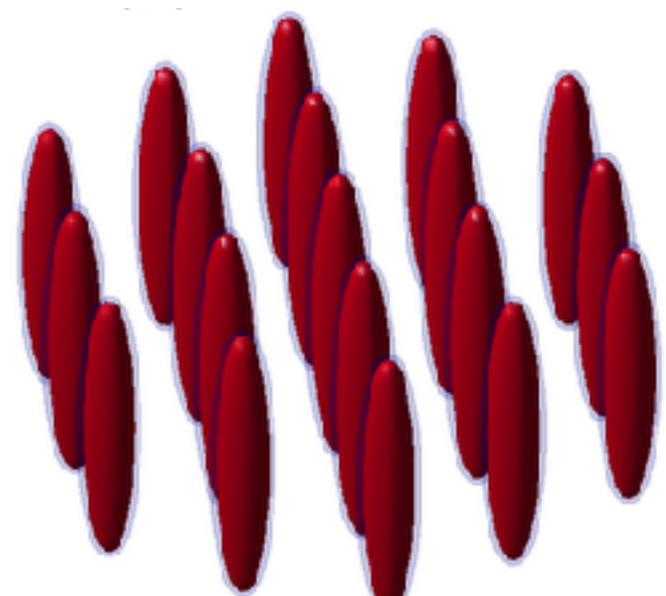
Computing droplet crystals of a magnetic quantum gas

Blair Blakie
Department of Physics, University of Otago, New Zealand
work with **Danny Baillie**



D. Baillie, R.M. Wilson, R.N. Bisset, & P.B. Blakie, PRA **94**, 021602(R) (2016).
D. Baillie, R. Wilson, and P.B. Blakie, PRL **119**, 255302 (2017)
D. Baillie and P. B. Blakie, PRL **121**, 195301 (2018)

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Outline

- Physics: ultra-dilute gases that behave like liquids and solids

- How we do what we do: computational physics

Gas… boring and simple right?

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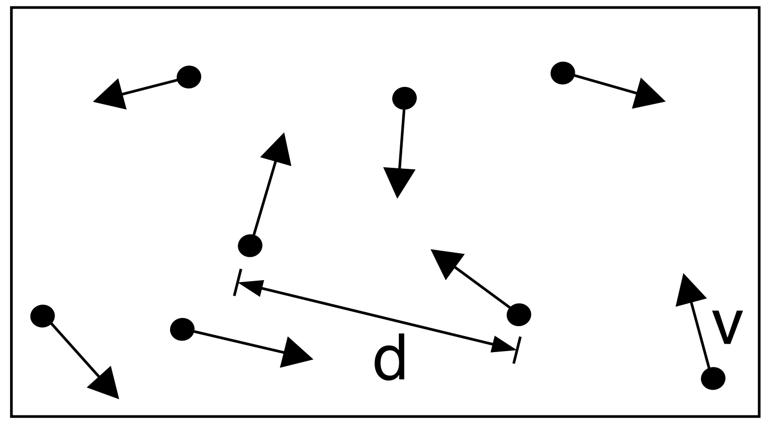

High Temperature T:

thermal velocity v

density d^{-3}

"Billiard balls"

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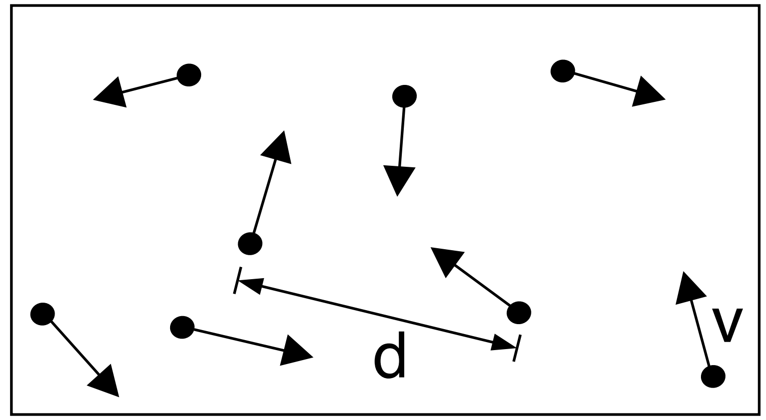

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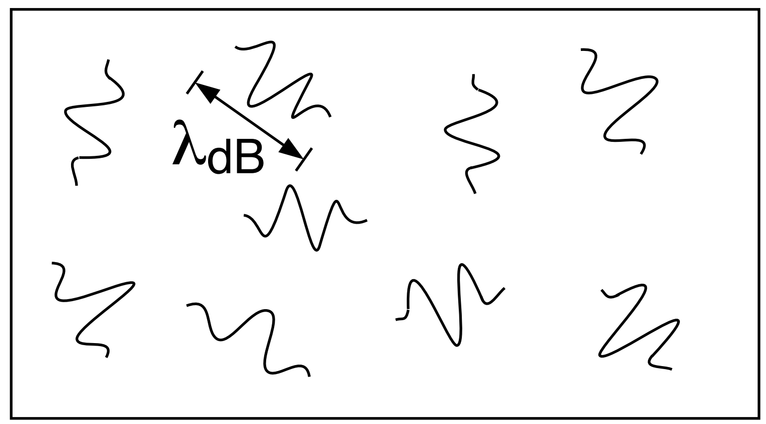

Low Temperature T:

De Broglie wavelength

$\lambda_{dB}=h/mv \propto T^{-1/2}$

"Wave packets"

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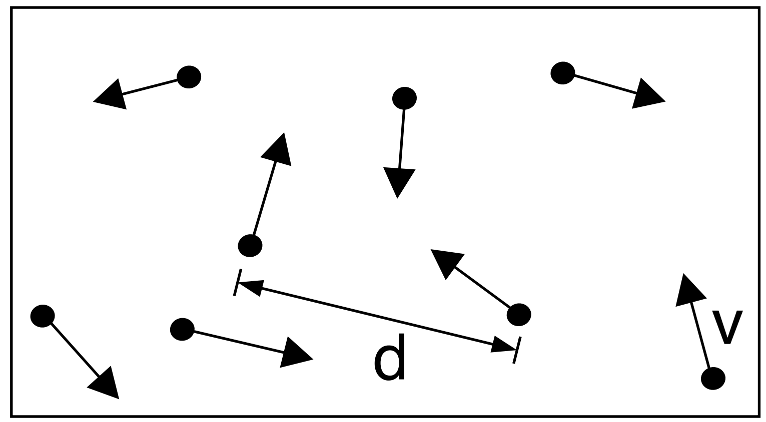

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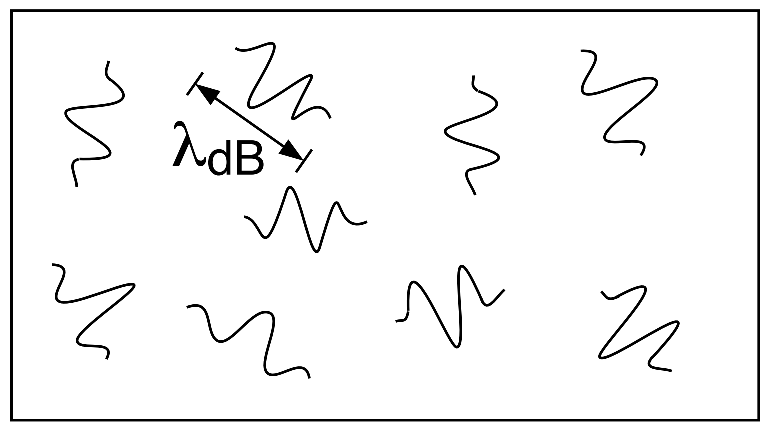

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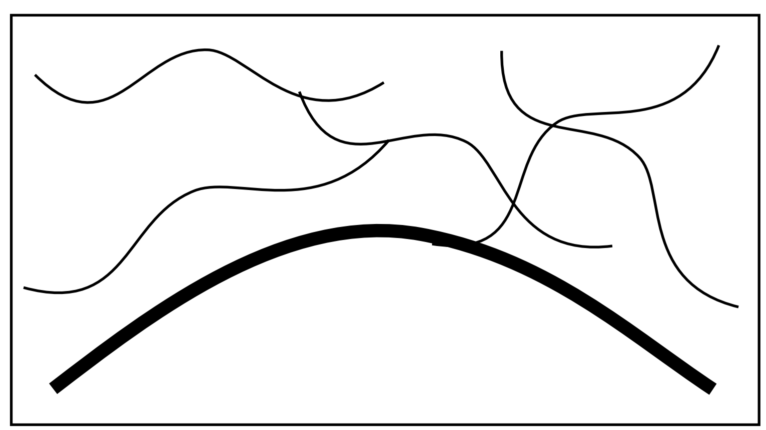

$T=T_C$:

BEC

$\lambda_{dB} \approx d$

"Matter wave overlap"

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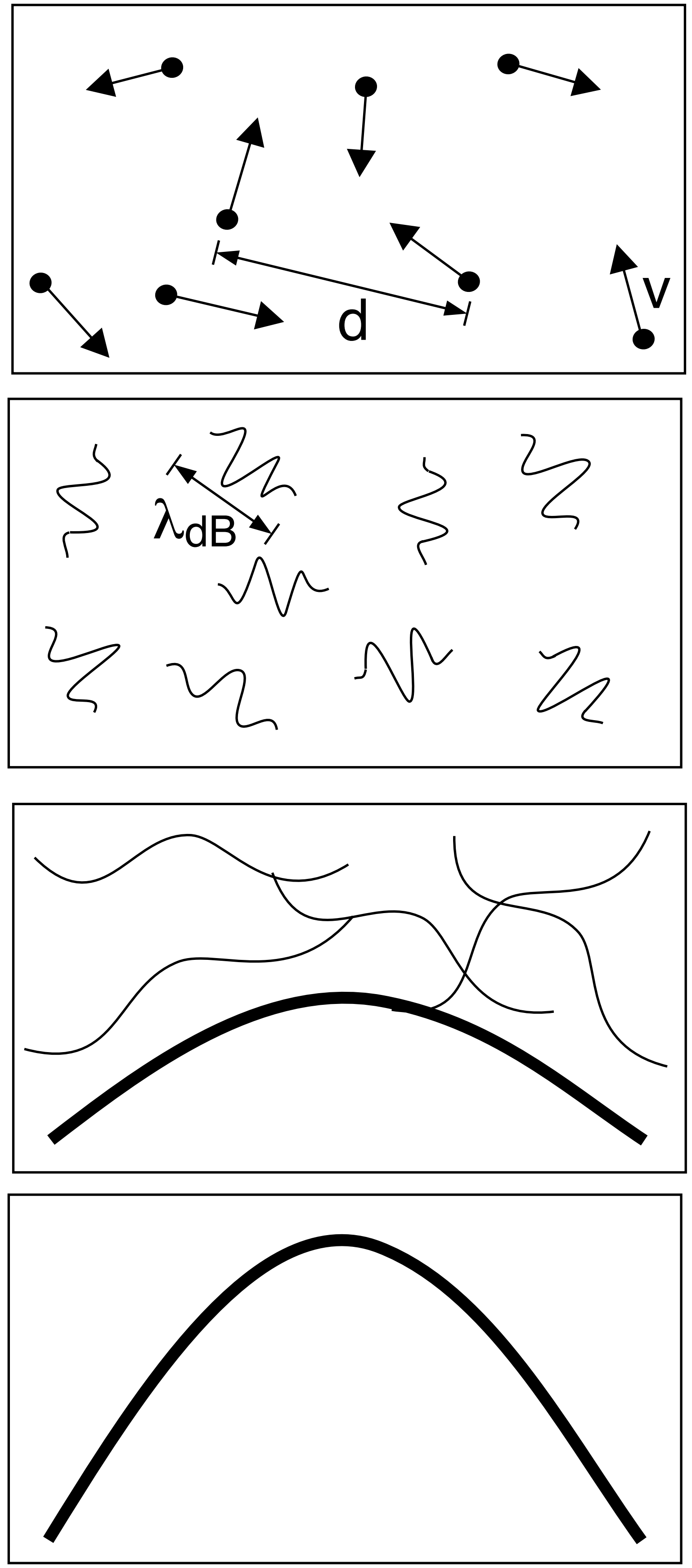

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"Wave packets"

$T=T_C$:

BEC

$\lambda_{dB} \approx d$

"Matter wave overlap"

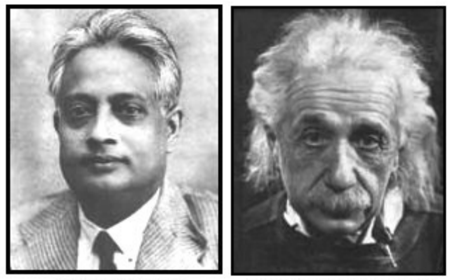
T=0:

Pure Bose condensate

"Giant matter wave"

Bose-Einstein condensation

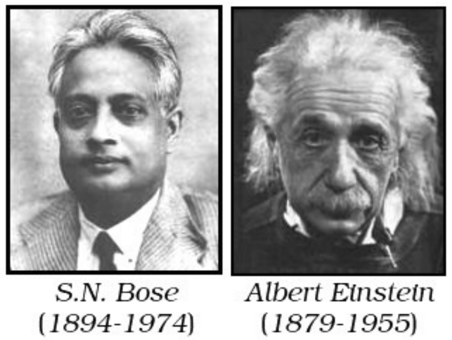
Bose-Einstein condensation



S.N. Bose (1894-1974) Albert Einstein (1879-1955)

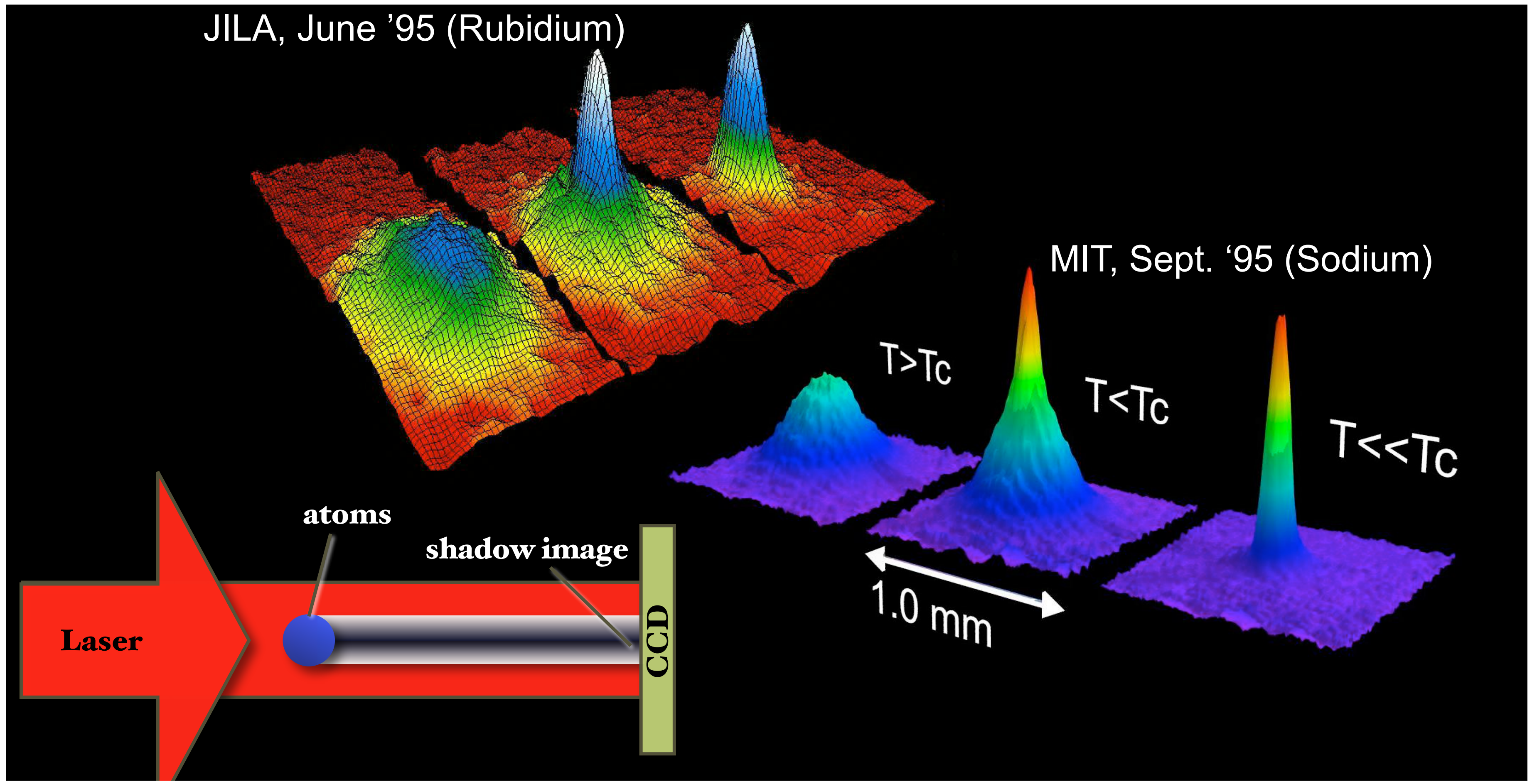
Predicted 1925

Bose-Einstein condensation



Predicted 1925

Produced in 1995!



Bose-Einstein condensation

S.N. Bose
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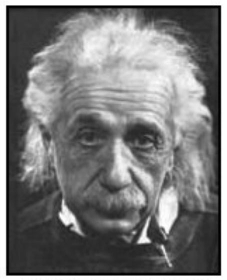

Albert Einstein
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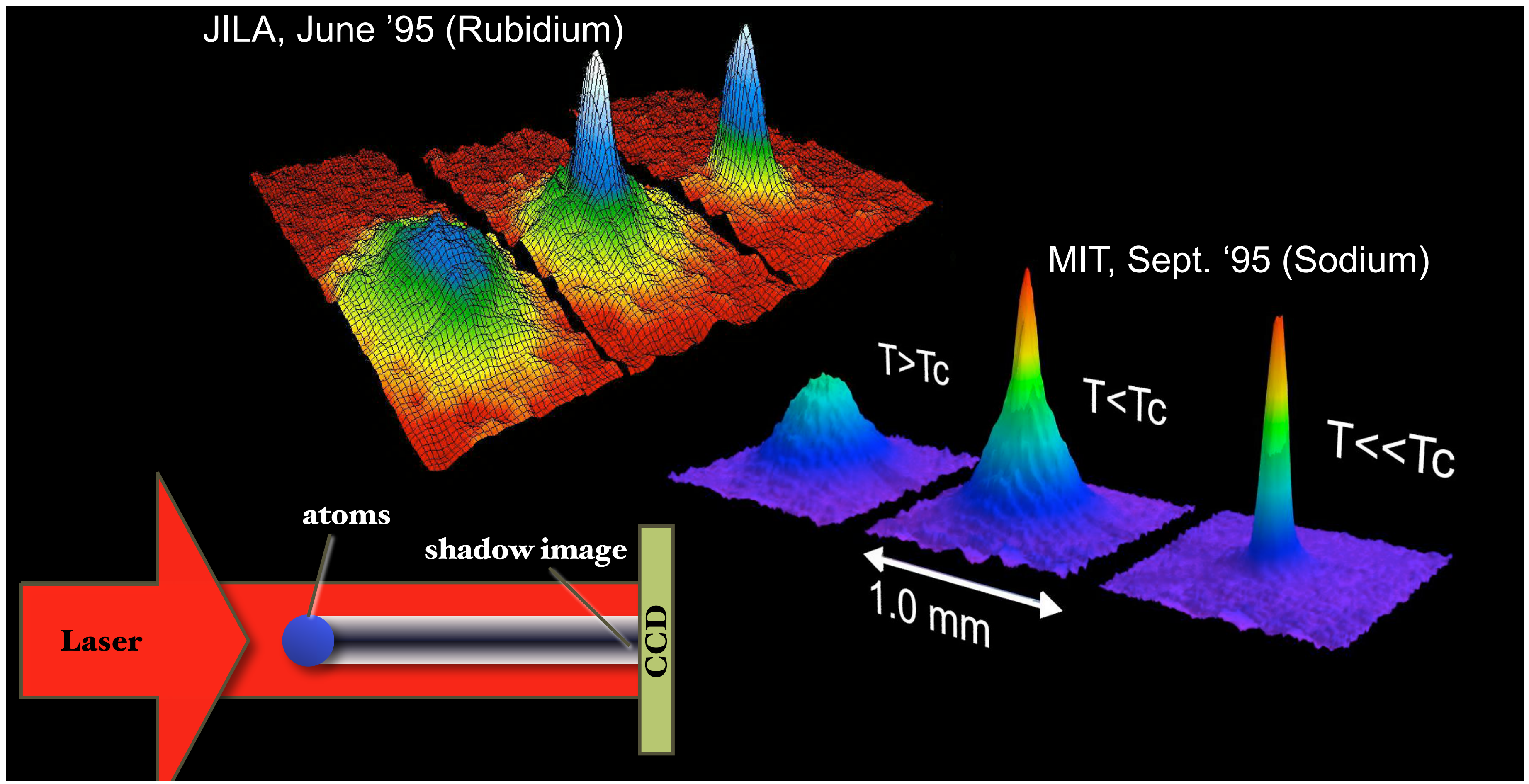


