Neural canonical transformation for m^* of electron gases

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https://wangleiphy.github.io

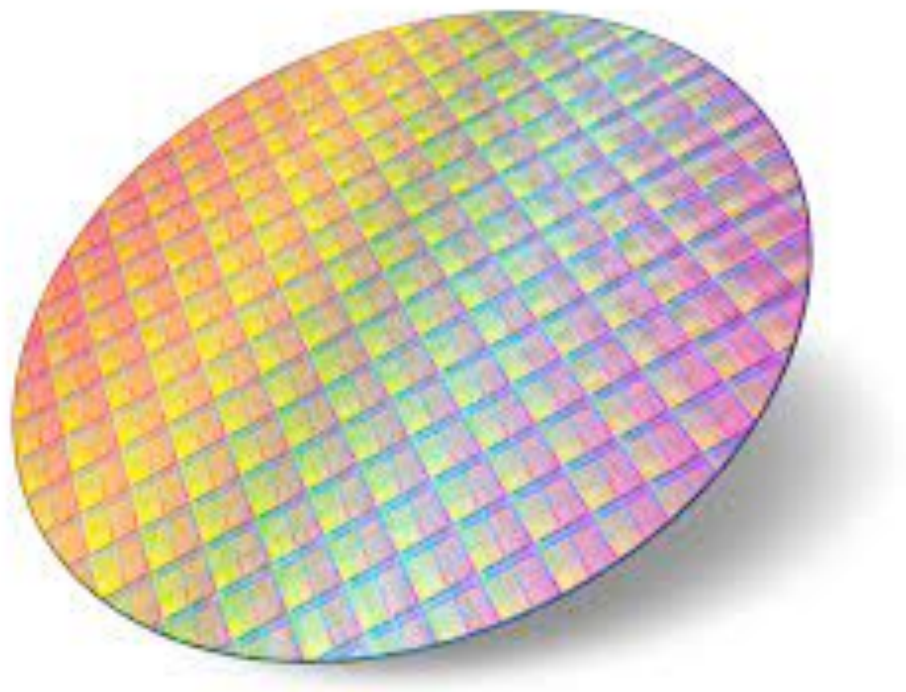
2105.08644
2201.03156

github.com/fermiflow/

Triumph of condensed matter physics

Insulators

Metals



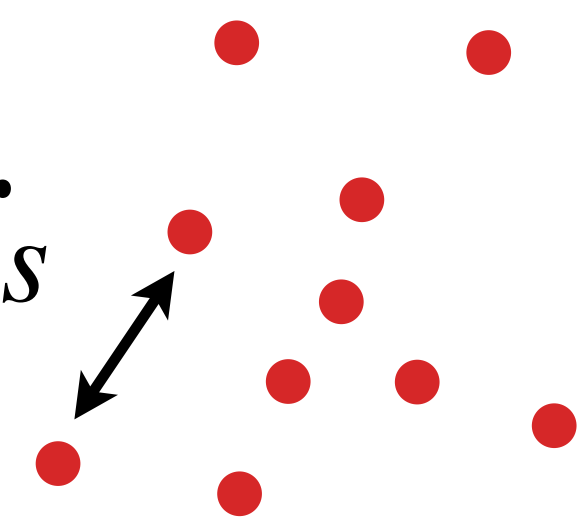
Semiconductors

Why metal is metal ?

$$H = -\sum_{i=1}^{N}\frac{\hbar^2\nabla_i^2}{2m} + \sum_{i<j}\frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

Uniform electron gas

$$\sim r_s^{-2} \qquad\qquad \sim r_s^{-1}$$



r_s

$r_s \ll 1$ High density: kinetic energy dominants

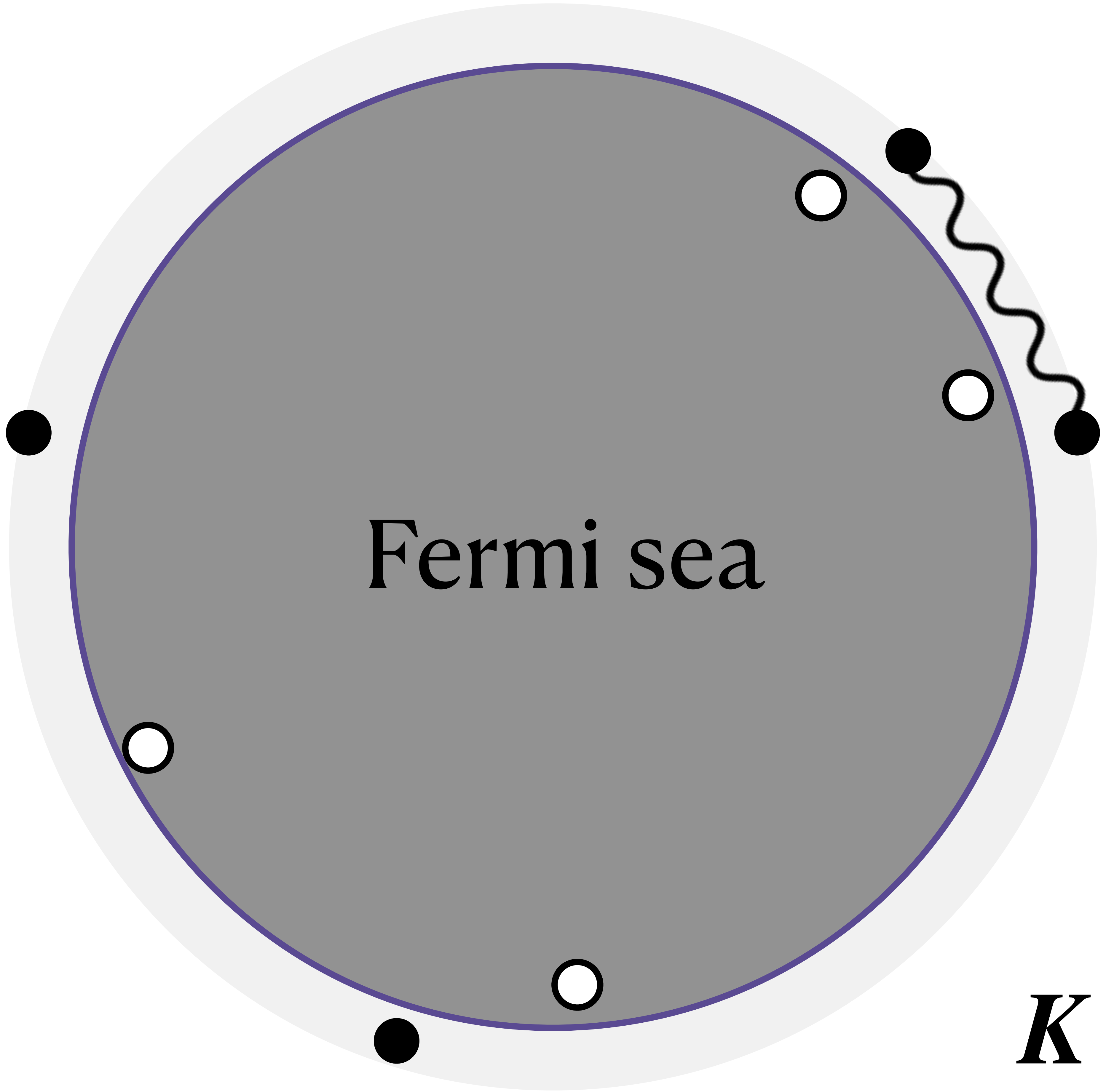
$2 < r_s < 6$ Metal density: Coulomb interaction is not perturbative compared to kinetic energy

$r_s \gg 1$ Low density: Coulomb interaction dominants

Richard Martin, *Electronic structure*

$Z = 1$	$Z = 2$	$Z = 1$	$Z = 2$	$Z = 3$	$Z = 4$
Li 3.23	Be 1.88			B	C 1.31
Na 3.93	Mg 2.65			Al 2.07	Si 2.00
K 4.86	Ca 3.27	Cu 2.67	Zn 2.31	Ga 2.19	Ge 2.08
Rb 5.20	Sr 3.56	Ag 3.02	Cd 2.59	In 2.41	Sn 2.39
Cs 5.63	Ba 3.69	Au 3.01	Hg 2.15	Tl	Pb 2.30

