A new Gross-Pitaevskil approach for exciton superfluids and incompressible supersolids

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Research Foundation Flanders
Opening new horizons

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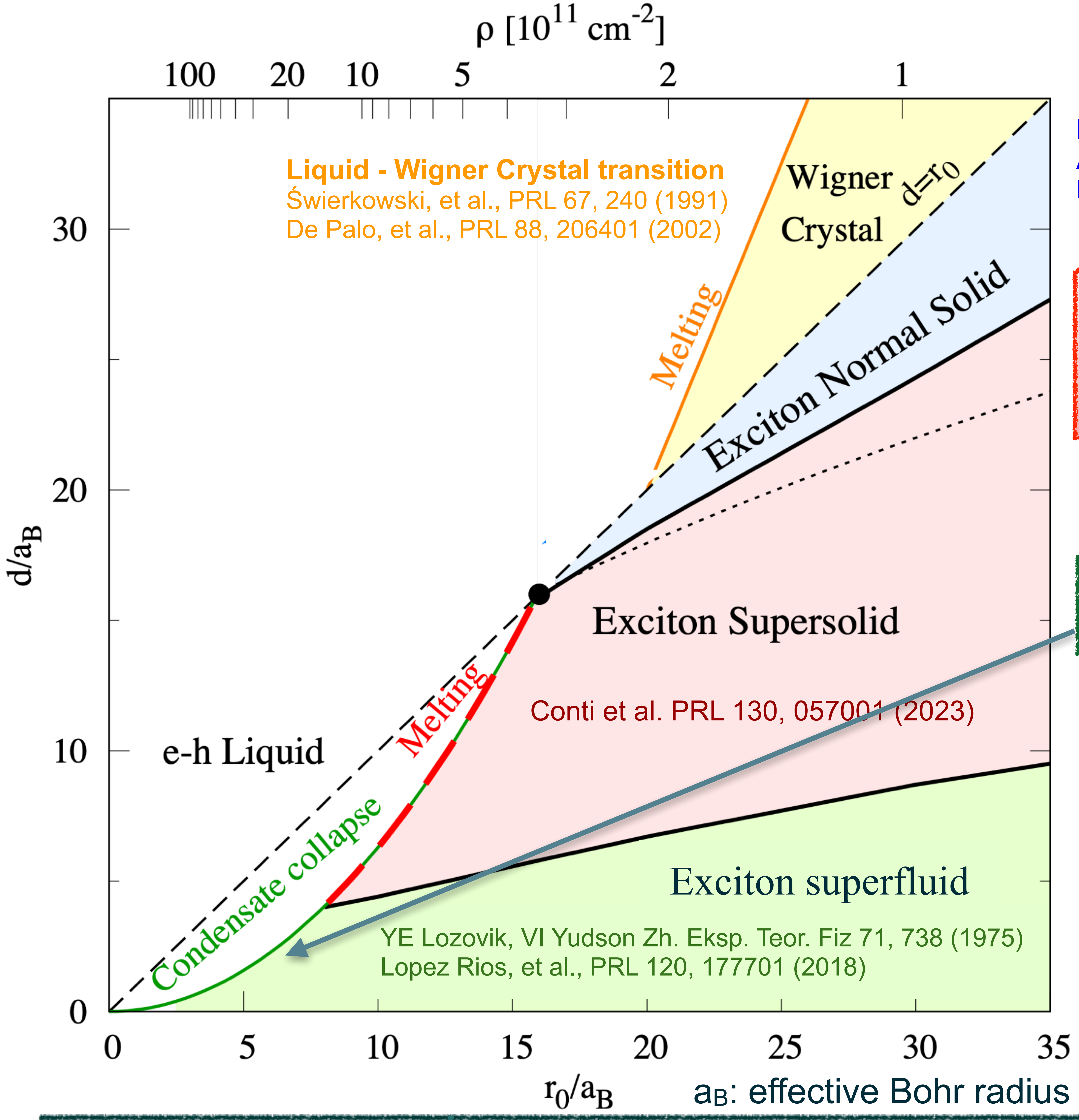
ELECTRON-HOLE PHASE DIAGRAM (T = 0)



aB: effective Bohr radius

Exciton liquid-solid transition
Astrakharchik et al. PRL 98, 060405 (2007);
Böning, et al., PRB 84, 075130 (2011)

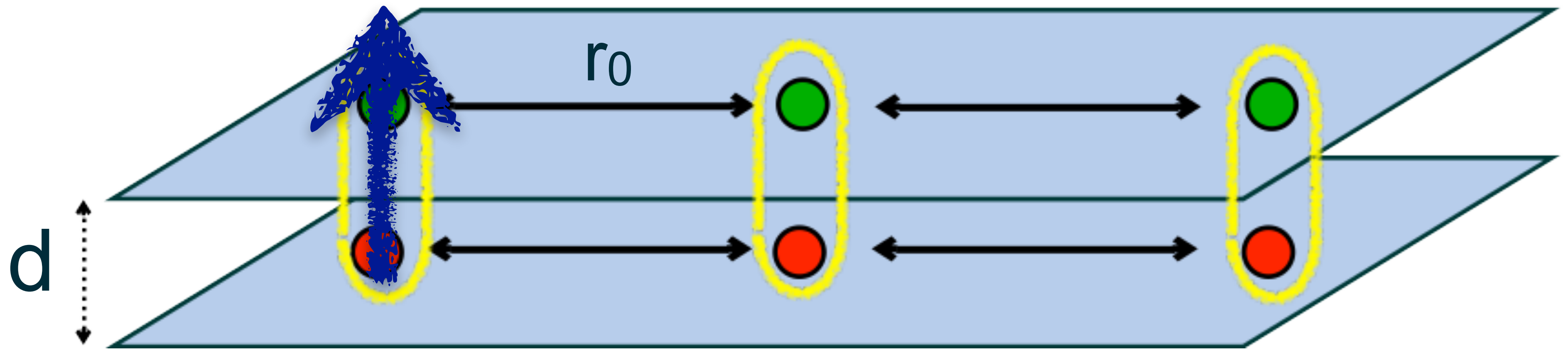
First example of **incompressible supersolid**:
- Spontaneous breaking of both symmetries
- One particle per site
- No vacancies needed

[A. J. Leggett, Phys. Rev. Lett. 25, 1543 (1970)]
[G. V. Chester, Phys. Rev. A 2, 256 (1970)]

Because of the **screening**, quantum coherence is suppressed at high density. Superfluidity confined to the **BEC regime.**

[F. Pascucci et al. Phys. Rev. B **109**, 094512 (2024)]

$$\langle V_{ee} \rangle = \langle V_{hh} \rangle \propto \frac{1}{r_0}$$



$$\langle V_{eh} \rangle \propto -\frac{1}{d}$$

THEORY FOR EXCITON SUPERSOLID

The Hamiltonian is,

$$H = \int d^2\mathbf{r}\,\Psi^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2M_\mathrm{X}}\right)\Psi(\mathbf{r}) + \frac{1}{2}\iint d^2\mathbf{r}d^2\mathbf{r}'\,\Psi^\dagger(\mathbf{r})\Psi^\dagger(\mathbf{r}')V_\mathrm{XX}(\mathbf{r}'-\mathbf{r})\Psi(\mathbf{r})\Psi(\mathbf{r}')$$

$$V_{XX}(r) = \frac{2\,e^2}{4\pi\epsilon}\left(\frac{1}{r} - \frac{1}{\sqrt{r^2+d^2}}\right)$$

Exciton-Exciton interaction (e-e, h-h, e-h Coulomb interactions)

- It is **purely REPULSIVE**!
- $d \ll r_0 \rightarrow V_{XX} \sim \dfrac{d^2}{r^3}$
- $d \gg r_0 \rightarrow V_{XX} = V_{ee} \sim \dfrac{1}{r}$

GROSS PITAEVSKII EQUATION

We can define the time-independent Gross-Pitaevskii equation (GPE) for $\Psi(\mathbf{r}, t) = \Psi(\mathbf{r}) e^{-i\mu t/\hbar}$

- For an exciton condensate with **non-local exciton-exciton interaction**.

$$-\frac{\hbar^2 \nabla^2}{2M_X} \Psi(\mathbf{r}) + \left(\int d^2\mathbf{r}' \, V_{XX}(\mathbf{r} - \mathbf{r}') \, |\Psi(\mathbf{r}')|^2 \right) \Psi(\mathbf{r}) = \mu \, \Psi(\mathbf{r}) \, .$$

This is still an incomplete picture:

- it does not include **exciton-exciton correlations**
- it incorrectly includes interaction of an exciton on a site with itself (**Self interaction**)

(i) TWO BODY CORRELATIONS

We work at very low exciton density: the short-range two-body correlations are known to be strong.

The exciton pair correlation function $g(\mathbf{r})$ vanishes across a region of small r.

[G. E. Astrakharchik, J. Boronat, I. L. Kurbakov, and Yu. E. Lozovik, Phys. Rev. Lett. 98, 060405 (2007)]

$V^{eff}_{XX}(\mathbf{r}) = g(\mathbf{r})V_{XX}(\mathbf{r})$ with $g(\mathbf{r})=0$ when $r < R_{HardCore.}$

We include the effect with an effective Hamiltonian.

$$\mathscr{H}^{\rm eff} = \int d^2\mathbf{r}\,\Psi^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2M_X}\right)\Psi(\mathbf{r}) + \frac{1}{2}\iint d^2\mathbf{r}d^2\mathbf{r}'\,\Psi^\dagger(\mathbf{r})\Psi^\dagger(\mathbf{r}')t_{XX}(\mathbf{r}'-\mathbf{r})\Psi(\mathbf{r})\Psi(\mathbf{r}')$$

The local t-matrix $t_{XX}(\mathbf{r})$ (multiple short-range two-body scattering) vanishes for $r < R_{HardCore.}$

(ii) THE TRUE BOSE SOLID

The "true Bose solid" ground state of the form,

$$|\Psi_0\rangle = \left(\prod_{i=1}^{N} c_i^\dagger\right)|\Psi_{\mathrm{vac}}\rangle$$

with

$$c_i^\dagger = \int d^2r\,\phi_i(\mathbf{r})\Psi^\dagger(\mathbf{r}); \qquad c_i = \int d^2r\,\phi_i(\mathbf{r})\Psi(\mathbf{r})$$

for a complete basis with fixed sites *i* of a periodic lattice hosting localized orbital $\phi_i(r)$.

The effective Hamiltonian can be written as

$$\mathscr{H}^{\mathrm{eff}} = \sum_{i,j} c_i^\dagger T_{ij}\, c_j + \frac{1}{2}\sum_{i,i',j,j'} c_i^\dagger c_{i'}^\dagger\, U^{XX}_{i,i',j,j'}\, c_j c_{j'}$$

$$T_{ij} = \int d^2\mathbf{r}\,\phi_i(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2M_{\mathrm{X}}}\right)\phi_j(\mathbf{r})$$

$$U^{XX}_{i,i',j,j'} = \iint d^2\mathbf{r}\,d^2\mathbf{r}'\,\phi_i(\mathbf{r})\,\phi_{i'}(\mathbf{r}')\,t_{XX}(\mathbf{r}'-\mathbf{r})\,\phi_j(\mathbf{r})\,\phi_{j'}(\mathbf{r}')$$

[P. W. Anderson, Basic notions of condensed matter physics (Addison-Wesley, Reading, Mass., 1997)]

(ii) HARTREE EQUATION

$$-\frac{\hbar^2 \nabla^2}{2M_\mathrm{X}}\phi_i(\mathbf{r}) + \int d^2\mathbf{r}'\phi_i(\mathbf{r})t_{XX}(|\mathbf{r}'-\mathbf{r}|)\sum_j |\phi_j(\mathbf{r}')|^2 - \int d^2\mathbf{r}'\phi_i(\mathbf{r})t_{XX}(|\mathbf{r}'-\mathbf{r}|)|\phi_i(\mathbf{r}')|^2 = \mu\phi_i(\mathbf{r})$$

- Only present when there is exactly one exciton per unit cell!
  - $c_i|\Psi_0\rangle = 0$ since the site *i* cannot be emptied twice.