The Nobel Prize in Physics 2001

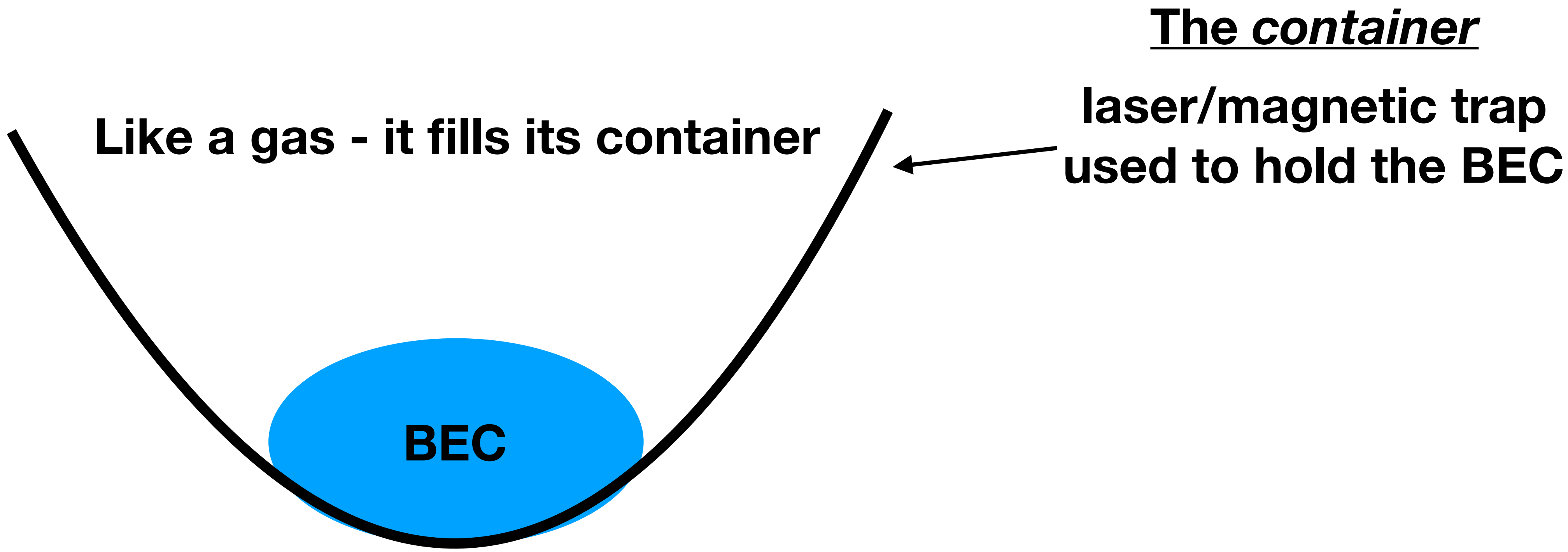
"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"

E. A. Cornell

W. Ketterle

C. E. Wieman

But BECs are still gases



It’s a Long story…

But thanks to some subtle quantum effects

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But thanks to some subtle quantum effects

$$\frac{E}{V} = \frac{1}{2} g_s n^2 \left[1 + \frac{128}{15\sqrt{\pi}} \sqrt{n a_s^3} \right]$$

Lee-Huang-Yang

L

H

Y

T.D. Lee and C.N. Yang, Phys. Rev. **105**, 1119 (1957).
T.D. Lee, K. Huang, and C.N. Yang, Phys. Rev. **106**, 1135 (1957)

Of highly magnetic atoms

Self-bound droplets

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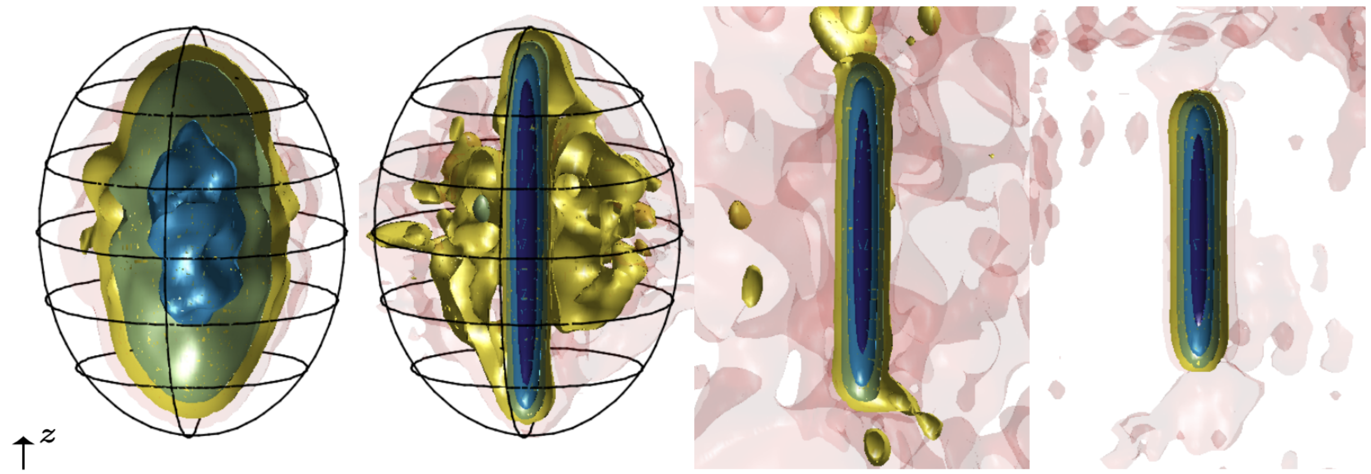

$t = 0\,\mathrm{ms}$
$a_s = 130a_0$
$\omega_\rho = 2\pi \times 70\,\mathrm{s}^{-1}$
$\lambda = 0.75$

$t = 10\,\mathrm{ms}$
$a_s = 80a_0$
$\omega_\rho = 2\pi \times 70\,\mathrm{s}^{-1}$
$\lambda = 0.75$

$t = 20\,\mathrm{ms}$
$a_s = 80a_0$
$\omega_\rho = \omega_z = 0$

$t = 30\,\mathrm{ms}$
$a_s = 80a_0$
$\omega_\rho = \omega_z = 0$

Of highly magnetic atoms

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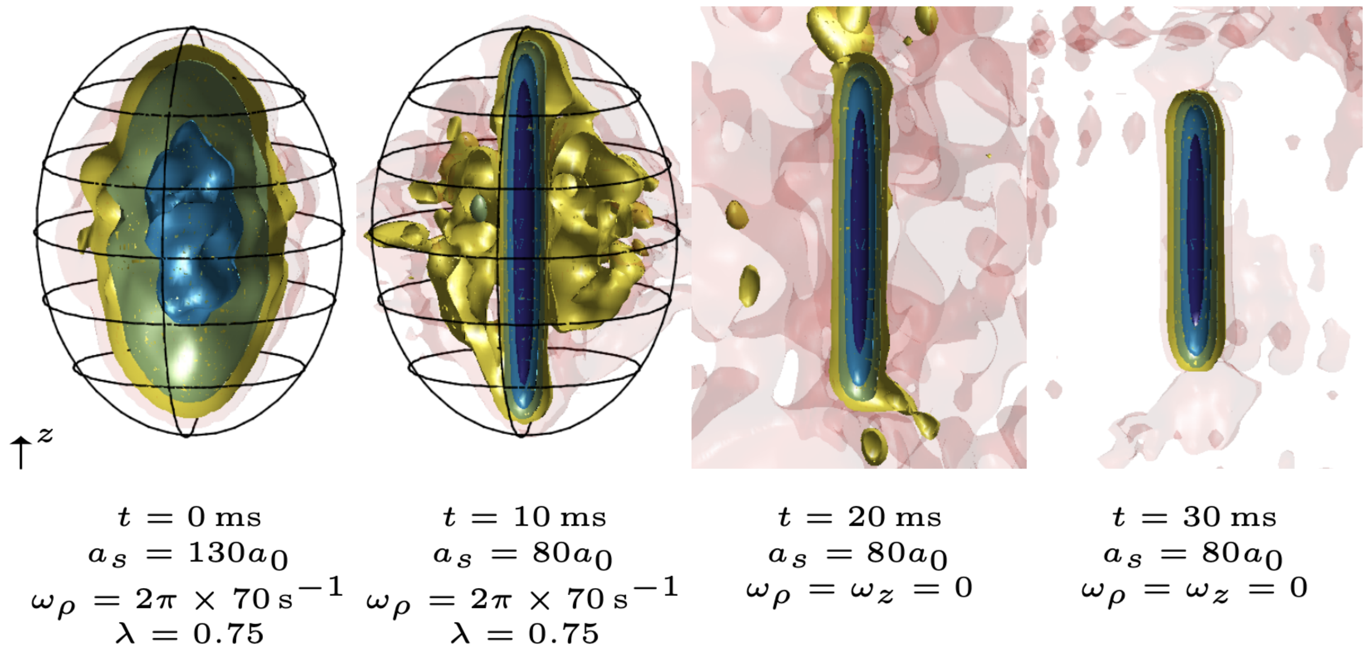

nature International weekly journal of science

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日本語要約

Self-bound droplets of a dilute magnetic quantum liquid

Matthias Schmitt, Matthias Wenzel, Fabian Böttcher, Igor Ferrier-Barbut & Tilman Pfau

Affiliations | Contributions | Corresponding authors

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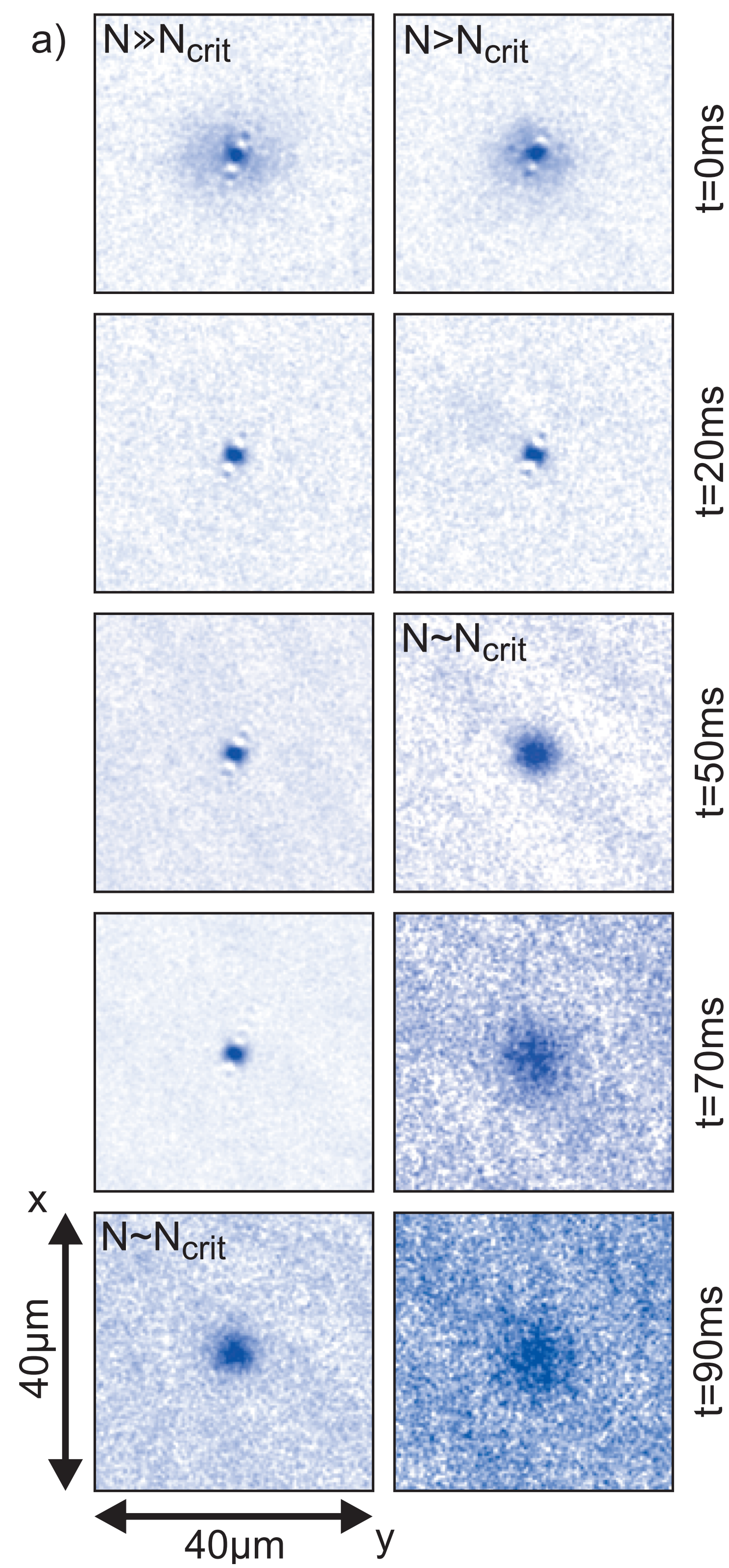

One or multiple droplets

- **Droplets behave like a liquid** (e.g. incompressible)**.**
- **Magnetic interactions cause droplets to repel each other**

P. B. Blakie, PRA 93, 033644 (2016),
also see I. Ferrier-Barbut, et al., PRA 97 011604 (2018); M. Wenzel, et al., PRA **96** 053630 (2017)

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Adding a trap?

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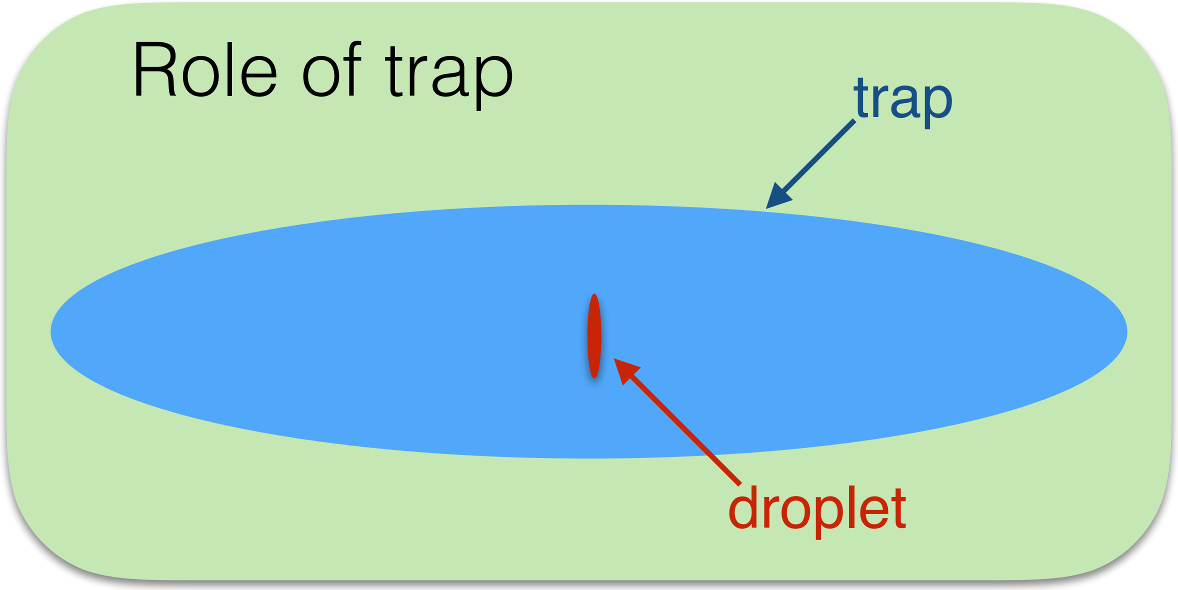

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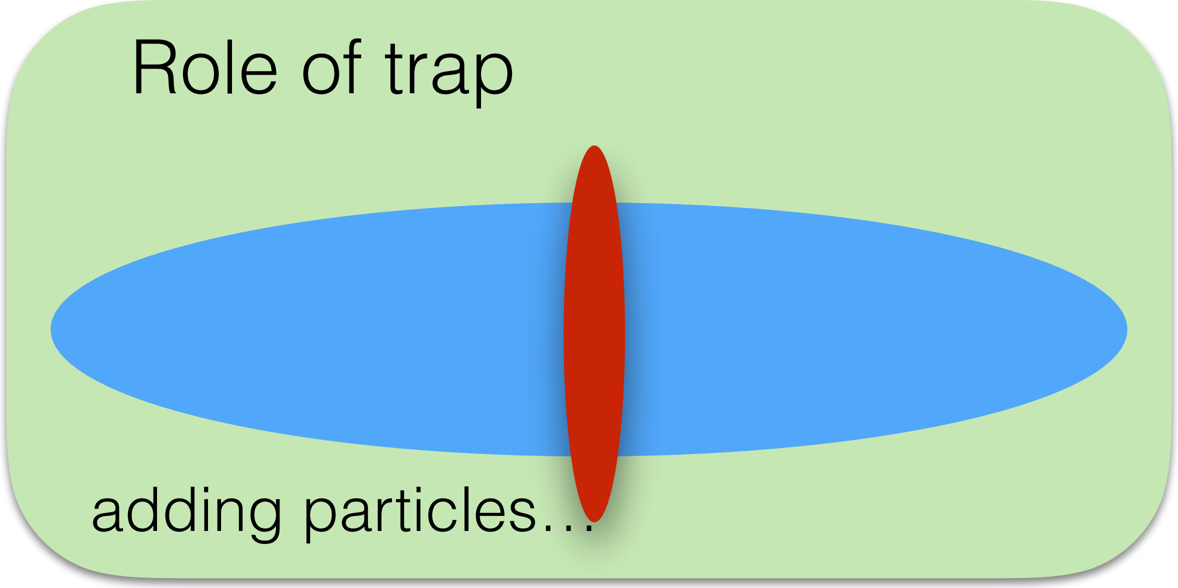

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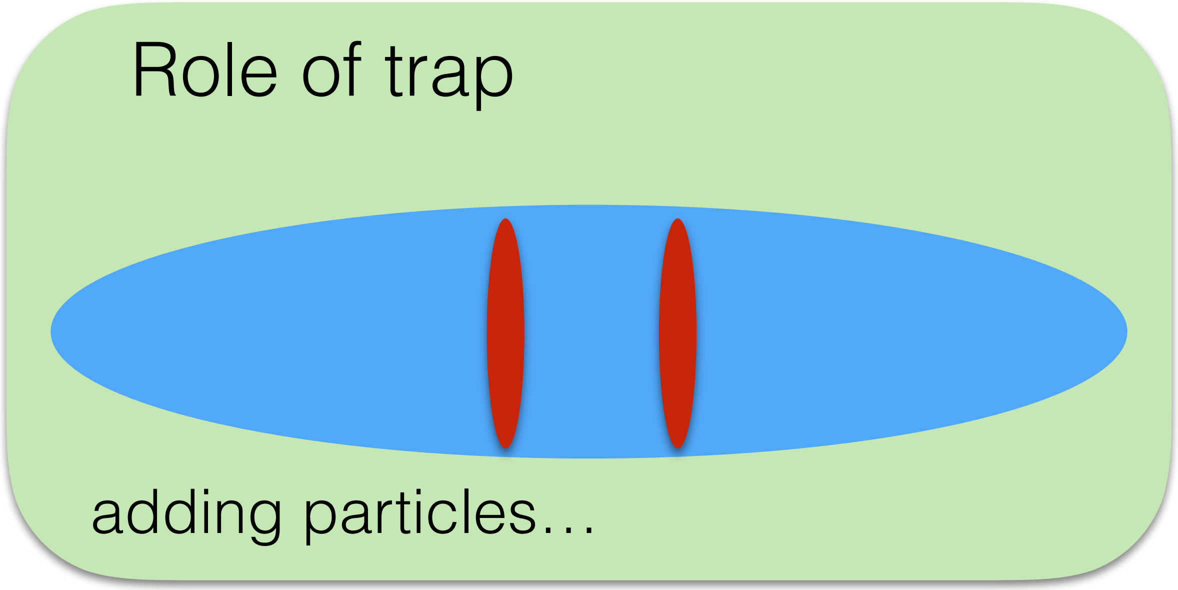

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Stationary states in a trap

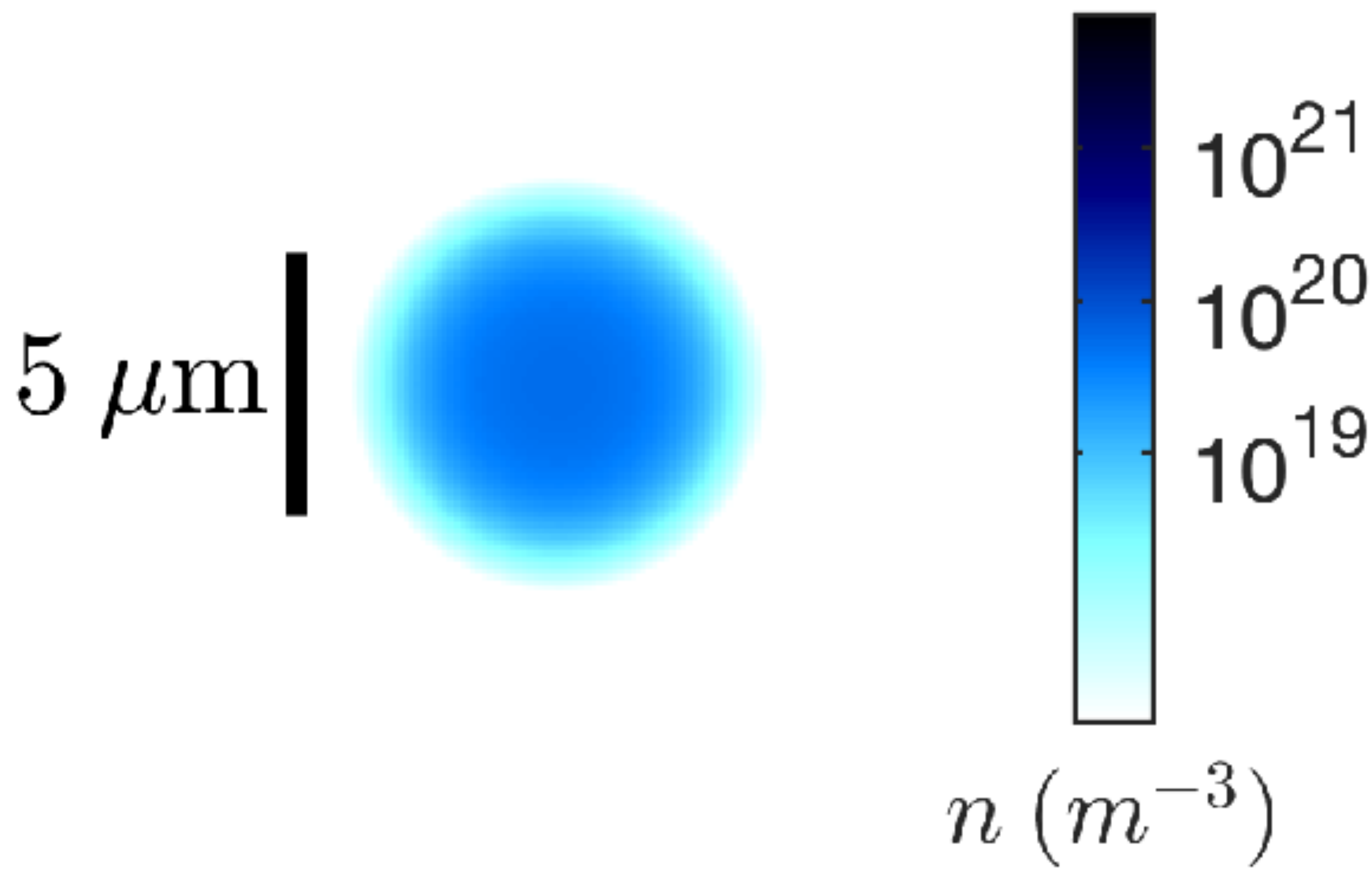
^{164}Dy atoms, $a_s = 70a_0, \quad (\omega, \omega_z) = 2\pi \times (60, 300)\,\mathrm{Hz}$ varying N

$$i\hbar\frac{\partial\psi}{\partial t} = \left[H_{\mathrm{sp}} + \int d\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\mathrm{QF}}|\psi|^3\right]\psi$$