Landau fermi liquid theory



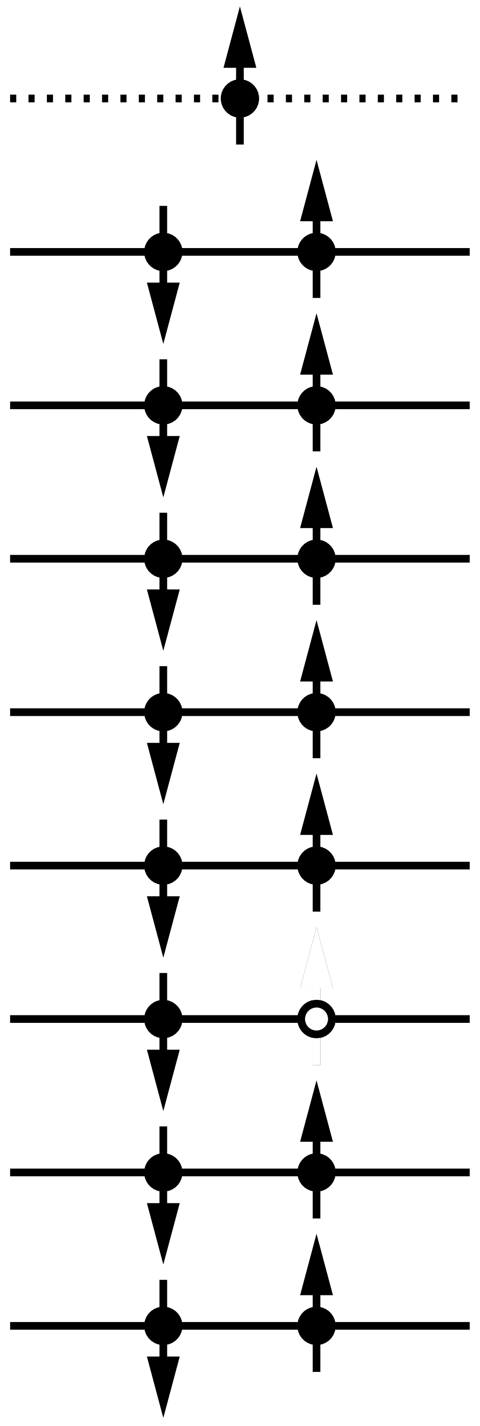
$$\frac{e^2}{r_s} \gtrsim E_F \gg T$$

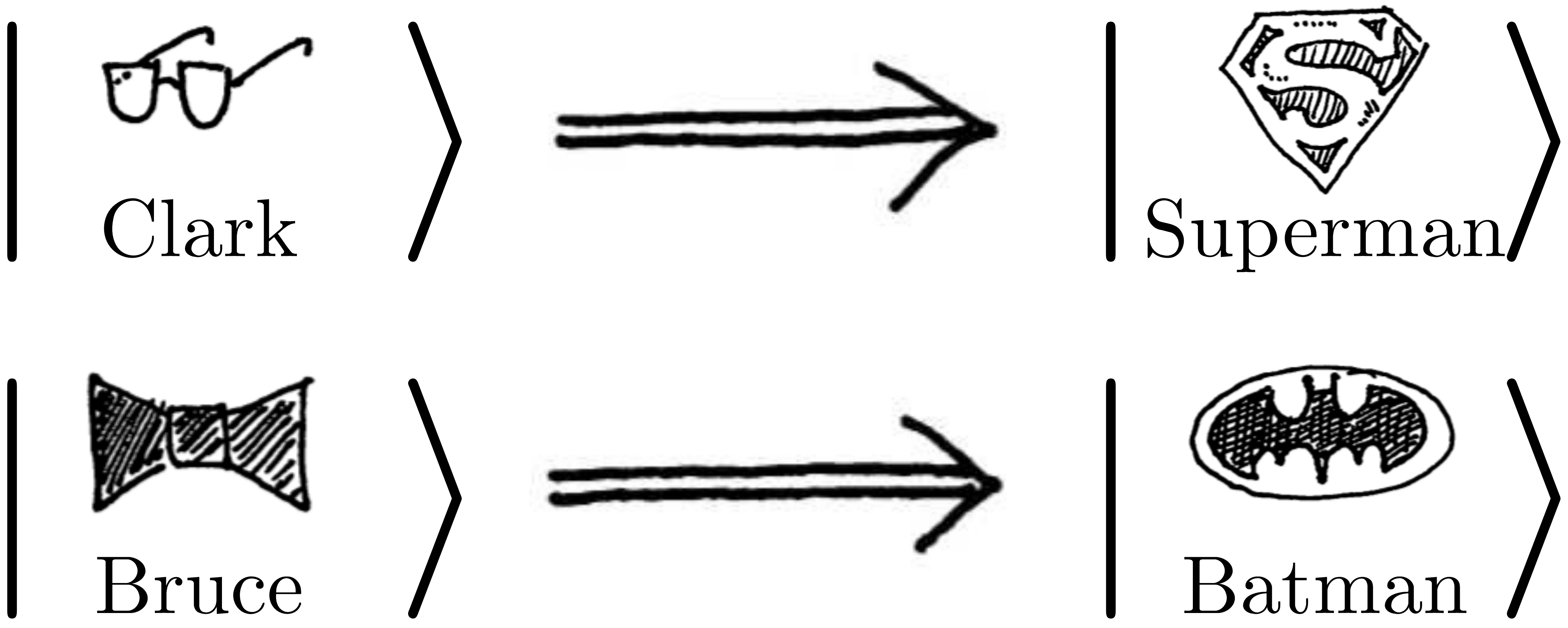
$$\boldsymbol{K} = \{\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_N\}$$

Physics happens around the Fermi surface with strongly constrained phase-space

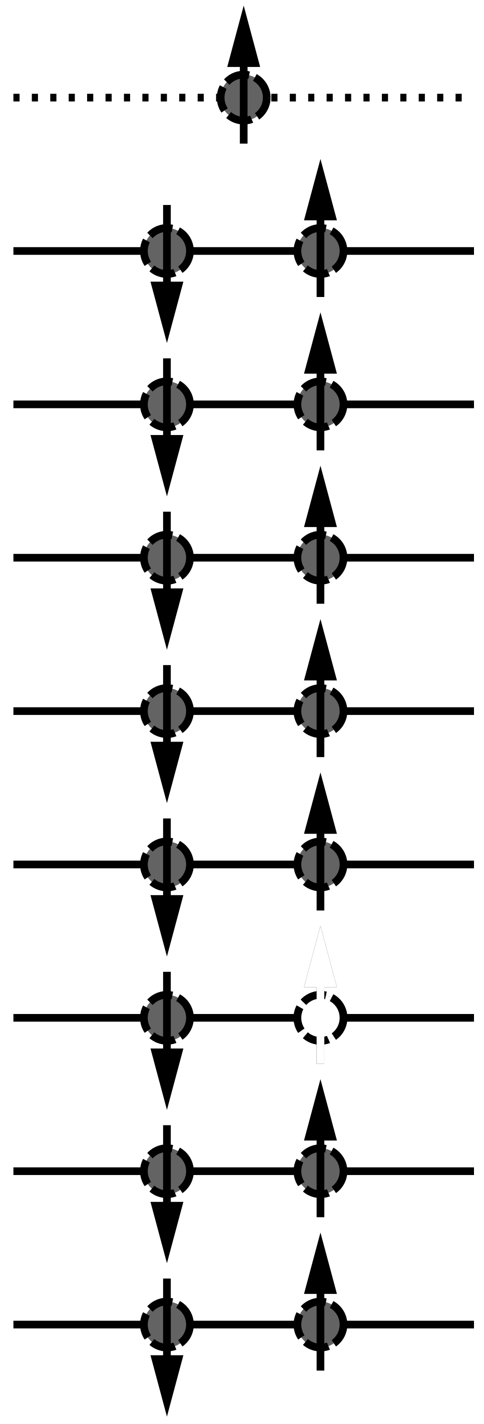
Landau fermi liquid theory

Adiabatic continuity





Lancaster & Blundell , QFT for the Gifted Amateur



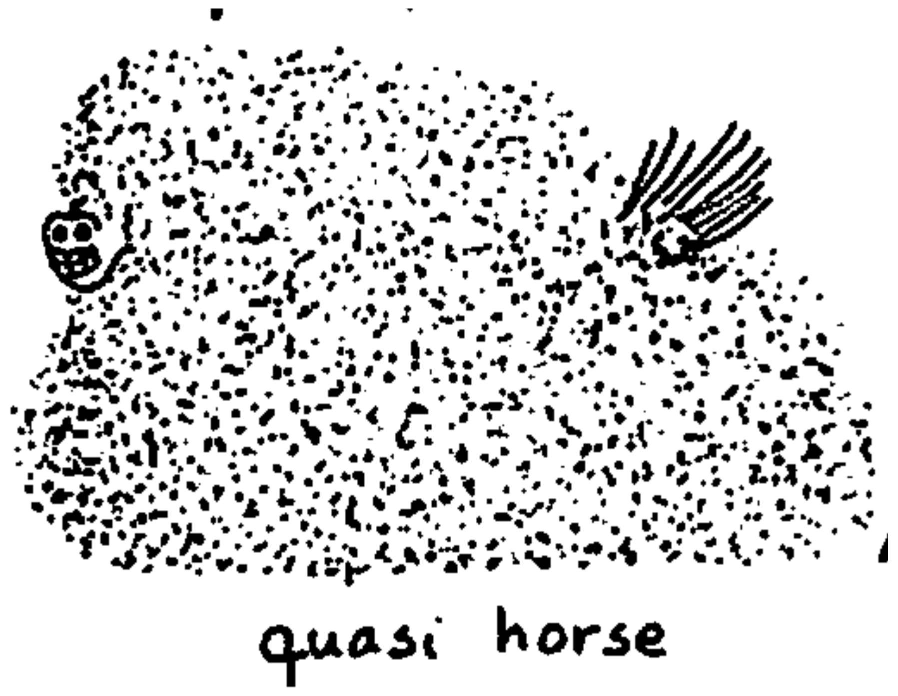
Noninteracting electrons

Interacting electrons

Predicts a large number of physical properties based on a few parameters

Quasi-particles effective mass

$$\frac{m^*}{m} =$$



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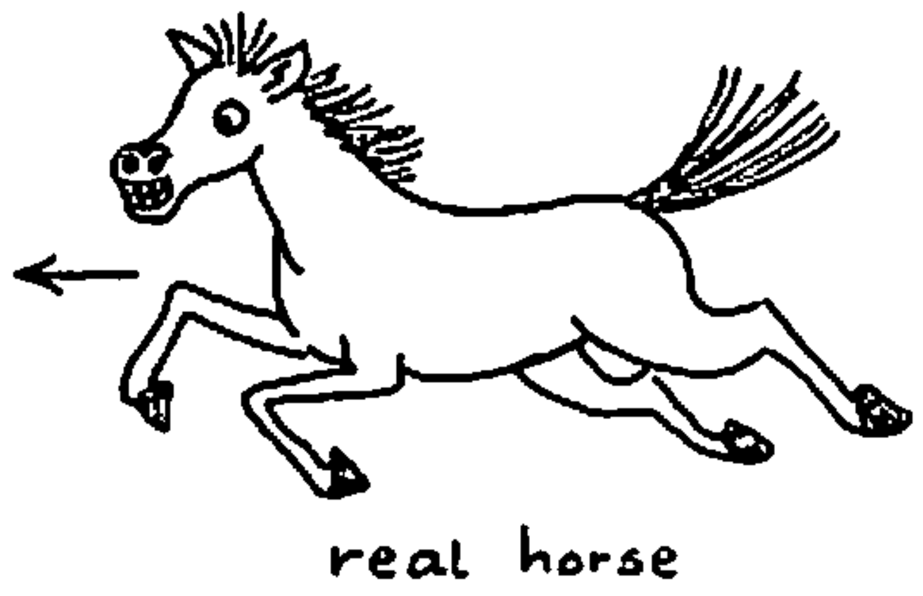


