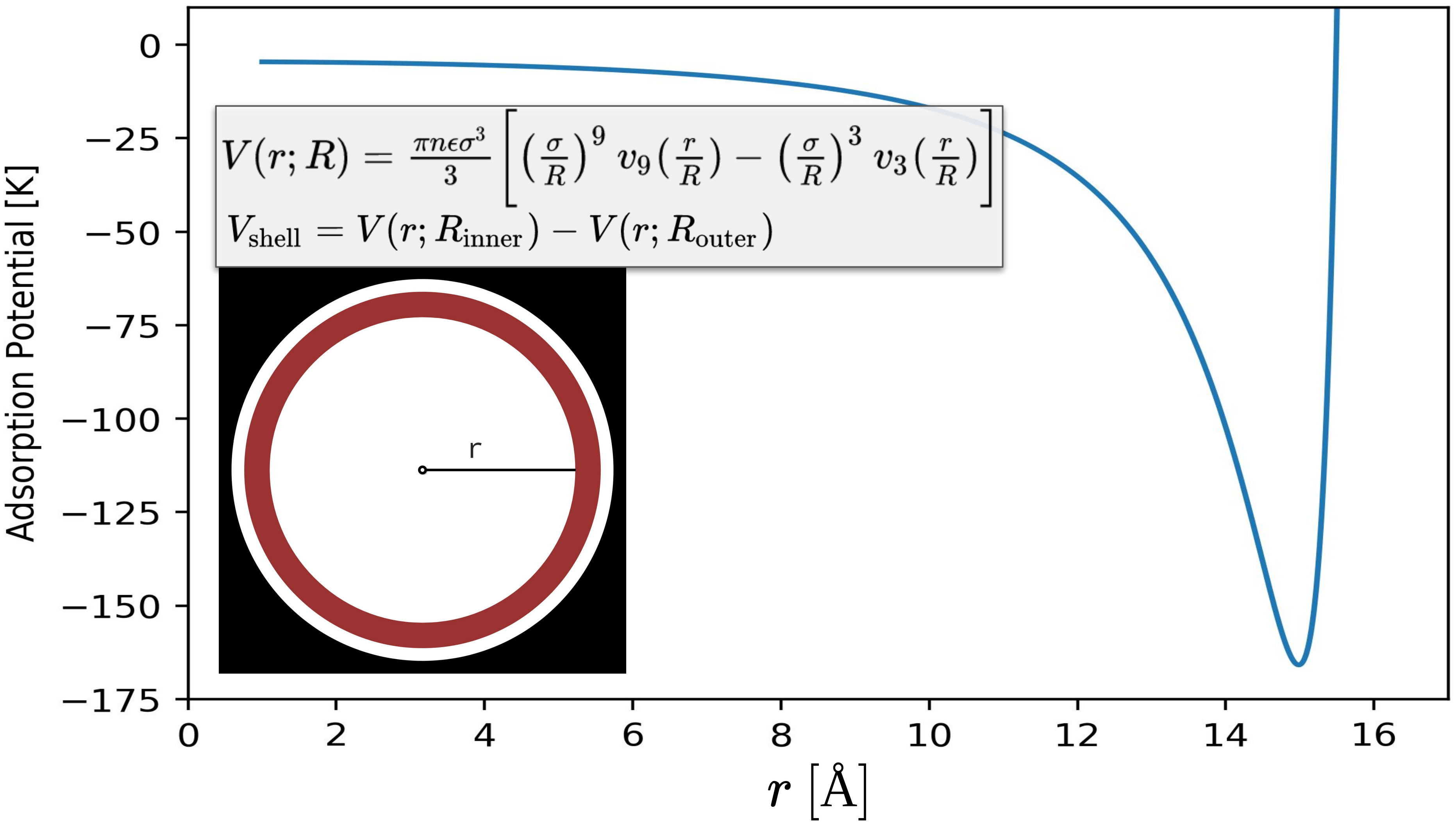
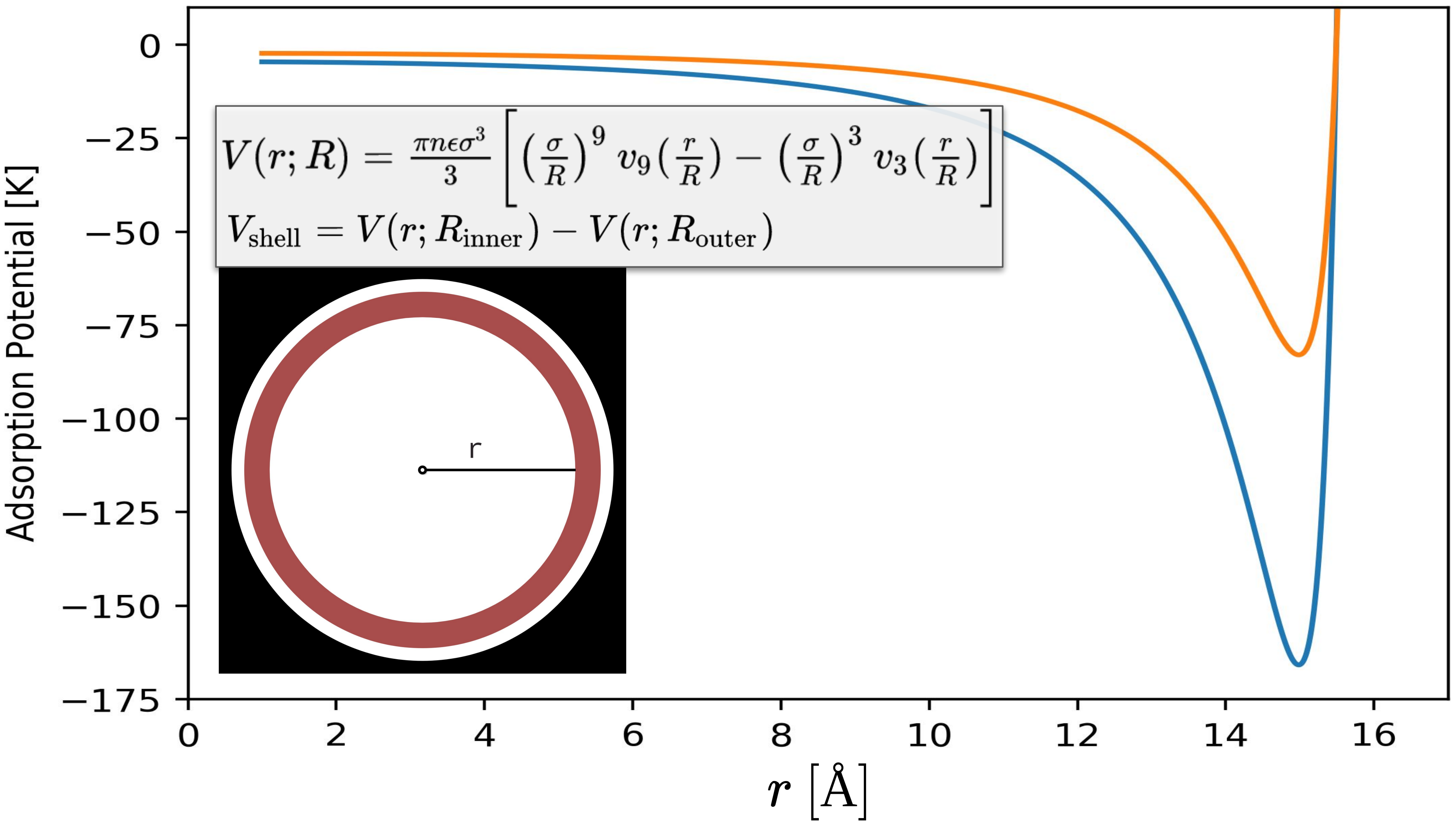


$V(r;R) = \frac{\pi n \epsilon \sigma^3}{3}\left[\left(\frac{\sigma}{R}\right)^9 v_9\left(\frac{r}{R}\right) - \left(\frac{\sigma}{R}\right)^3 v_3\left(\frac{r}{R}\right)\right]$
$V_{\mathrm{shell}} = V(r; R_{\mathrm{inner}}) - V(r; R_{\mathrm{outer}})$
r
Adsorption Potential [K]
0
−25
−50
−75
−100
−125
−150
−175
0
2
4
6
8
10
12
14
16
r [Å]



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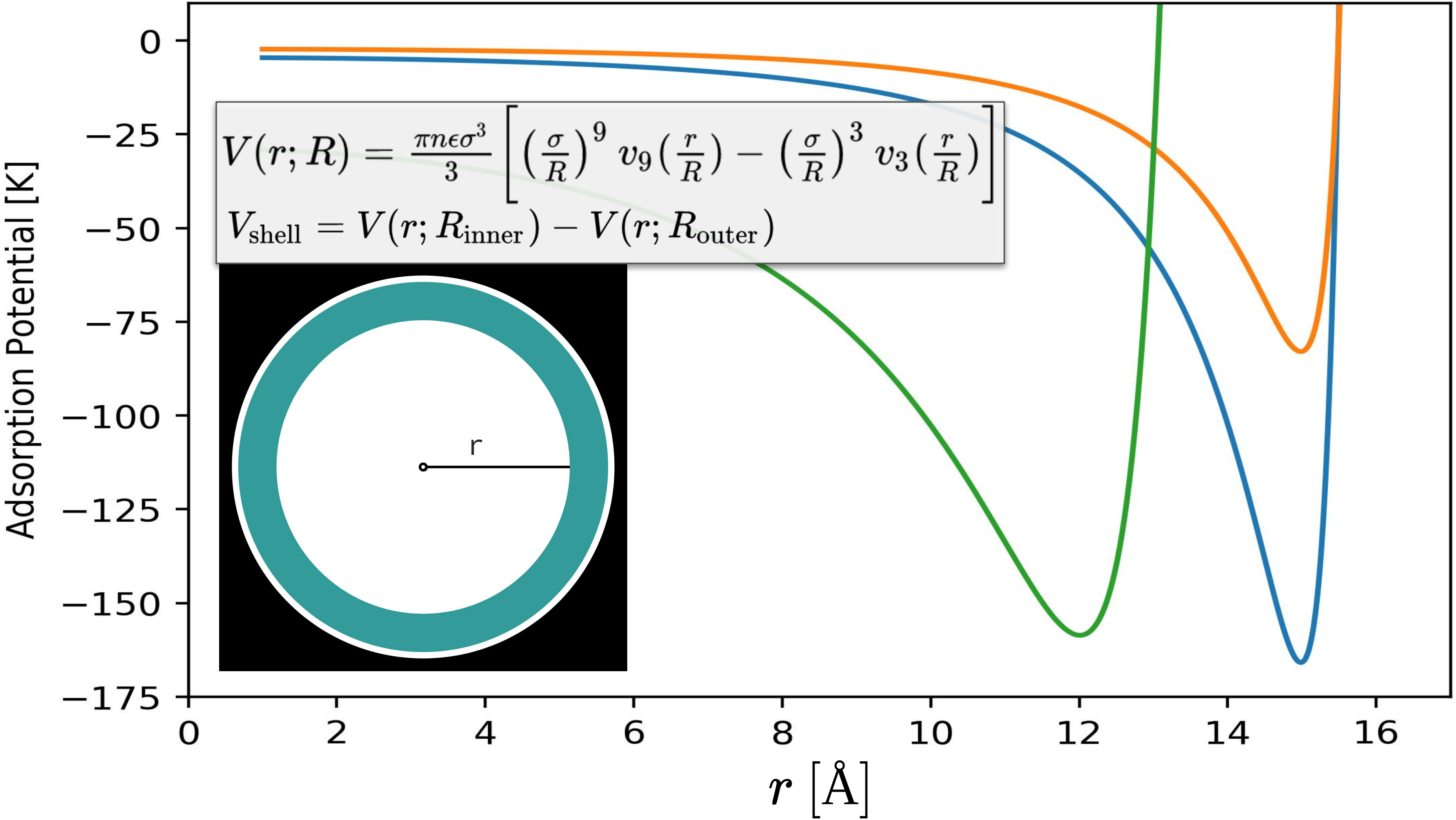