Stationary states in a trap

^{164}Dy atoms, $a_s = 70a_0$, $(\omega, \omega_z) = 2\pi \times (60, 300)\,\mathrm{Hz}$ varying N

(a) $\nu = 0,\ N = 1 \times 10^3$



$$i\hbar\frac{\partial\psi}{\partial t} = \left[H_{\mathrm{sp}} + \int d\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\mathrm{QF}}|\psi|^3\right]\psi$$

Stationary states in a trap

^{164}Dy atoms, $a_s = 70a_0$, $(\omega, \omega_z) = 2\pi \times (60, 300)$ Hz varying N

$(b)\ \nu = 1,\ N = 3.98 \times 10^3$

$$i\hbar\frac{\partial\psi}{\partial t} = \left[H_{\mathrm{sp}} + \int d\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\mathrm{QF}}|\psi|^3\right]\psi$$

Stationary states in a trap

^{164}Dy atoms, $a_s = 70a_0$, $(\omega, \omega_z) = 2\pi \times (60, 300)$ Hz varying N

(c) $\nu = 2,\ N = 10 \times 10^3$

$$i\hbar\frac{\partial\psi}{\partial t} = \left[H_{\rm sp} + \int d\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\rm QF}|\psi|^3\right]\psi$$

Stationary states in a trap

^{164}Dy atoms, $a_s = 70a_0$, $(\omega, \omega_z) = 2\pi \times (60, 300)\,\mathrm{Hz}$ varying N

(d) $\nu = 3,\ N = 15.8 \times 10^3$

$$i\hbar\frac{\partial\psi}{\partial t} = \left[H_{\mathrm{sp}} + \int d\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\mathrm{QF}}|\psi|^3\right]\psi$$

Stationary states in a trap

^{164}Dy atoms, $a_s = 70a_0$, $(\omega, \omega_z) = 2\pi \times (60, 300)\,\mathrm{Hz}$ varying N

$$\text{(e)}\ \nu = 4,\ N = 22.4 \times 10^3$$

$$i\hbar \frac{\partial \psi}{\partial t} = \left[H_{\mathrm{sp}} + \int d\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\mathrm{QF}}|\psi|^3 \right] \psi$$

Stationary states in a trap

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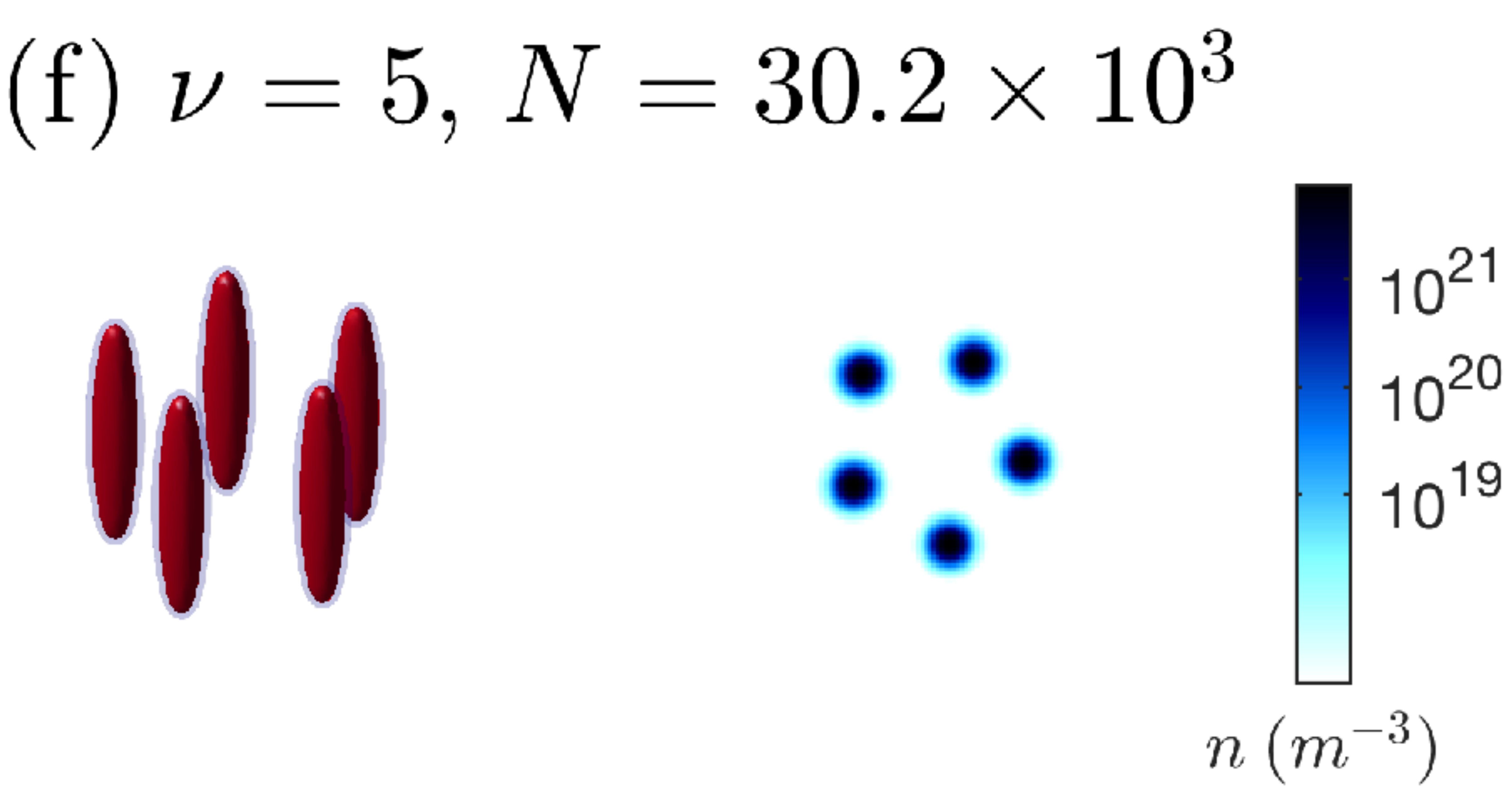

$$i\hbar\frac{\partial\psi}{\partial t} = \left[H_{\mathrm{sp}} + \int d\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\mathrm{QF}}|\psi|^3\right]\psi$$

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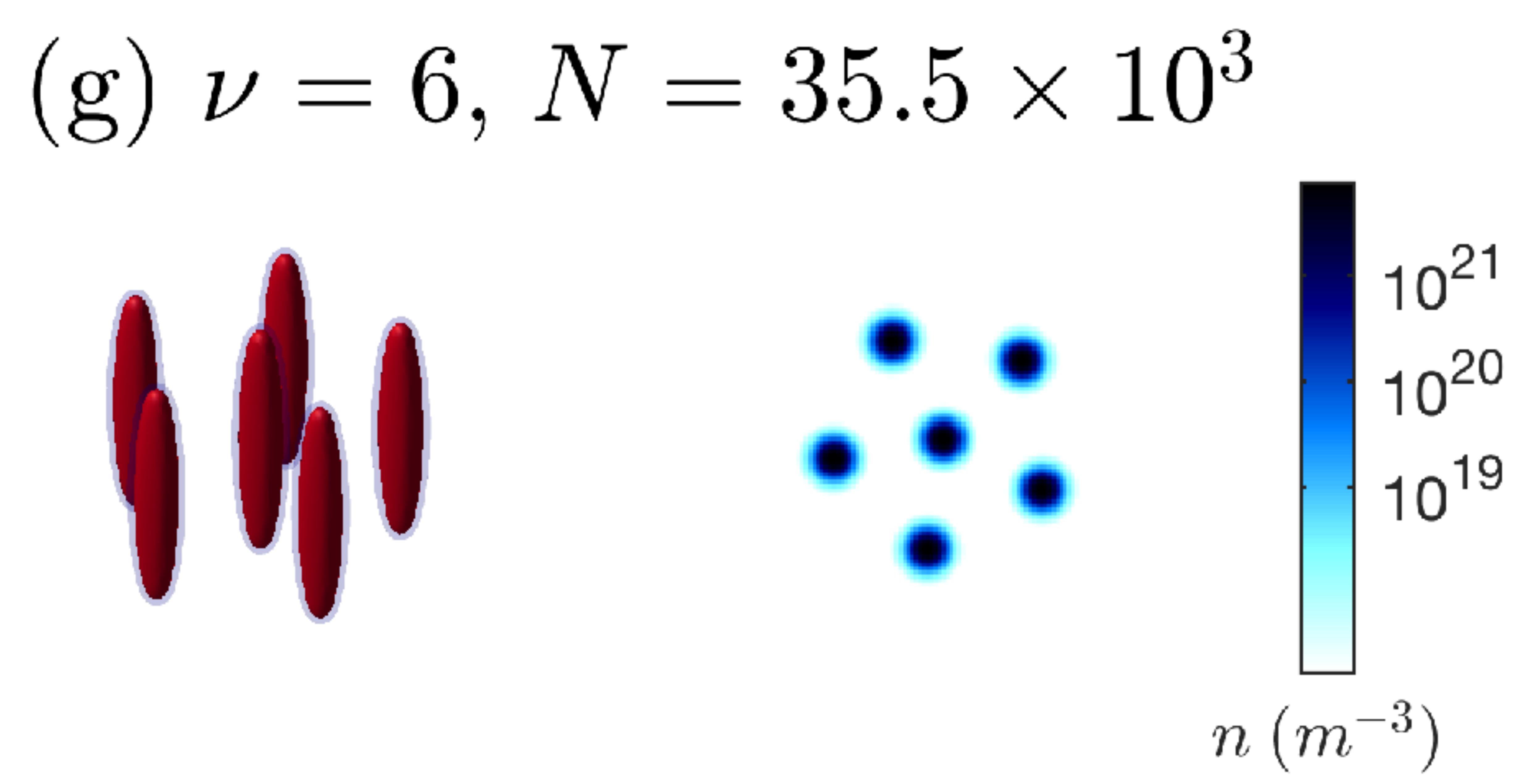

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Stationary states in a trap

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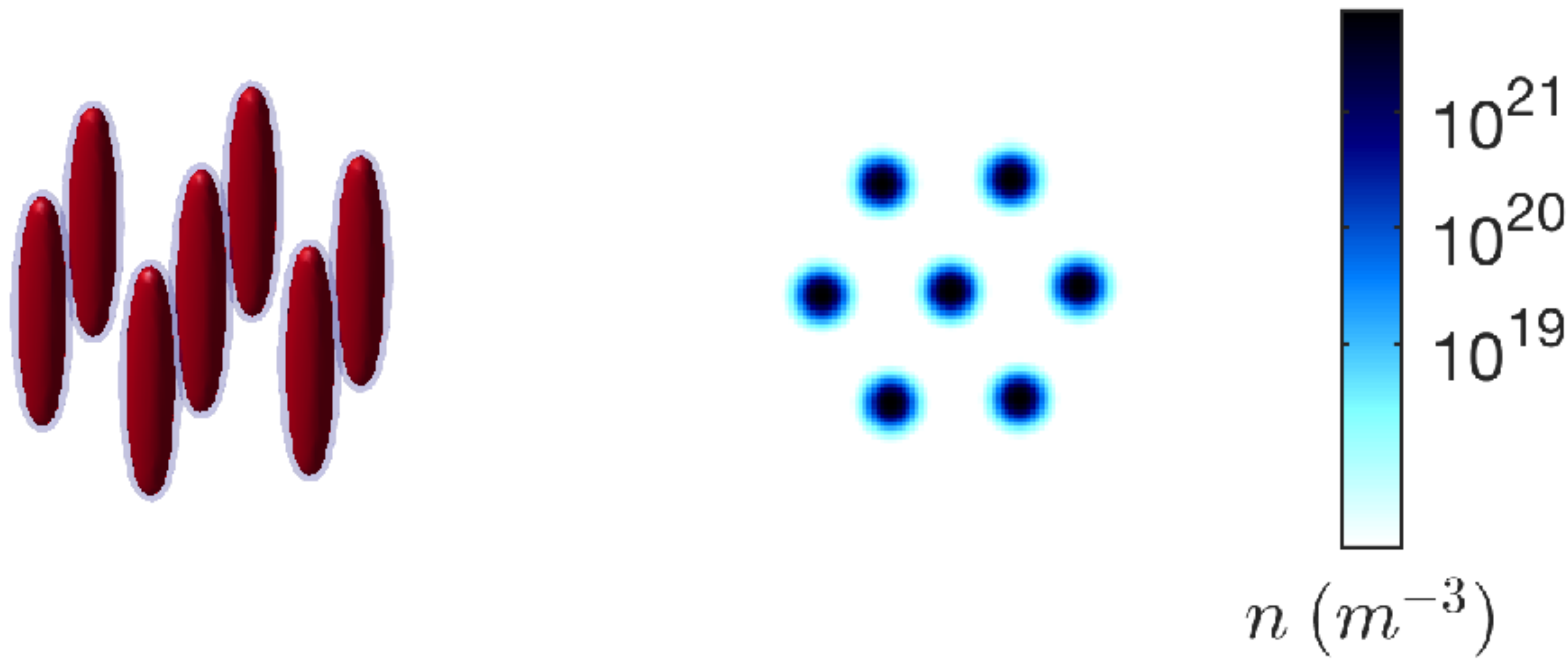
$$(\mathrm{h})\ \nu = 7,\ N = 39.8 \times 10^3$$

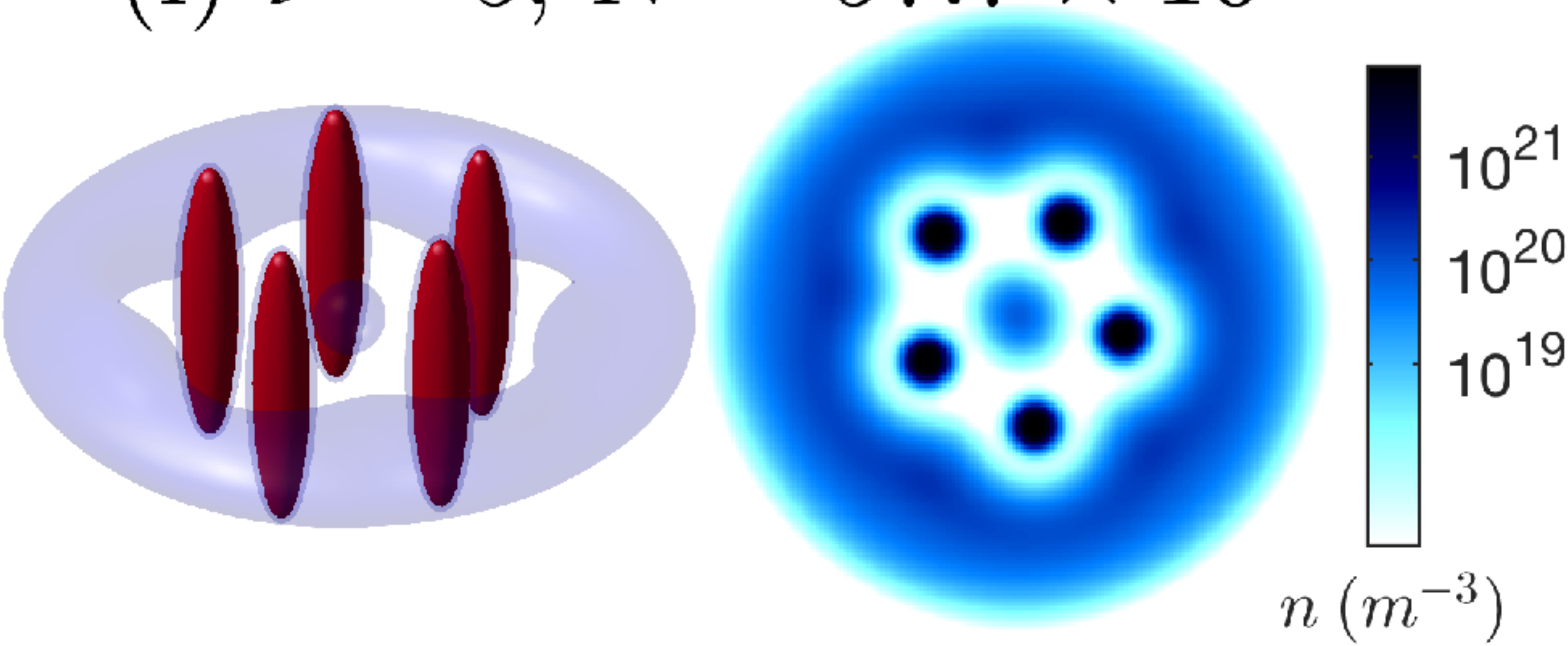


$$i\hbar\frac{\partial\psi}{\partial t} = \left[H_{\mathrm{sp}} + \int d\mathbf{r}'\,U(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\mathrm{QF}}|\psi|^3\right]\psi$$

Stationary states in a trap

^{164}Dy atoms, $a_s = 70a_0$, $(\omega, \omega_z) = 2\pi \times (60, 300)$ Hz varying N

(i) $\nu = 5$, $N = 97.7 \times 10^3$



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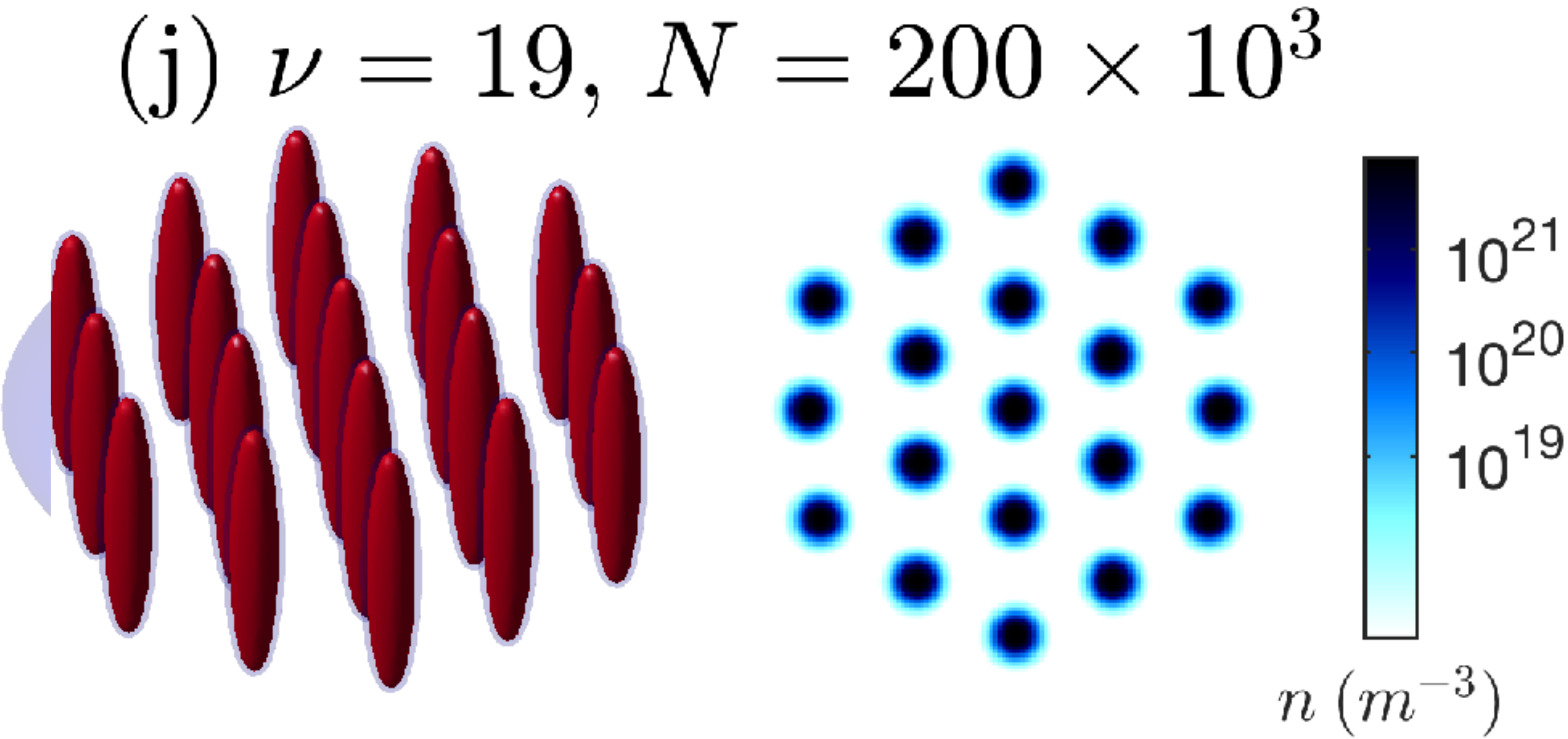

