

The mathematical engine behind quantum chemistry

Density-functional theory at OsloMet

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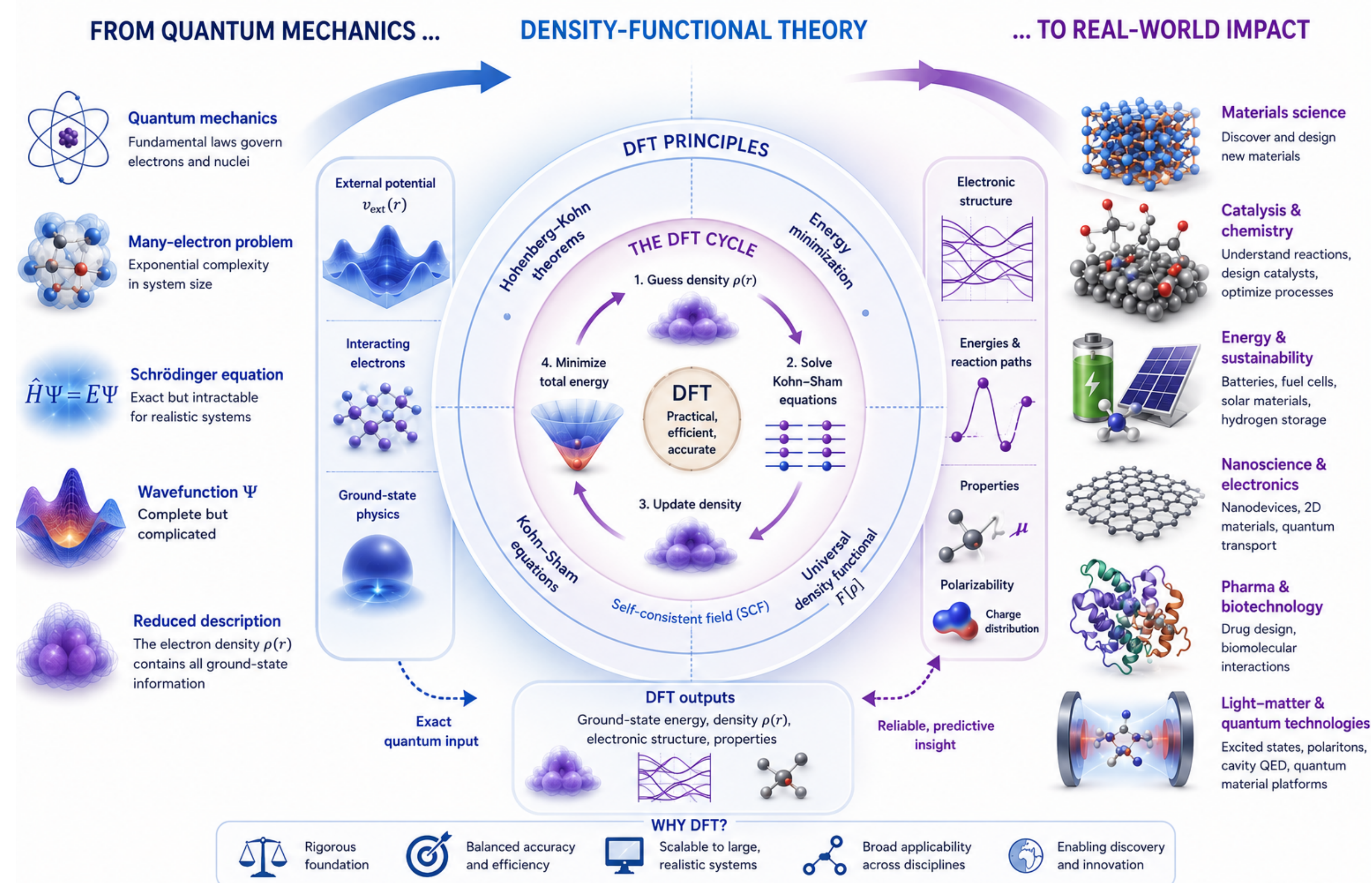
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DFT & quantum chemistry calculations