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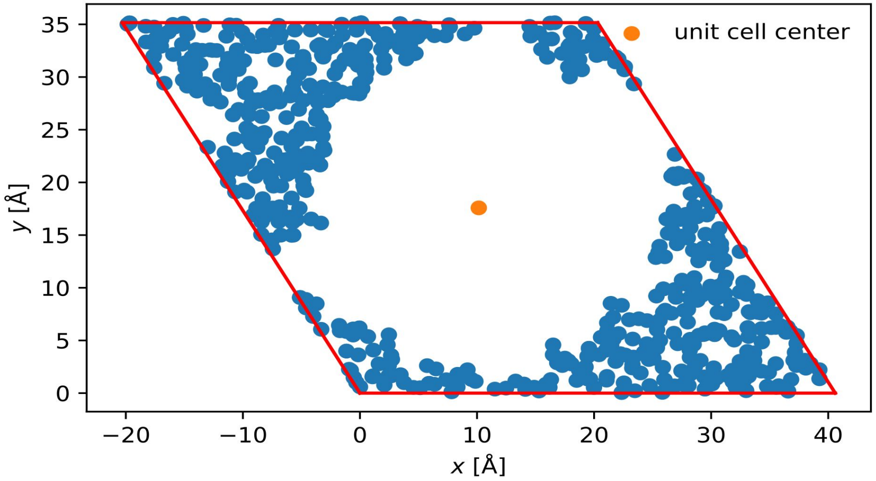
r [Å]

calculating the effective many-body potential

- sum of Lennard-Jones

$$U(\vec{r}) = \sum U_{\mathrm{LJ}}(|\overrightarrow{r_i} - \vec{r}|, \sigma_i, \epsilon_i)$$

Atom pair	σ [Å]	$\epsilon / k_{\mathrm{B}}$ [K]
Si-Si	3.804	155.858
O-O	3.033	48.115
H-H	2.846	0.0503
He-He	2.640	10.9

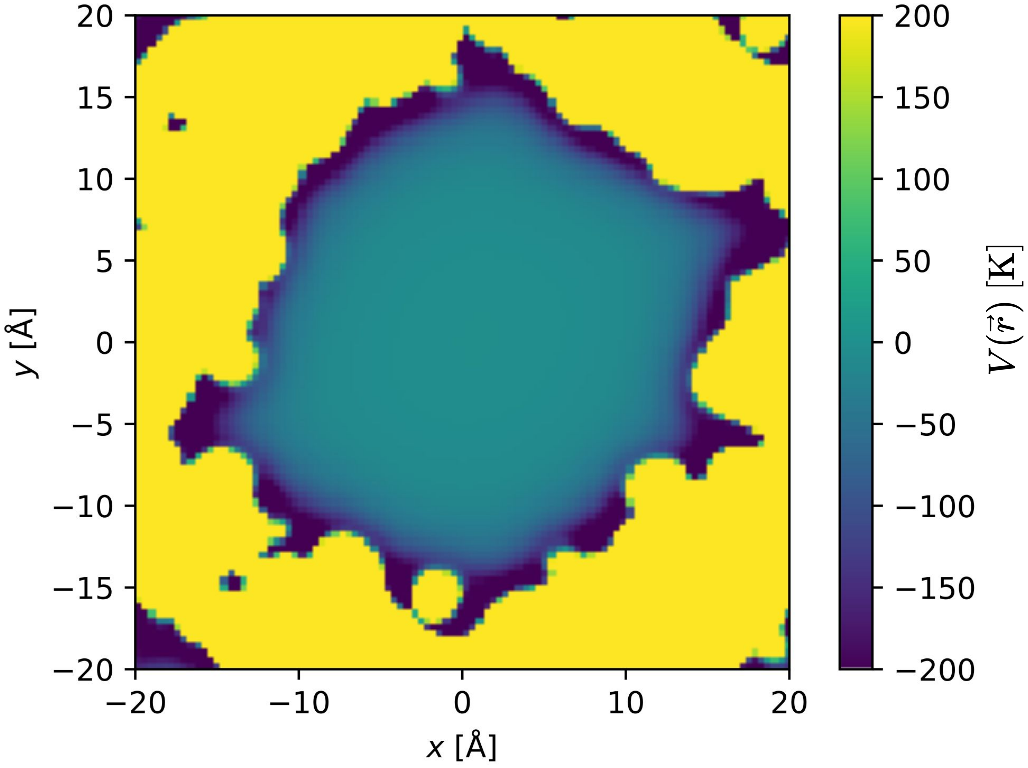


$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$$

$$\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$$

Chang *et al.* (2015) 10.1016/j.apsusc.2015.01.084
Talu and Myers (2001) 10.1016/S0927-7757(01)00628-8

effective many-body potential inside the pore



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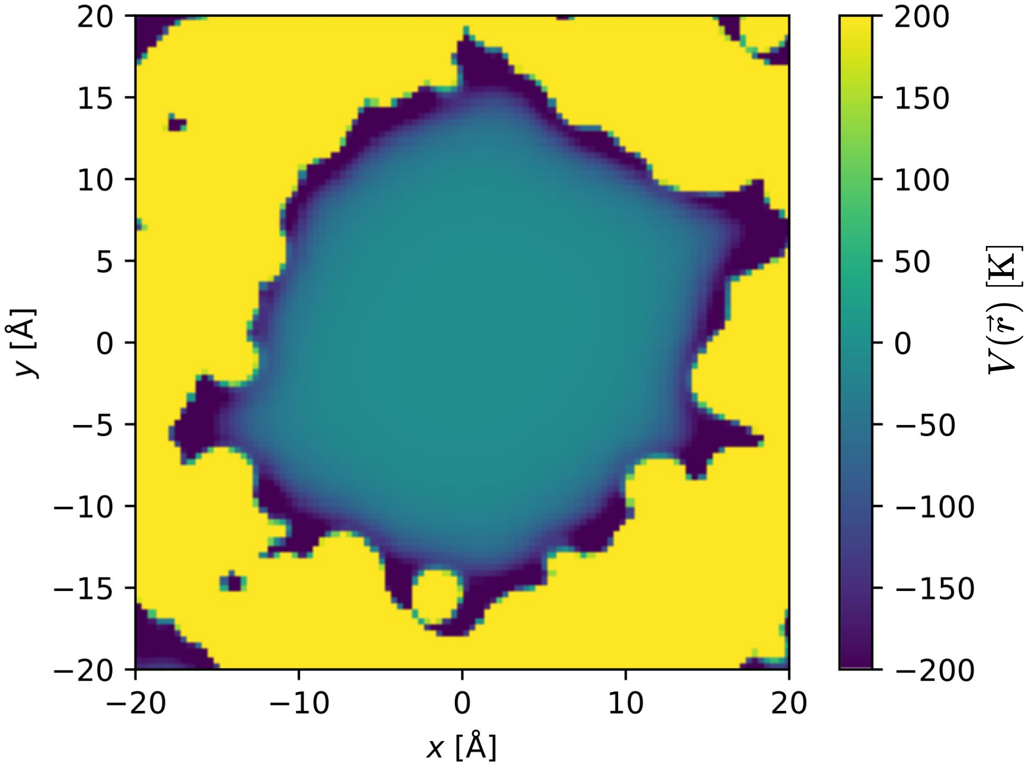
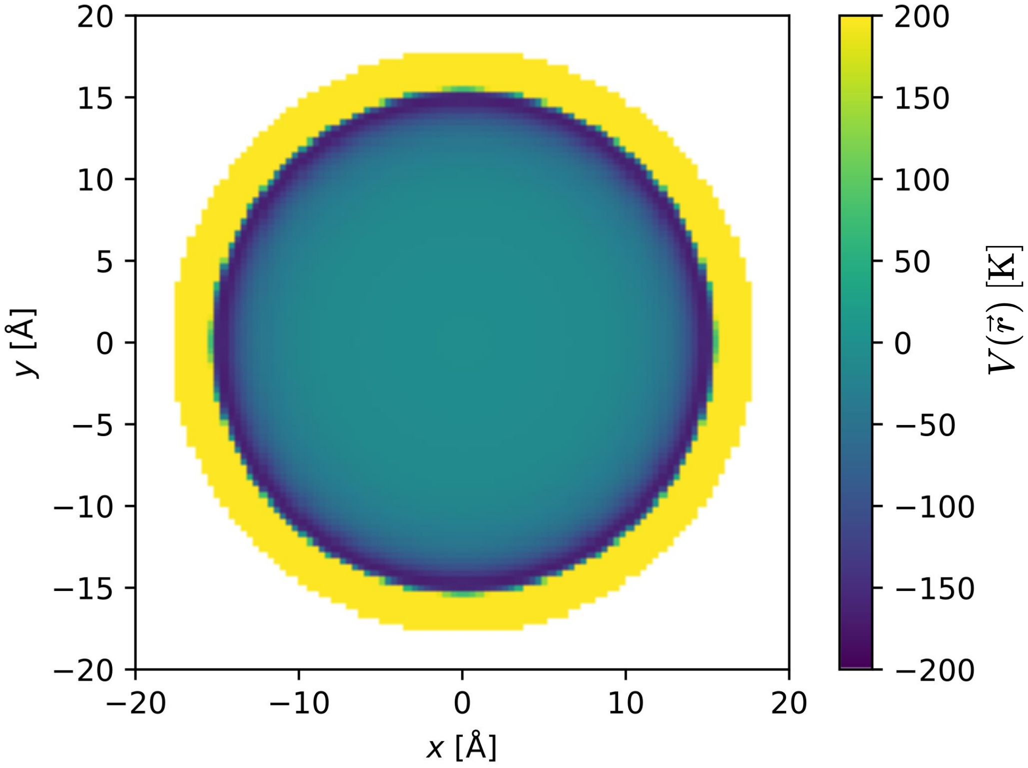
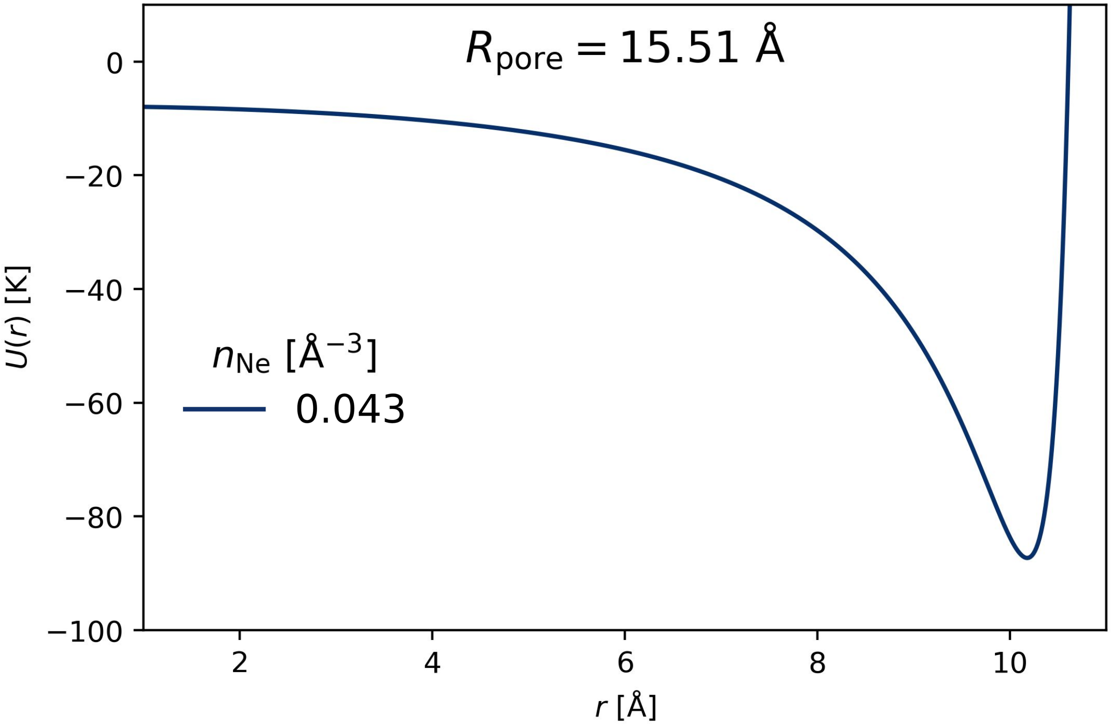