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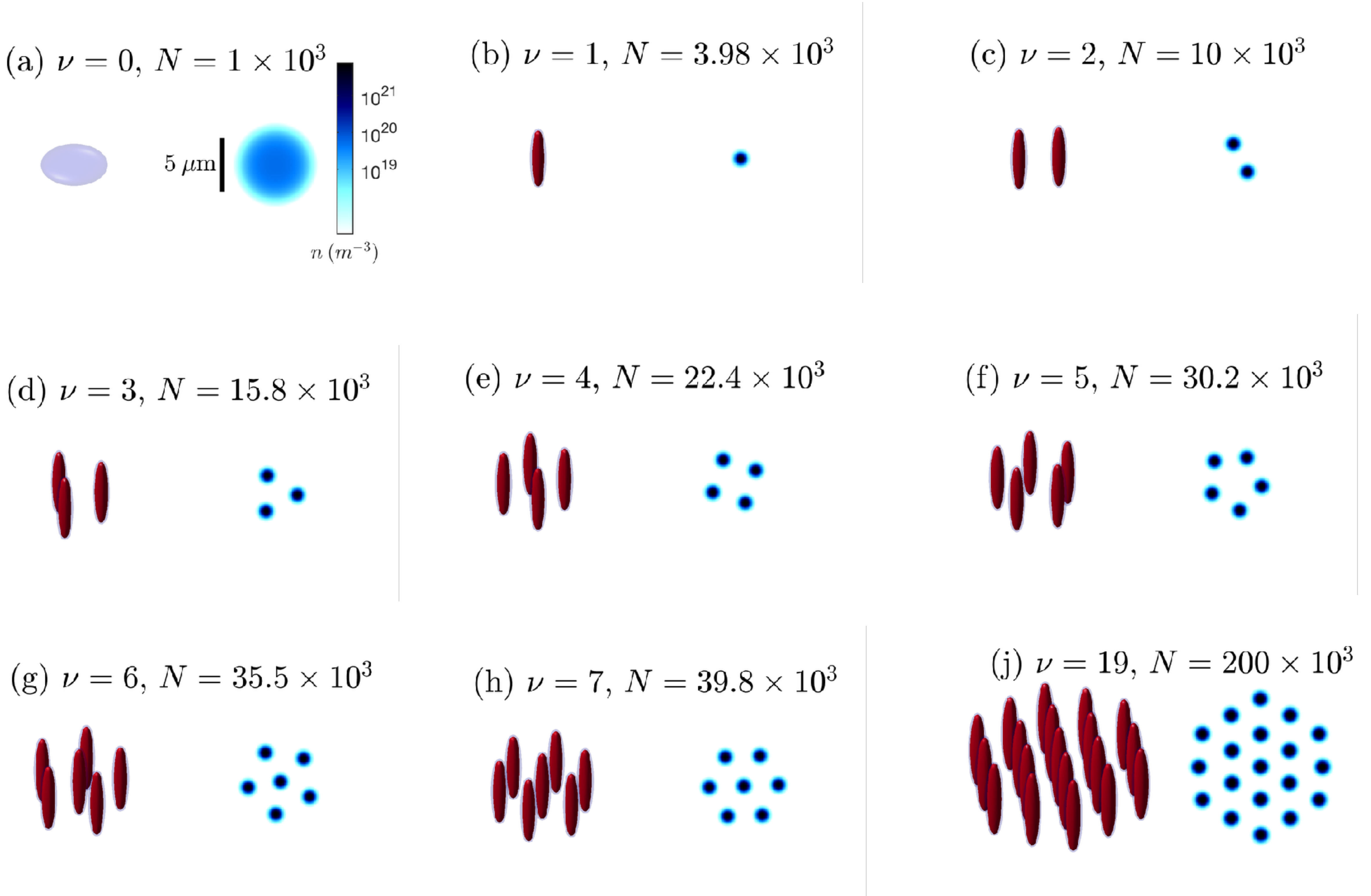
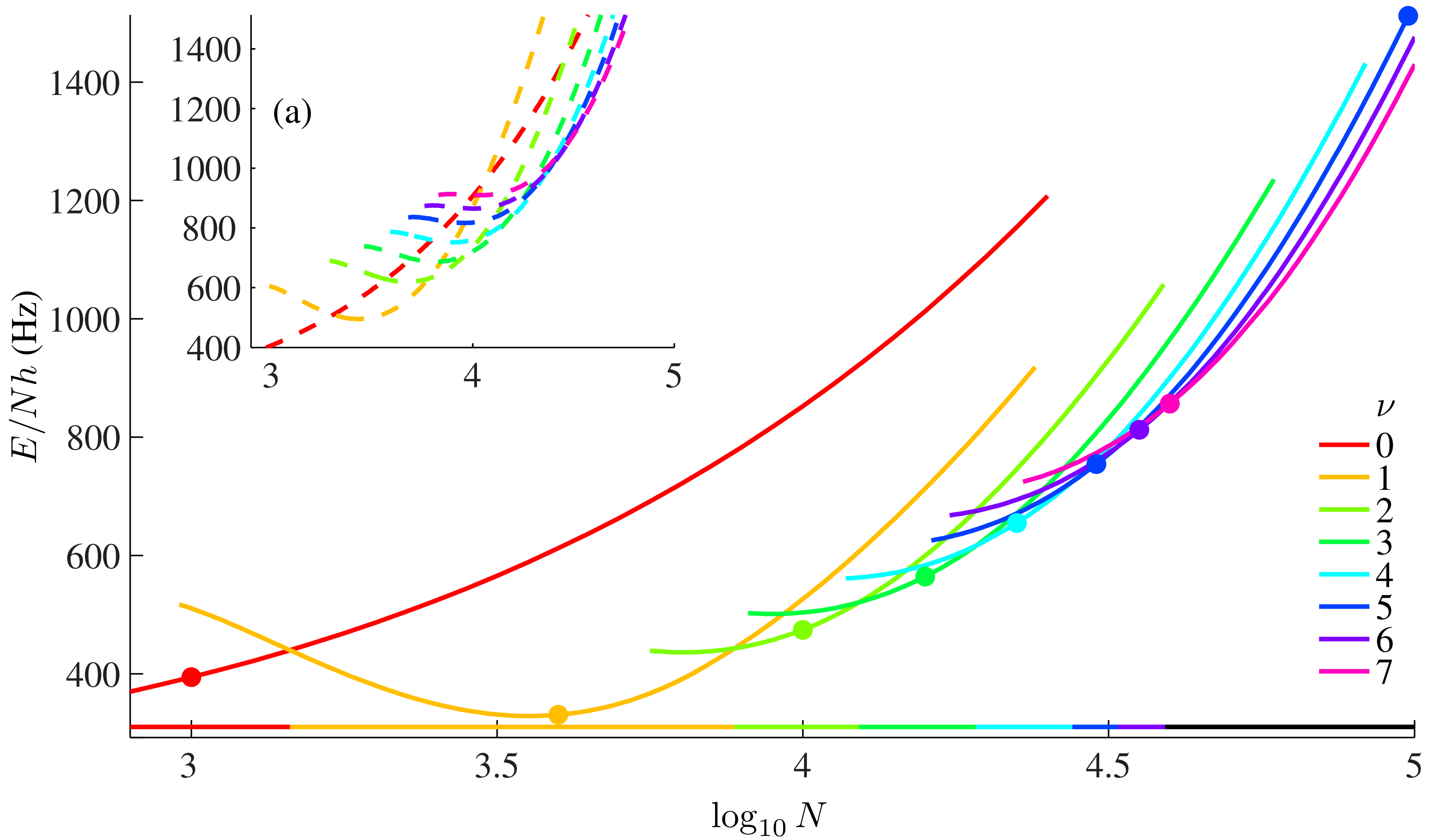


Dy-164 $a_s = 70a_0$, trap: radial=60Hz, axial=300Hz

Stationary state energies



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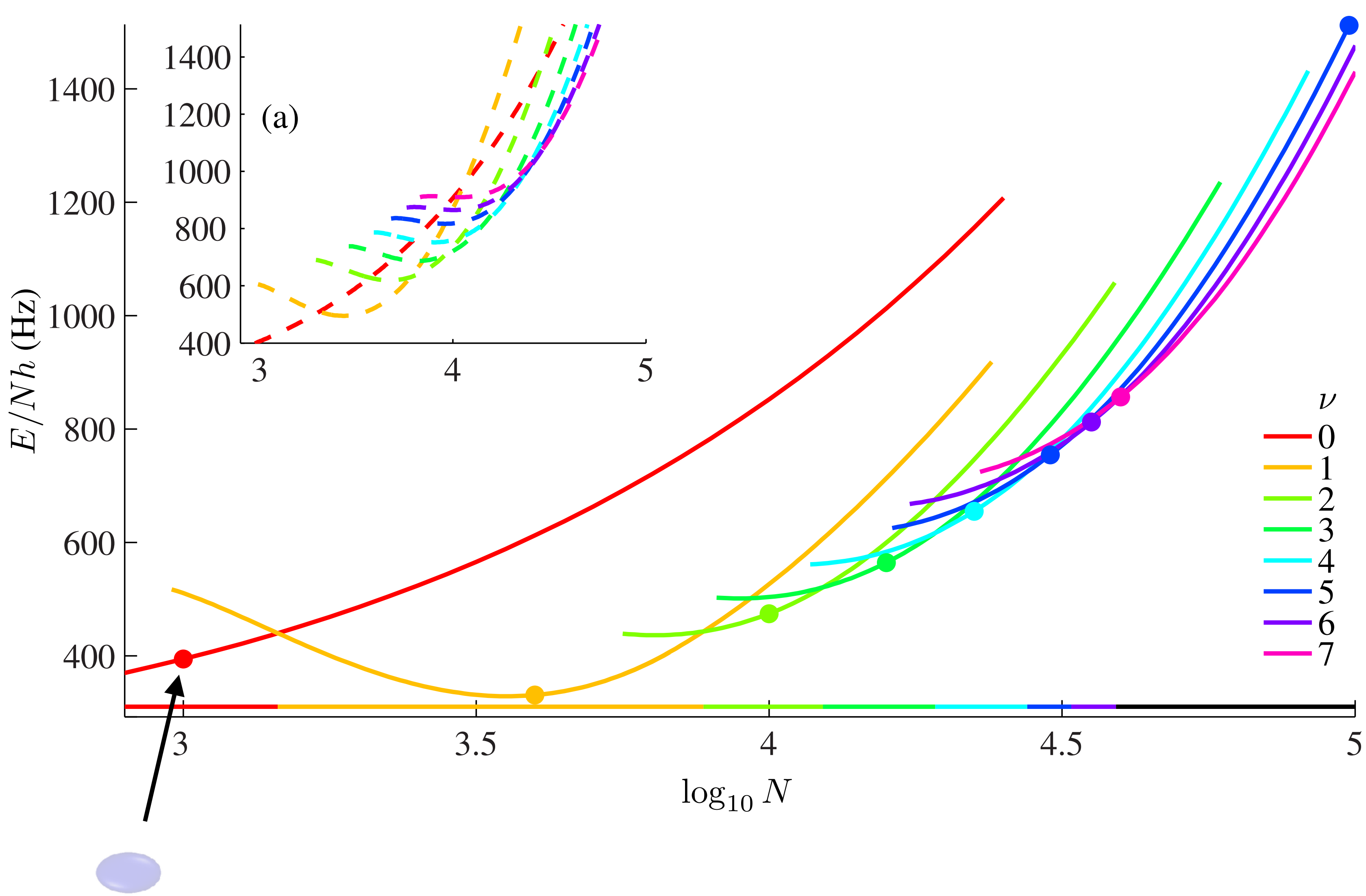

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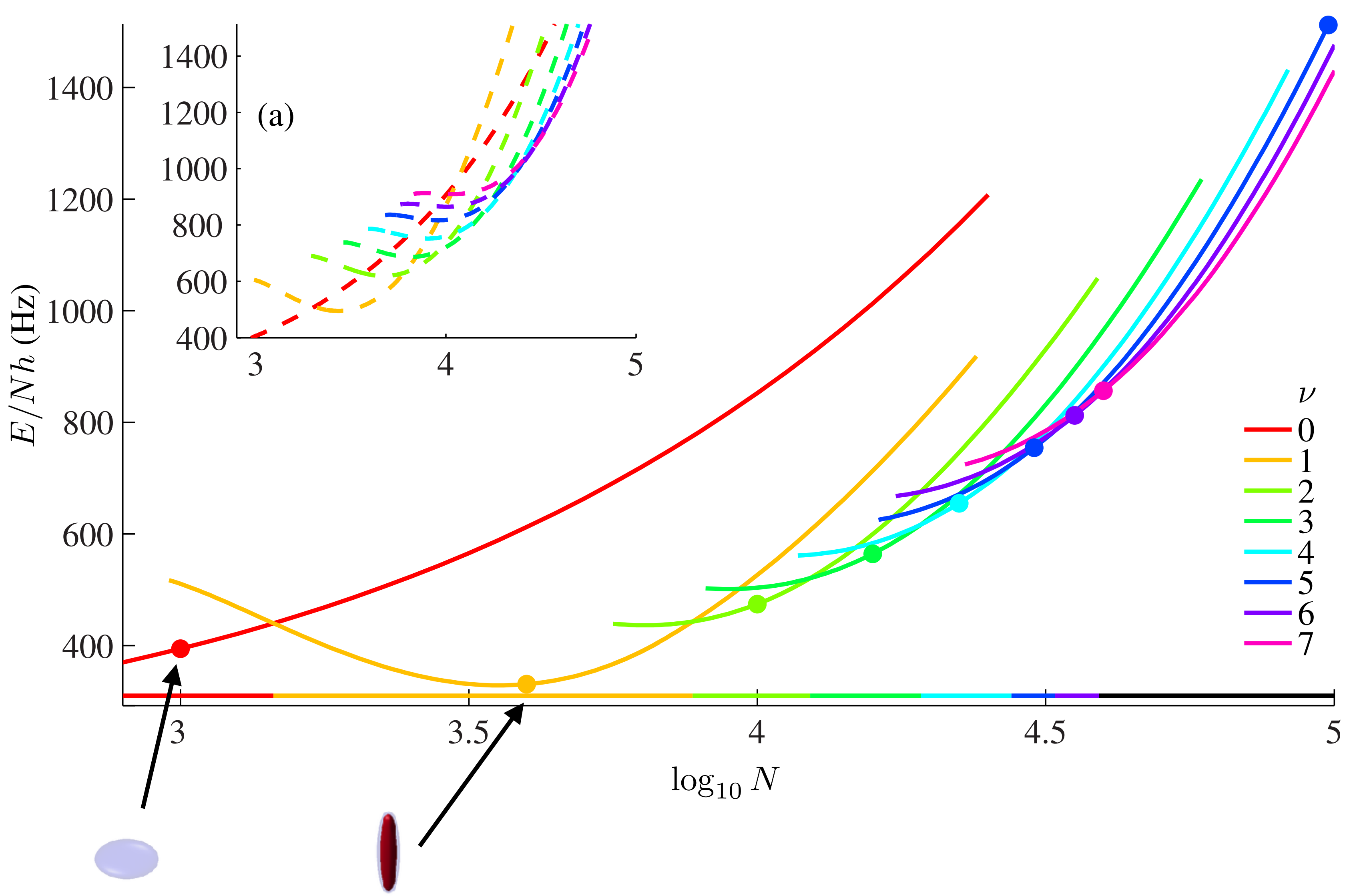

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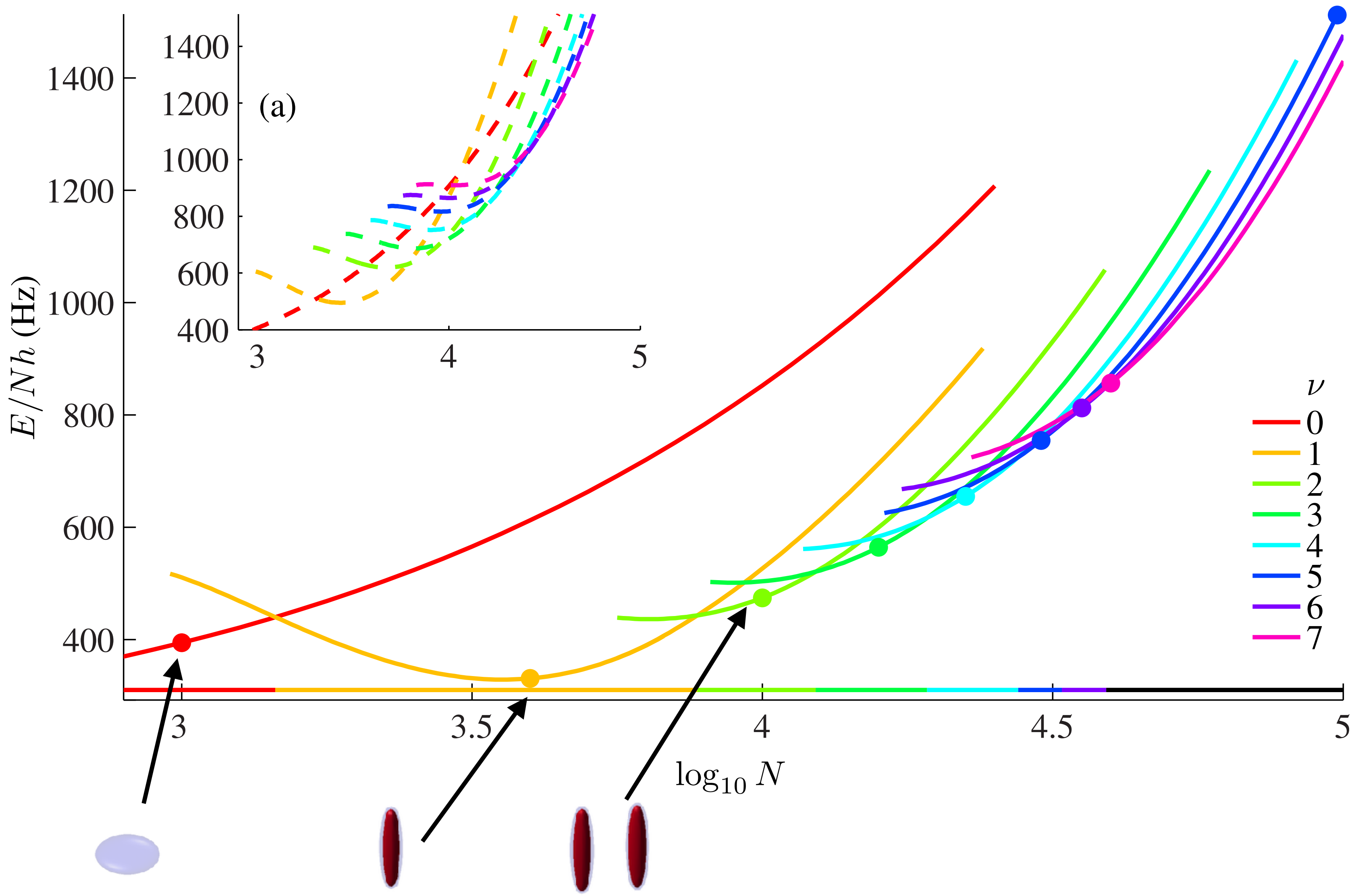

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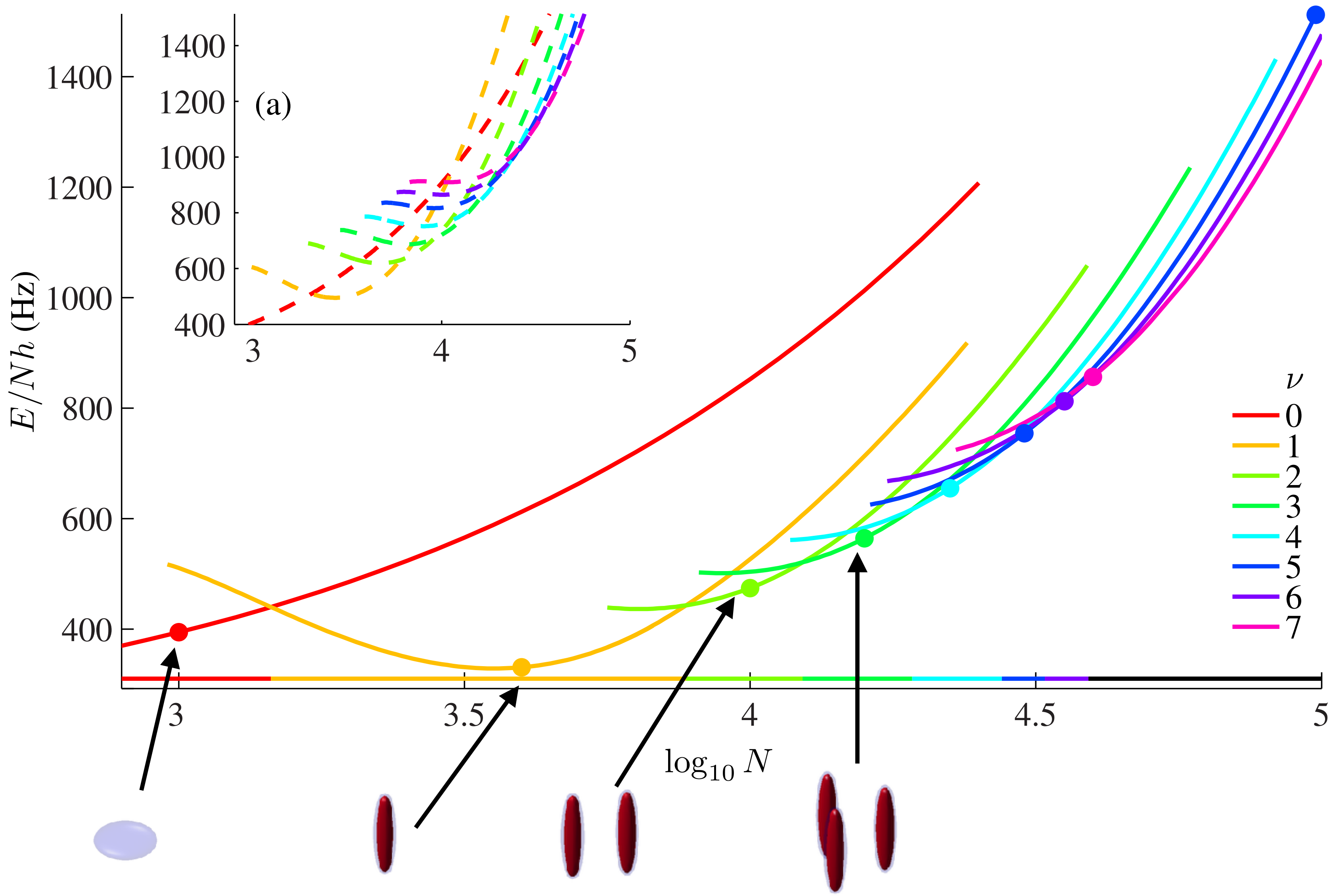