- **Attractive interaction** generated from the property that an exciton on a site feels the repulsions from its neighbours on other sites but not its own potential.

- The **absence of these self-interactions** acts like a potential well centered on the site.

- If V_{XX} is strong enough (large d), the potential wells can be deep enough to form bound-states.

- The potential wells **make the solid incompressible**!

EXTENDED GROSS PITAEVSKII EQUATION

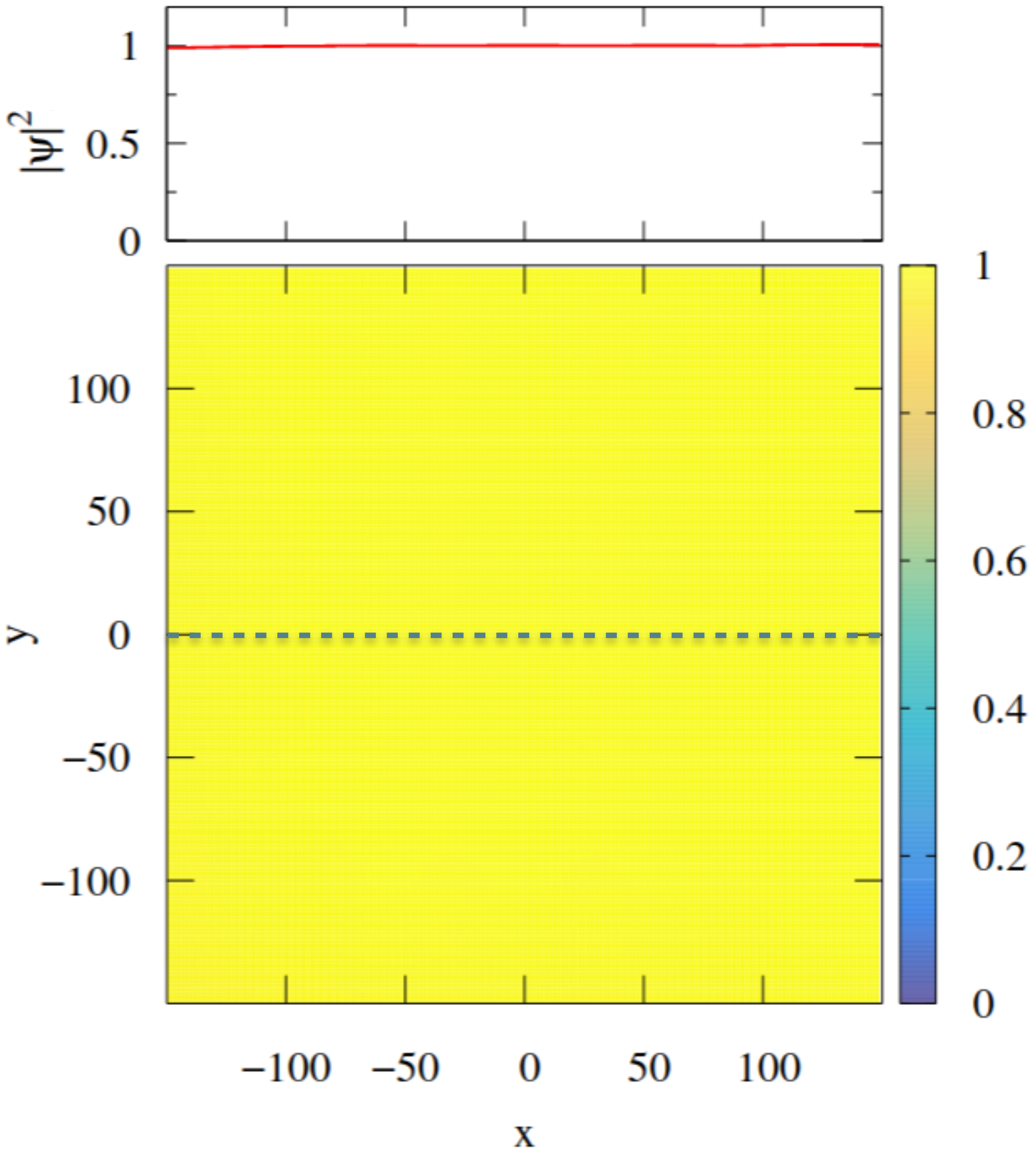
- For an exciton condensate with **non-local exciton-exciton interaction, correlations** and without **self-interaction**.

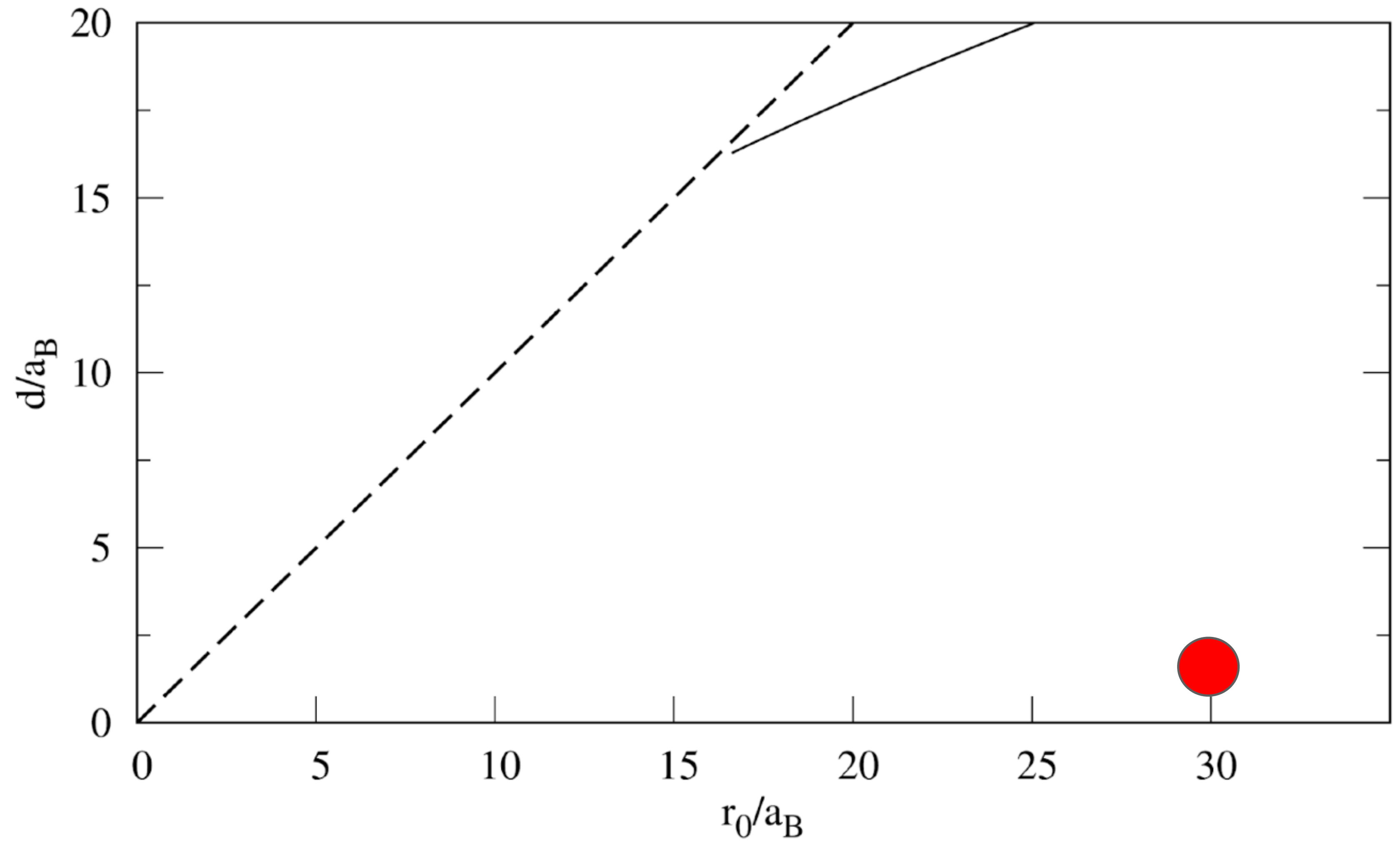
$$-\frac{\hbar^2\nabla^2}{2M_X}\Psi(\mathbf{r})+\left(\int d^2\mathbf{r}'\,t_{XX}(\mathbf{r}-\mathbf{r}')\,|\Psi(\mathbf{r}')|^2\right)\Psi(\mathbf{r})-\boxed{\left(\int_{\mathbf{r}'\in j_{\mathbf{r}}} d^2\mathbf{r}'\,t_{XX}(\mathbf{r}-\mathbf{r}')\,|\Psi(\mathbf{r}')|^2\right)\Psi(\mathbf{r})}=\mu\,\Psi(\mathbf{r})$$

Self interaction at site $j_{\mathbf{r}}$

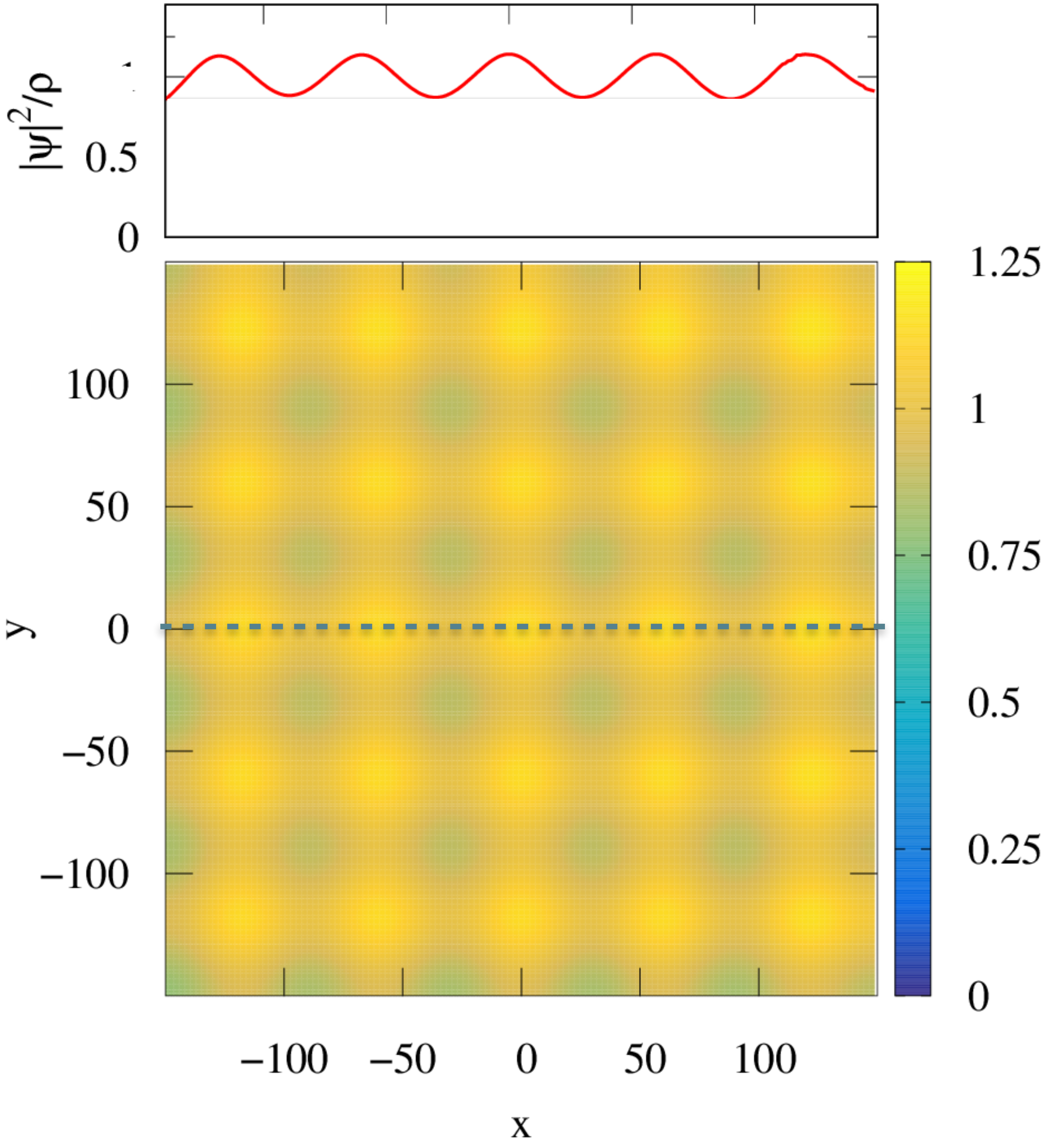
The **absence of self-interaction** for a particle on a site with itself leads to an **incompressible supersolid** (true Bose solid).