cylindrical pore in continuous media



helium in preplated MCM-41

Material	σ [Å]	ϵ/k_B [K]
MCM-41	3.44	1.59
Ar	3.02	36.14
Ne	2.71	20.16



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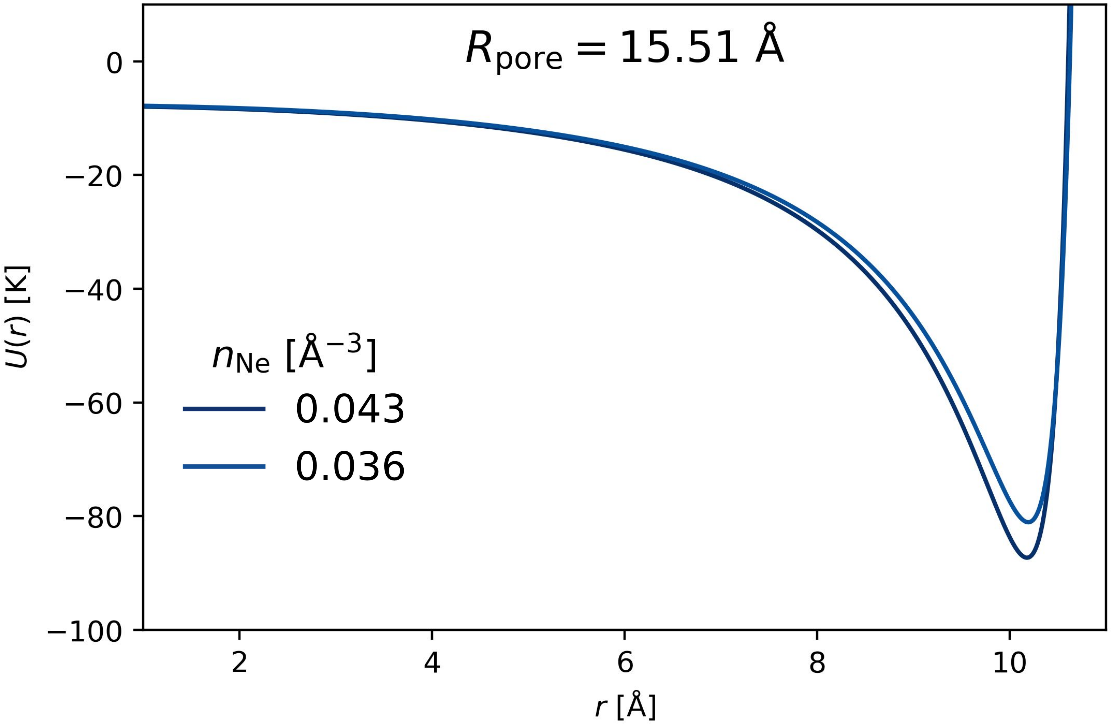

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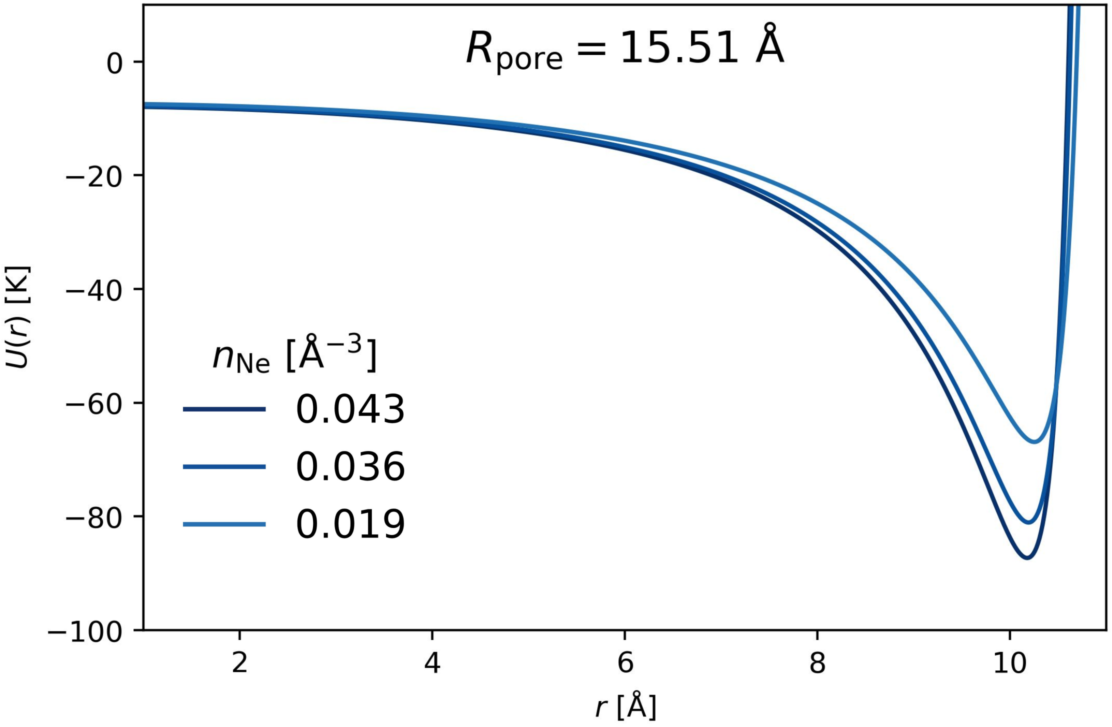

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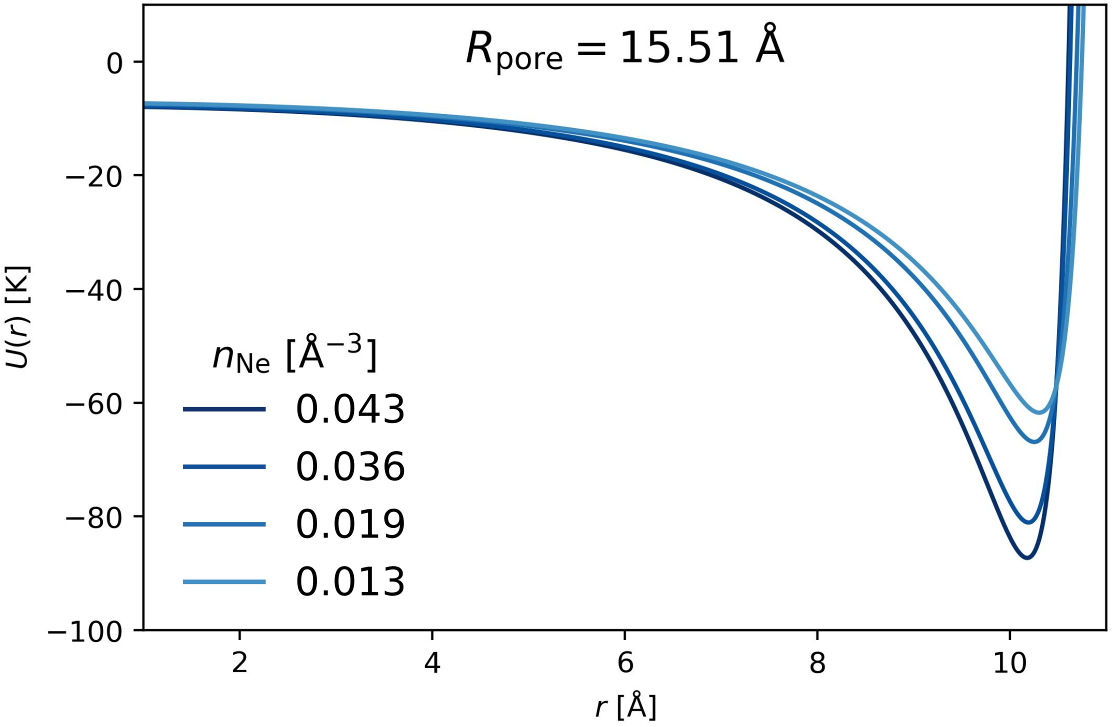

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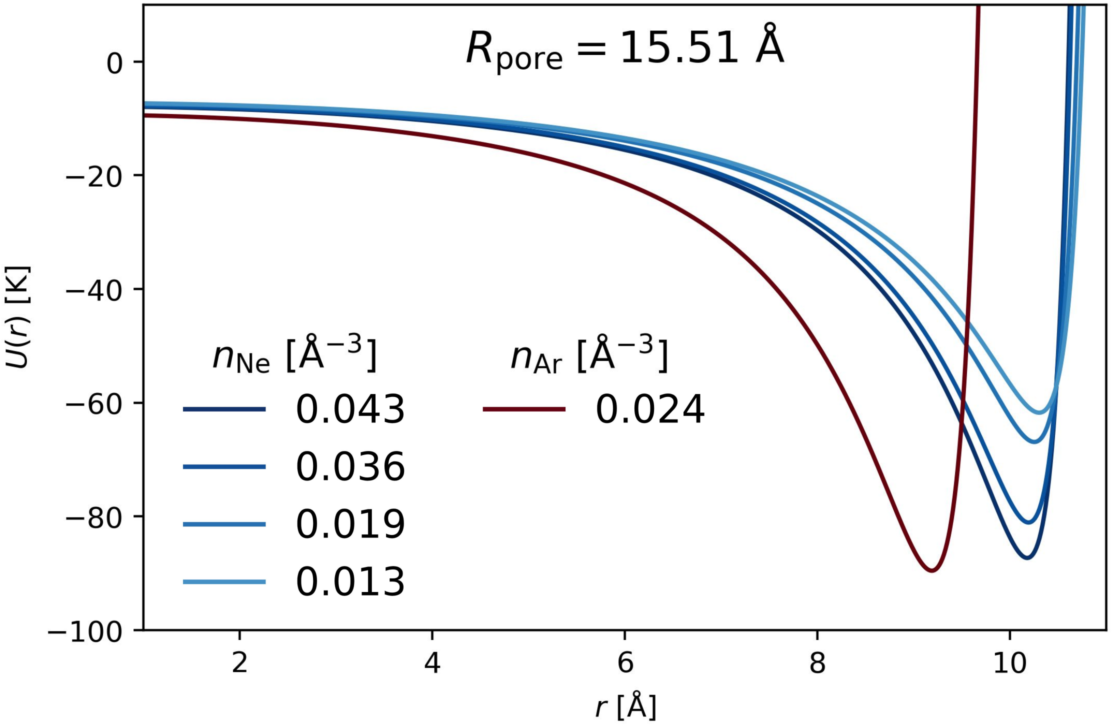