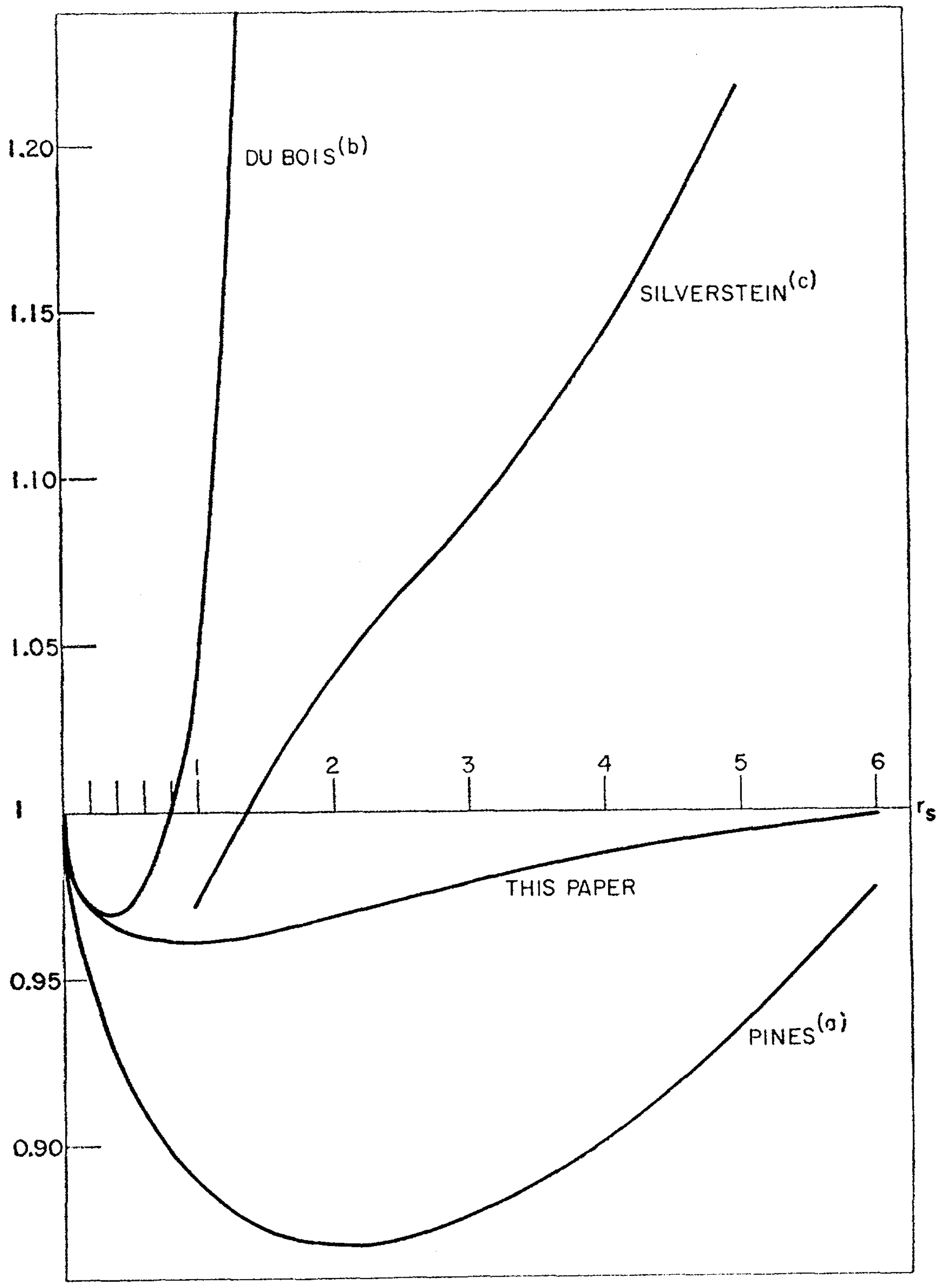
Richard D. Mattuck,
A Guide to Feynman Diagrams in the Many-body Problem

A fundamental quantity appears in nearly all physical properties of a Fermi liquid

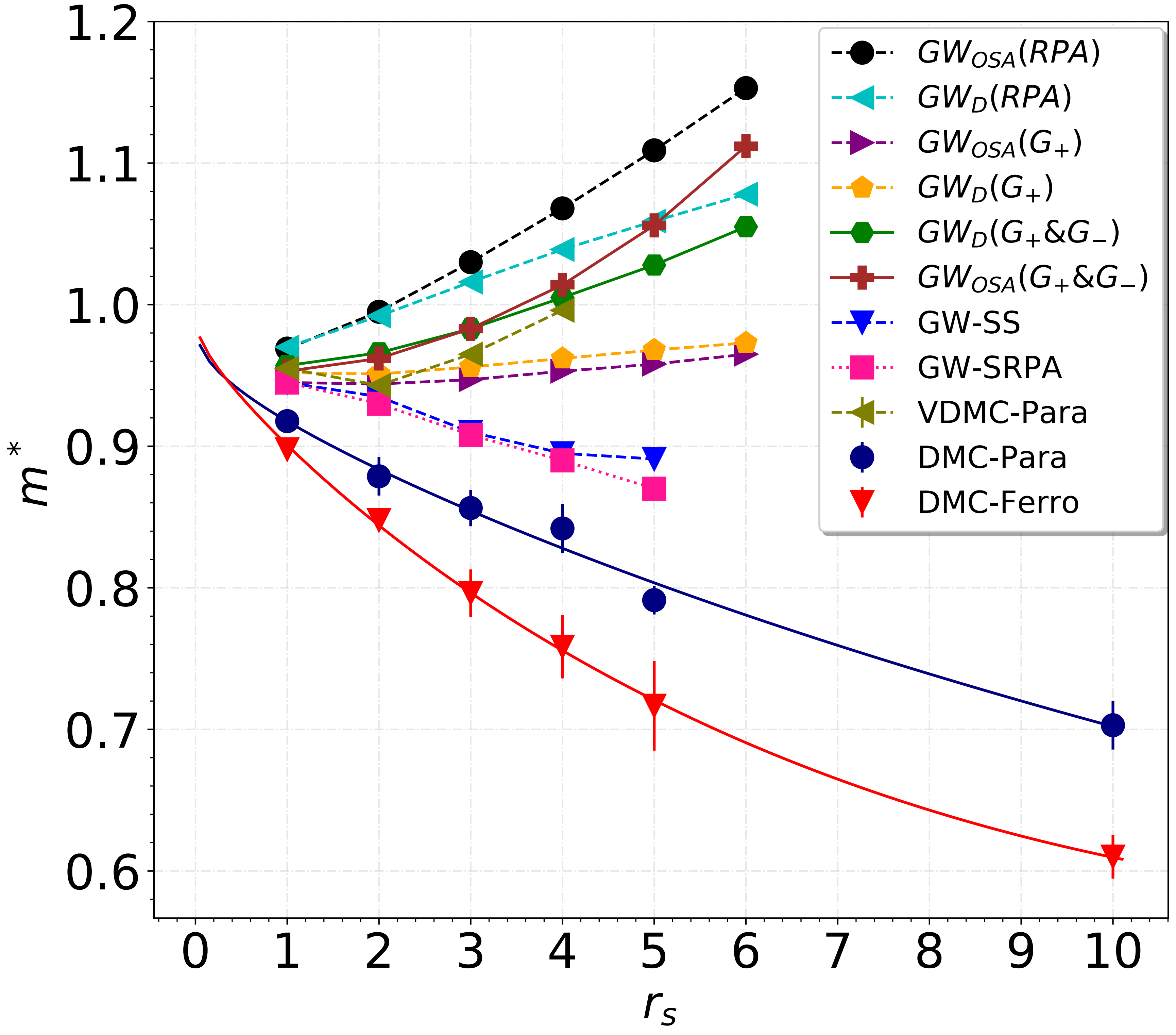
$N(0)$	s	c_V	χ
Density of states	entropy	specific heat	magnetic susceptibility

Quasi-particles effective mass of 3d electron gas

Hedin Phy. Rev. 1965



Azadi, Drummond, Foulkes, PRL 2021



> 50 years of conflicting results !

Two dimensional electron gas experiments

VOLUME 91, NUMBER 4 PHYSICAL REVIEW LETTERS week ending 25 JULY 2003

Spin-Independent Origin of the Strongly Enhanced Effective Mass in a Dilute 2D Electron System

A. A. Shashkin,* Maryam Rahimi, S. Anissimova, and S.V. Kravchenko
Physics Department, Northeastern University, Boston, Massachusetts 02115, USA

V. T. Dolgopolov
Institute of Solid State Physics, Chernogolovka, Moscow District 142432, Russia

T. M. Klapwijk
Department of Applied Physics, Delft University of Technology, 2628 CJ Delft, The Netherlands
(Received 13 January 2003; published 24 July 2003)

$m^*/m > 1$

PRL **101**, 026402 (2008) PHYSICAL REVIEW LETTERS week ending 11 JULY 2008

Effective Mass Suppression in Dilute, Spin-Polarized Two-Dimensional Electron Systems

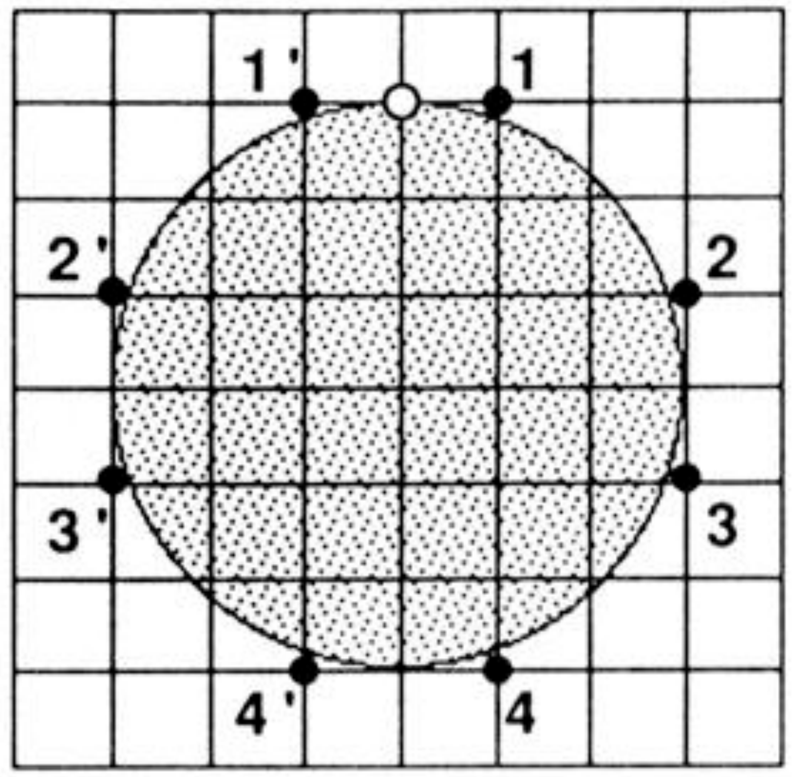
Medini Padmanabhan, T. Gokmen, N. C. Bishop, and M. Shayegan
Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA
(Received 19 September 2007; published 7 July 2008)