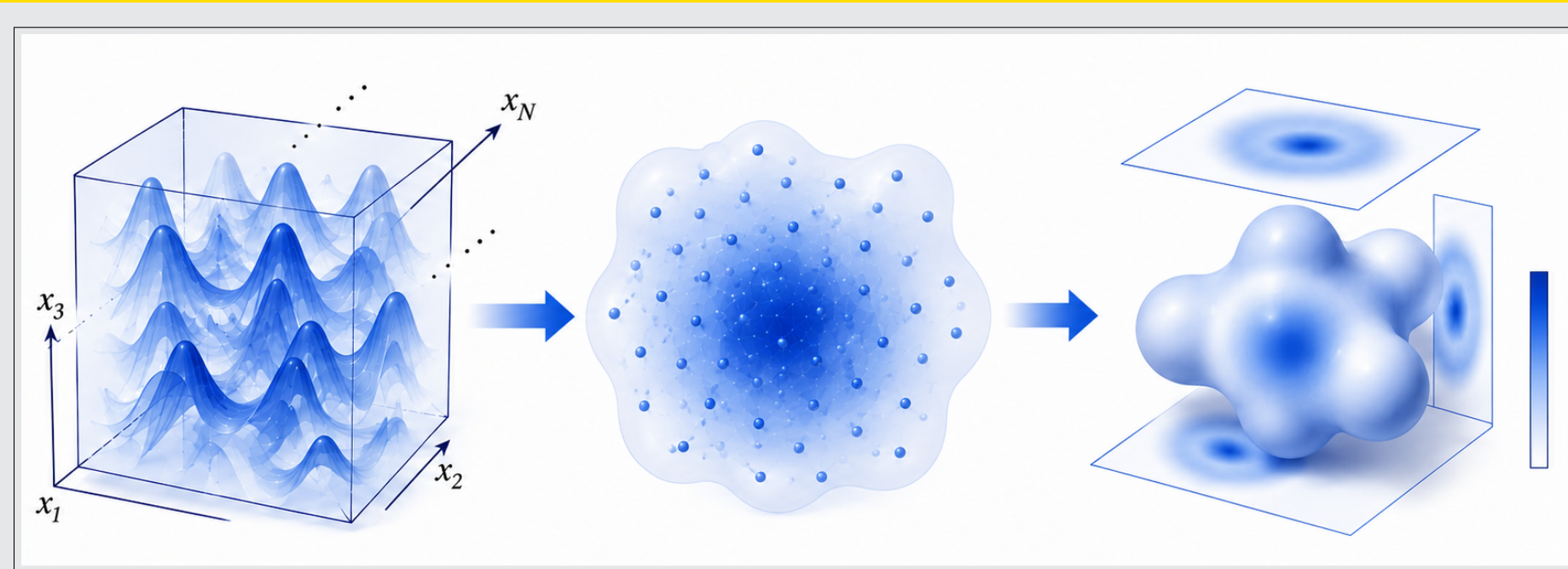
Quantum technologies need reliable ways to predict properties of matter, light, and their interaction.

Density-functional theory is one of the most successful routes from quantum mechanics to usable simulations of molecules and materials.

REGAL develops mathematical tools that make this route more well-founded and stable, as well as practical algorithms.



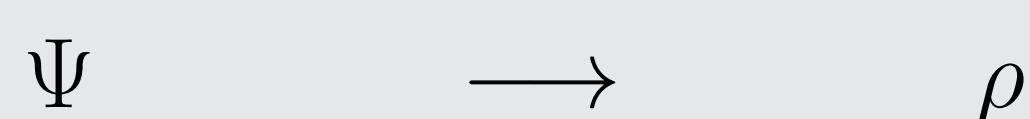
Density-functional theory



DFT is a workhorse of quantum simulation

- Over 50 000 scientific papers per year.
- 1/3 of all supercomputing resources.