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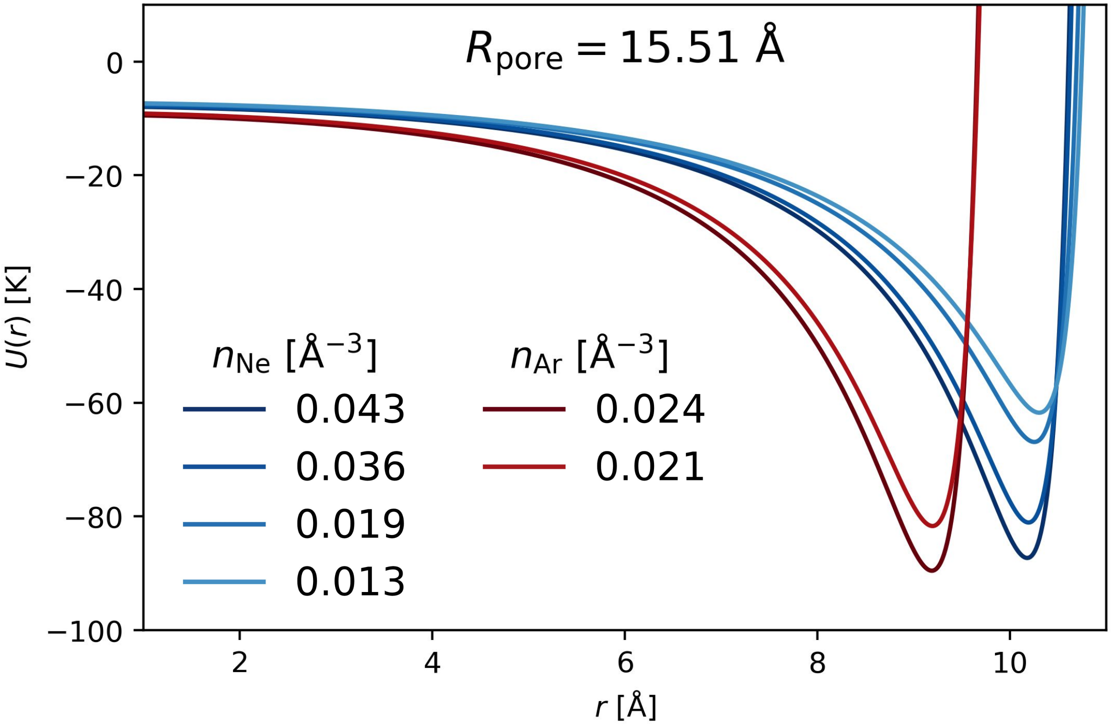

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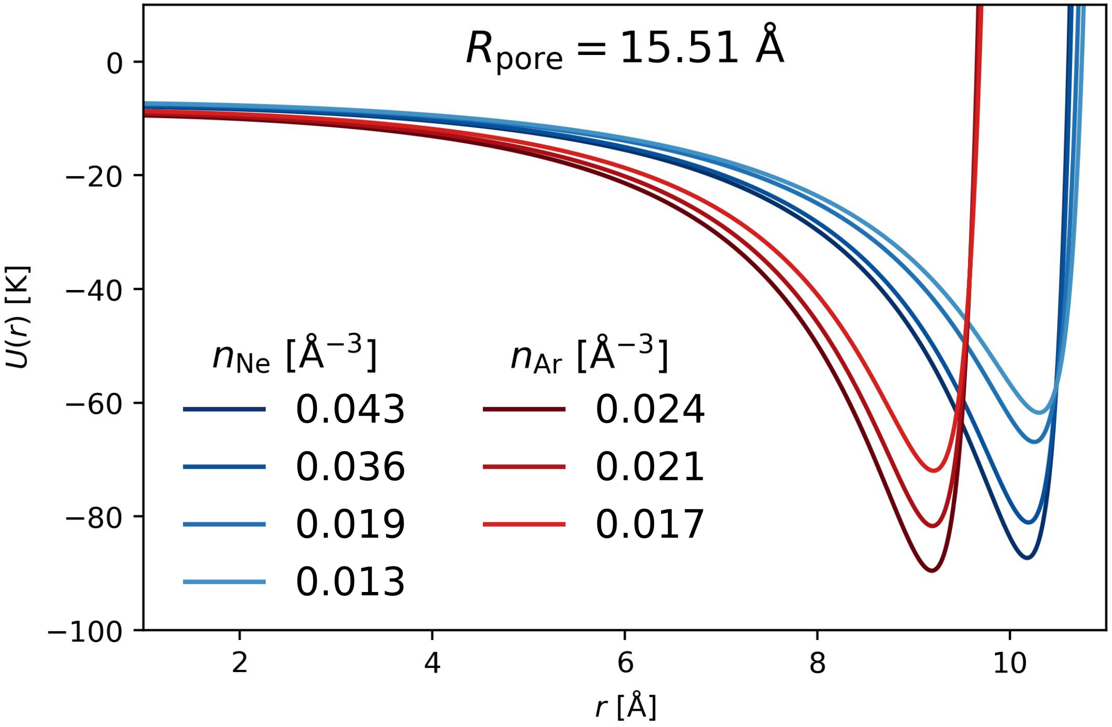


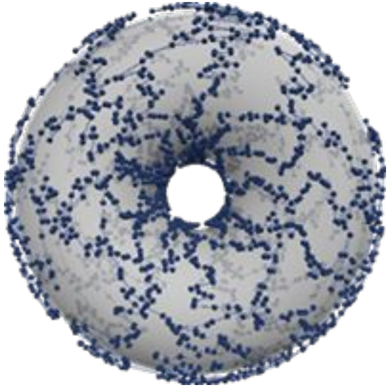
How is internal structure of the helium affected?

PIMC Summary

$$\mathcal{Z}(\beta) = \lim_{M\to\infty} \int dR_1 \ldots dR_M e^{-\sum_{t=1}^{M} S(R_{t-1},R_t;\beta/M)}$$

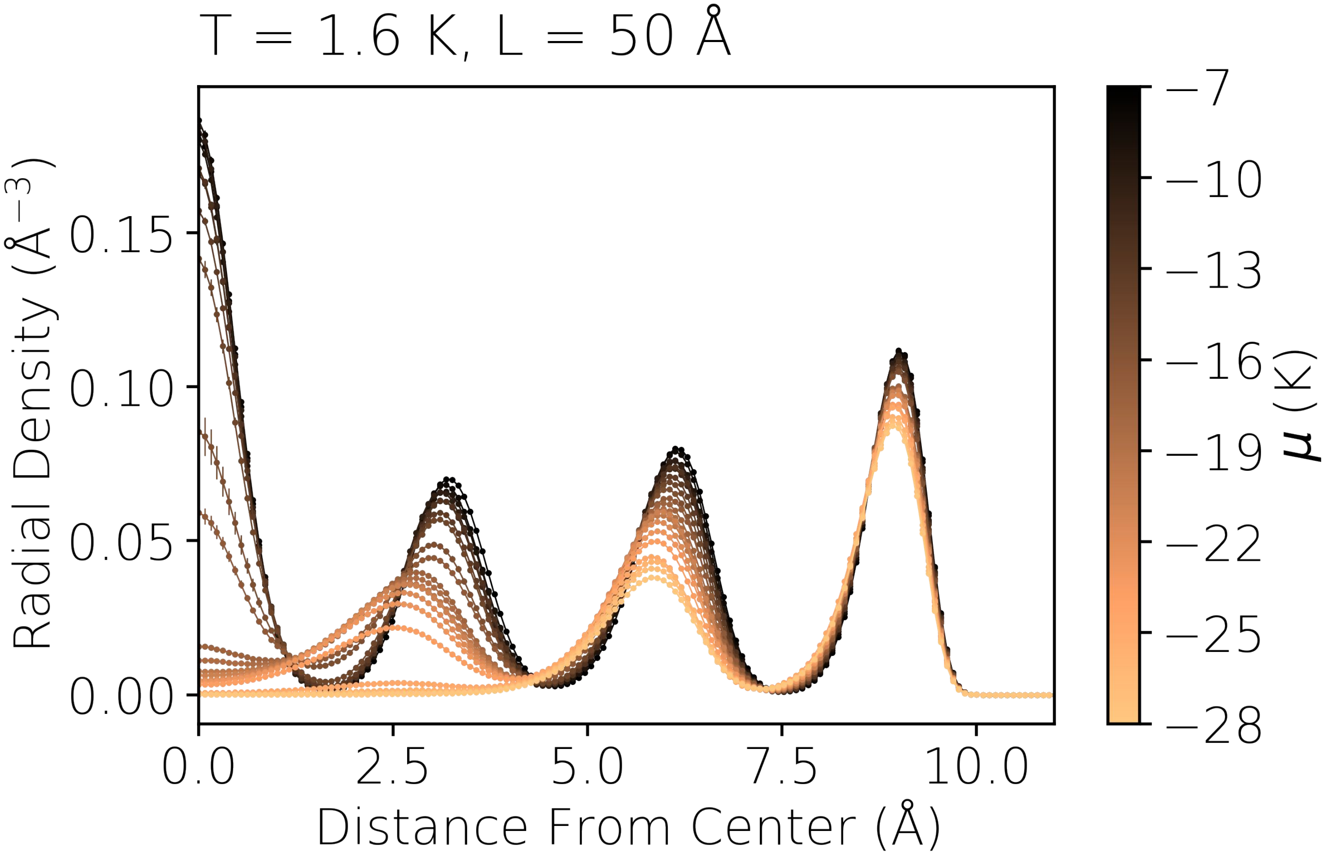
$$\langle O \rangle = \mathcal{Z}^{-1} \int d\mathbf{R} d\mathbf{R}' \rho(\mathbf{R},\mathbf{R}';\beta) \langle \mathbf{R}|O|\mathbf{R}' \rangle$$