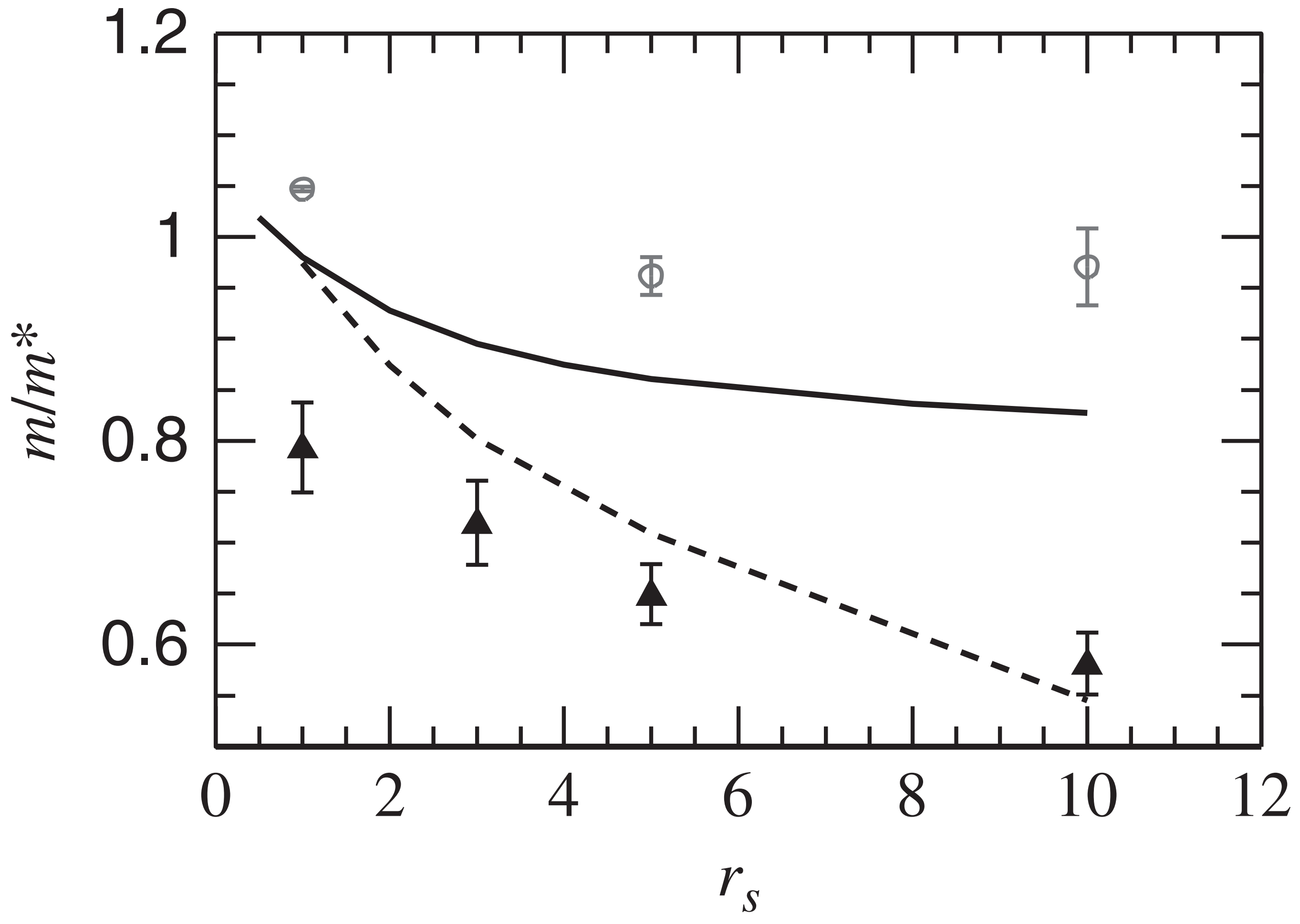
$m^*/m < 1$

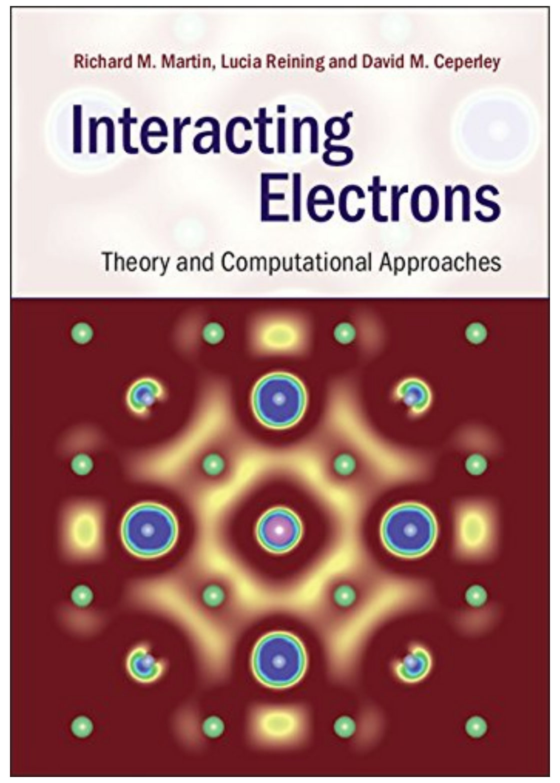
Layer thickness, valley, disorder, spin-orbit coupling...

m* of 2d electron gas

Two quite different QMC results for the 2D HEG are shown in Fig. 23.3 and compared with screened RPA and local field method results. The two different QMC calculations were done in a similar way, but the effective mass differs because of the way it is calculated from the QMC energies.







Martin, Reining, Ceperley, *Interacting Electrons* ‘16

Conflicting results even from the SAME numerical method

Effective mass from thermodynamics

Eich, Holzmann, Vignale, PRB ‘17

$$s = \frac{\pi^2 k_B}{3}\frac{m^*}{m}\frac{T}{T_F}$$

$$\Rightarrow \frac{m^*}{m} = \frac{s}{s_0}$$

Interacting/Noninteracting entropy ratio

However, low temperature calculation was challenging

Entropy was not directly accessible to many methods

A variational density-matrix approach

The variational free-energy

$$F = \frac{1}{\beta}\mathrm{Tr}(\rho \ln \rho) + \mathrm{Tr}(H\rho) \geq -\frac{1}{\beta}\ln Z$$

$$Z = \mathrm{Tr}(e^{-\beta H})$$

How to represent variational density-matrix so it is physical & optimizable ?

$\mathrm{Tr}\rho = 1 \qquad \rho \succ 0 \qquad \rho^\dagger = \rho \qquad \langle \boldsymbol{R} | \rho | \boldsymbol{R}' \rangle = (-)^{\mathscr{P}} \langle \mathscr{P}\boldsymbol{R} | \rho | \boldsymbol{R}' \rangle$

Variational density-matrix ansatz

$$\rho = \sum_{\boldsymbol{K}} p(\boldsymbol{K}) \left| \Psi_{\boldsymbol{K}} \rangle \langle \Psi_{\boldsymbol{K}} \right|$$

Normalized probability distribution

Orthonormal many-electron states

$$\sum_{\boldsymbol{K}} p(\boldsymbol{K}) = 1 \qquad \langle \Psi_{\boldsymbol{K}} | \Psi_{\boldsymbol{K}'} \rangle = \delta_{\boldsymbol{K},\boldsymbol{K}'}$$

How to represent them ???

Generative machine learning + physical considerations

Discriminative learning

$$y = f(\boldsymbol{x})$$

or $p(y \mid \boldsymbol{x})$

Generative learning

$$p(\boldsymbol{x}, y)$$

Generative models and their physics genes

Generative modeling

Known: samples

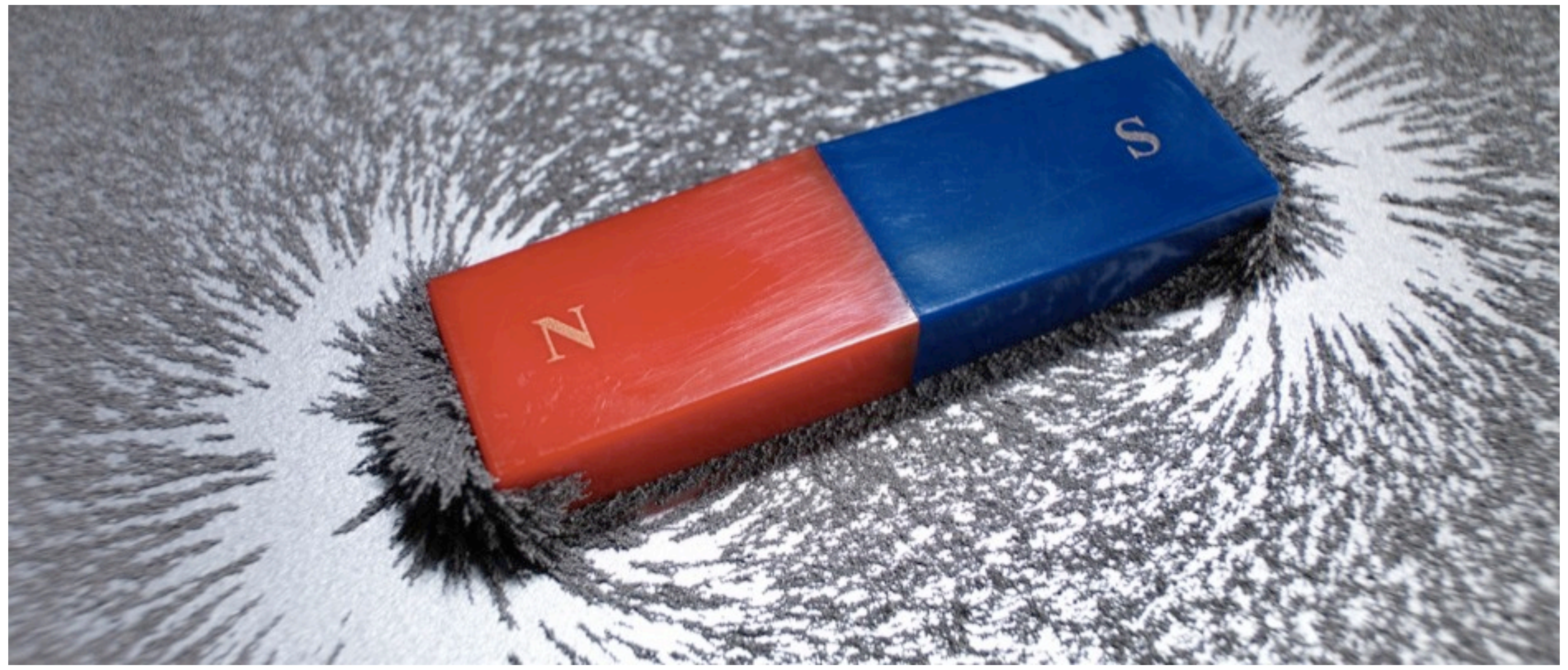
Unknown: generating distribution

Density estimation

"learn from data"

$$\mathscr{L} = -\,\mathbb{E}_{\boldsymbol{x}\sim \text{dataset}} \left[\ln p(\boldsymbol{x})\right]$$