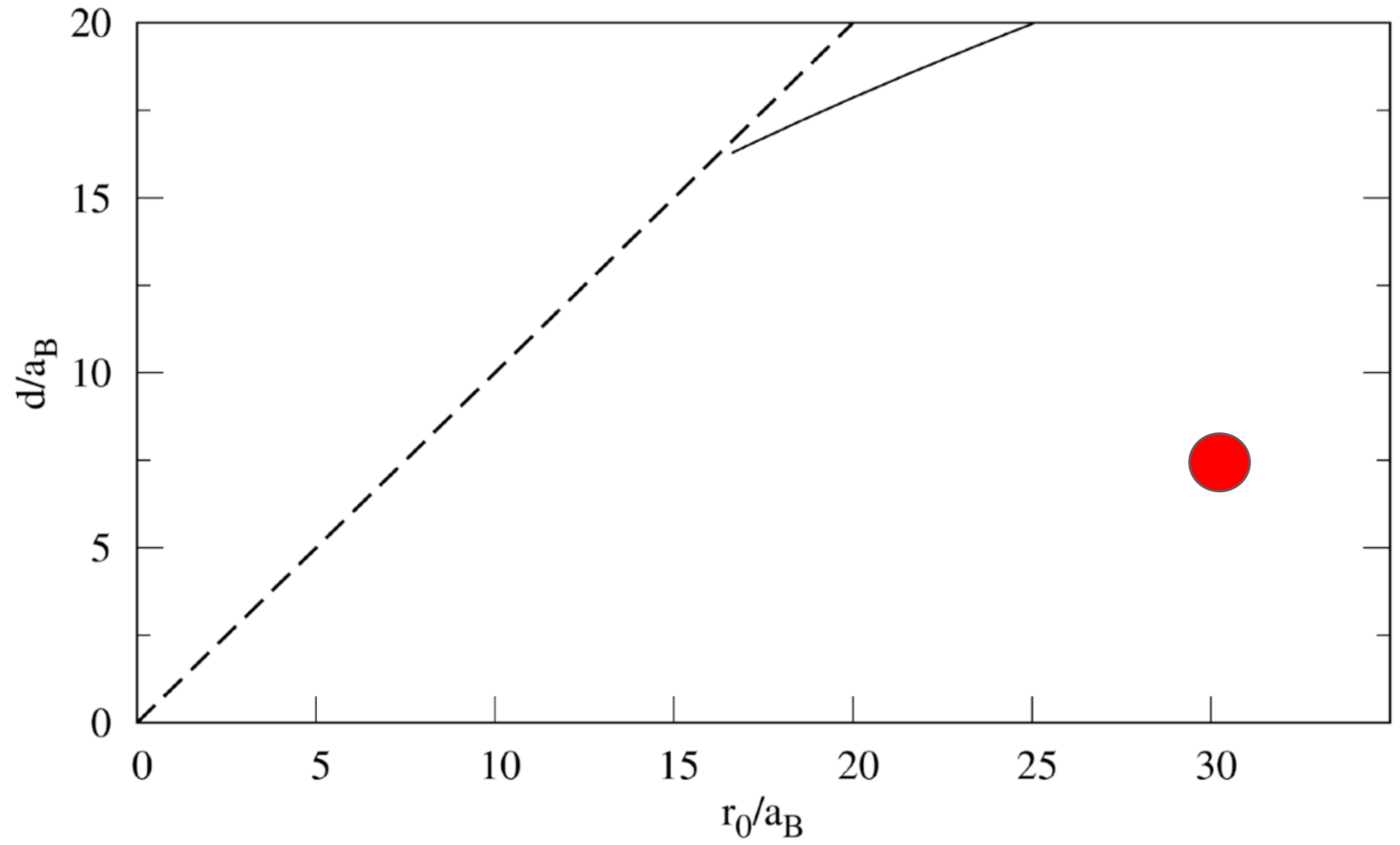
GPE for d=1 Superfluid homogeneous solution





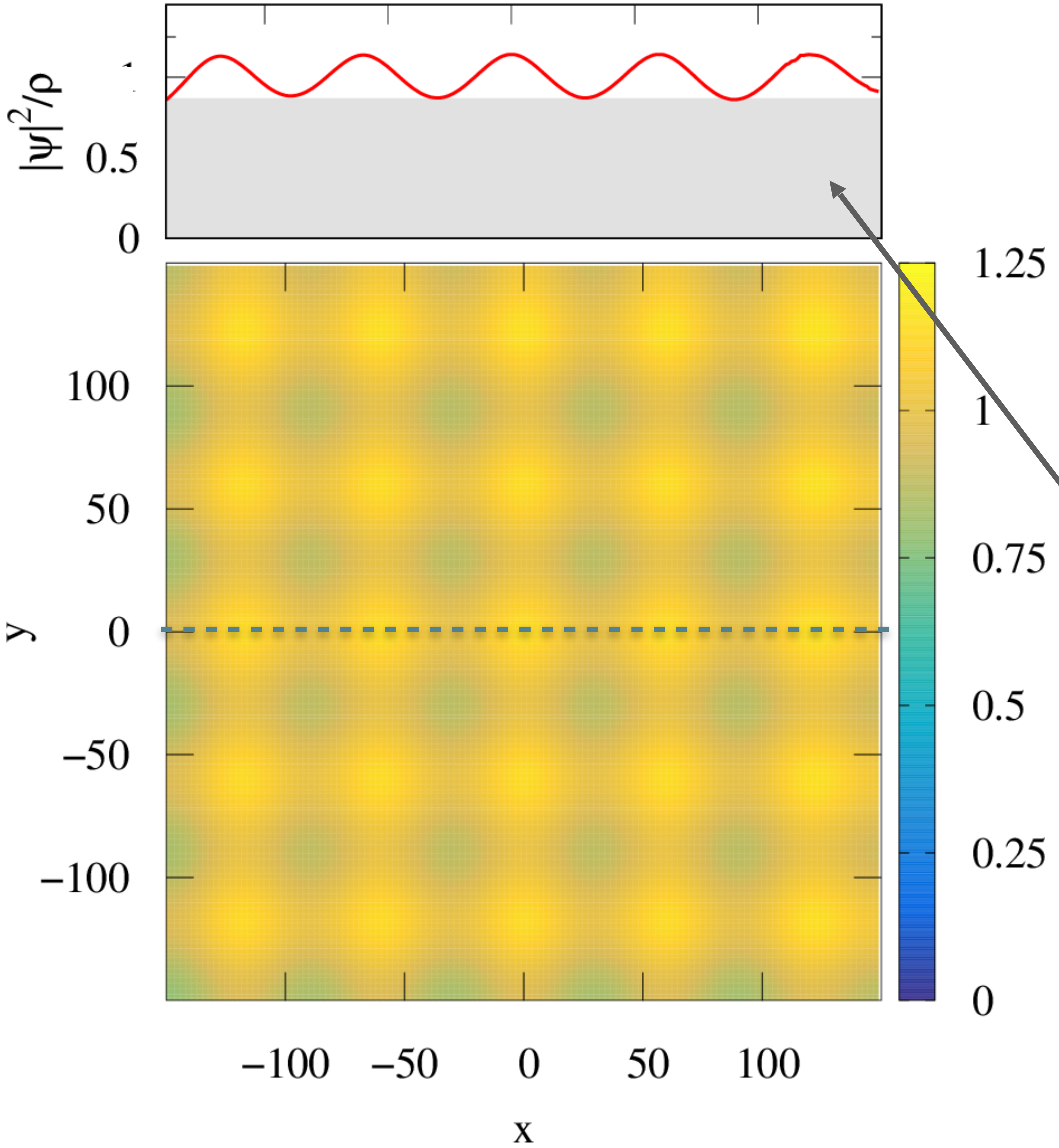
GPE for d=8 Supersolid solution

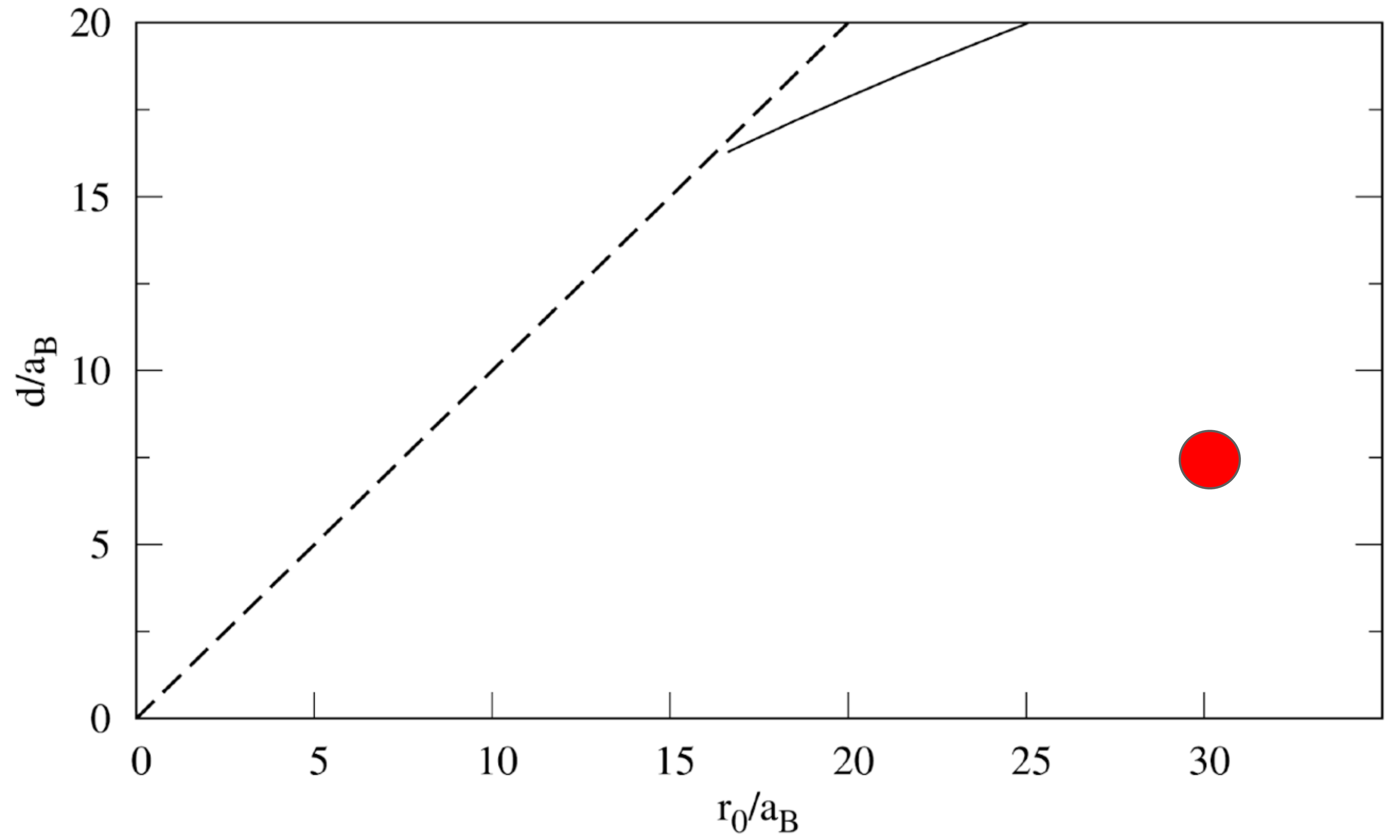




Note this is not a density wave!
This is an incompressible supersolid with one particle per site