code.delmaestro.org

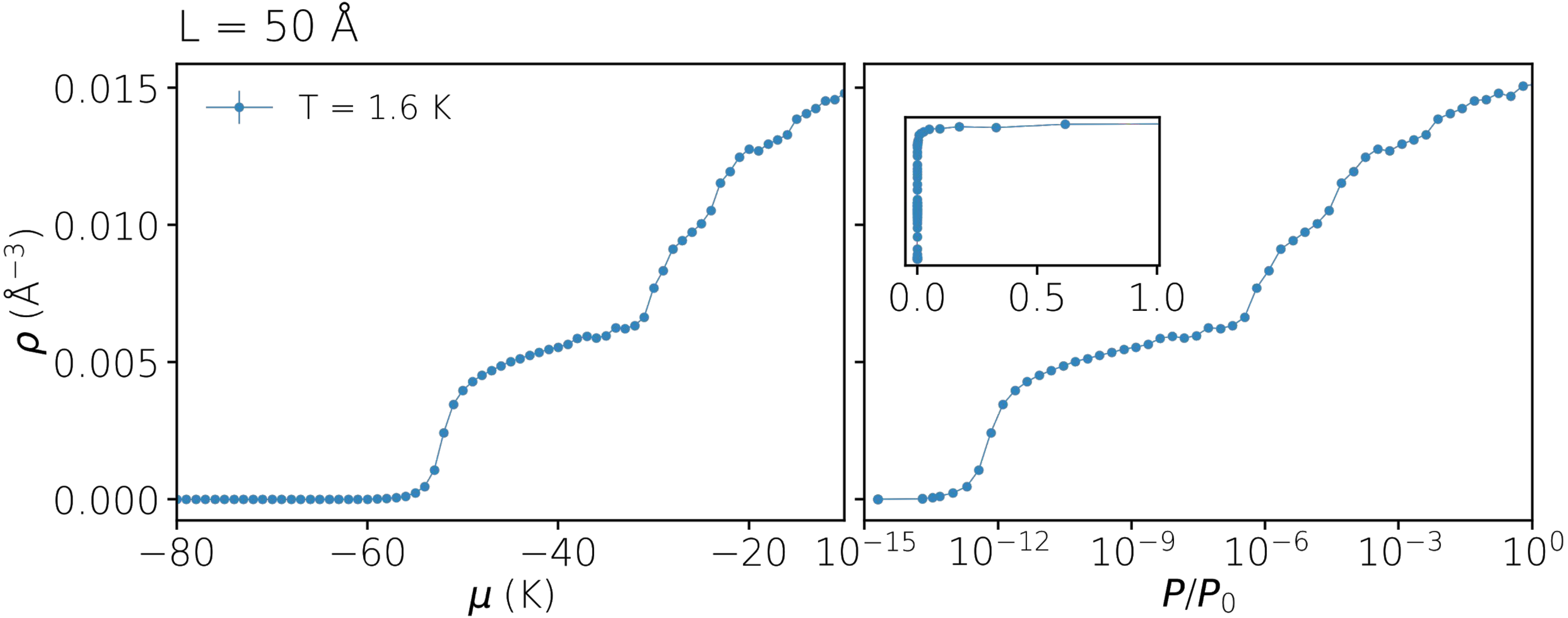


Ceperley (1995) 10.1103/RevModPhys.67.279
Boninsegni (2006) 10.1103/PhysRevE.74.036701

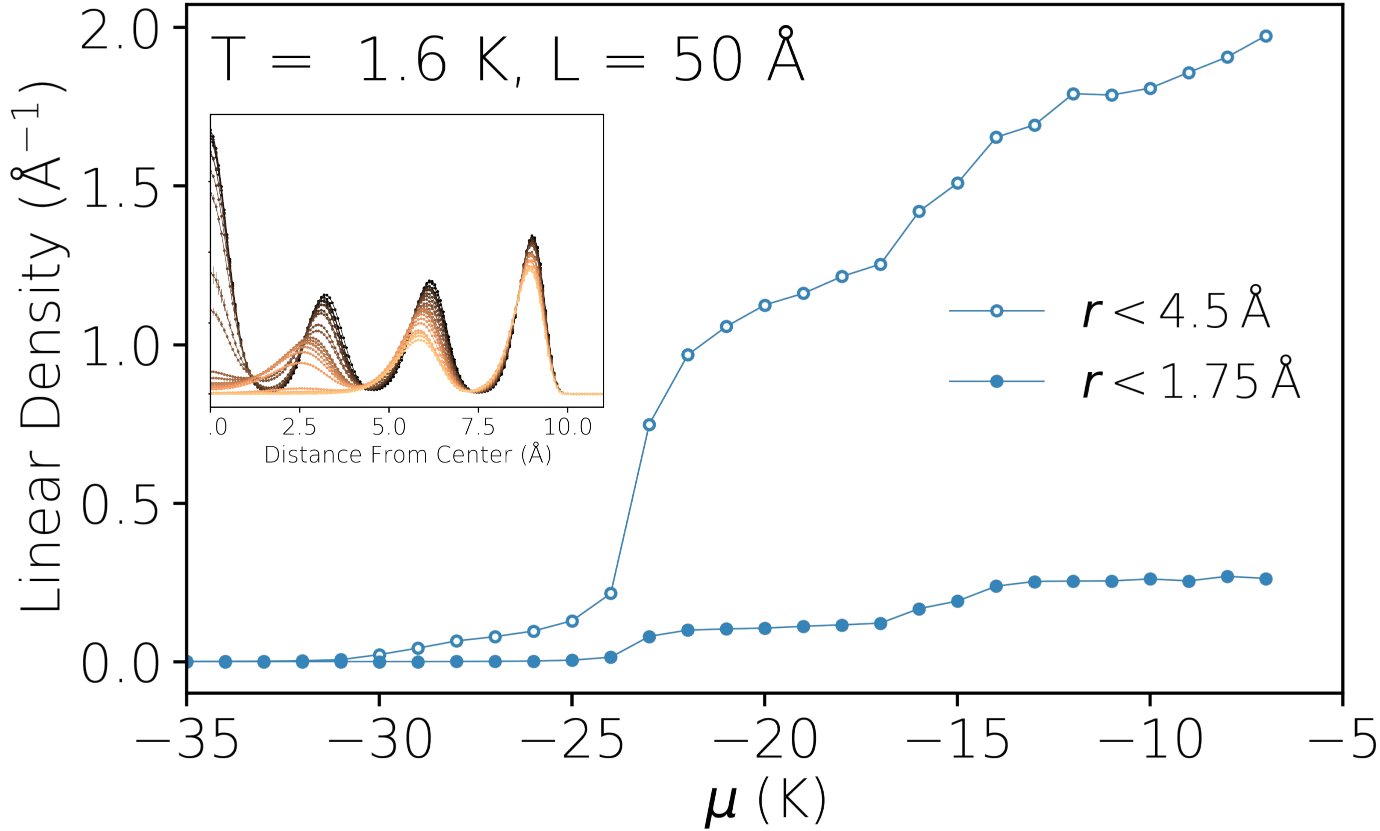
radial density of helium in pore



filling the pore

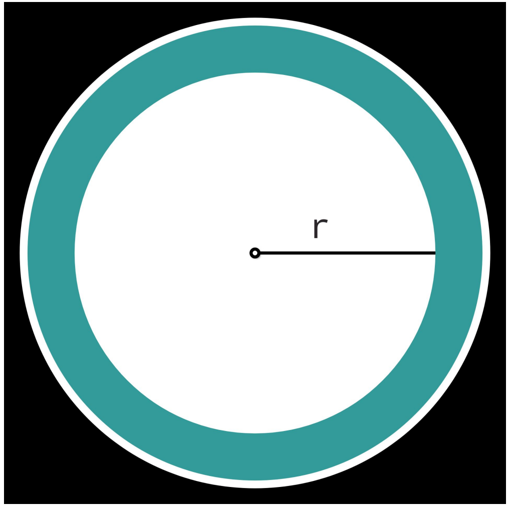


linear density of the central channel



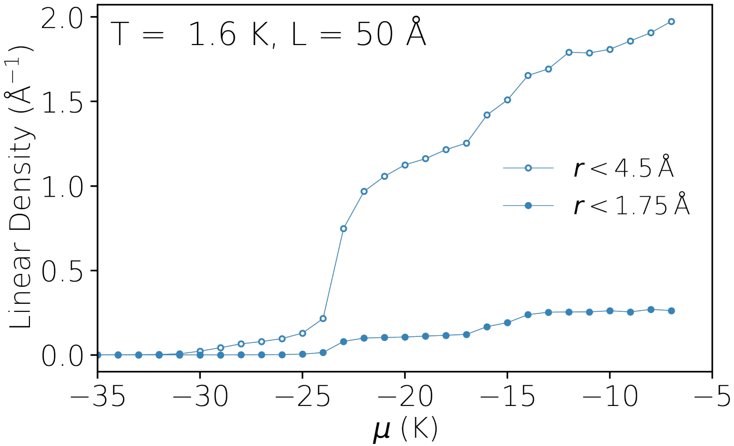
summary

- tunability of confining potential
  - pore size
  - plating material
- interesting structural effects
  - linear density
  - pore filling