Statistical physics



Known: energy function

Unknown: samples, partition function

Variational calculation

"learn from Hamiltonian"

$$F = \mathbb{E}_{\boldsymbol{x}\sim p(\boldsymbol{x})} \left[\frac{1}{\beta}\ln p(\boldsymbol{x}) + H(\boldsymbol{x})\right]$$

see, e.g., Wu, LW, Zhang, PRL '19

Generative models

Normalizing flow

Glow 1807.03039

https://blog.openai.com/glow/

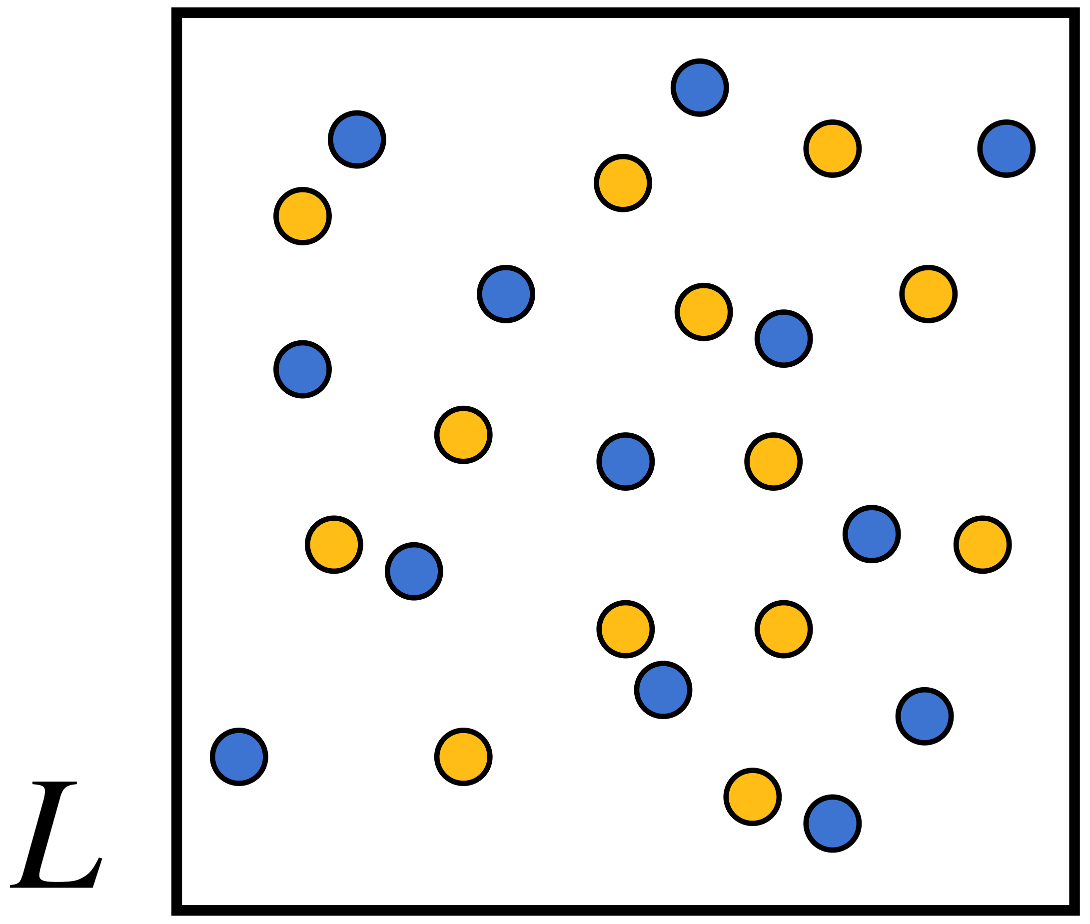
Autoregressive network

WaveNet 1609.03499 1711.10433

https://deepmind.com/research/case-studies/wavenet

Normalizing flow for $|\Psi_K\rangle$

$\boldsymbol{R} = \{\boldsymbol{r}_i\} \leftrightarrow \boldsymbol{\zeta} = \{\boldsymbol{\zeta}_i\}$

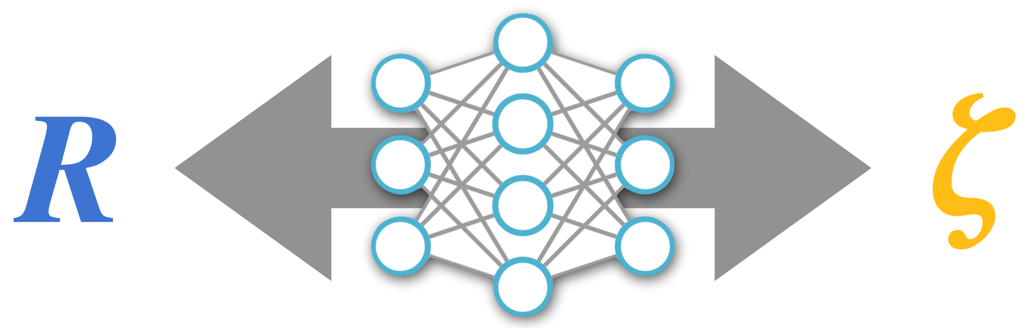


$$\Psi_K(\boldsymbol{R}) = \frac{\det(e^{i\boldsymbol{k}_i \cdot \boldsymbol{\zeta}_j}/L)}{\sqrt{N!}} \cdot \left| \det\left(\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{R}}\right) \right|^{\frac{1}{2}}$$

Electron coordinates

Quasi-particle coordinates

Jacobian of a bijective neural network



ensures orthonormality

$$\langle \Psi_K | \Psi_{K'} \rangle = \delta_{K,K'}$$

The flow implements a many-body unitary transformation

Eger & Gross 1963

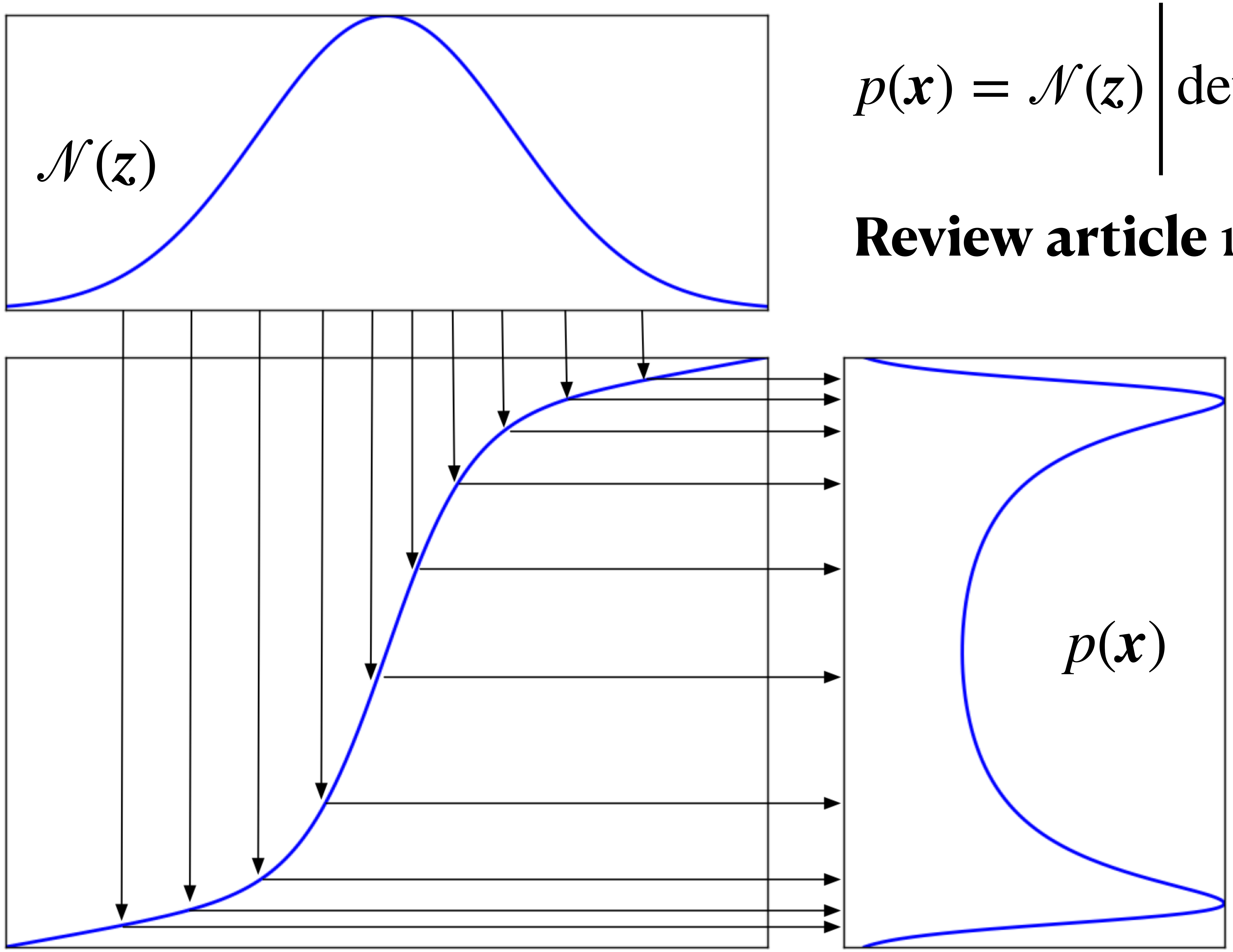
Normalizing flow in a nutshell

$$p(\boldsymbol{x}) = \mathcal{N}(z) \left| \det \left(\frac{\partial z}{\partial \boldsymbol{x}} \right) \right|$$