GPE for d=8 Supersolid solution

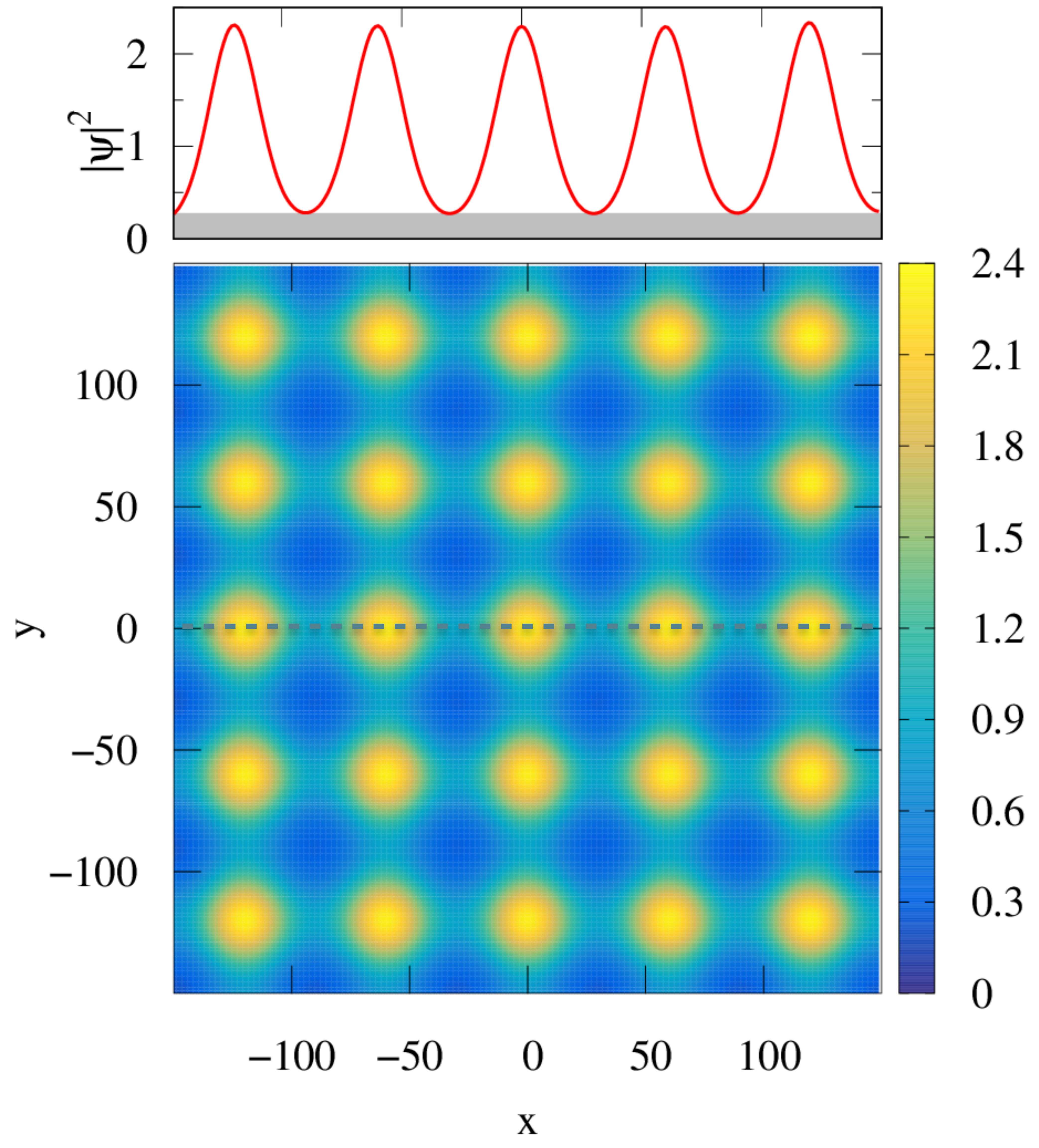


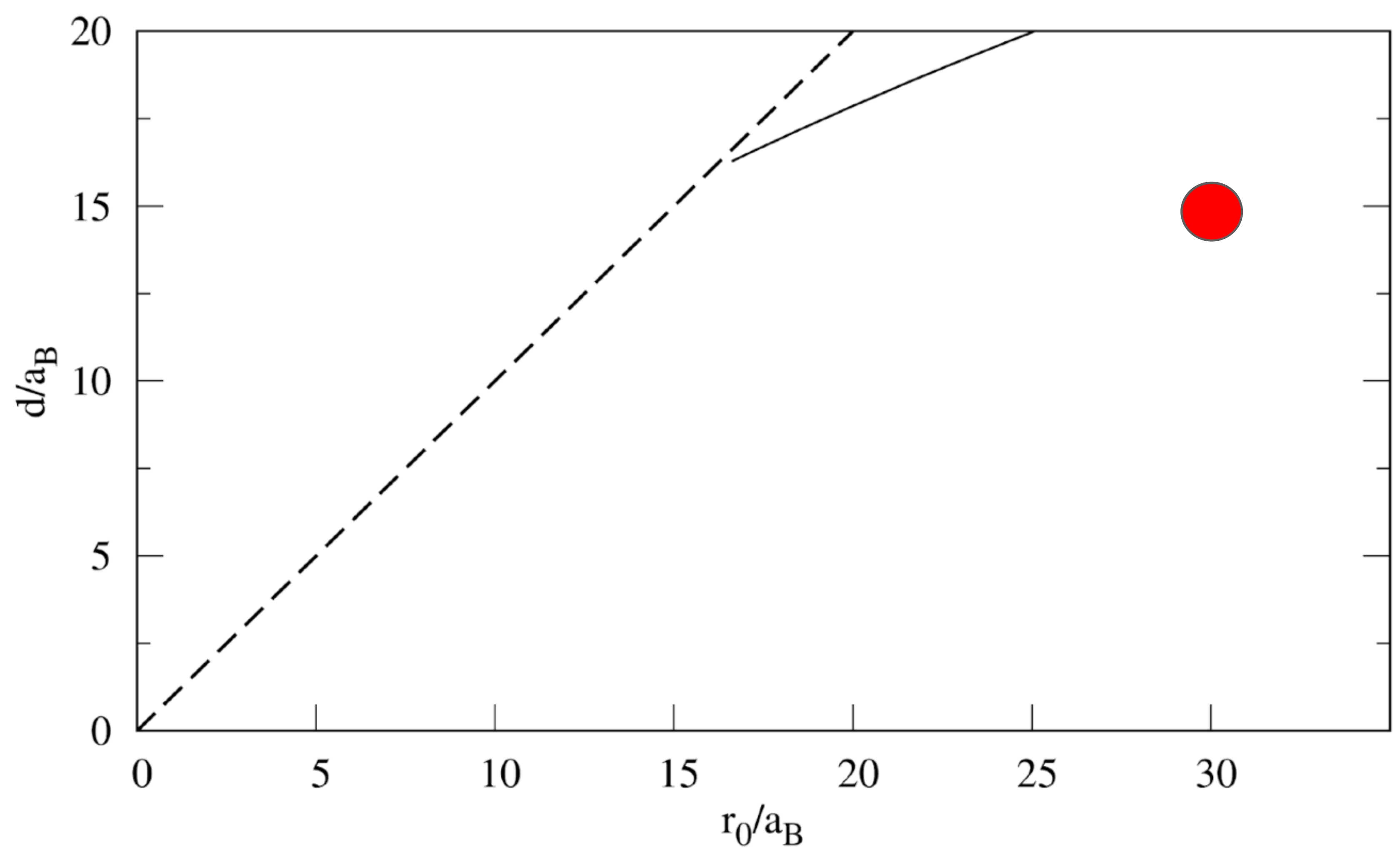


$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{N}}\left(\sqrt{\rho_B} + \sum_{i=1}^{N} G(\mathbf{r}-\mathbf{r}_i)\right)$$

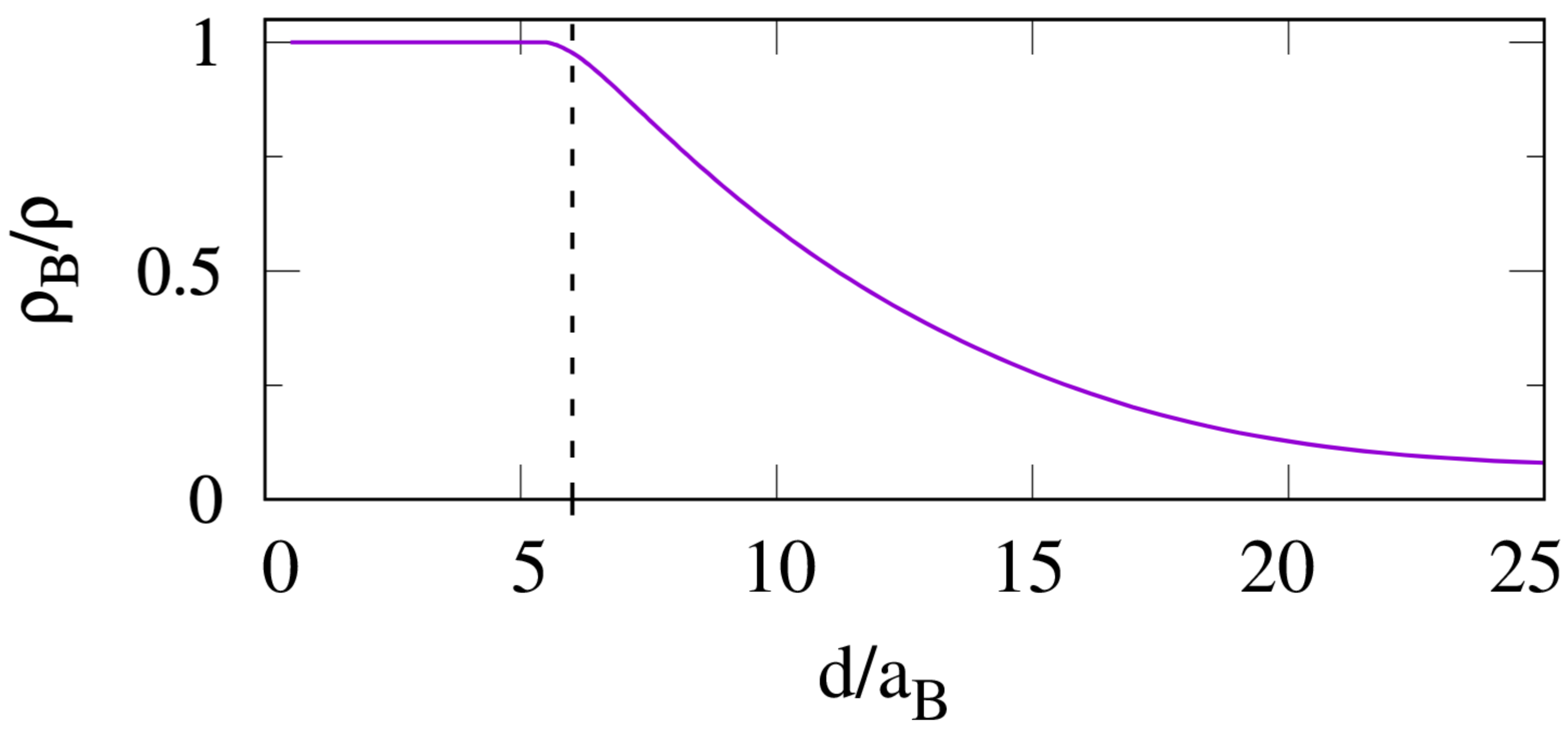
Grey area is a background contribution to the supersolid order parameter
(strong Leggett exchange term).
[A. J. Leggett, Phys. Rev. Lett. 25, 1543(1970)]