Simplification:



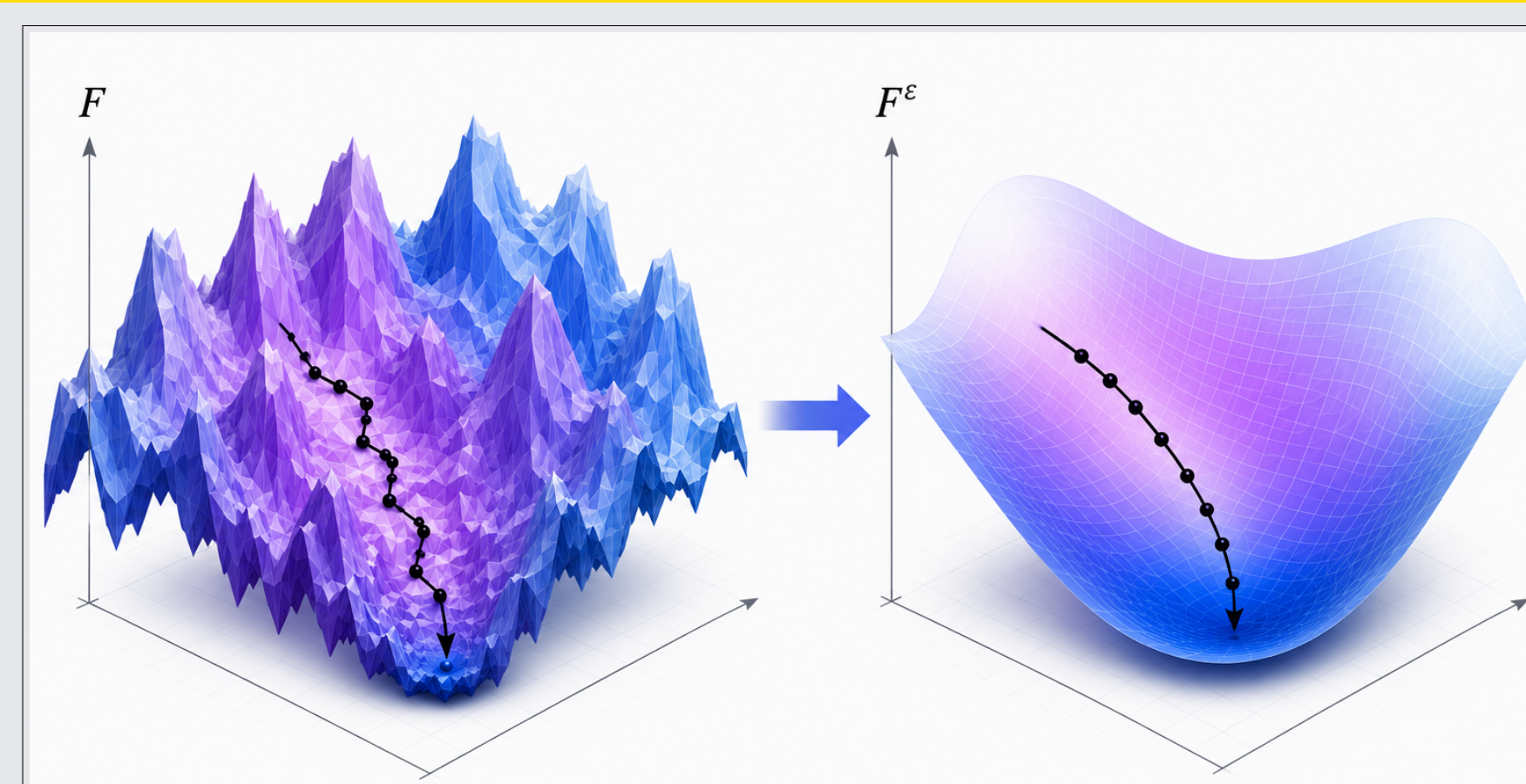
quantum wavefunction the electronic density

This makes otherwise impossible calculations feasible for real materials and molecules.

Example: penicillin (41 atoms)

- An “exact” calculation would require more bytes of memory than there are atoms in the universe.
- DFT lets us calculate quantities of interest.
- Quantum computing?