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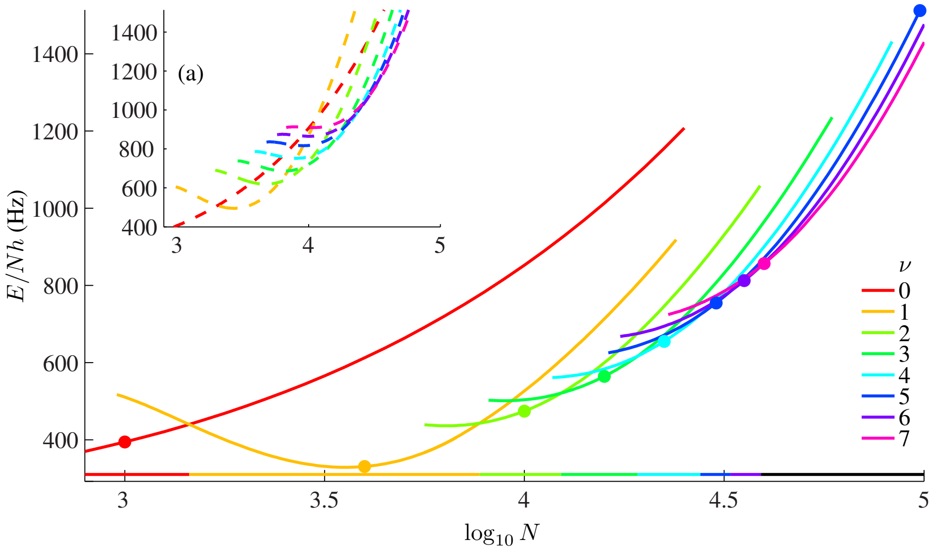

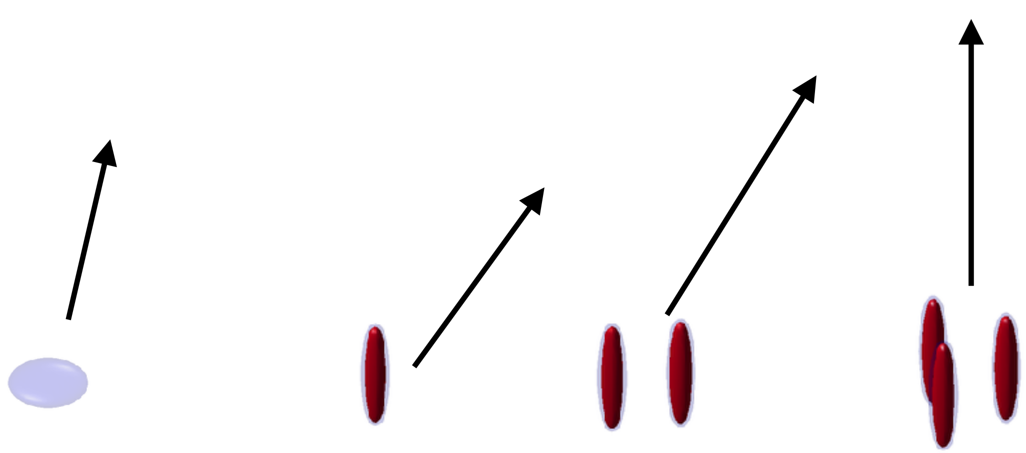

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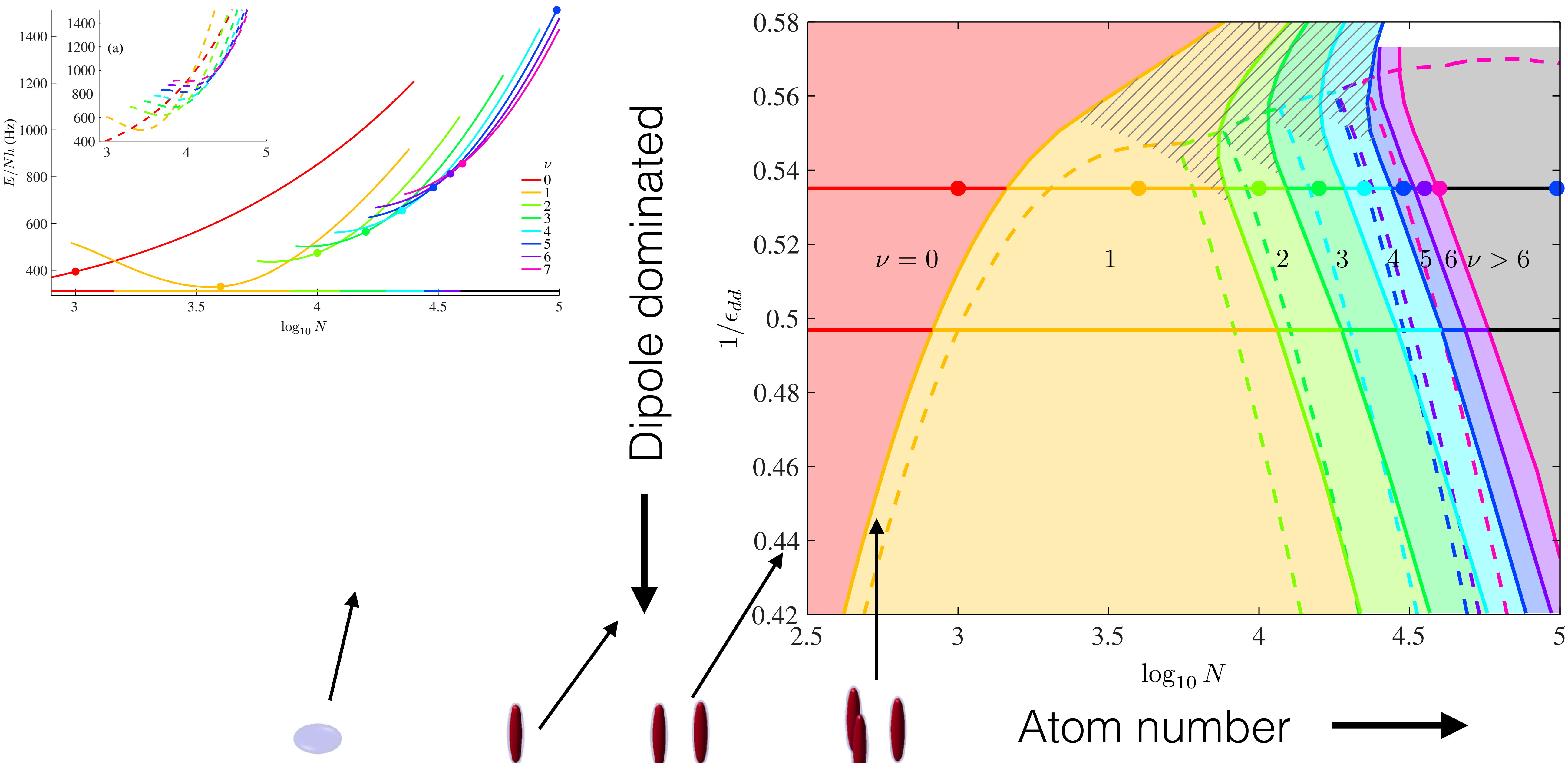

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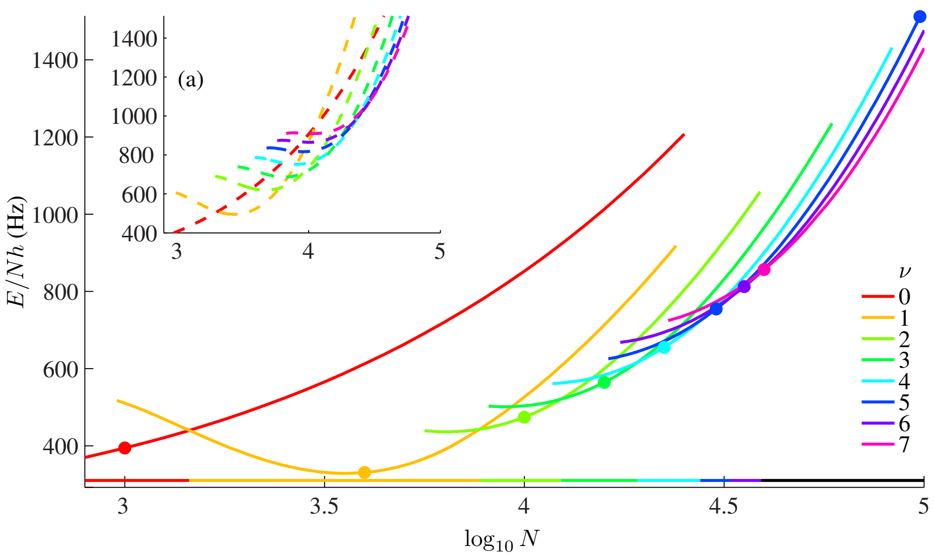
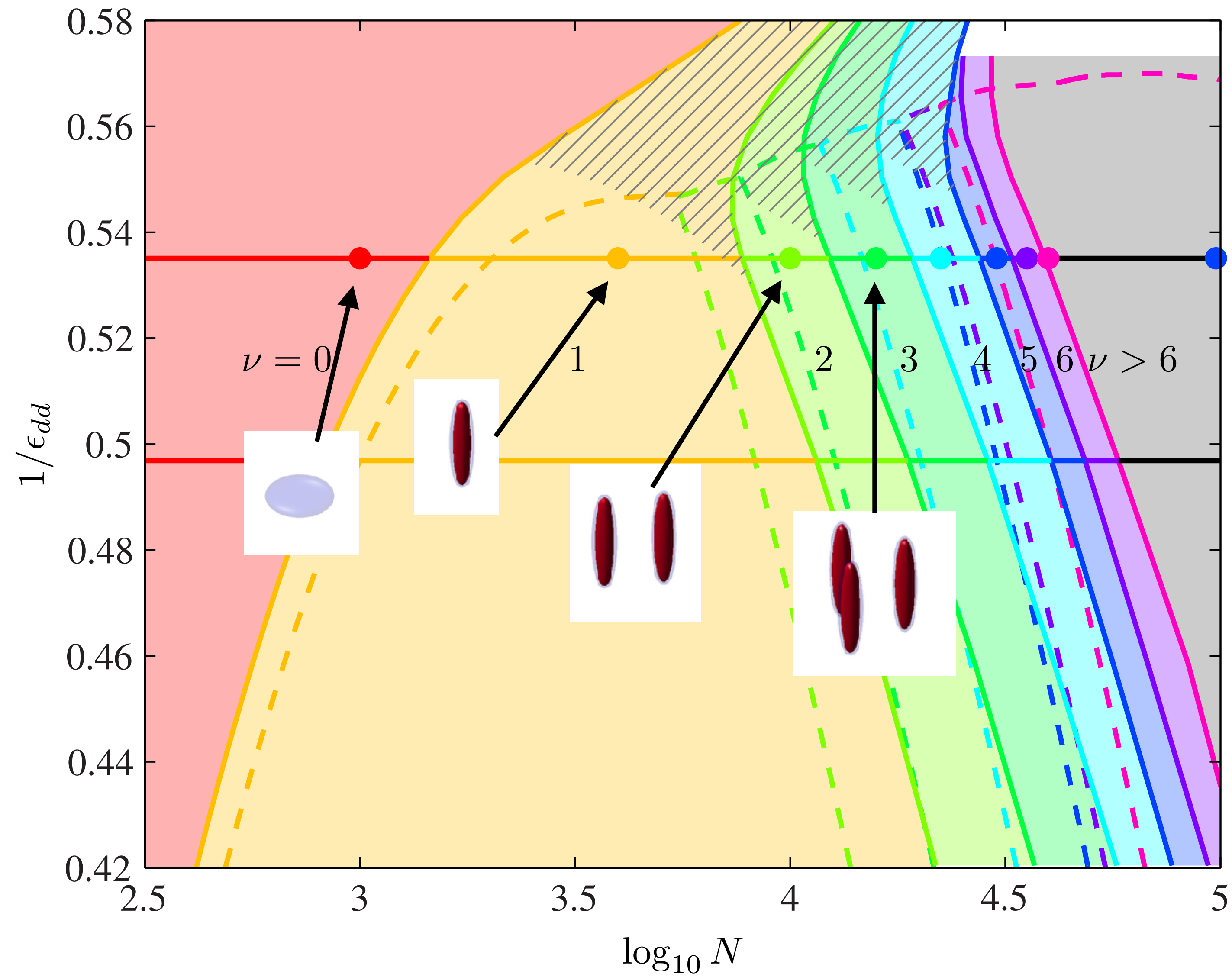


Dipole dominated



Atom number

Dy-164 $a_s = 70a_0$, trap: radial=60Hz, axial=300Hz

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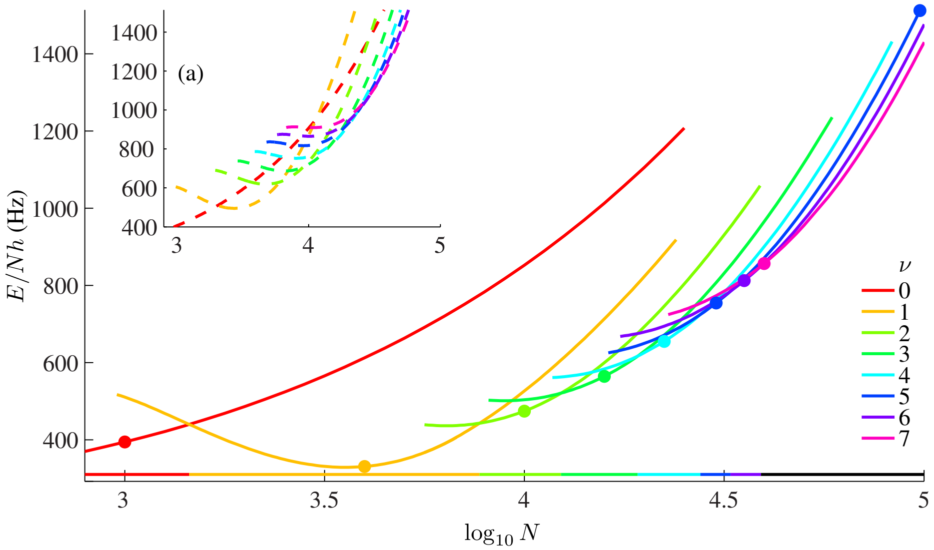

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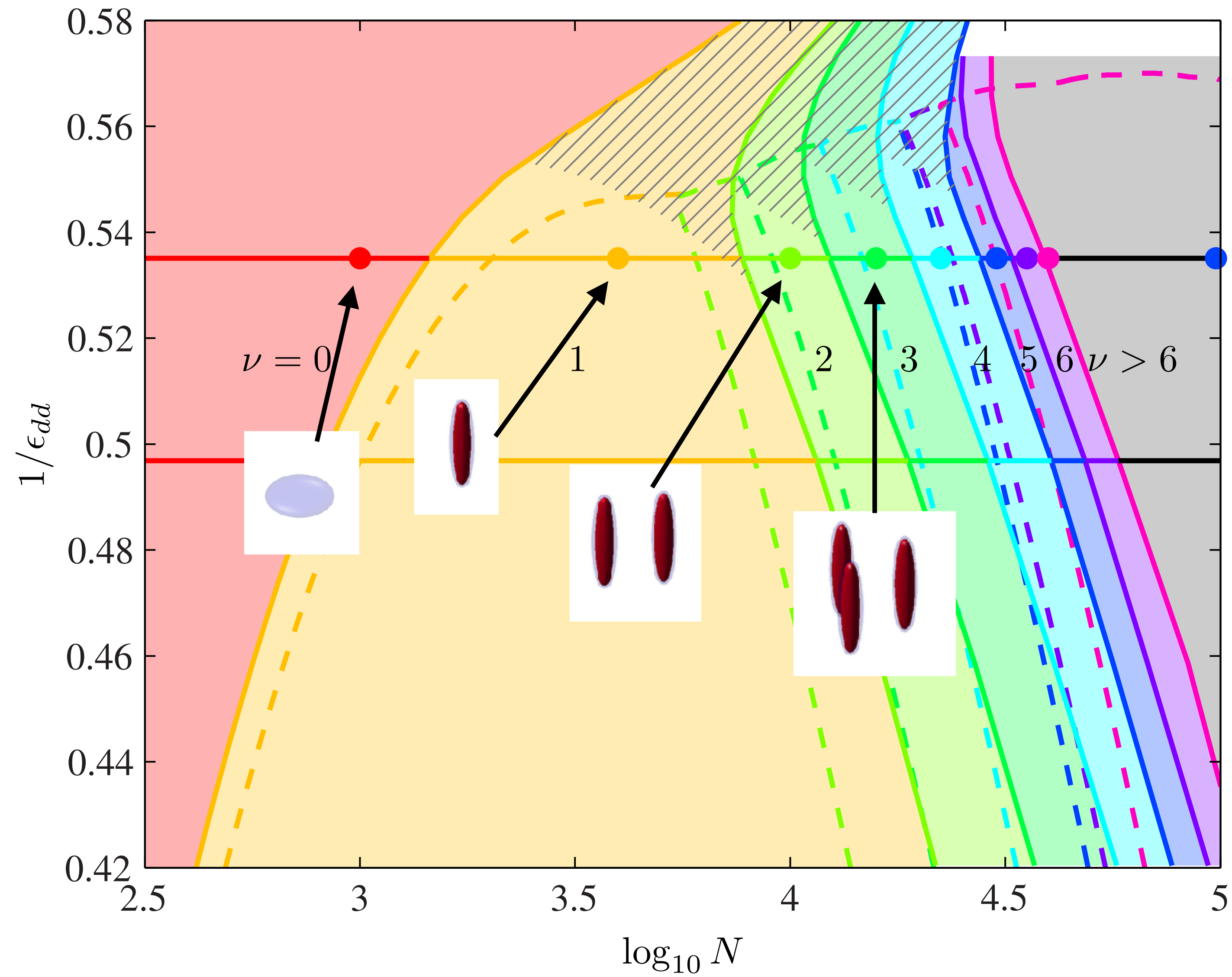

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D. Baillie and P. B. Blakie, PRL **121**, 195301 (2018)

Computational physics behind our work

Nonlinear differential equations

- Droplet crystals are solutions of the dipolar Gross-Pitaevskii equation (nonlinear eigenvalue equation)

Linear parts

Nonlinear parts

$$\mu\Psi = \Bigg[\underbrace{-\frac{\hbar^2\nabla^2}{2M} + V_{\mathrm{tr}}}_{\text{Linear parts}} + \underbrace{g_s|\Psi|^2 + \int d\mathbf{x}'\, U_{dd}(\mathbf{x}-\mathbf{x}')|\Psi(\mathbf{x}')|^2 + \gamma_{\mathrm{QF}}|\Psi|^3}_{\text{Nonlinear parts}}\Bigg]\Psi$$

Subject to the constraint $\int d\mathbf{x}\,|\Psi|^2 = N$

$$V_{\mathrm{tr}} = \frac{1}{2}M\omega_\rho^2(x^2+y^2+\lambda^2 z^2),$$

$$U_{dd}(\mathbf{r}) = \frac{3g_{dd}}{4\pi}\frac{1-3\cos^2\theta}{r^3},$$

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$$U_{dd}(\mathbf{r}) = \frac{3g_{dd}}{4\pi}\frac{1-3\cos^2\theta}{r^3},$$

- The field has been working for 20 years with *simpler* forms of this equation

Nonlinear differential equations

- Droplet crystals are solutions of the dipolar Gross-Pitaevskii equation (nonlinear eigenvalue equation)

Linear parts

Nonlinear parts

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Today's focus

Linear parts

Nonlinear parts

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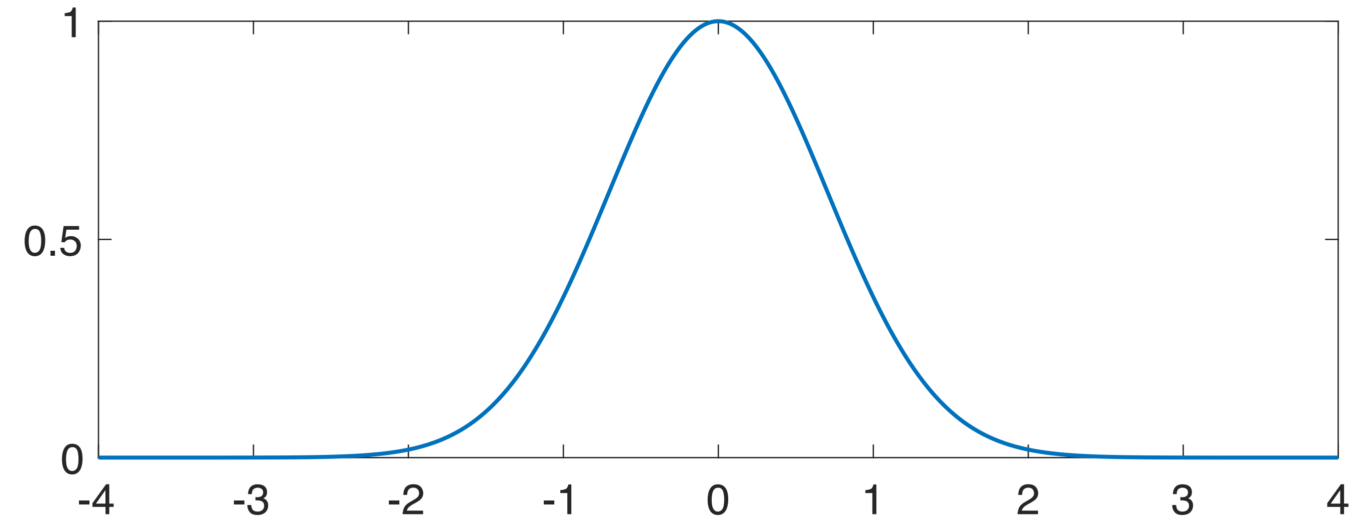
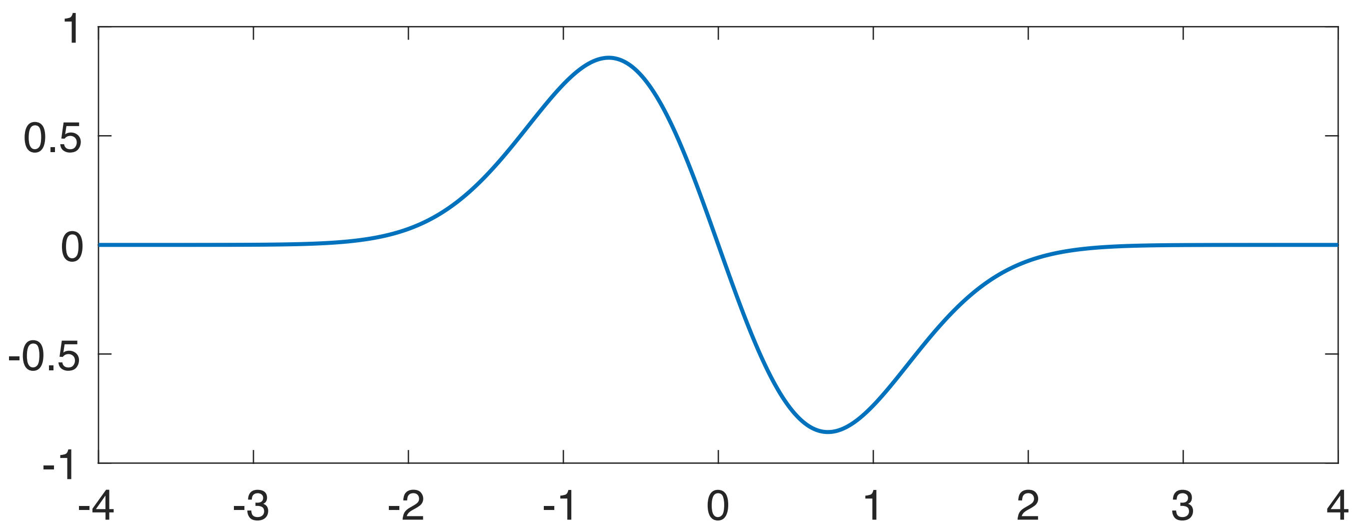
Derivatives