GPE for d=15 Supersolid solution

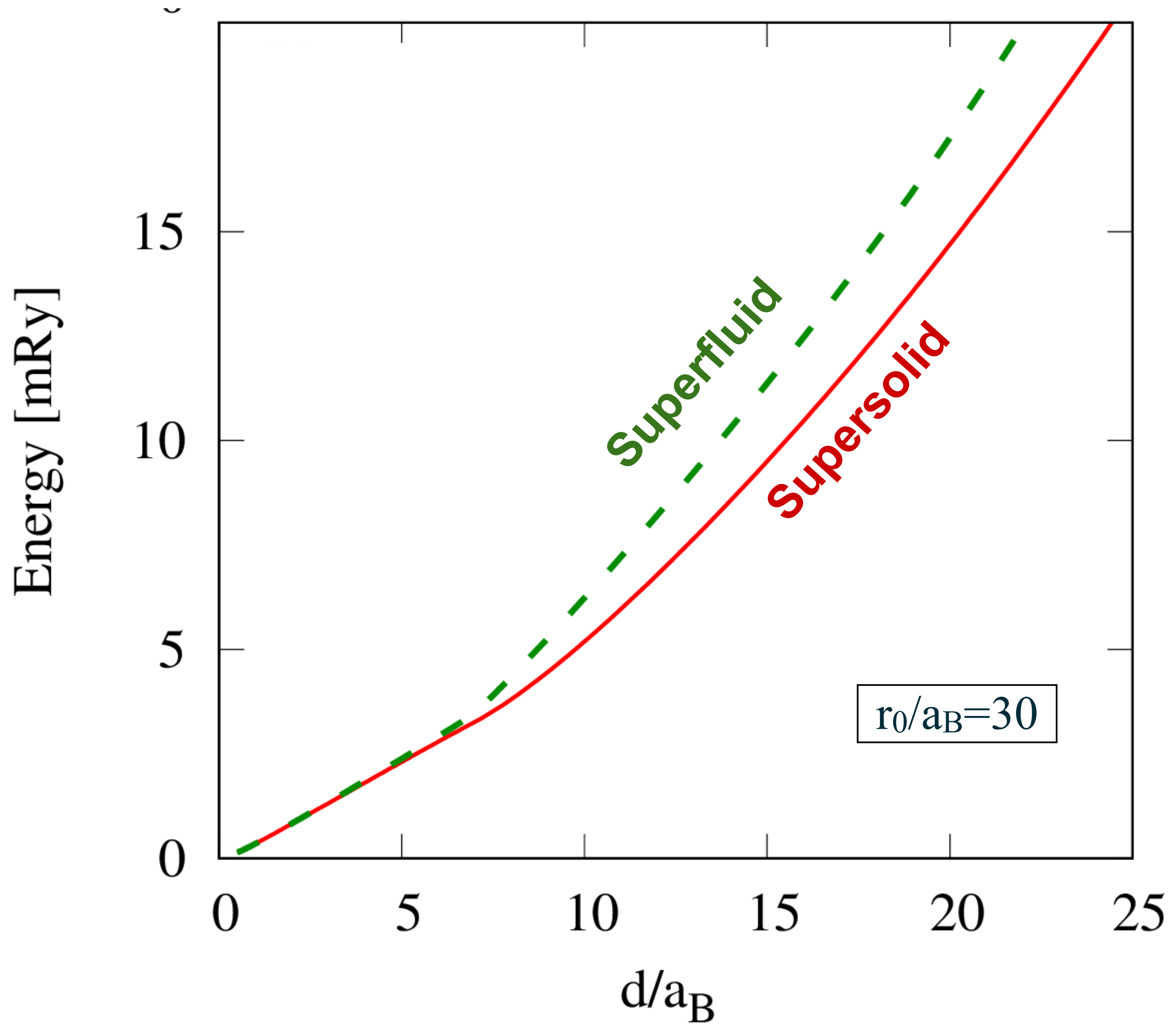


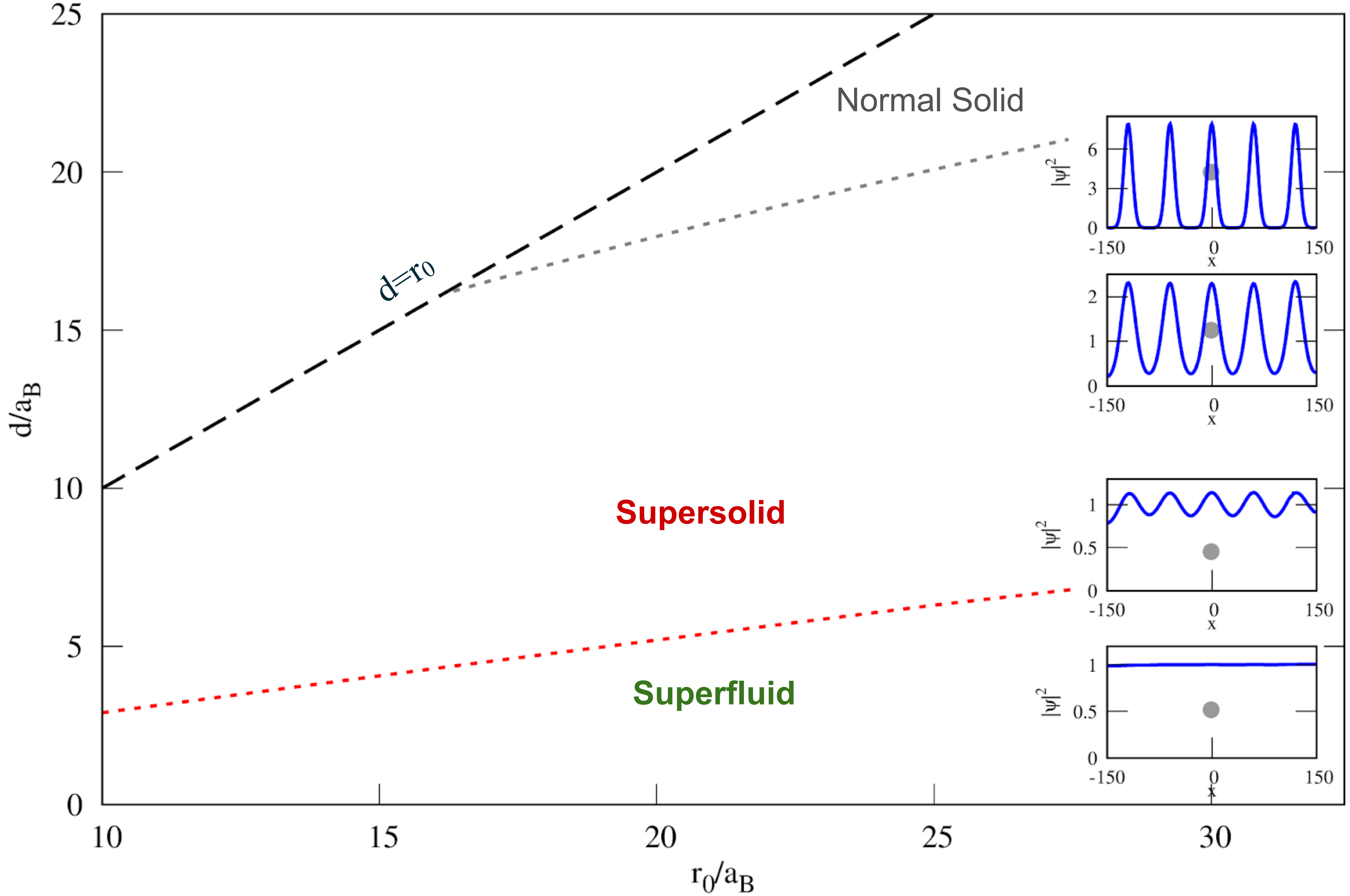


The background contribution (BG) in the Ψ(r) decreases by increasing d.



SUPERFLUID TO SUPERSOLID TRANSITION





- For small d the GPE gives the superfluid solution.
- As d increases there is a **Superfluid to Supersolid transition**. [Conti et al. PRL 130, 057001 (2023)]

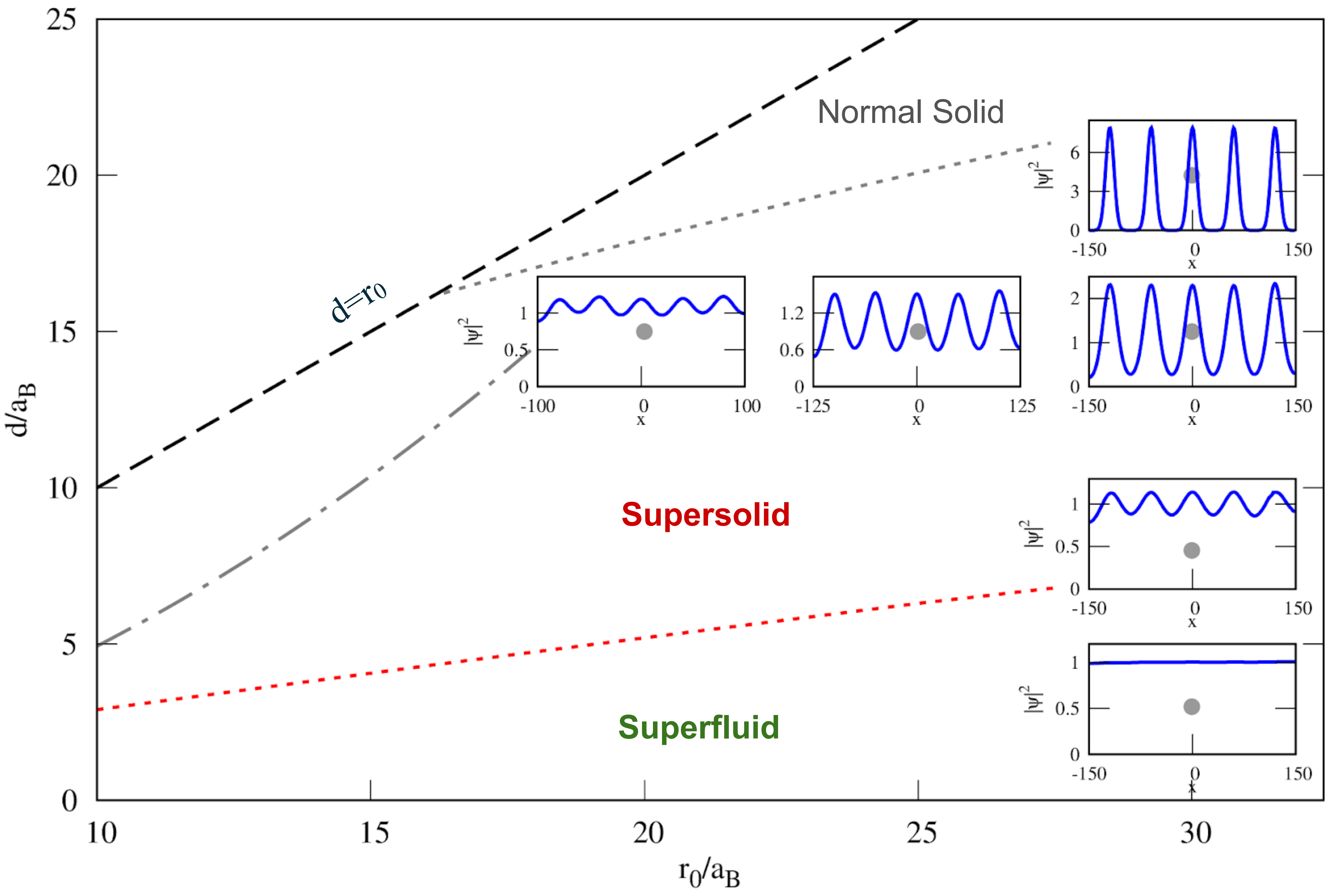
MELTING OF THE SUPERSOLID

As r_0 decreases (density increases):

- V_{xx} goes from dipolar-like to Coulomb-like interaction:
  ***V_{xx}* cannot support solidification.**
[J. Böning, et al. Phys. Rev. B 84, 075130 (2011)]