Review article 1912.02762

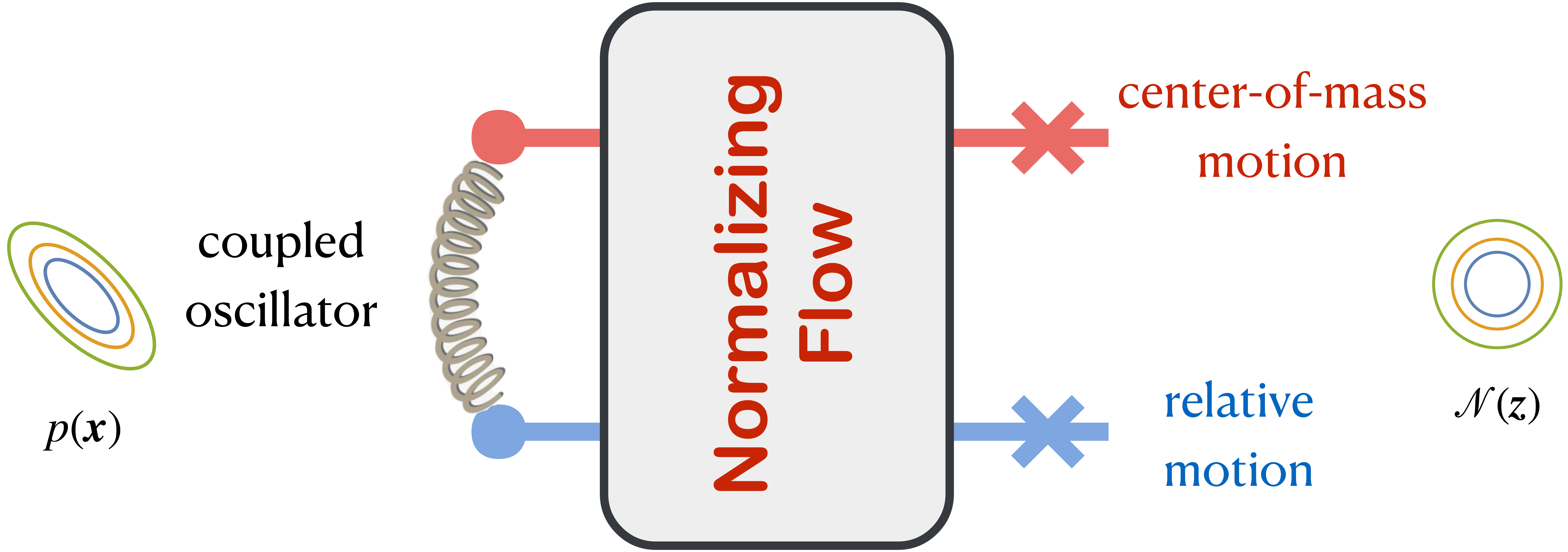
latent space

“neural net” with 1 neuron



physical space

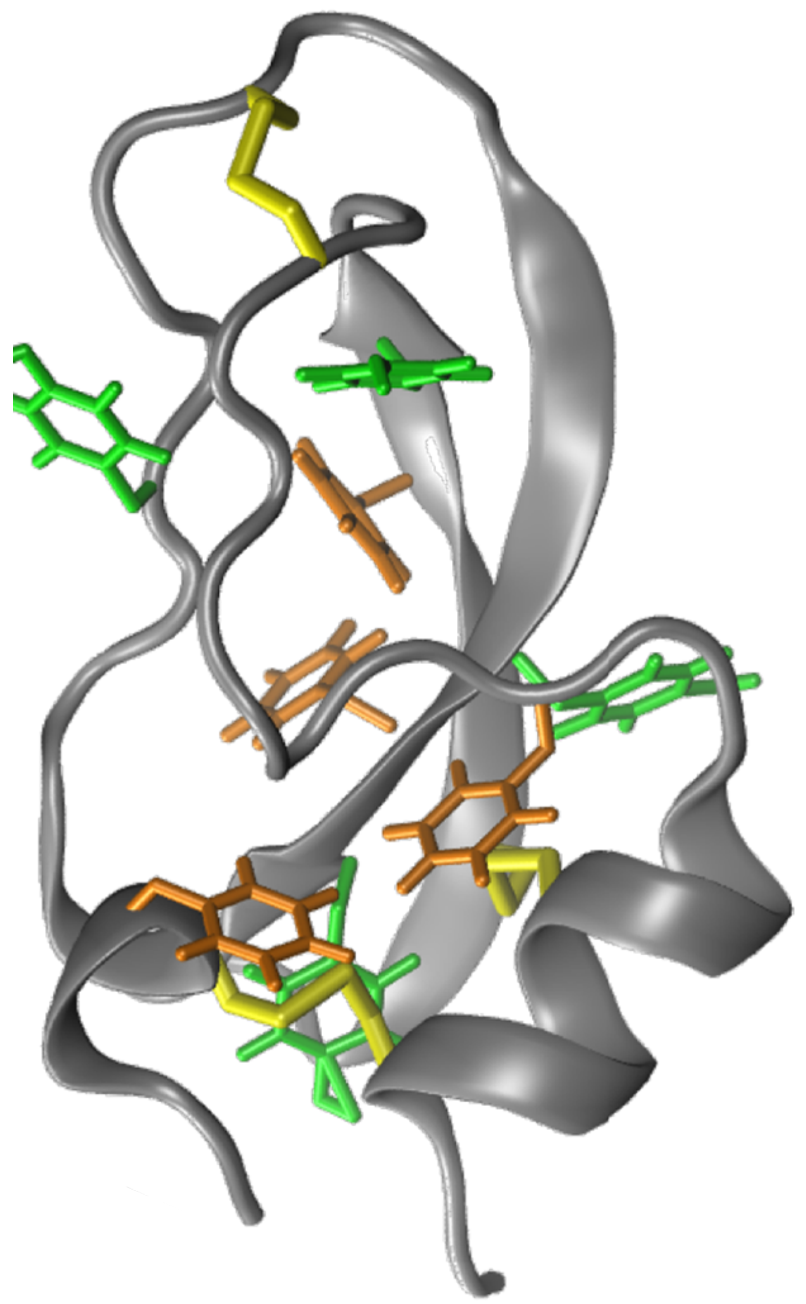
Normalizing flow for physics



Neural renormalization group, Li, LW, PRL '18
Neural canonical transformation, Li, Dong, Zhang, LW, PRX '20