Derivatives



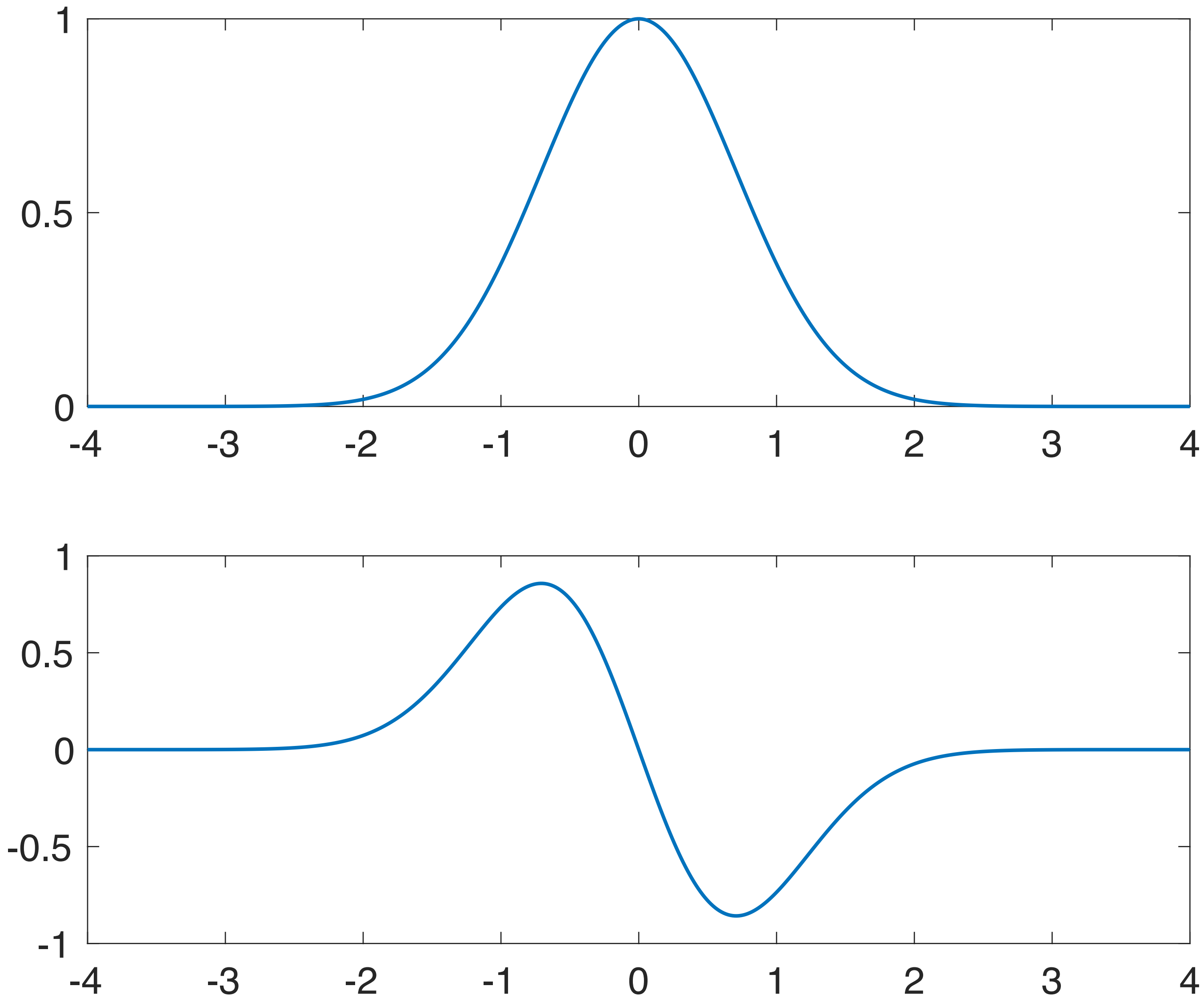
$$f(x) = e^{-x^2}$$



$$\frac{df}{dx} = -2xe^{-x^2}$$

Derivatives

Finite Difference Approach



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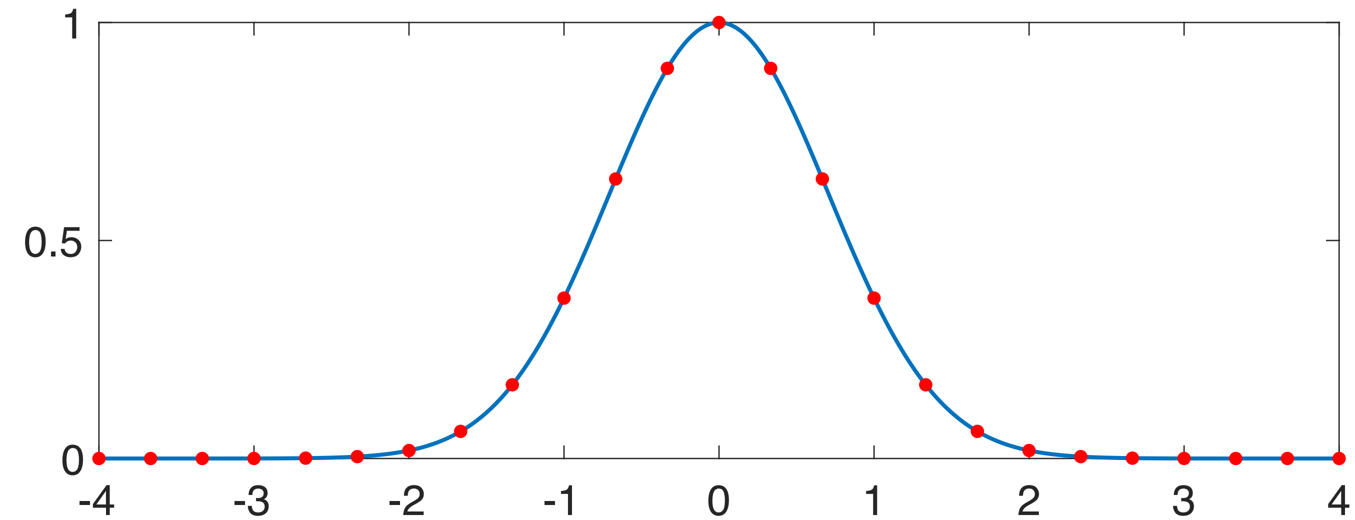
Derivatives

Finite Difference Approach

Sample with 25 points



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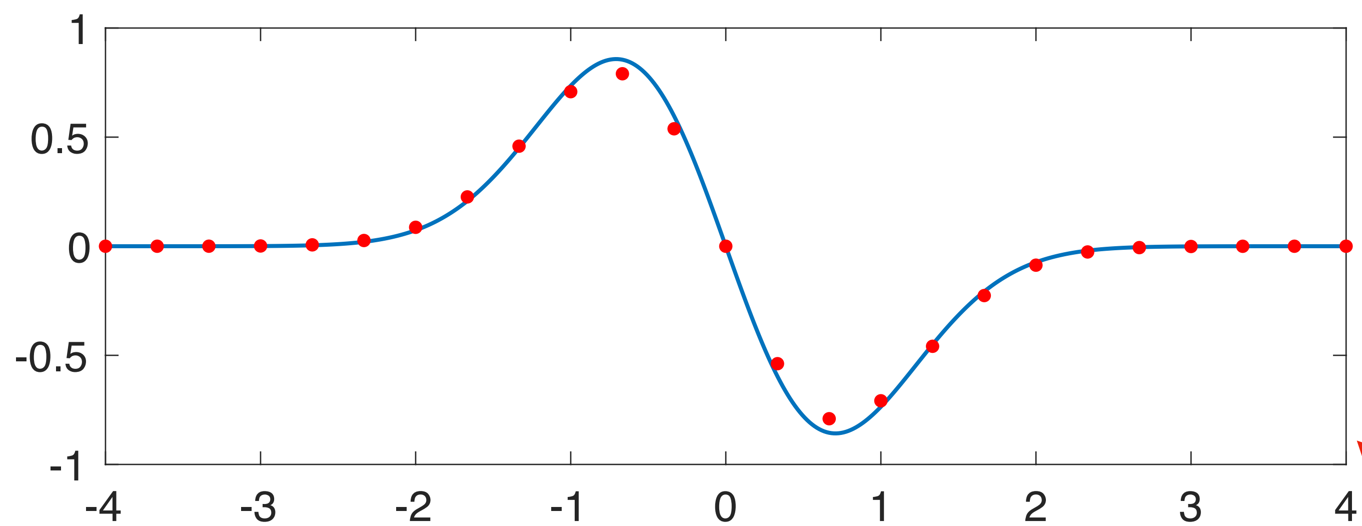