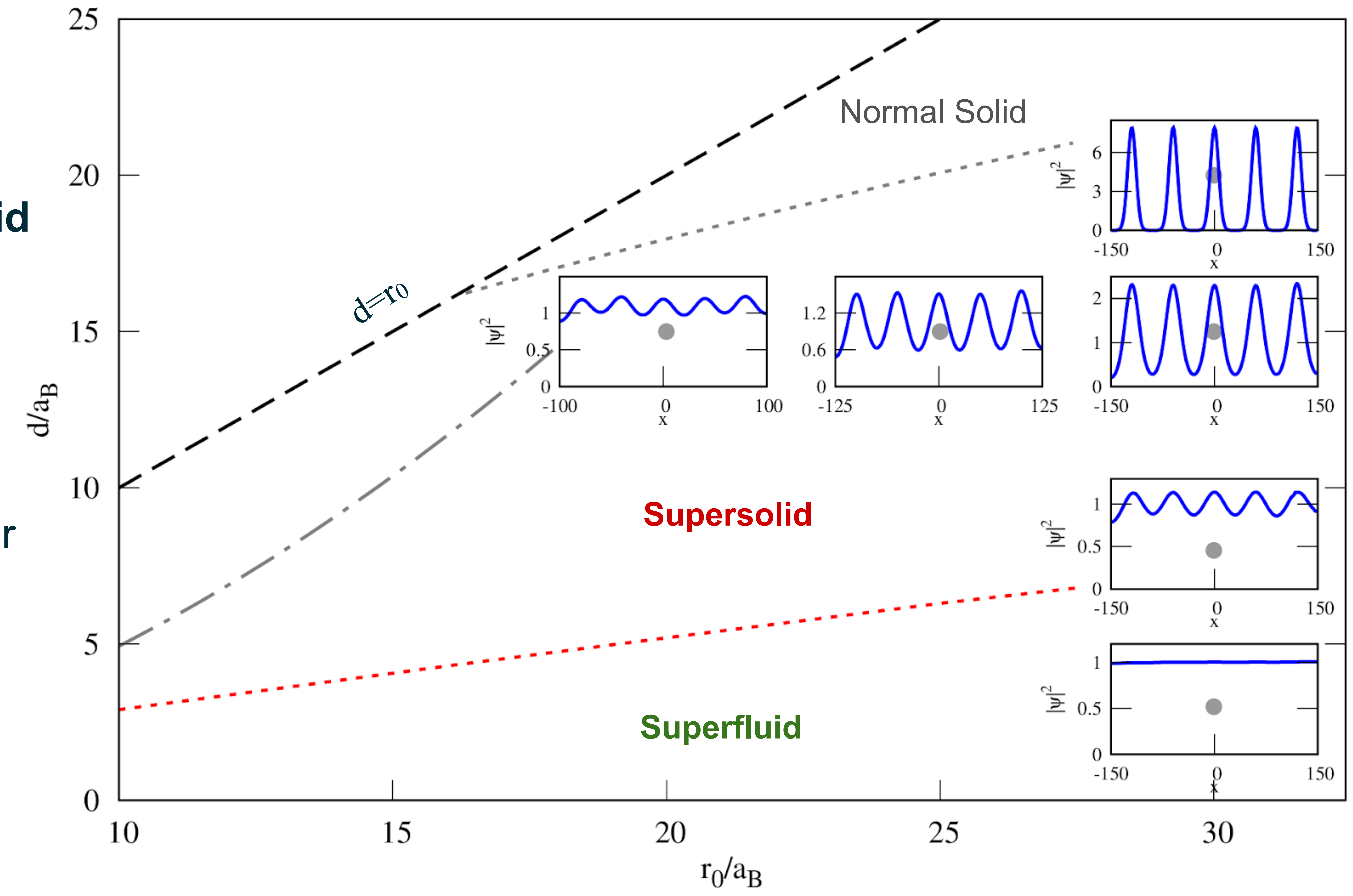
- Screening and intralayer correlations become stronger:
  the quantum coherence collapses.
[F. Pascucci et al. Phys. Rev. B **109**, 094512 (2024)]

Melting of the supersolid!



First step… but more to do

- **The absent self-interactions** for one particle on each site leads to an **incompressible supersolid**.
- GPE predicts a **superfluid to supersolid transition**.
- GPE well describes the evolution of the supersolid ground state throughout the phase diagram.
- We set the foundations to explore further supersolid properties, eg: vortices



[ArXiv:2507.20236]

Vortices to detect the existence of superfluidity and supersolidity.

- Collective modes

Filippo Pascucci

THEORY: SINGLE VORTEX IN EXCITON SUPERFLUID

We solve the time-independent Gross-Pitaevskii equation for $\Psi_{SF}(\mathbf{r}) = \sqrt{N}\,\psi_{SF}(r)\,e^{i\ell\theta(\mathbf{r})}$

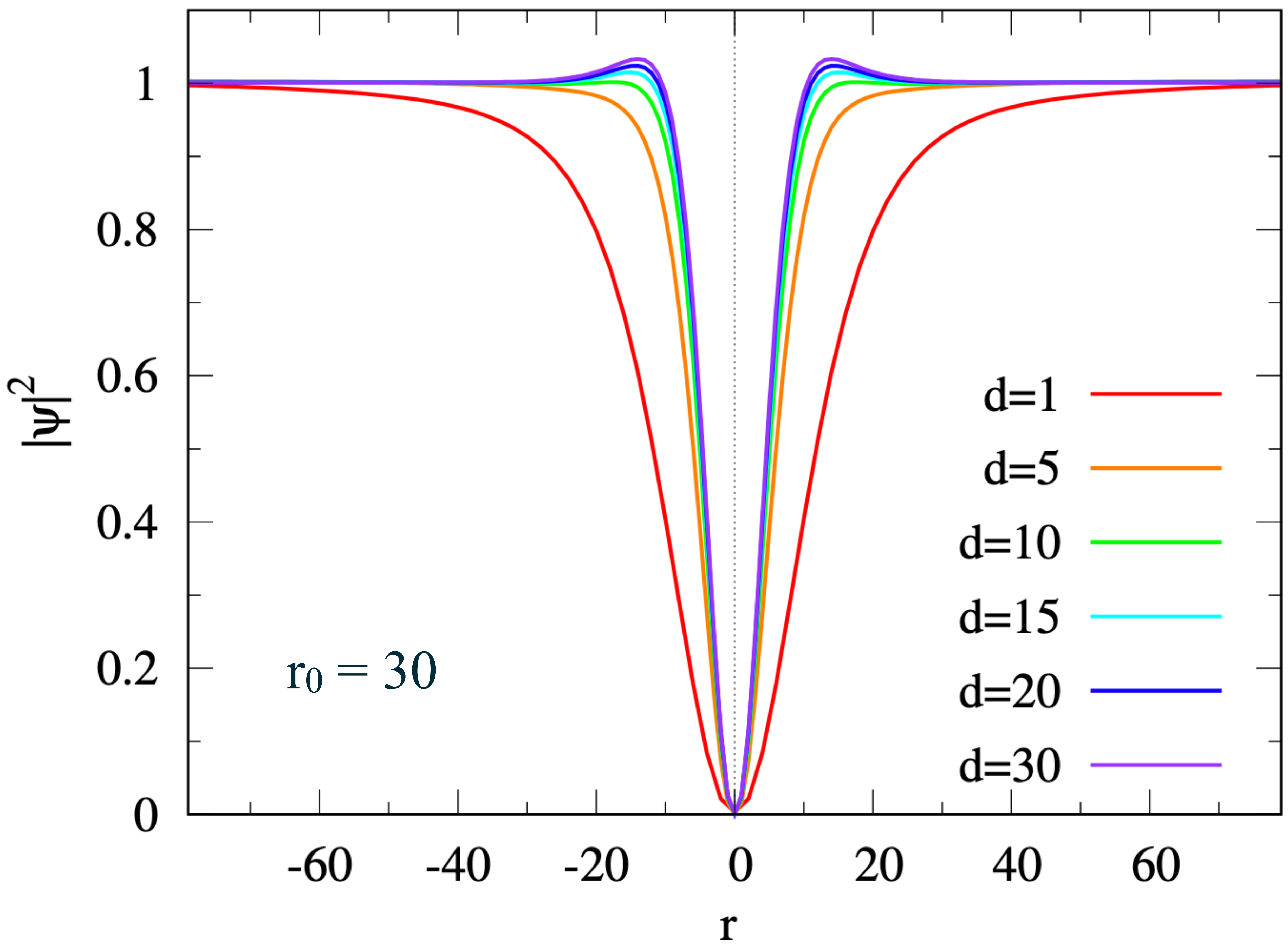
N number of particles

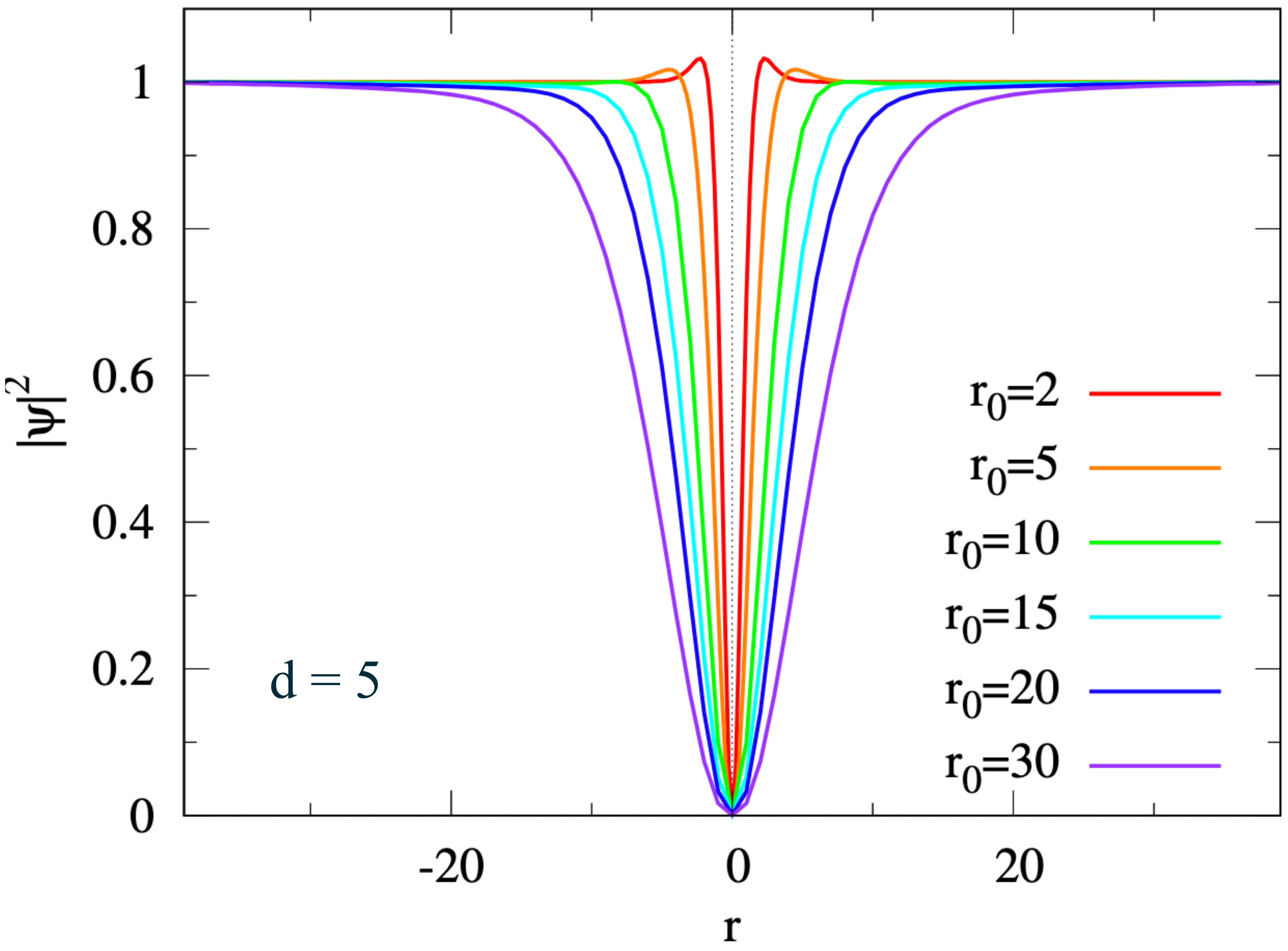
ℓ=*1* vortex degeneracy

$\theta = \tan^{-1}[y/x]$ Phase

$$\frac{\hbar^2\nabla^2}{2M_X}\,\psi_{SF}(\mathbf{r}) + \frac{\ell^2\hbar^2}{2M}\frac{1}{r^2}\psi_{SF}(r) + \left(\int d^2\mathbf{r}'\,V_{XX}(\mathbf{r}-\mathbf{r}')\,|\psi_{SF}(\mathbf{r}')|^2\right)\psi_{SF}(\mathbf{r}) = \mu\;\psi_{SF}(\mathbf{r})\,.$$

SINGLE VORTEX PROFILE





- **Healing length** ξ (radius of vortex) decreases by increasing the dipole strength and density and **saturates**.
- A **density pileup peak appears** at the vortex edge when *d* increases or the density increases.