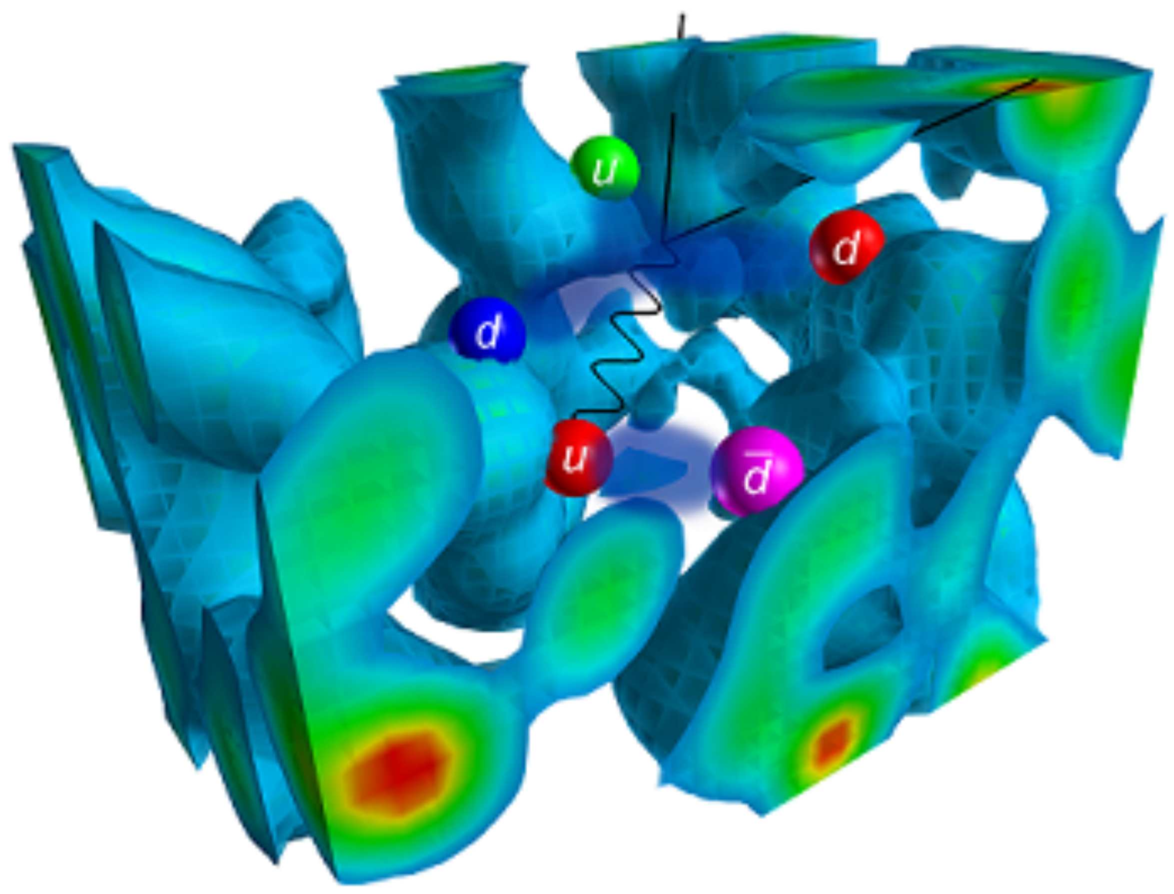
Normalizing flow for physics

Molecular simulation



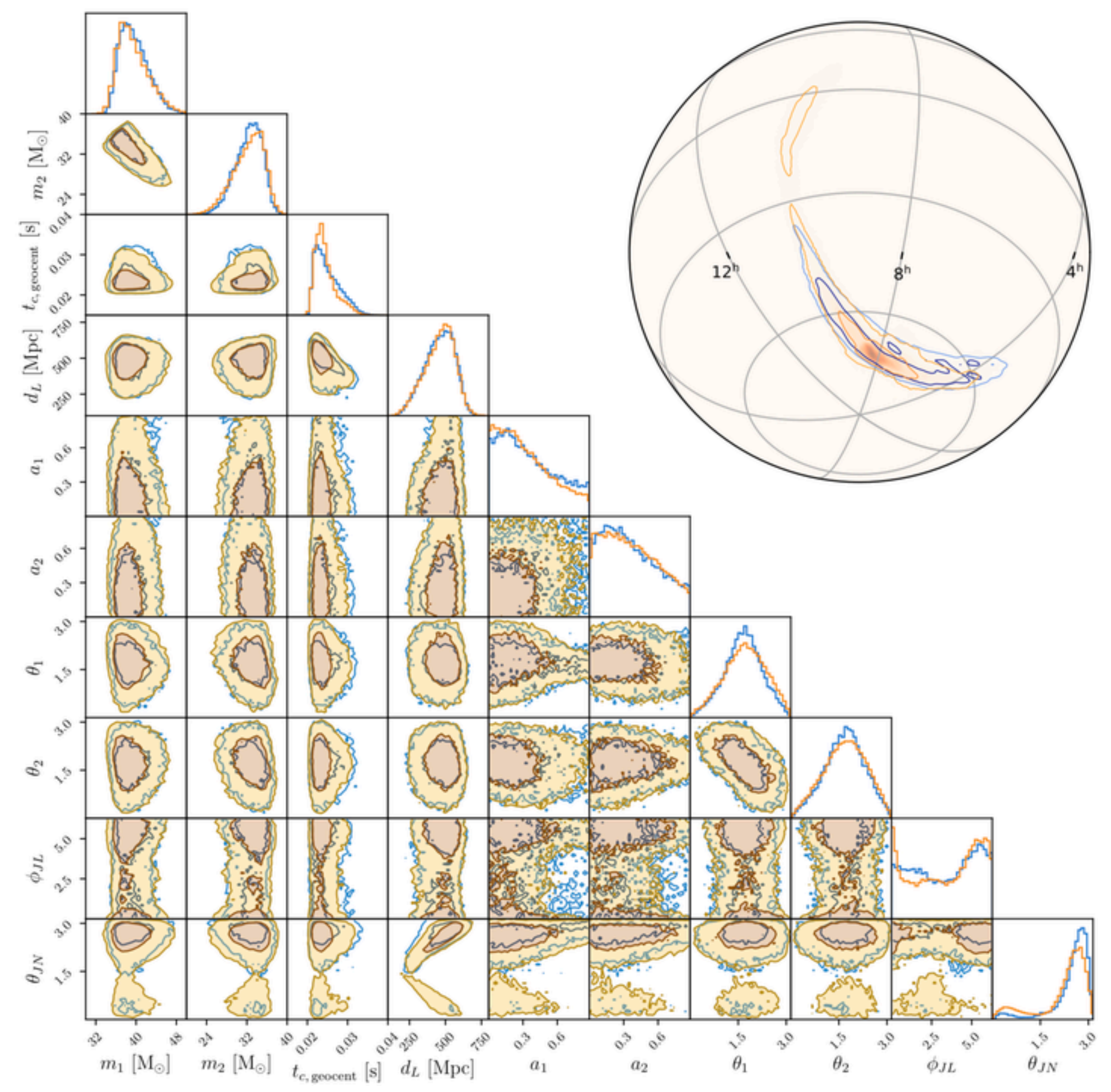
Noe et al, Science '19
Wirnsberger et al, JCP '20

Lattice field theory



Albergo et al, PRD '19
Kanwar et al, PRL '20

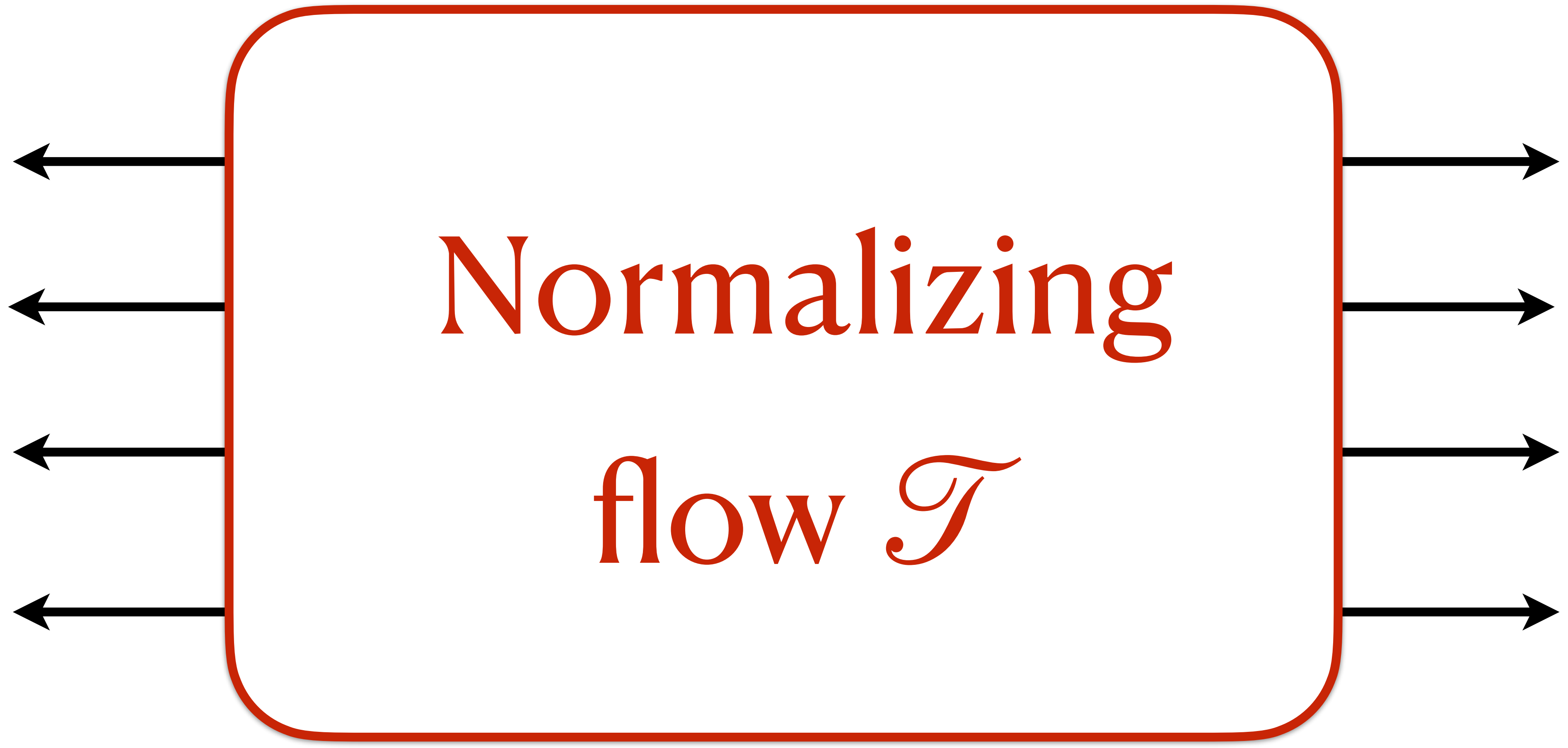
Gravitational wave detection



Green et al, MLST '21
Dex et al, PRL '21

Flow of electron coordinates

Electron coordinates $\boldsymbol{R}$



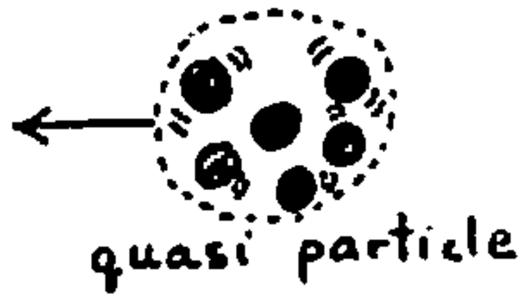
Quasiparticle coordinates $\boldsymbol{\zeta}$

$$\mathscr{T} \circ \mathscr{P}(\boldsymbol{R}) = \mathscr{P} \circ \mathscr{T}(\boldsymbol{R})$$

Flow should be equivariant to preserve physical symmetries

we use equivariant FermiNet layers Pfau et al, 1909.02487

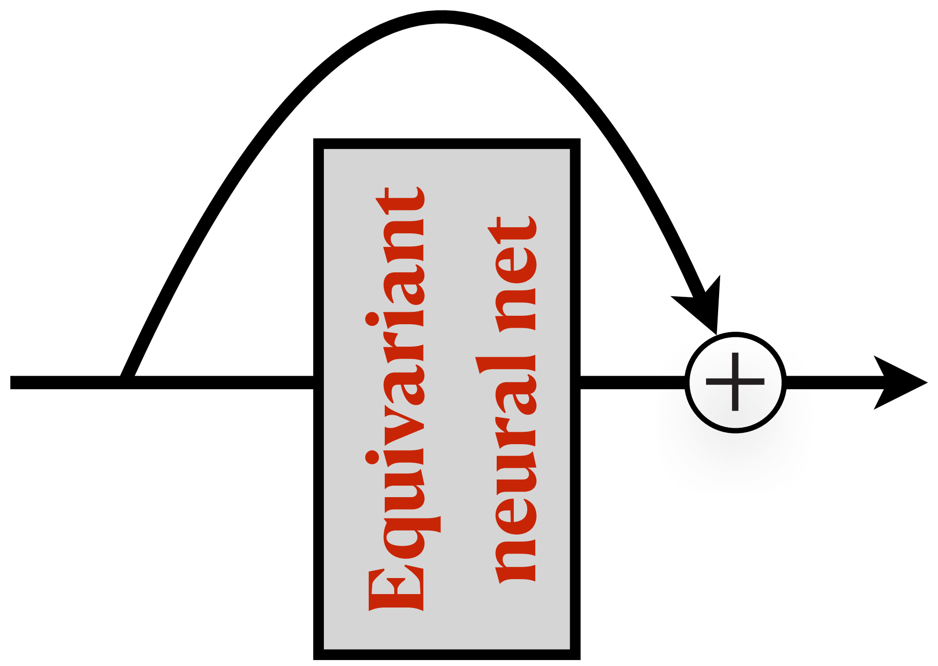
Backflow as a normalizing flow



$$\zeta_i = \boldsymbol{r}_i + \sum_{j \neq i} \eta(|\boldsymbol{r}_i - \boldsymbol{r}_j|)(\boldsymbol{r}_j - \boldsymbol{r}_i)$$

Wigner & Seitz 1934, Feynman 1954, ...