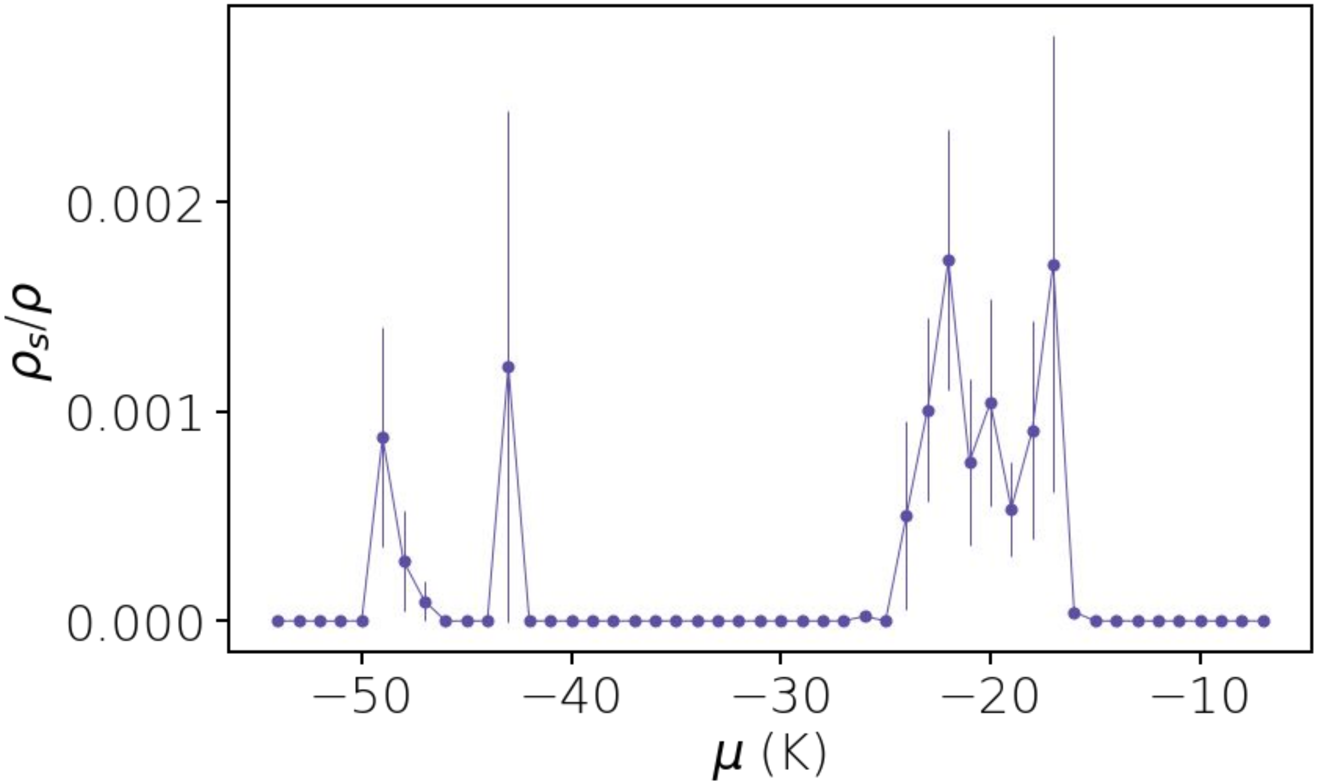


future work

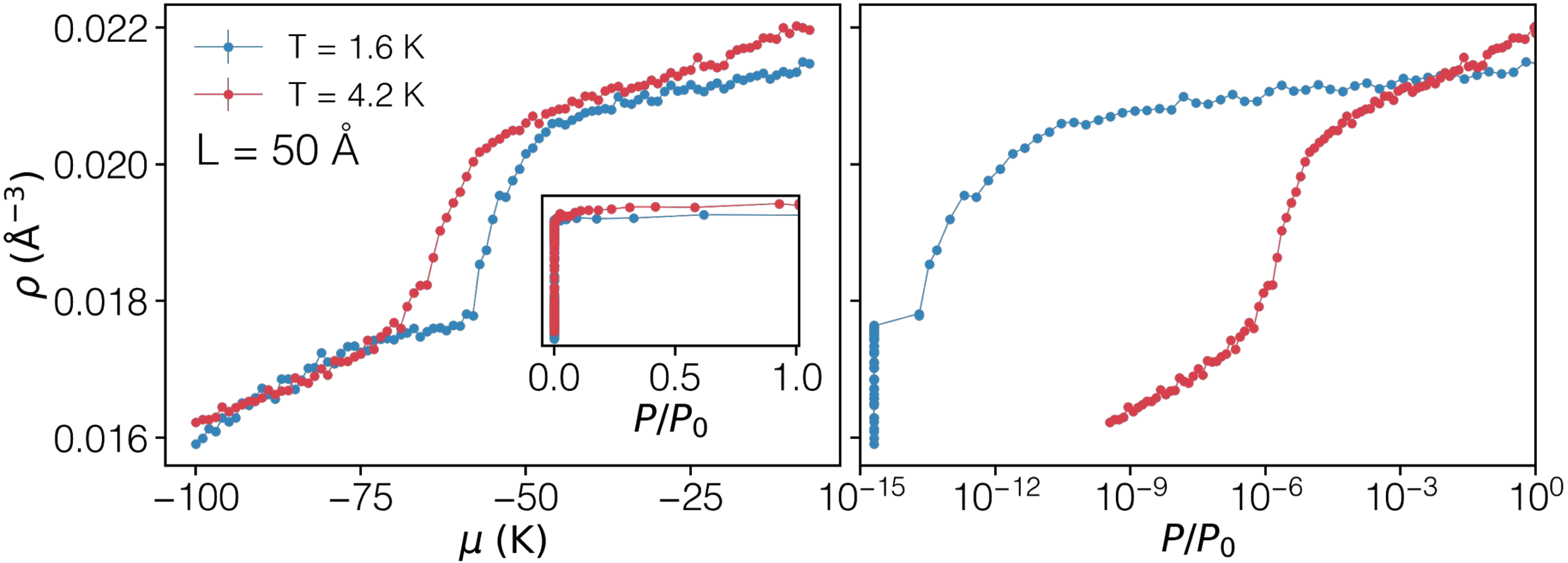
- superfluidity measurements
- evaluate dynamic structure factor
  - connect to neutron scattering experiments
- different plating material