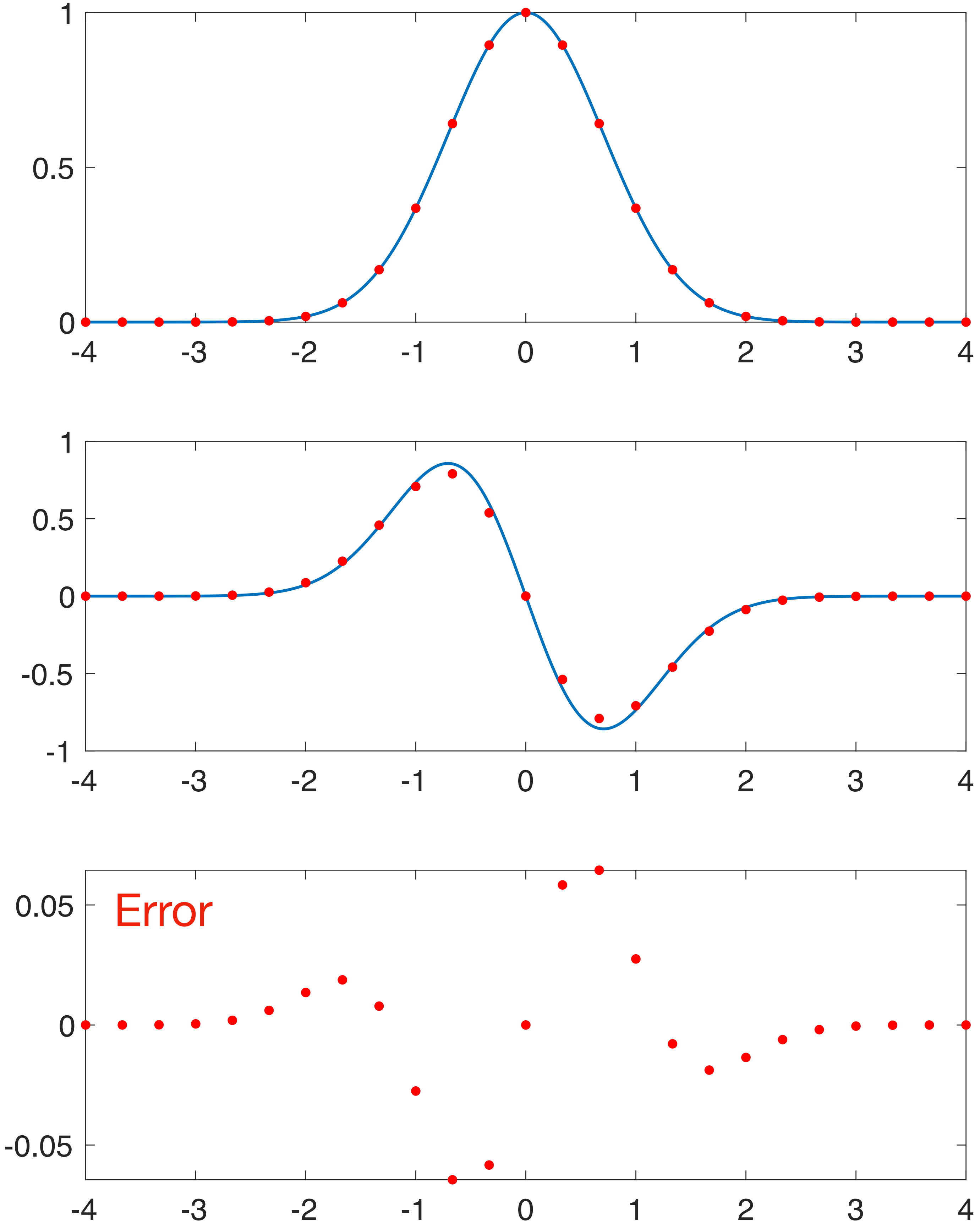
$$\frac{df}{dx} = -2xe^{-x^2}$$

Finite difference derivative

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$$

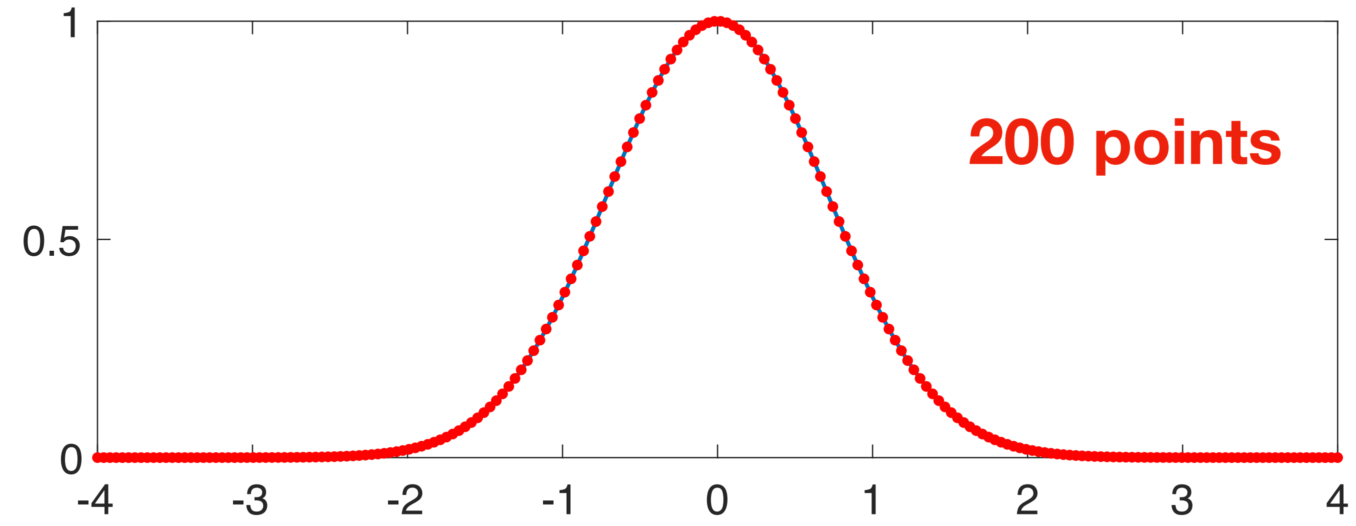
Derivatives

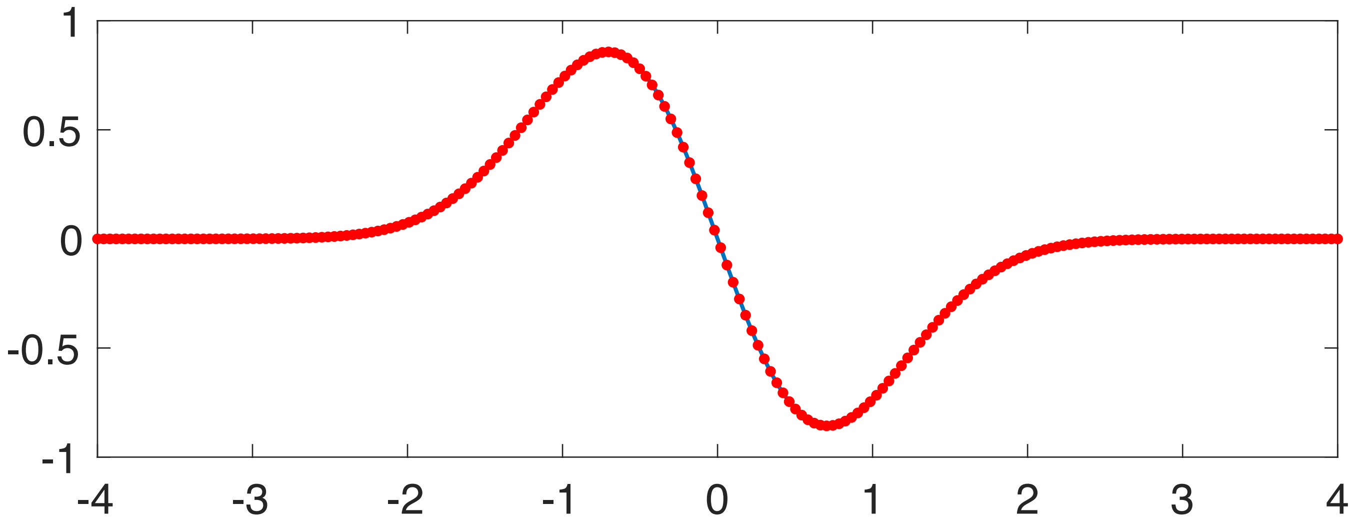
Finite Difference Approach



Derivatives

Finite Difference Approach





Derivatives

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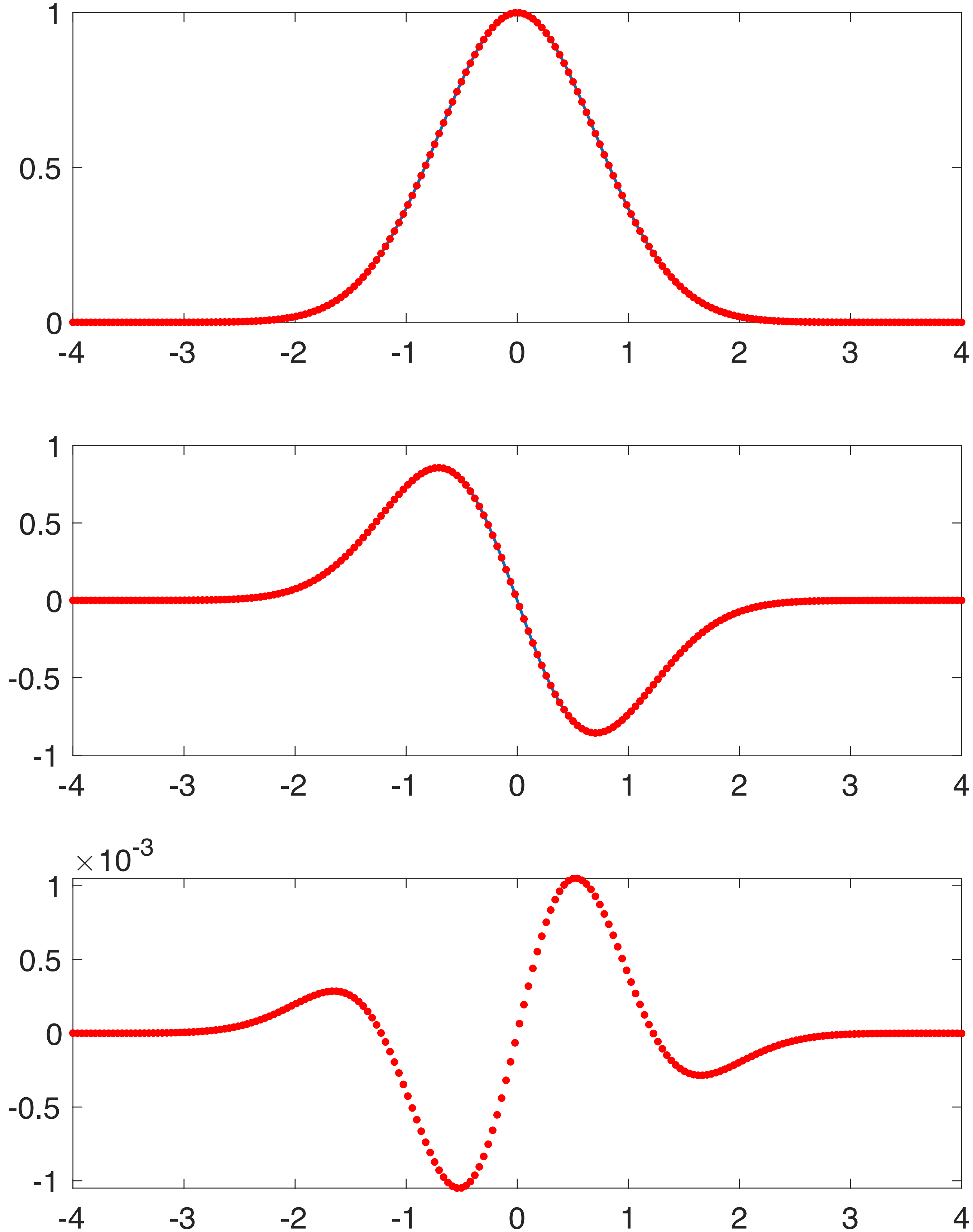
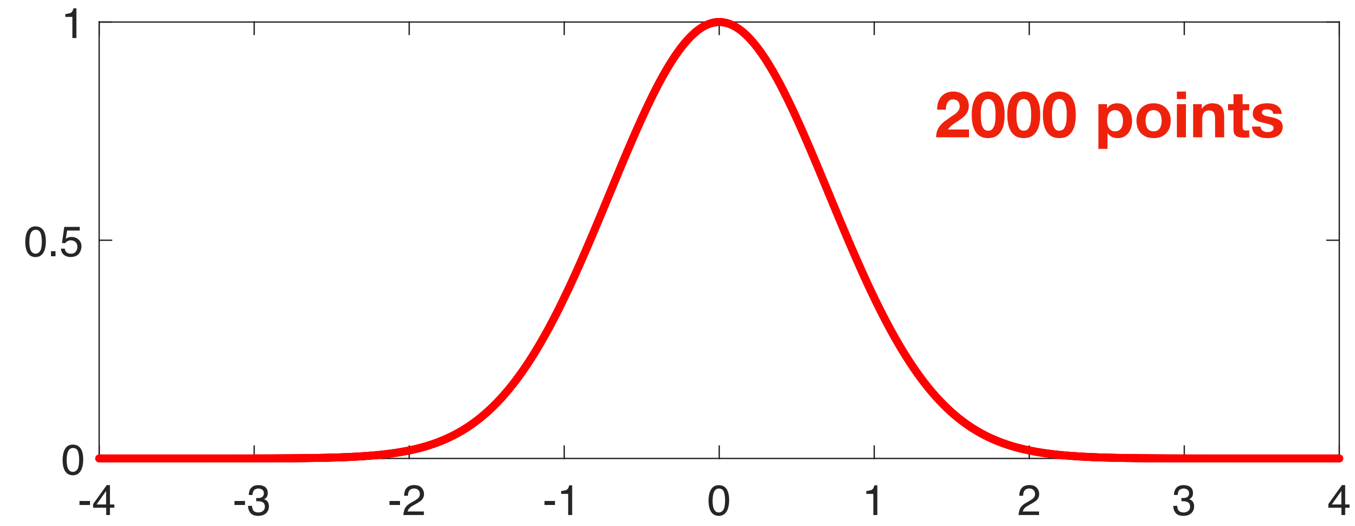
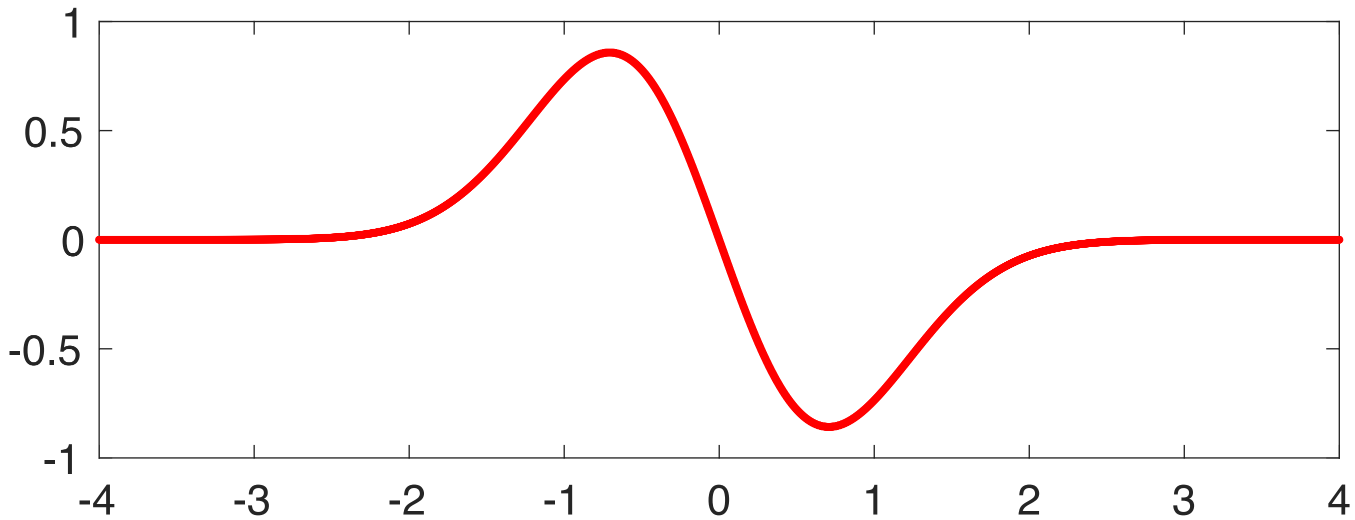


Derivatives

Finite Difference Approach





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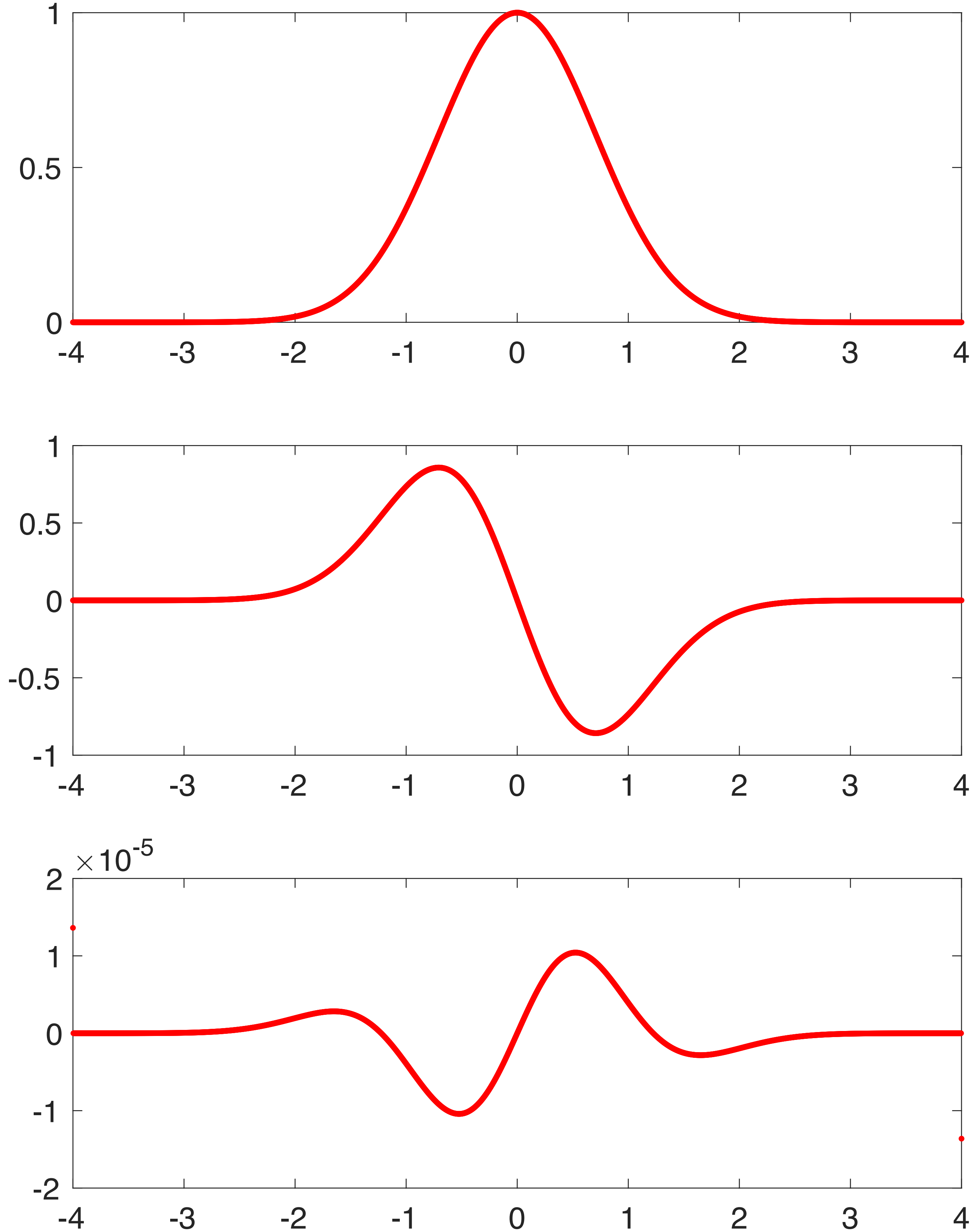
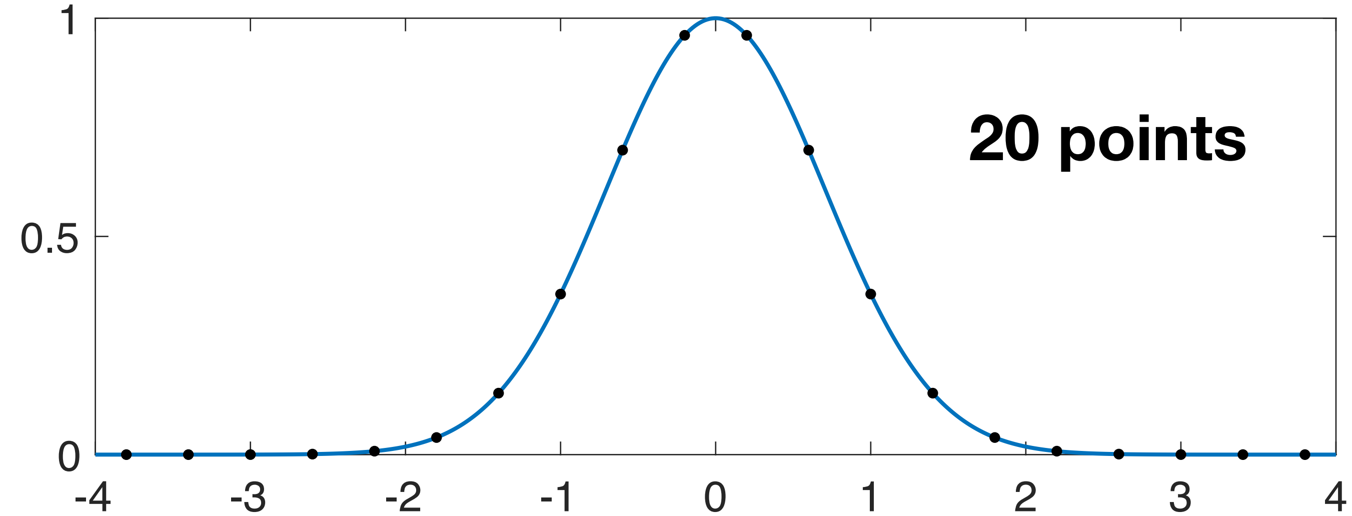
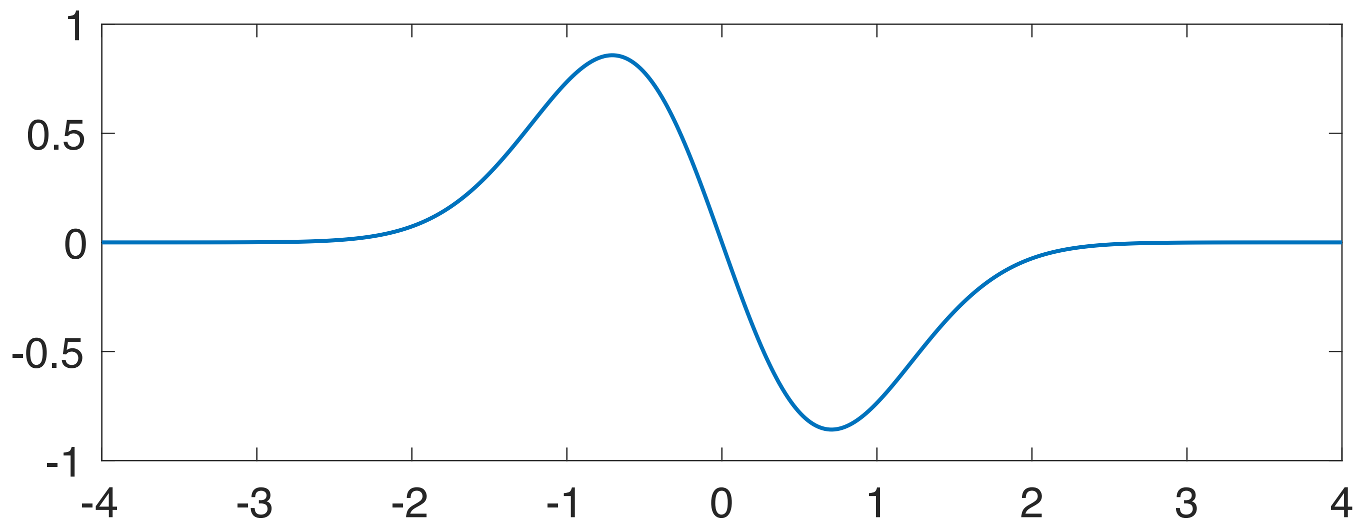


Derivatives

Fourier Approach





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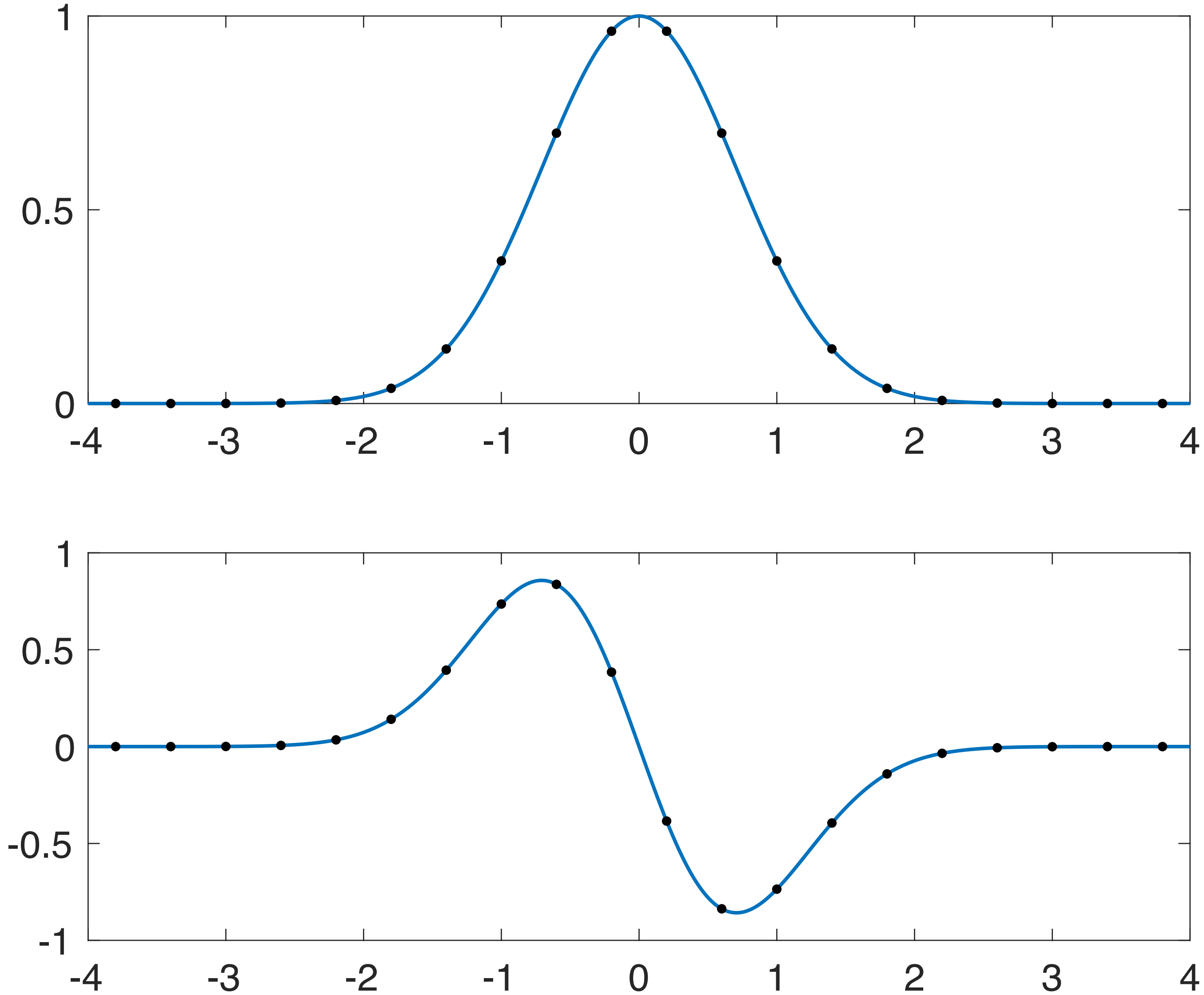
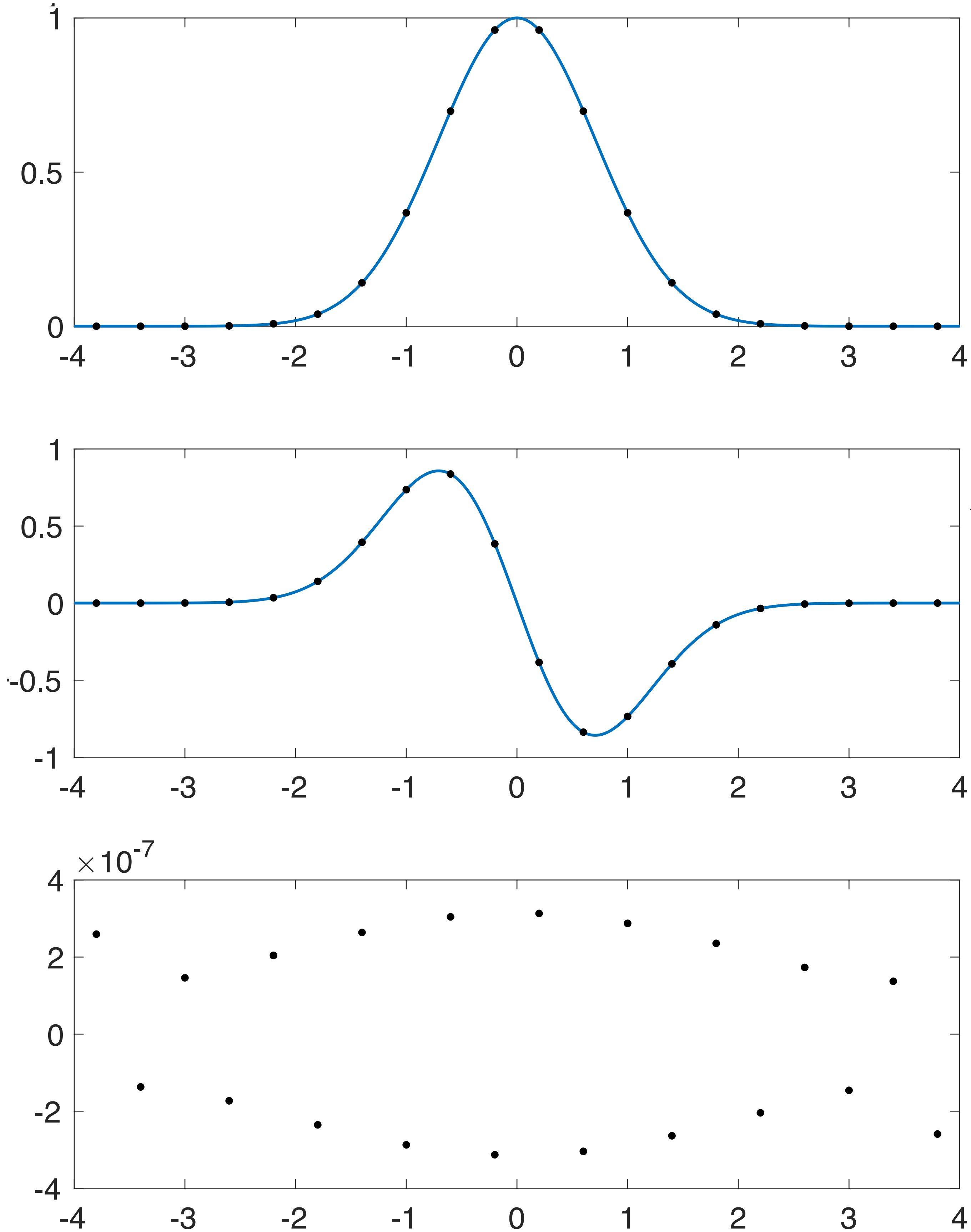