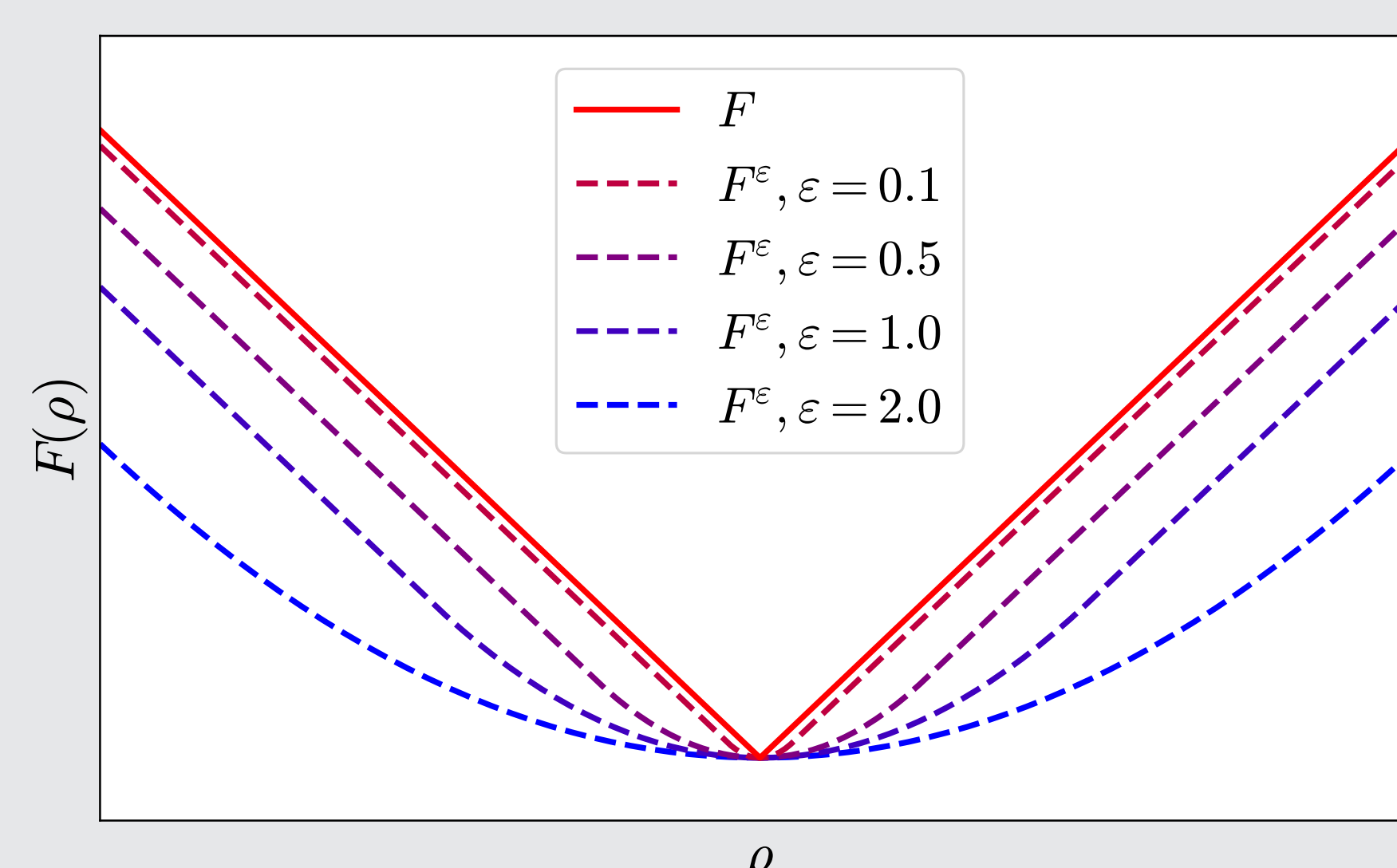
REGAL’s core theme



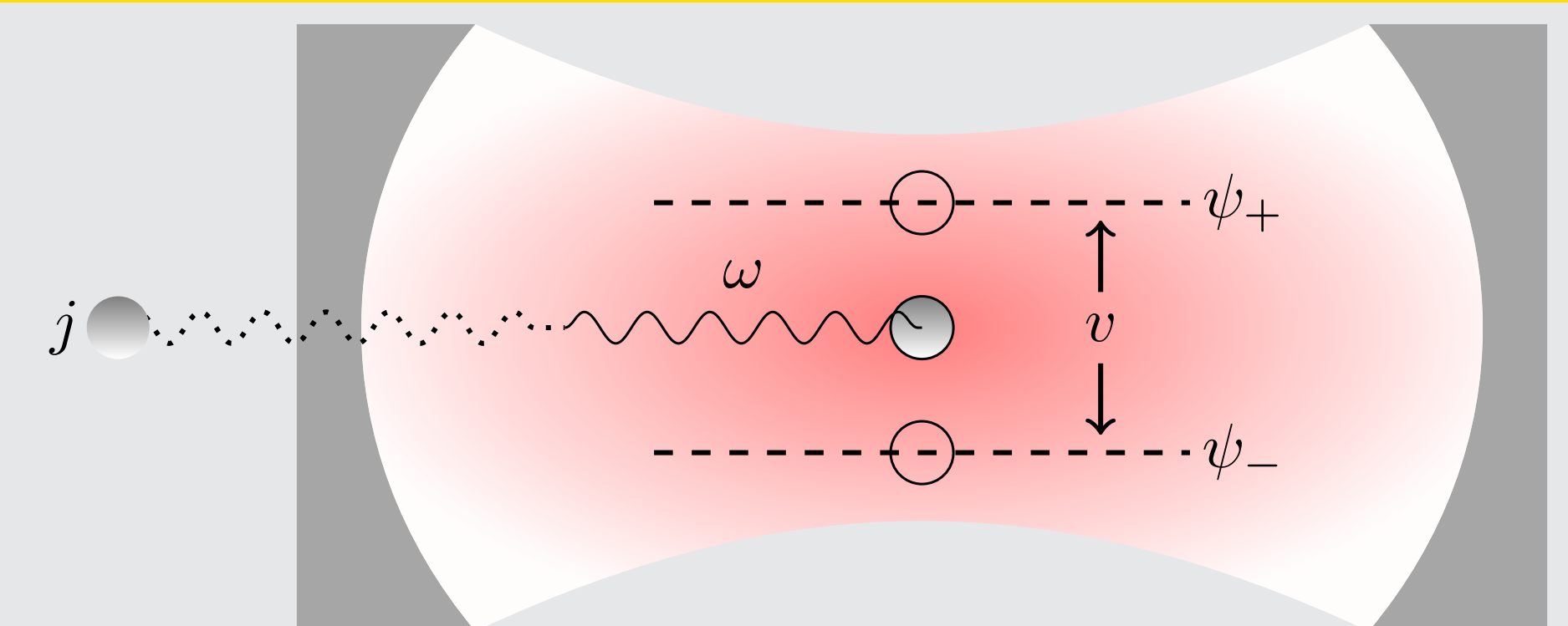
REGularized density-functional anALysis

The central object of DFT, the *universal density functional*, is hard to work with.

Moreau–Yosida regularization smooths the problem.



The QEDFT testing ground



Quantum-Electrodynamical Density-Functional Theory

Quantized light and matter as a model laboratory.

We study minimal models such as the **quantum Rabi model** and the **multi-mode Dicke model**.

- Light-matter interactions at low energy.
- How can DFT be applied to such systems?
- Laser-induced and polaritonic chemistry.
- Does Moreau–Yoshida regularization have a physical interpretation?
- ⇒ Light-matter interactions are highly relevant for technological applications.

Density-potential inversion

Can we reconstruct the potential from the density?

In DFT, the electronic density contains the essential ground-state information.

Density–potential inversion asks which potential gives rise to a given density.

REGAL approach

Moreau–Yosida regularization makes inverse Kohn–Sham calculations more stable.

- sounder Kohn–Sham foundations
- improved functional development
- more reliable quantum simulations

Collaborations

- MPI: Structure and Dynamics of Matter
- EPFL, Lausanne
- RWTH Aachen
- University of Oslo
- University of Fribourg
- University of Stuttgart
- Rensselaer Polytechnic Institute