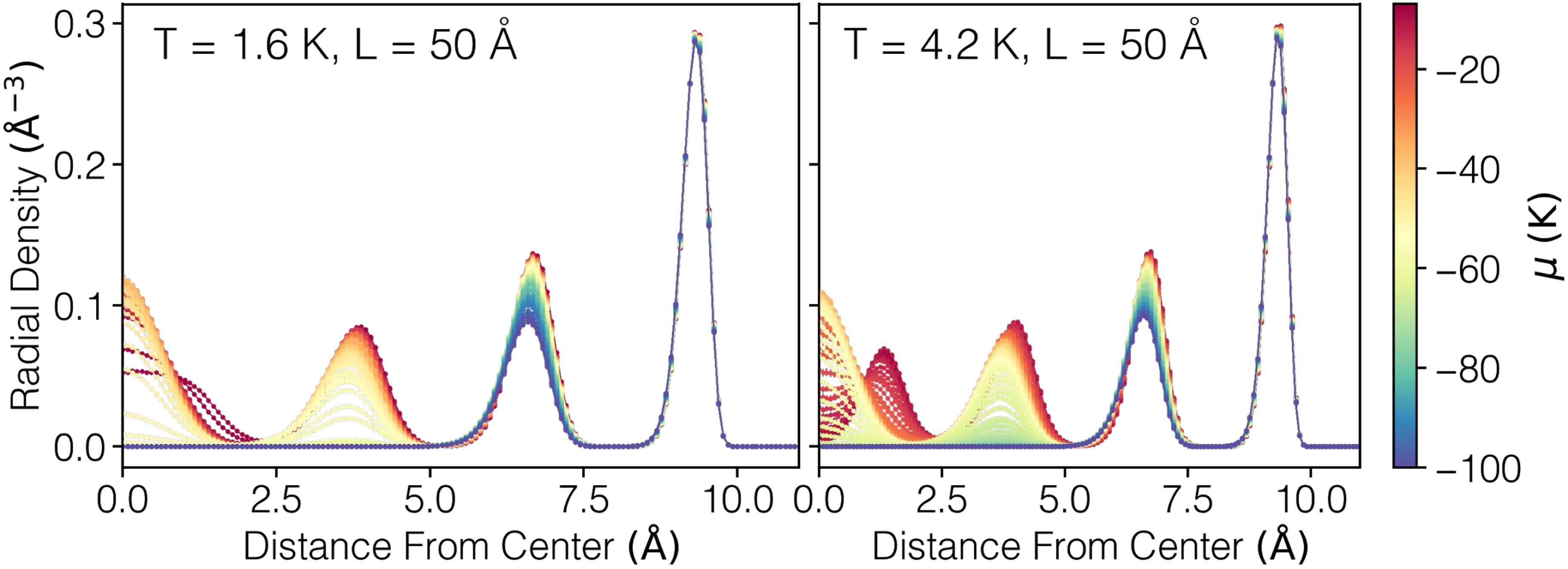
superfluidity



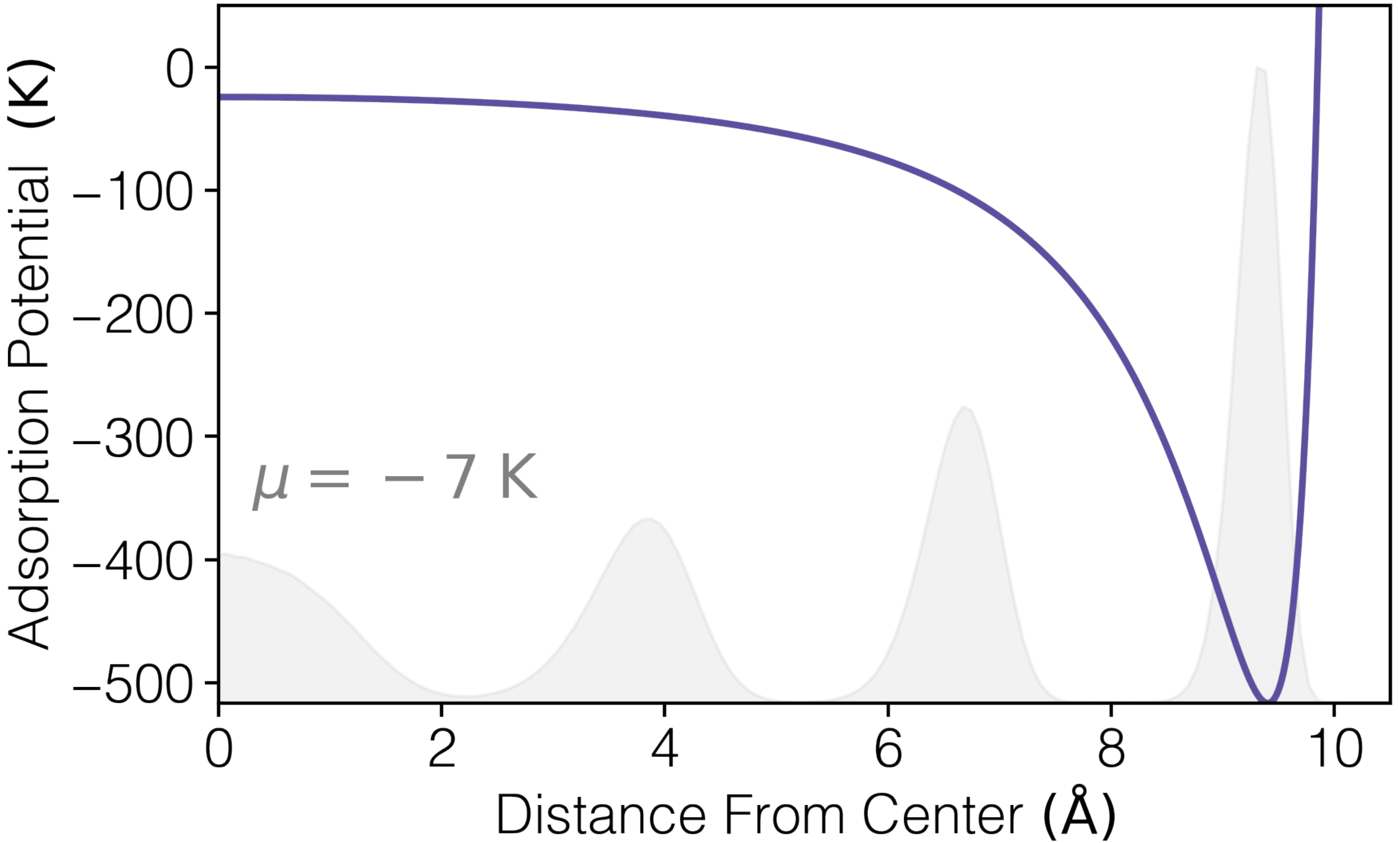
filling the pore



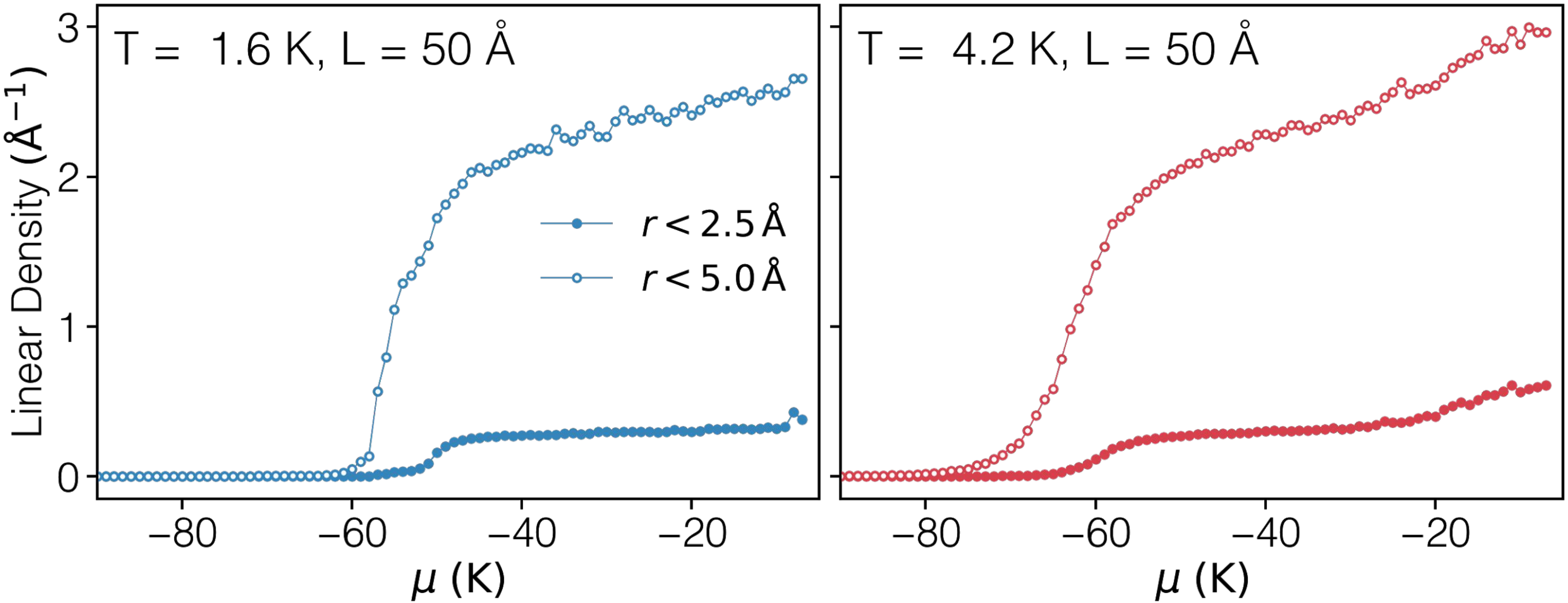
radial density



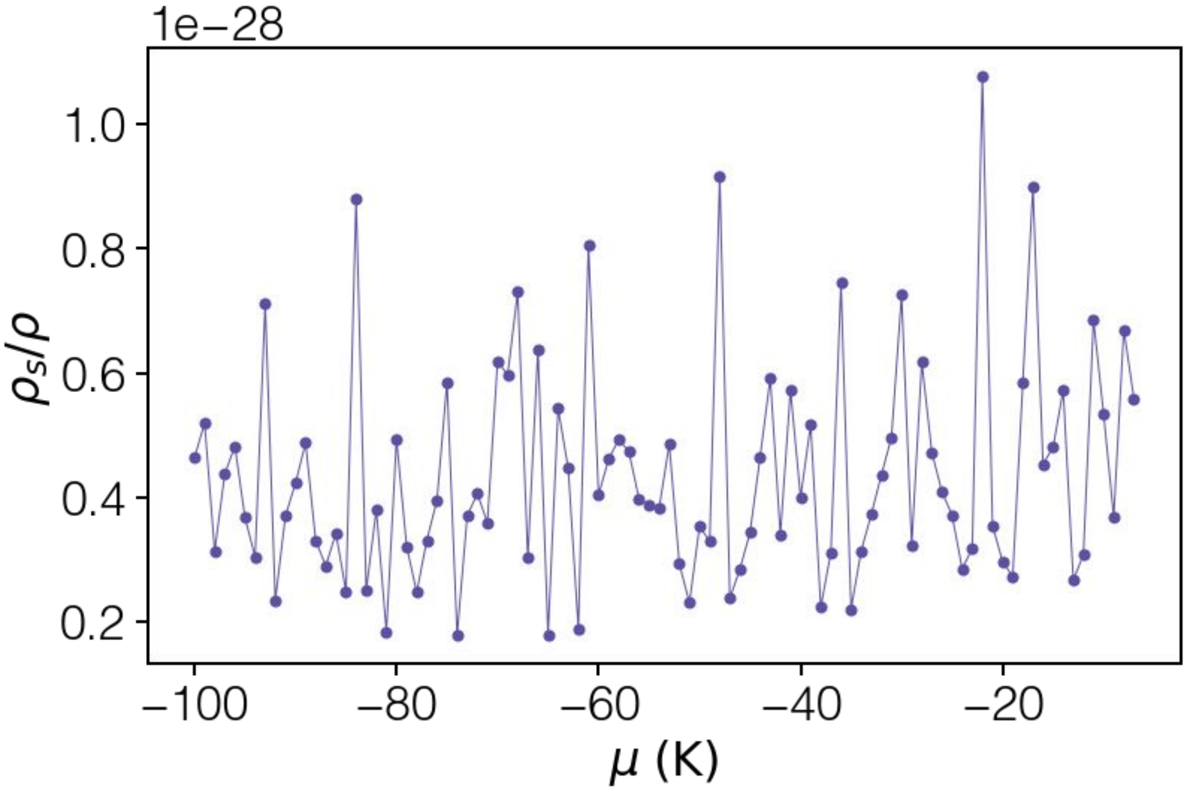
radial density with external potential



linear density



superfluidity



cavity in an infinite medium

$$V(\vec{r};R) = n \int_{\vec{r}' \notin \mathcal{C}_R} d^3r' \; U(|\vec{r} - \vec{r}'|)$$

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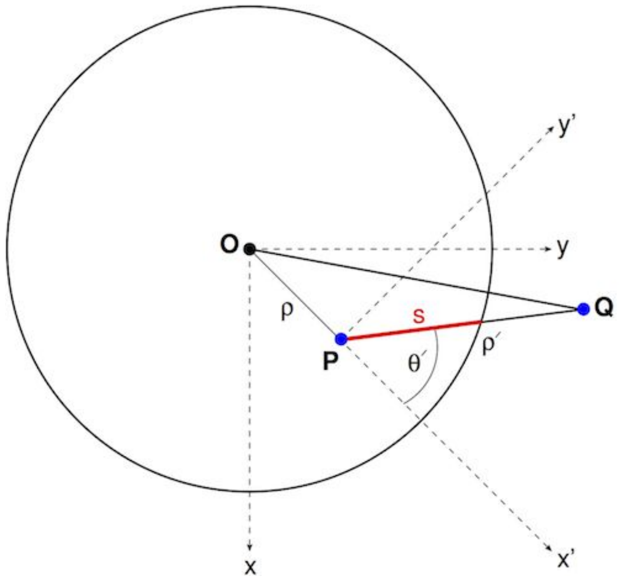
$$V(\rho; R) = n \iiint d\theta' \, dz' \, d\rho' \, \rho' U \left(\sqrt{z'^2 + \rho'^2} \right)$$



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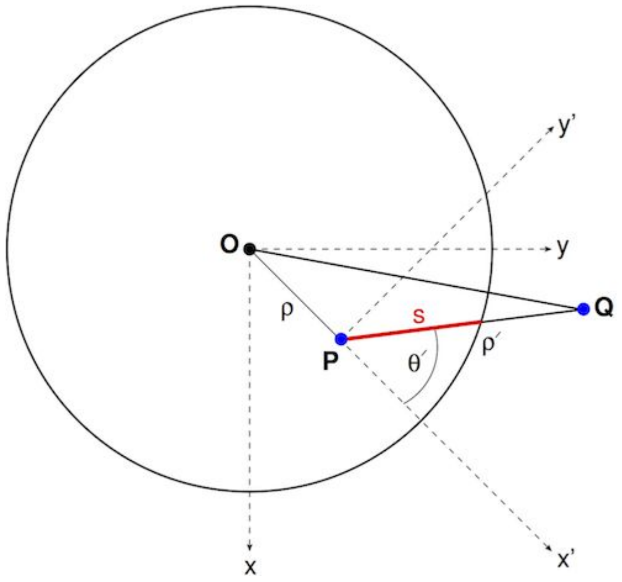

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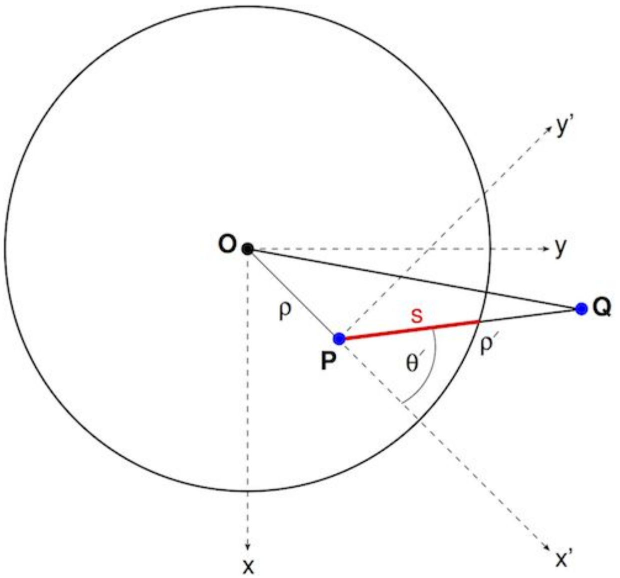

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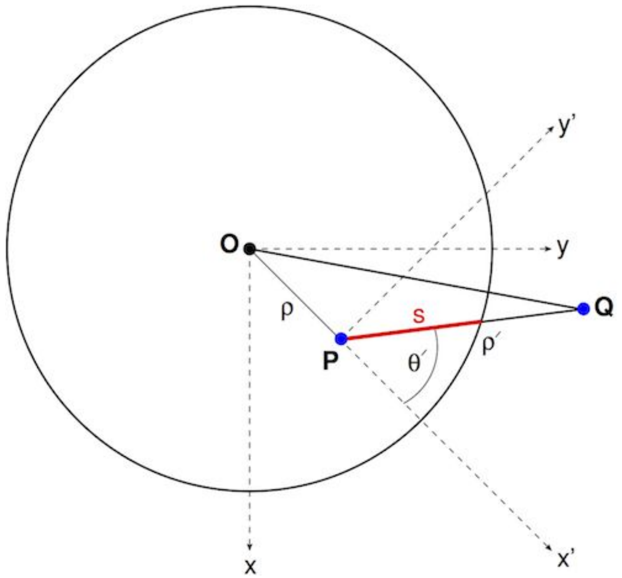

$$v_9(x) = \frac{1}{240(1-x^2)^9} \left[(1091 + 11156x^2 + 16434x^4 + 4052x^6 + 35x^8) E(x) \right.$$
$$\left. - 8(1-x^2)(1+7x^2)(97 + 134x^2 + 25x^4) K(x) \right]$$

$$v_3(x) = \frac{2}{(1-x^2)^3} \left[(7 + x^2) E(x) - 4(1-x^2) K(x) \right]$$

cavity in an infinite medium

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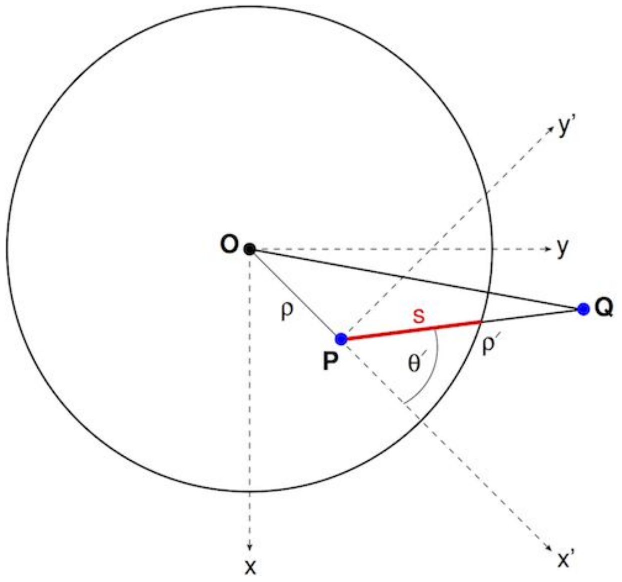
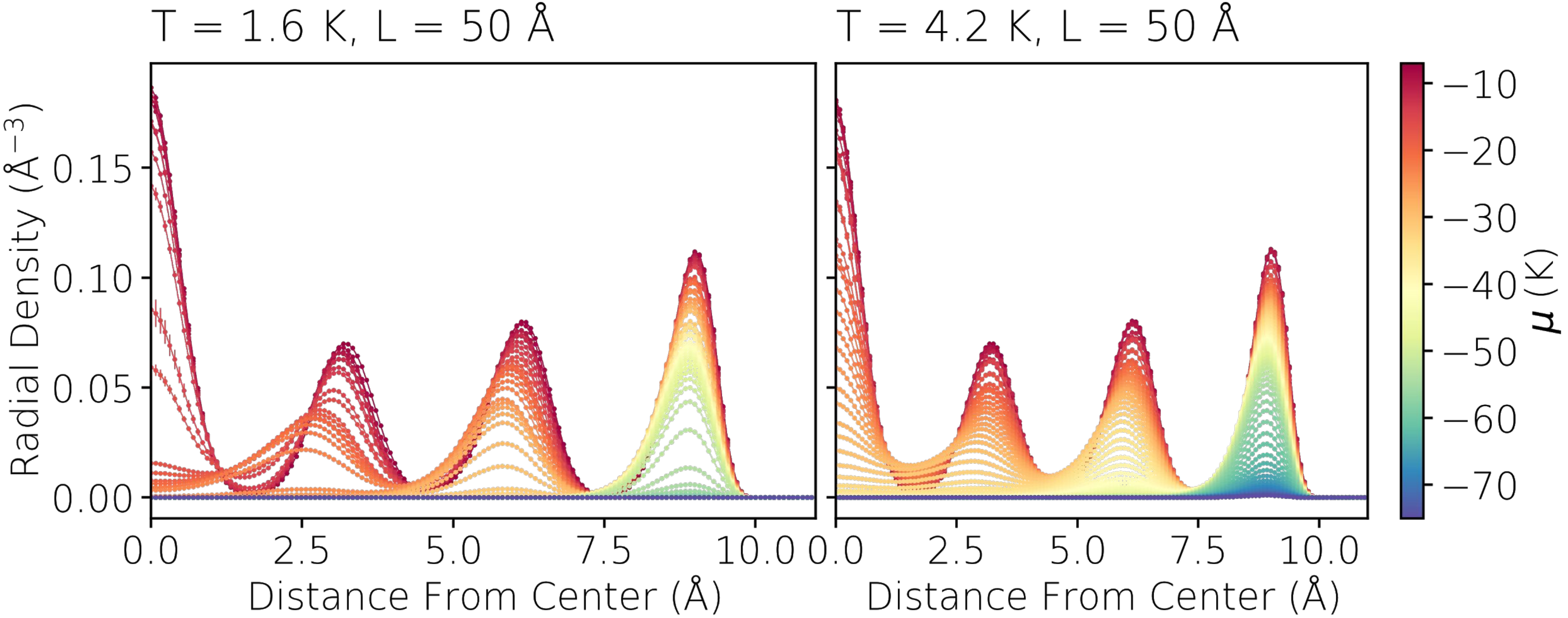