Implemented as a FFT

$$\frac{df}{dx} \approx a_{11}f(x_1) + a_{12}f(x_2) + \ldots a_{1N}f(x_N)$$

Derivatives

<u>Fourier Approach</u>



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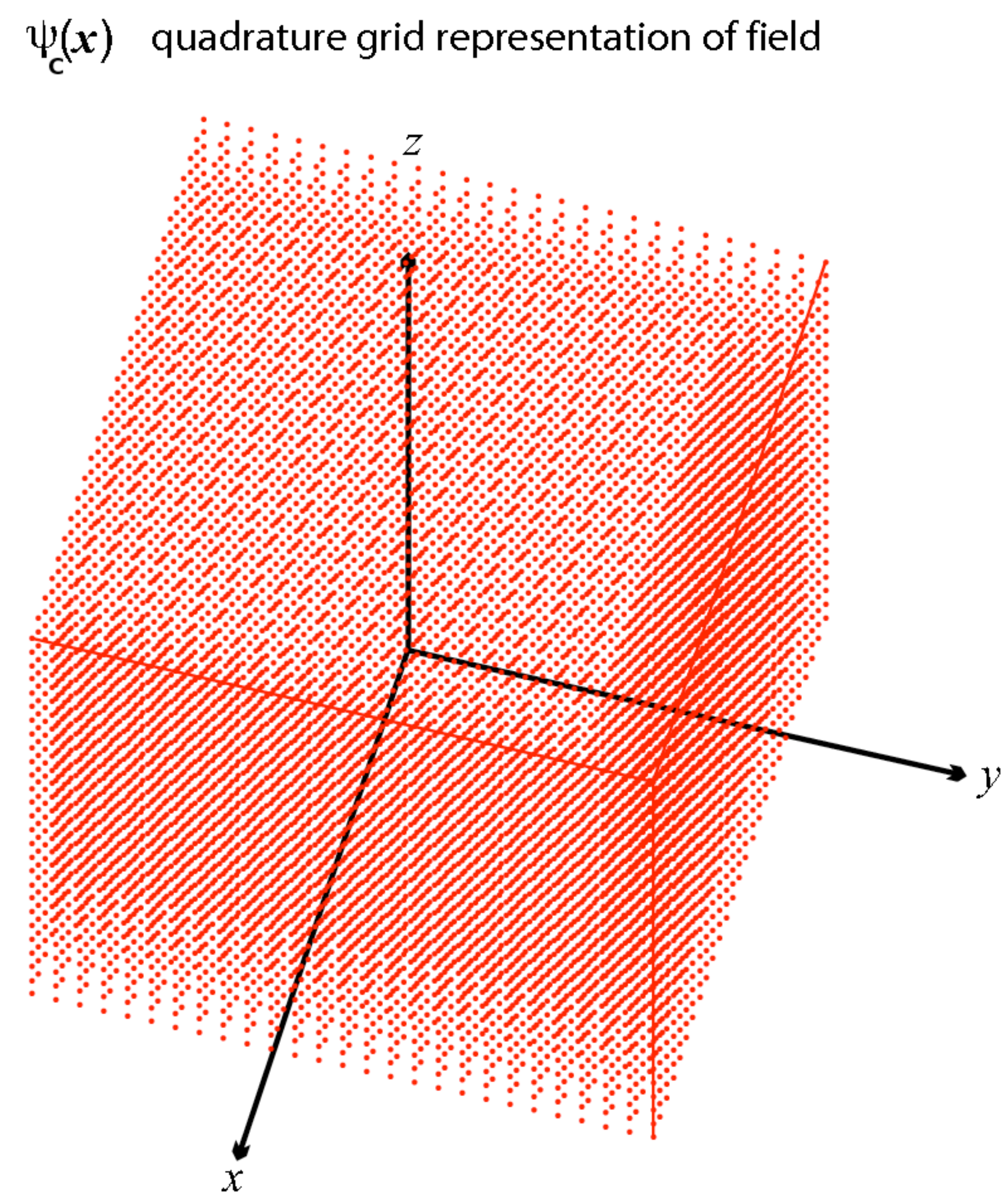
Spectral methods

1000×1000×1000

Vs

100×100×100



Spectral methods

- Extremely efficient and accurate representations

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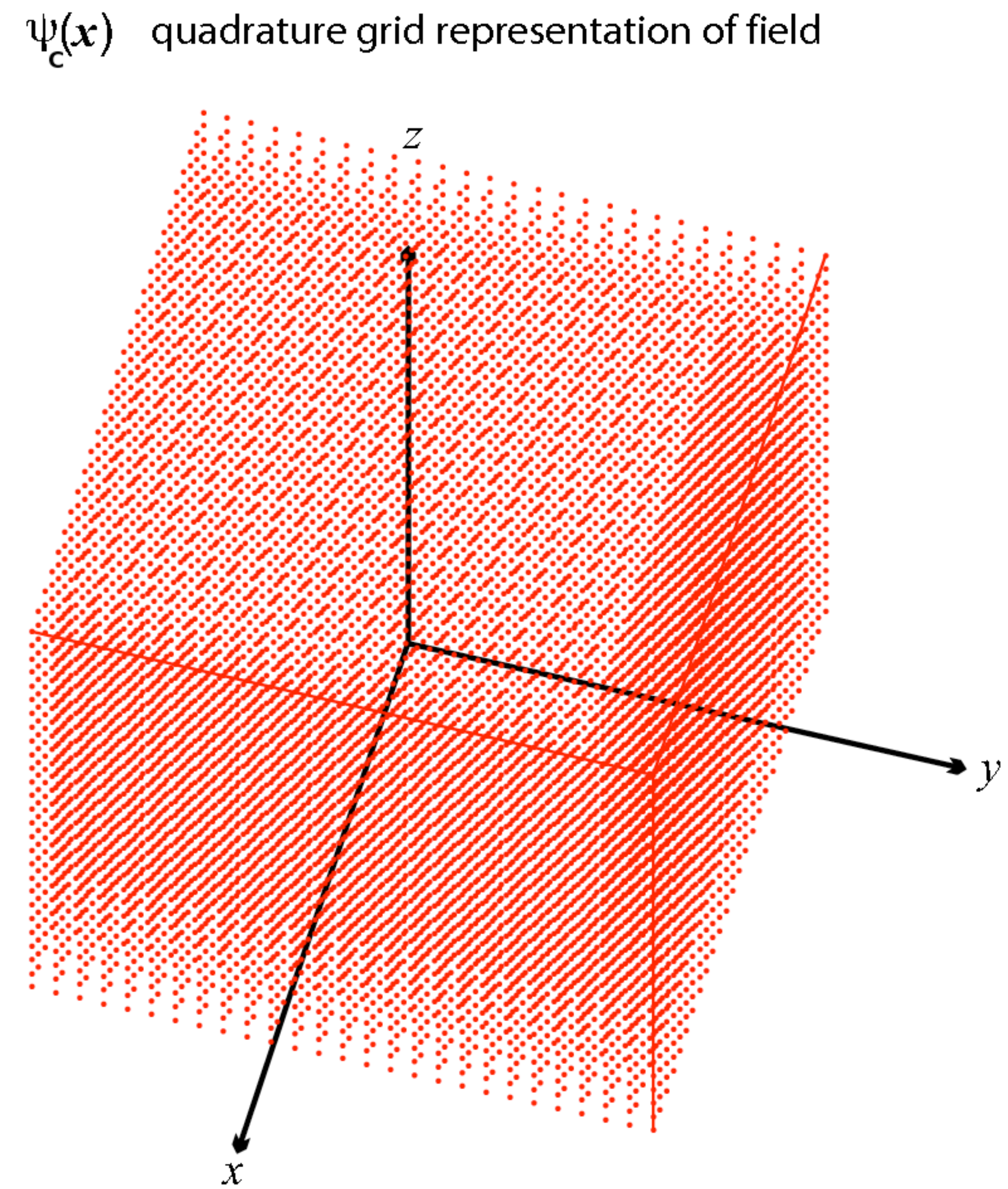

Spectral methods

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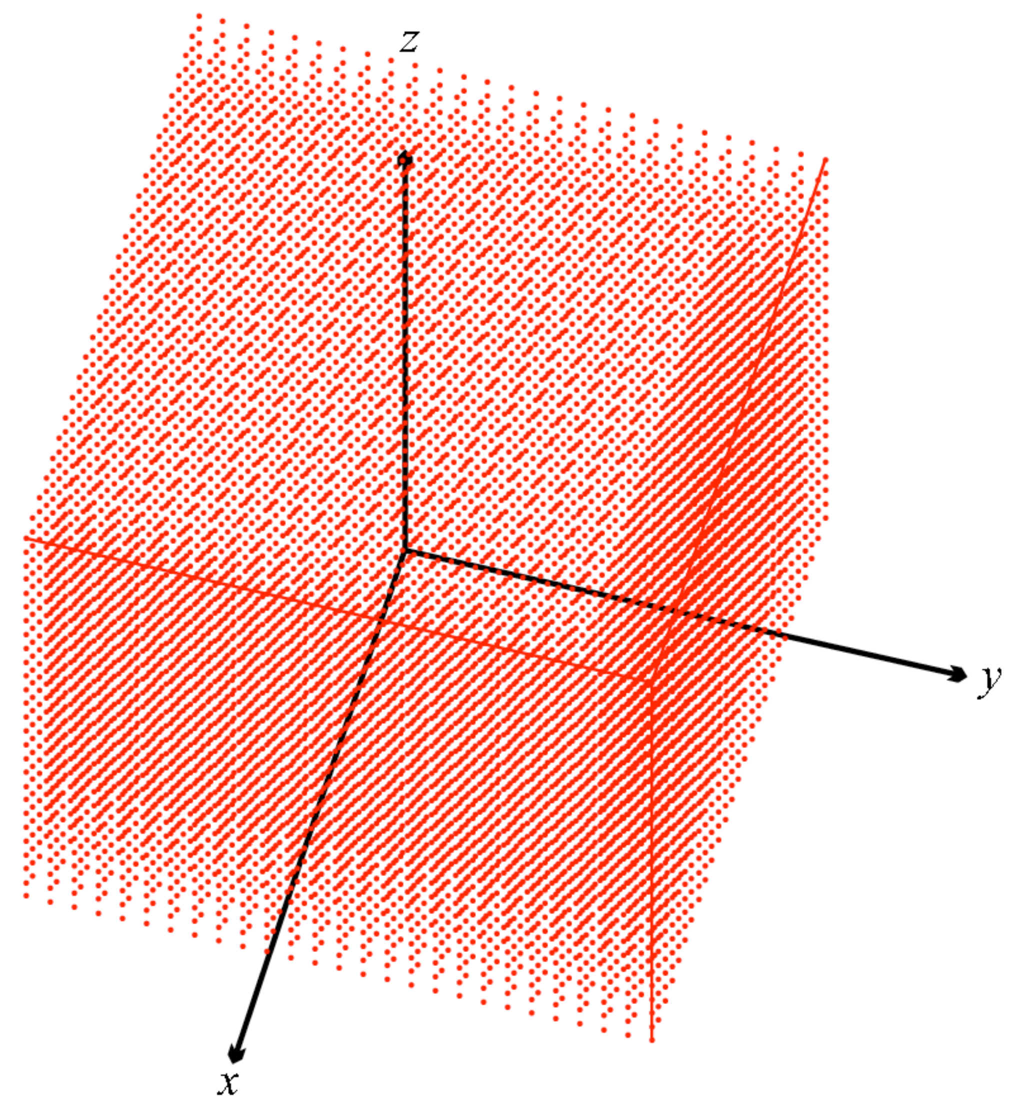
- Great for integration + interpolation

$\psi_c(x)$ quadrature grid representation of field



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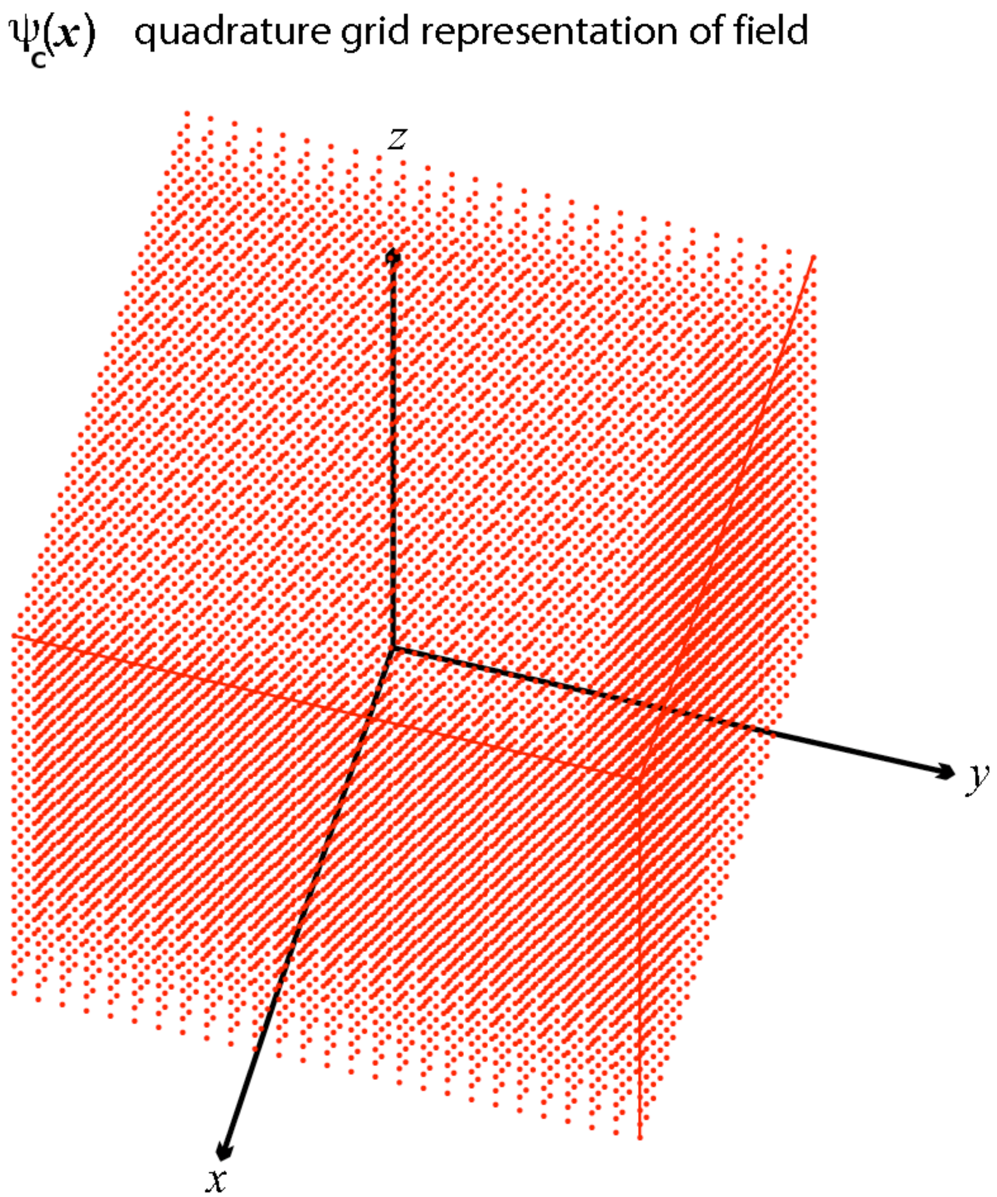

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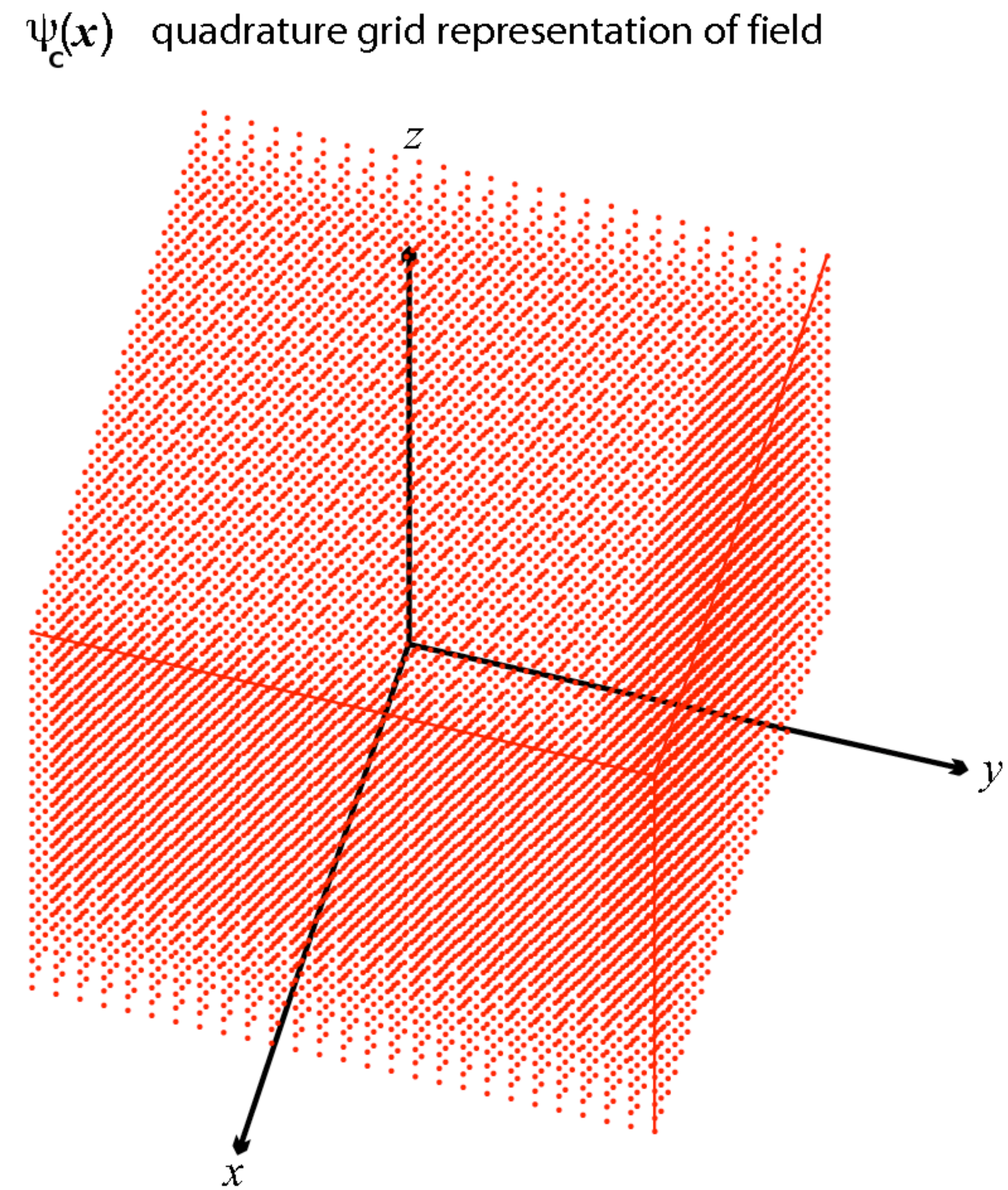

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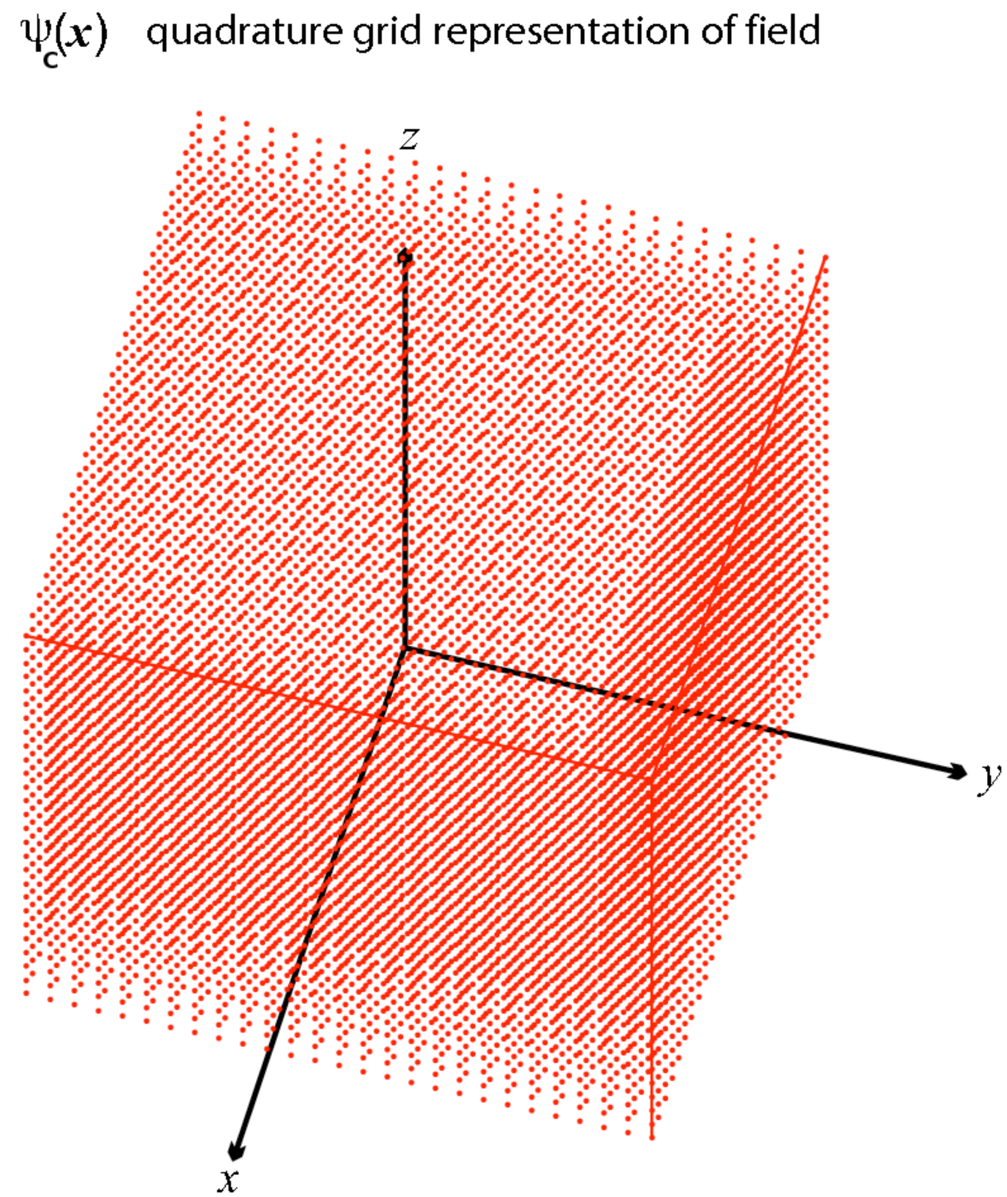

Key to accurate answers (e.g. >5SF) and tractable calculations in 3D

Code

- Group members write bespoke code for their research projects.
- Most code written in MatLab
  - Good for development and execution in single node environments
  - Surprisingly (?) good performance on GPUs
  - Supported on NeSI via Otago Site licence

Hardware Performance*

		Time (s)
Mahuika	Tesla P100 GPU	**25**
	CPU 12 Cores	230
	CPU 24 Cores	165
	CPU 36 Cores	154
iMac Pro	CPU 8 Cores	180
Thunderbirds (Otago Cluster)	3.3GHz CPU 10 Cores	181
	2.7GHz CPU 6 Cores	195
	Titan Black GPU	35
	Titan V GPU	**13**

Titan V
Volta architecture
12GB HBM2
5120 CUDA cores
~$3k USD

***Tentative numbers from a test**
3D GPE evolution 192×192×192 size

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Conclusion

- Quantum physics research is a niche user of HPC resources in NZ
- Our students are in demand in “big data” for their modelling, visualization, analysis and coding expertise.
- MORE GPUs!!!!!!