THEORY: VORTEX LATTICE

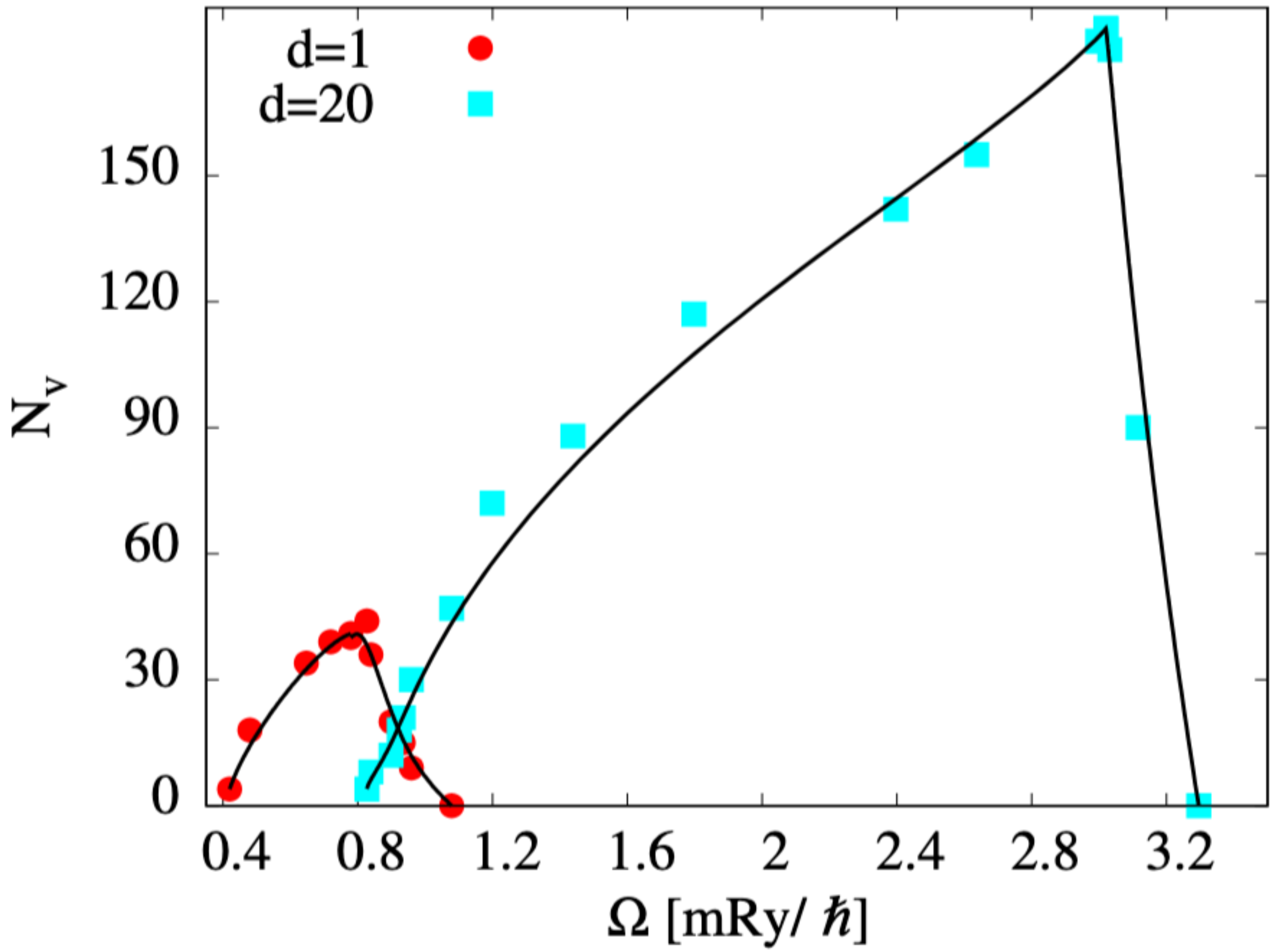
We solve the time-independent Gross-Pitaevskii equation in the rotating frame

$$-\frac{\hbar^2}{2M}\nabla^2\,\Psi(\mathbf{r}) + \phi_{XX}(\mathbf{r})\Psi(\mathbf{r}) - \boldsymbol{\Omega}\cdot\mathbf{L}\,\Psi(\mathbf{r}) = \mu\Psi(\mathbf{r})\,.$$

Ω is the angular velocity

$\mathbf{L} = -i\hbar\,\mathbf{r}\times\nabla$ is the angular momentum

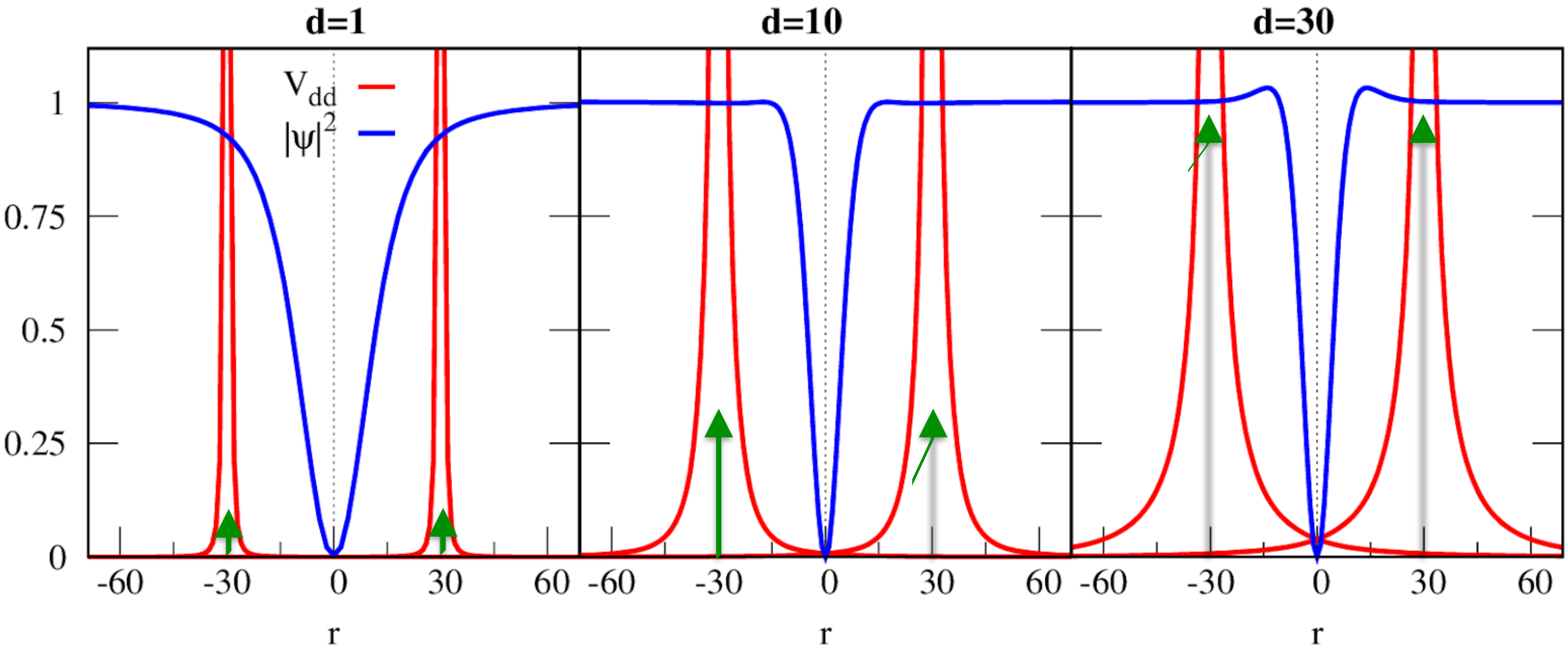
✳There is a critical (minimum) Ω that depends on the dipole moment *d*