radial density



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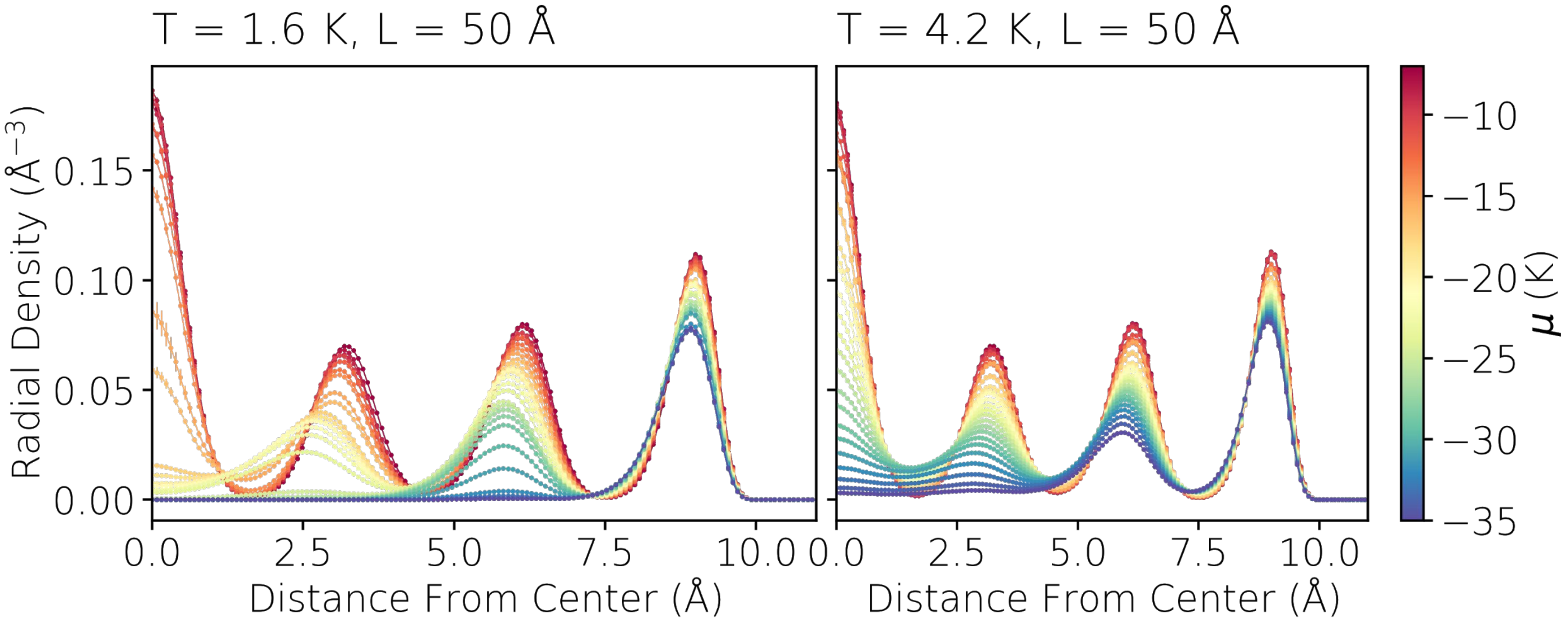
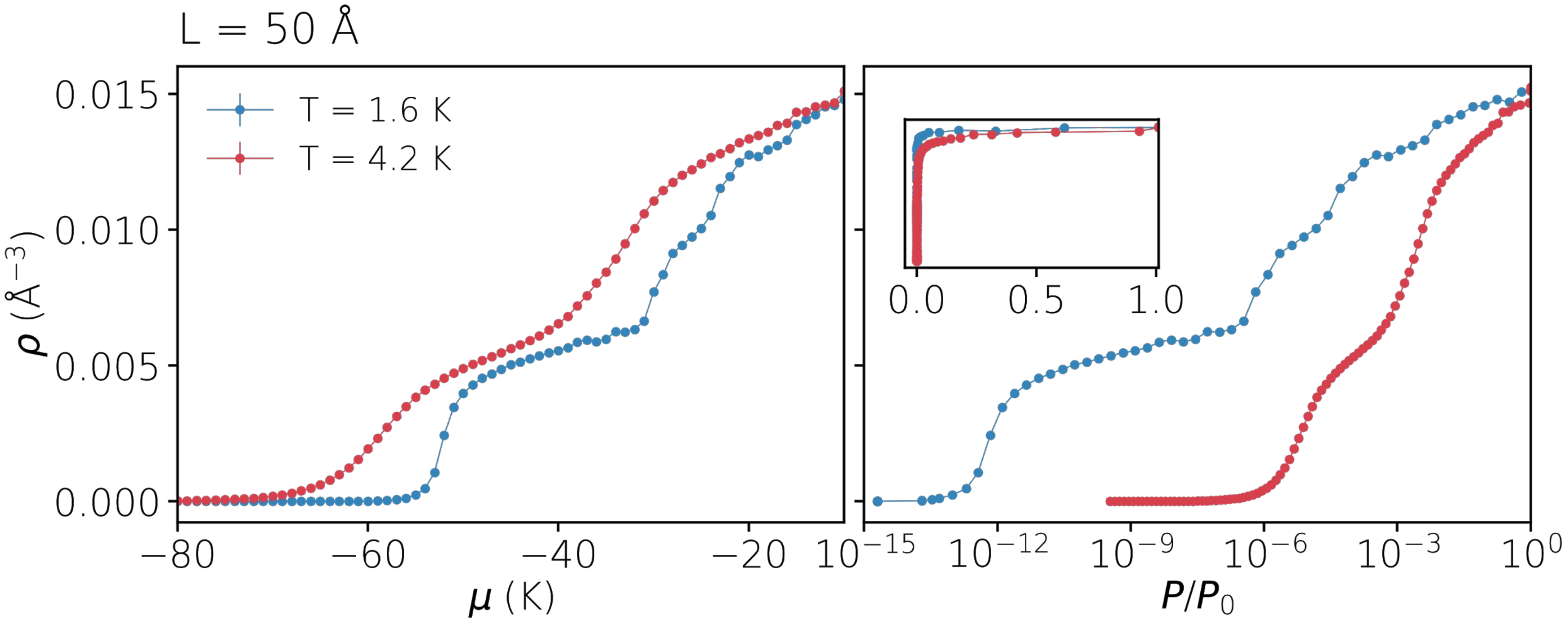
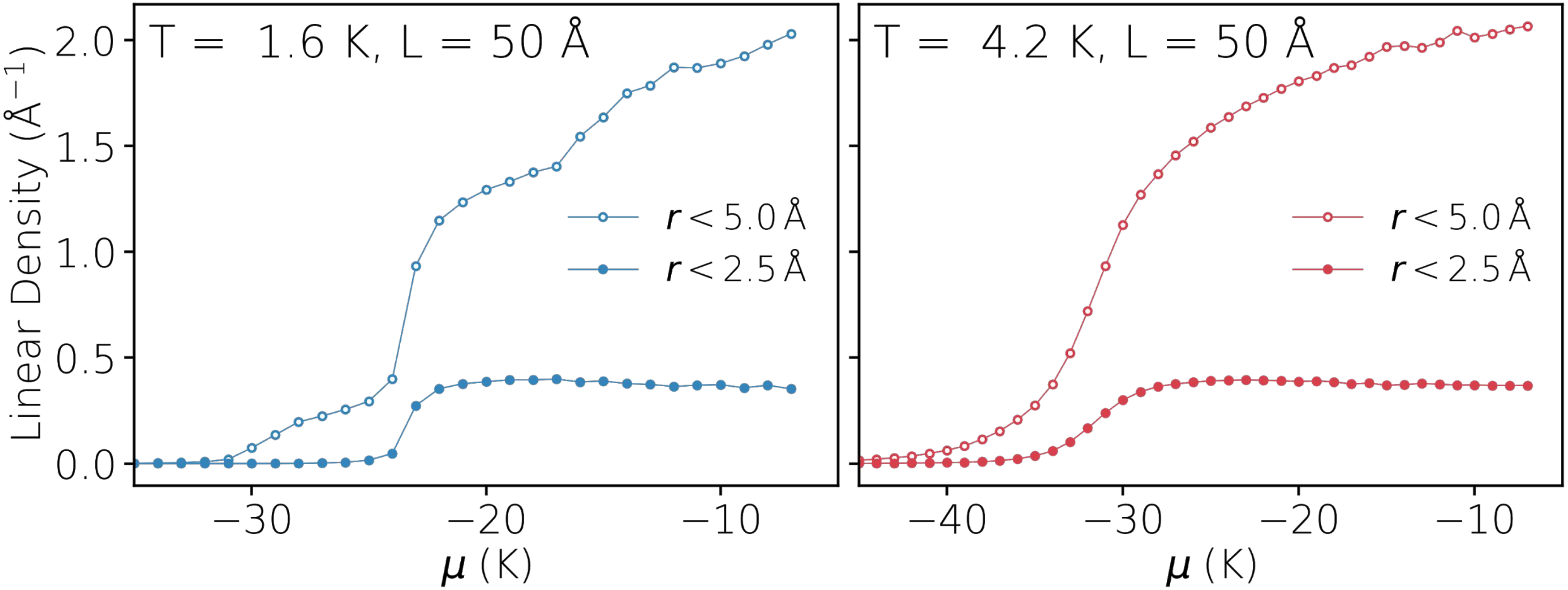


filling the pore



linear density



radial density with external potential