VORTEX LATTICE

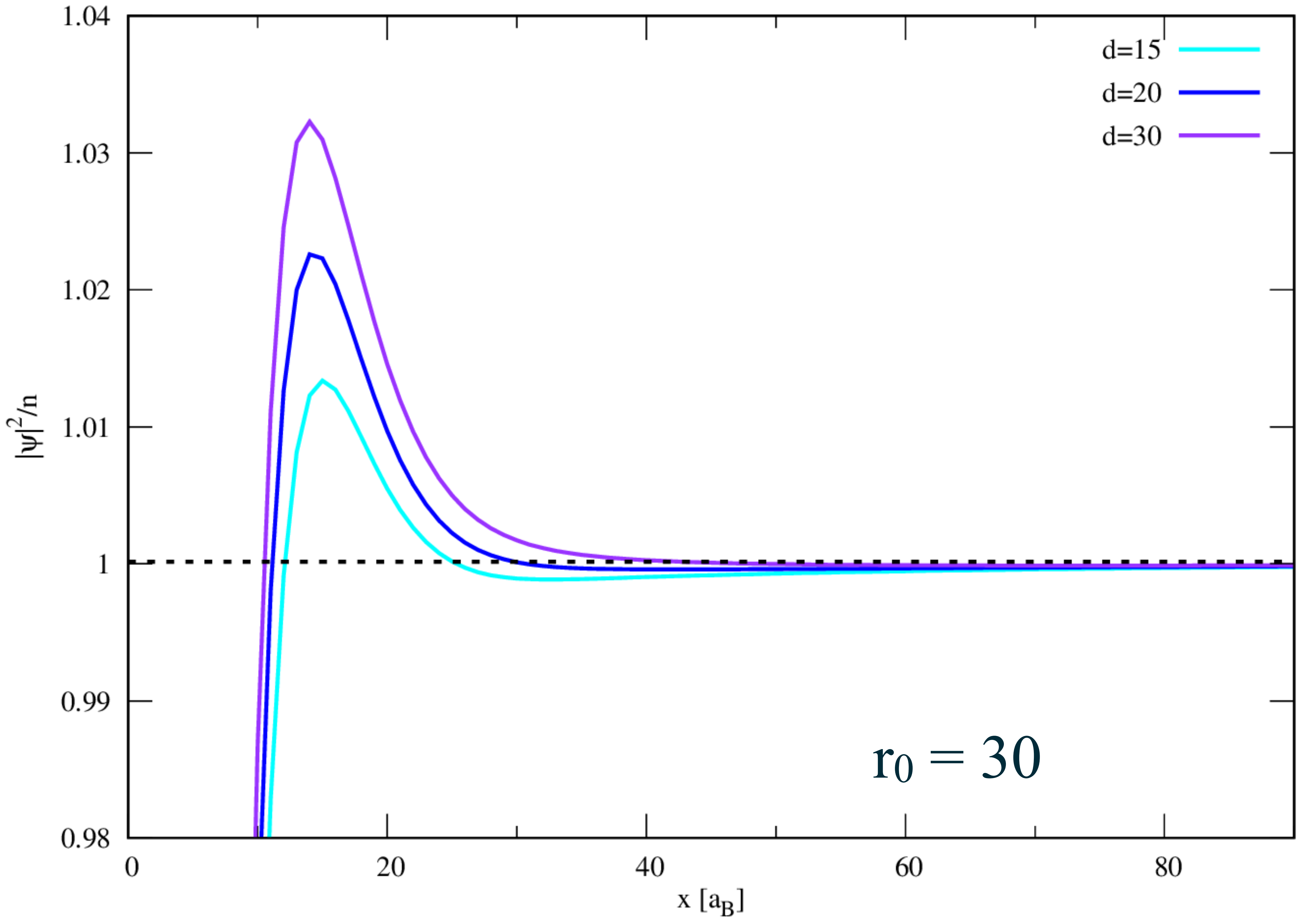
$r_0 = 30$

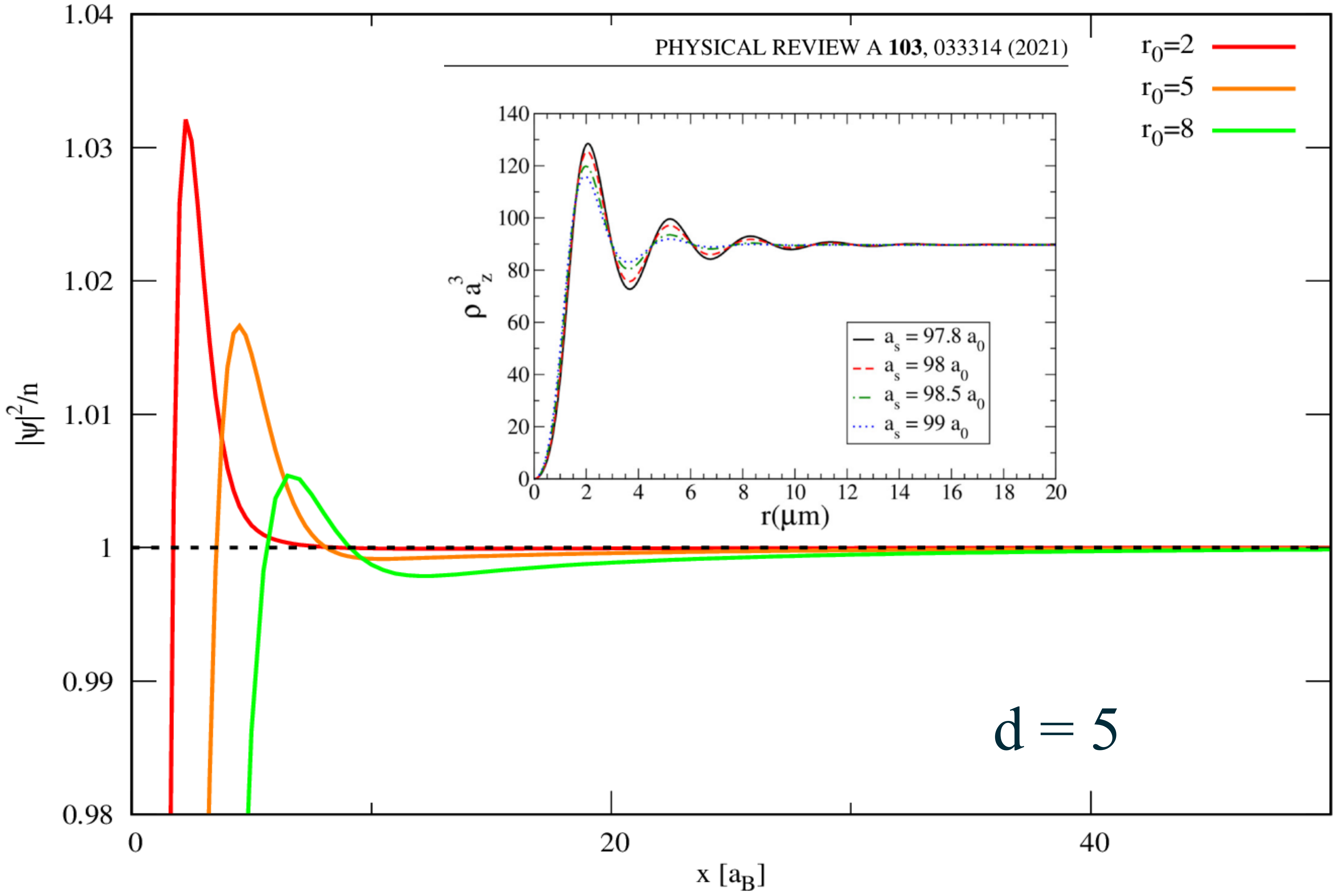
DENSITY PILEUP



The accumulation of density at the vortex edge is a result from competition between the outward **centrifugal force** and the inward **repulsion** from neighbouring dipoles.

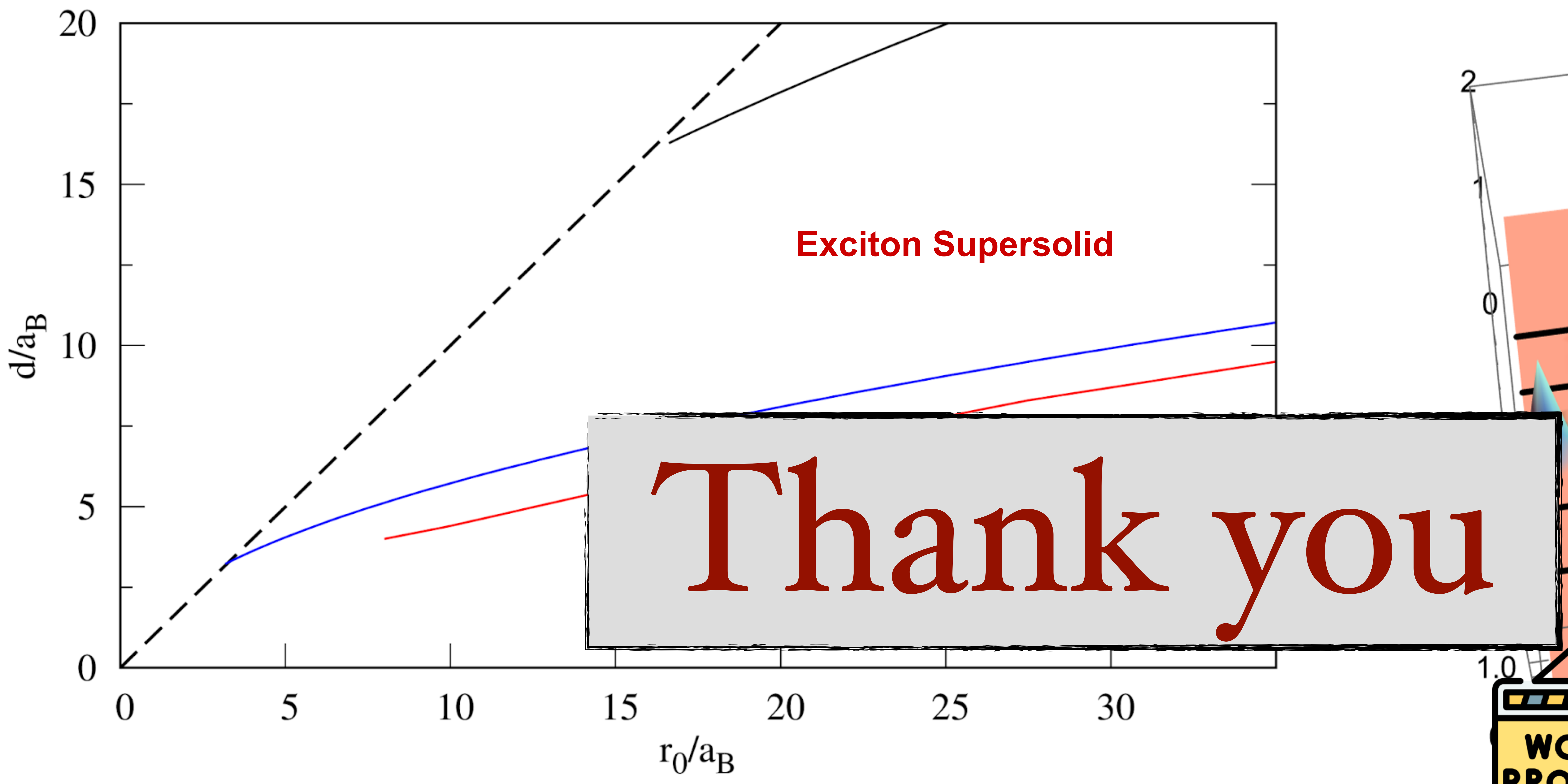
SINGLE VORTEX PROFILE

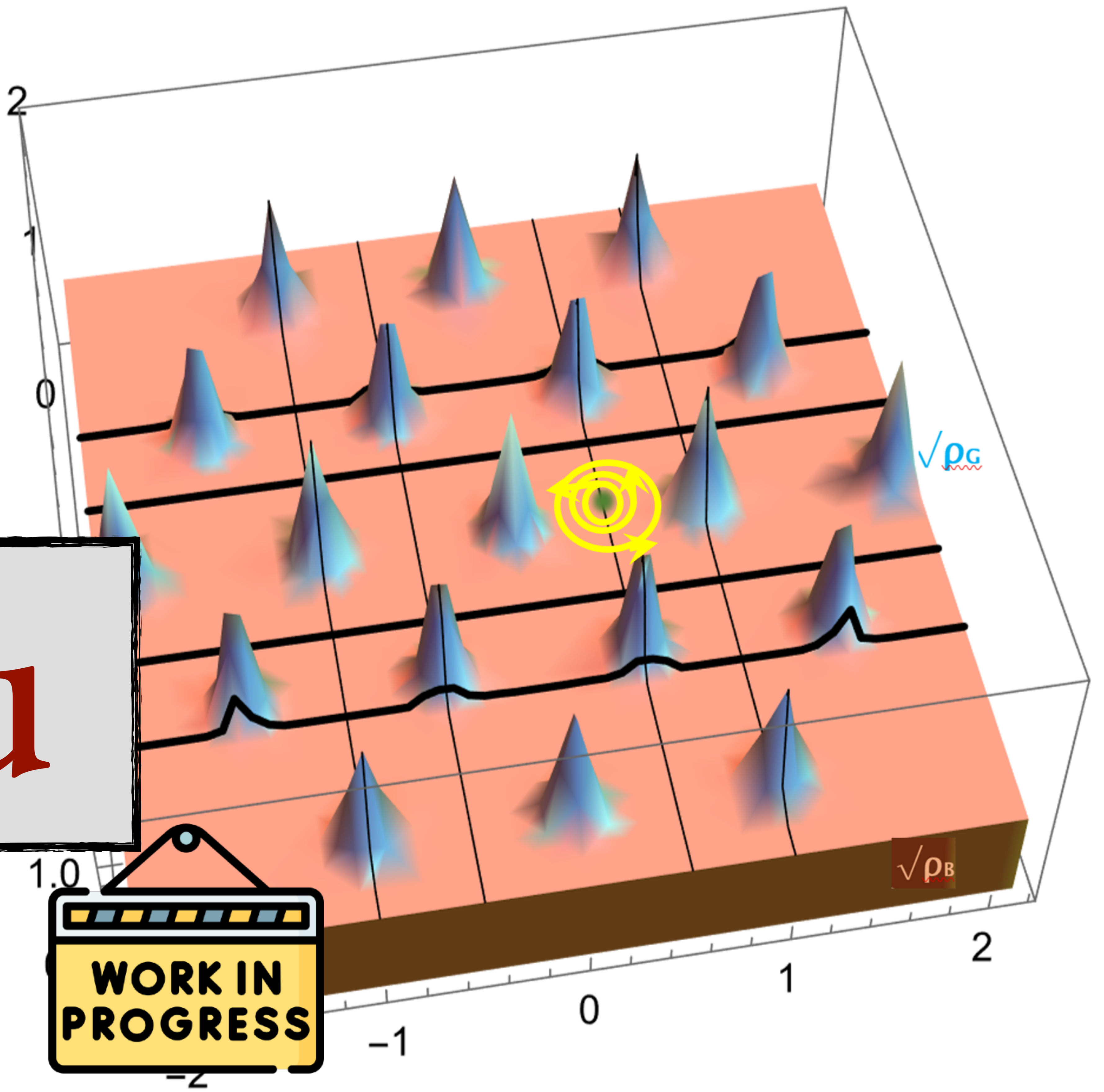




- In cold atoms the peak is accompanied by oscillations – associated with a low-lying roton collective excitation.
- However here there are **no oscillations.** ⟷ **NO ROTON!**

SUMMARY





BLUE LINE: density pileup appears on vortex.

RED LINE: superfluid to supersolid transition with GPE.

Both effects occur when the effective range of the exciton-exciton interaction becomes of same order as r_0.

[ArXiv:2507.15561]