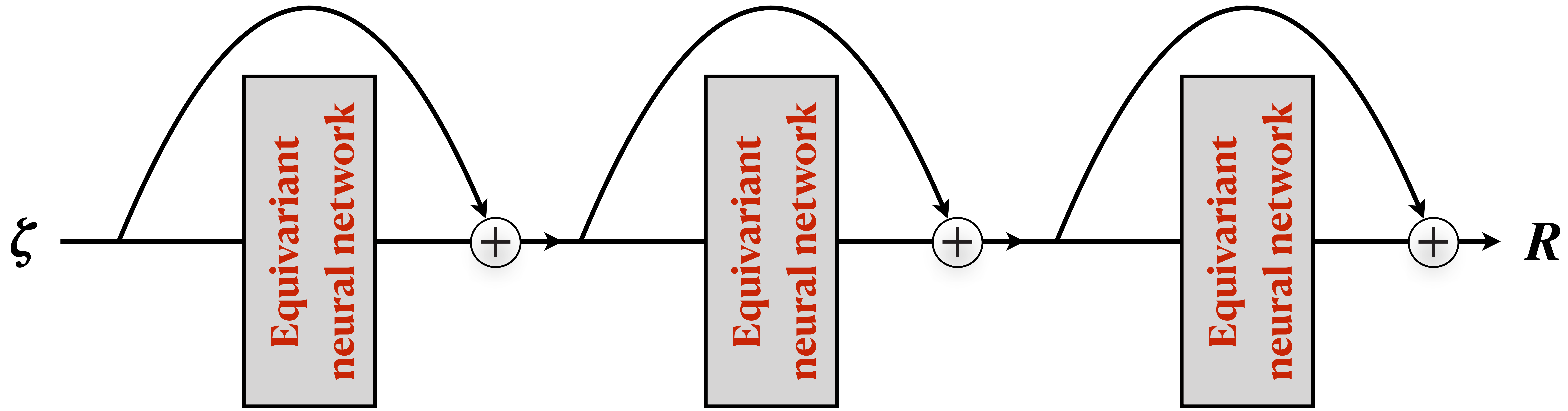
① Backflow is an equivariant residual flow



Behrmann et al, 1811.00995
Chen et al, 1906.02735

② Backflow can be made unitary (if we track its Jacobian)

Neural backflow transformations

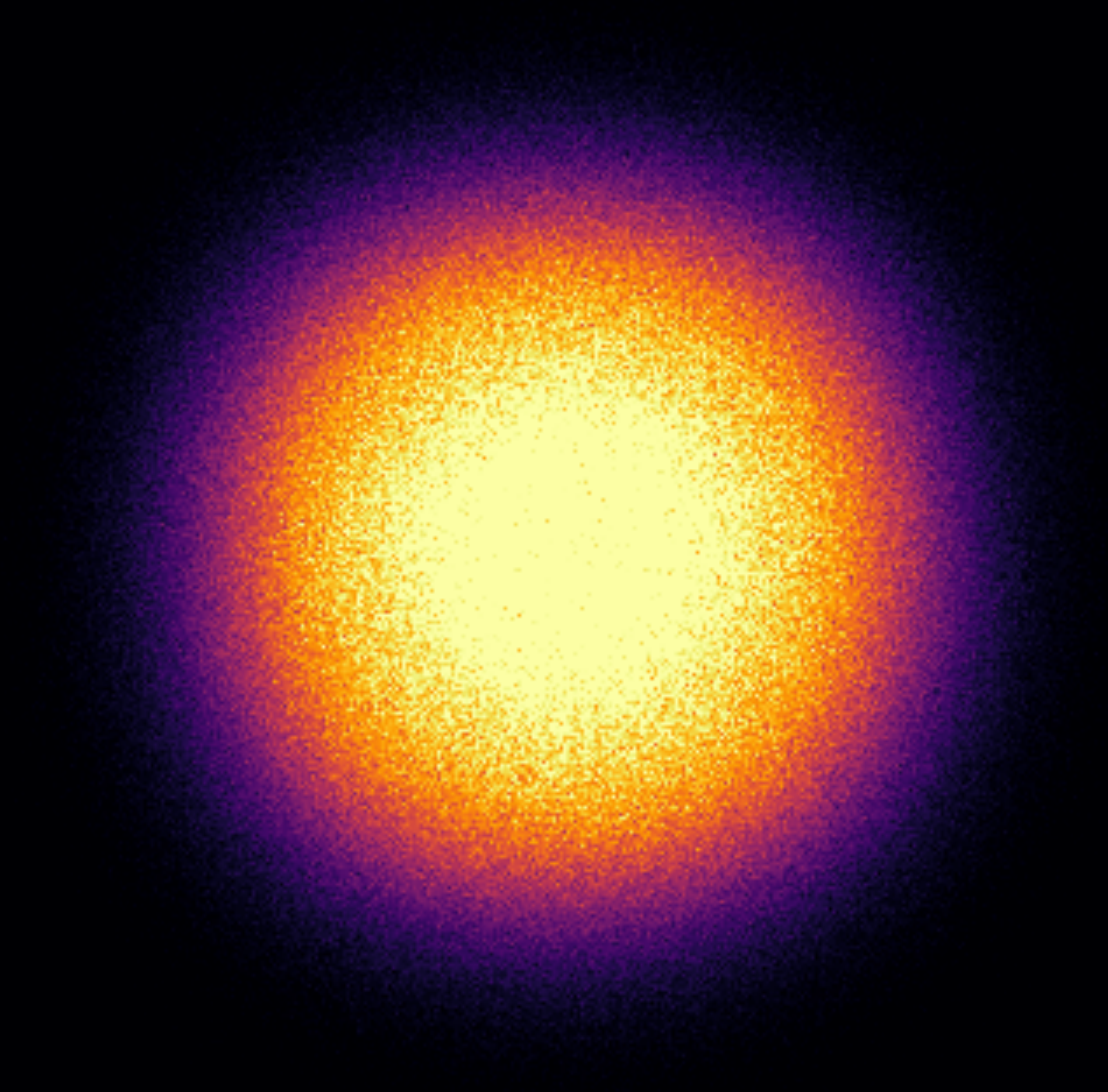


Composition of residual blocks has an
interesting connection to continuous dynamics

E Commun. Math. Stat 17', Harbor el al 1705.03341, Lu et al 1710.10121, Chen et al, 1806.07366

Electron density in a 2D quantum dot

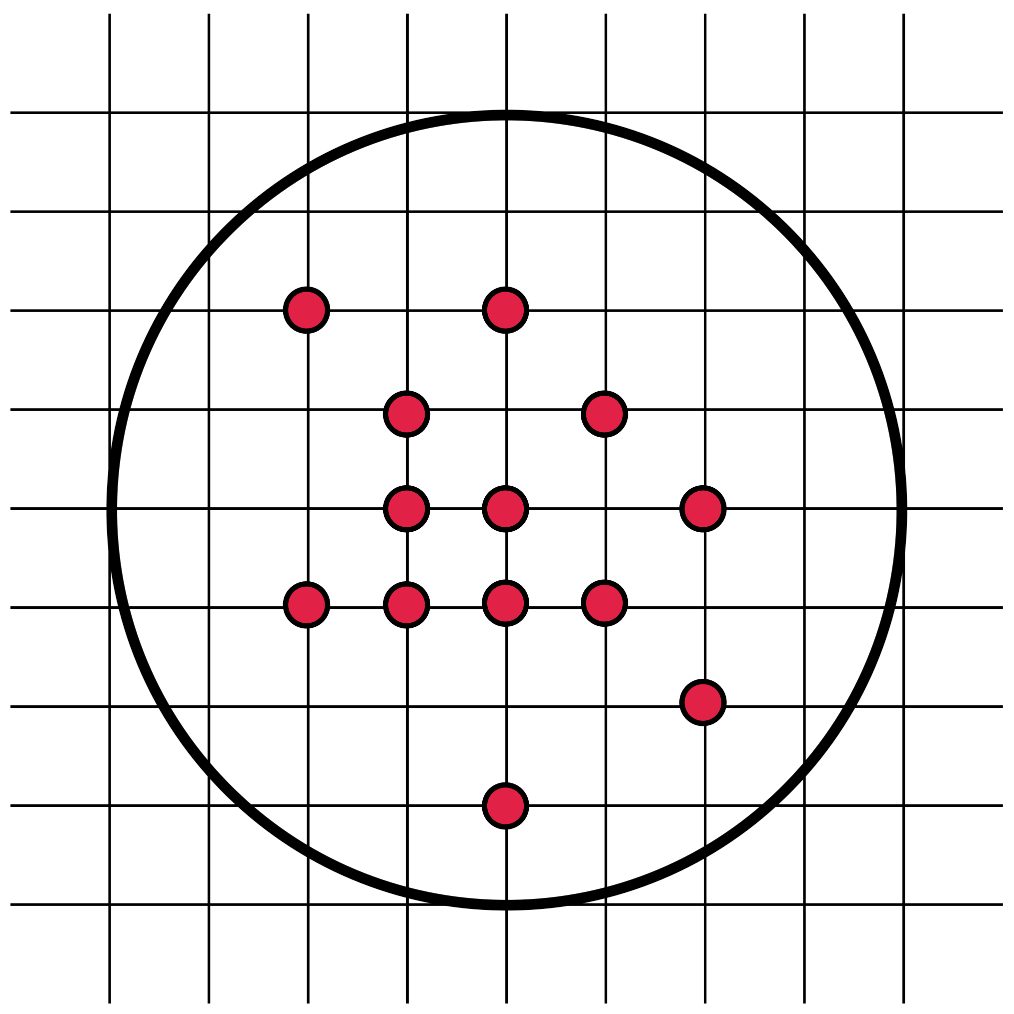
Xie, Zhang, LW, 2105.08644



Continuous flow from noninteracting density to Wigner molecule

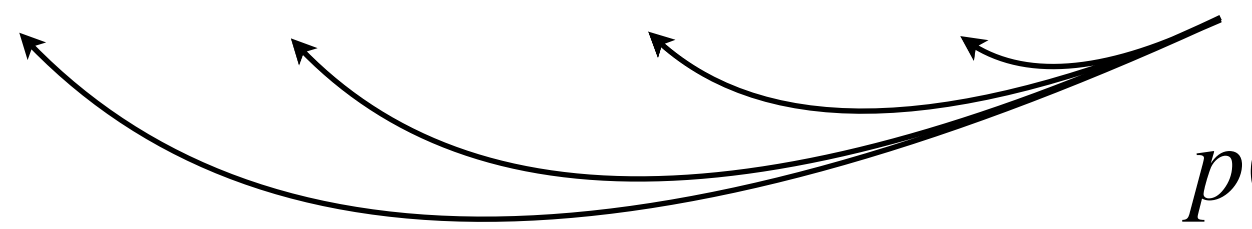
Autoregressive model for $p(\boldsymbol{K})$

$\boldsymbol{K} = \{\boldsymbol{k}_i\}$



$$p(\boldsymbol{K}) = p(\boldsymbol{k}_1)p(\boldsymbol{k}_2 | \boldsymbol{k}_1)p(\boldsymbol{k}_3 | \boldsymbol{k}_1, \boldsymbol{k}_2)\cdots$$

"... quick brown fox jumps ..."



$p(jumps | \ldots)$

$\binom{M}{N}$ possibilities

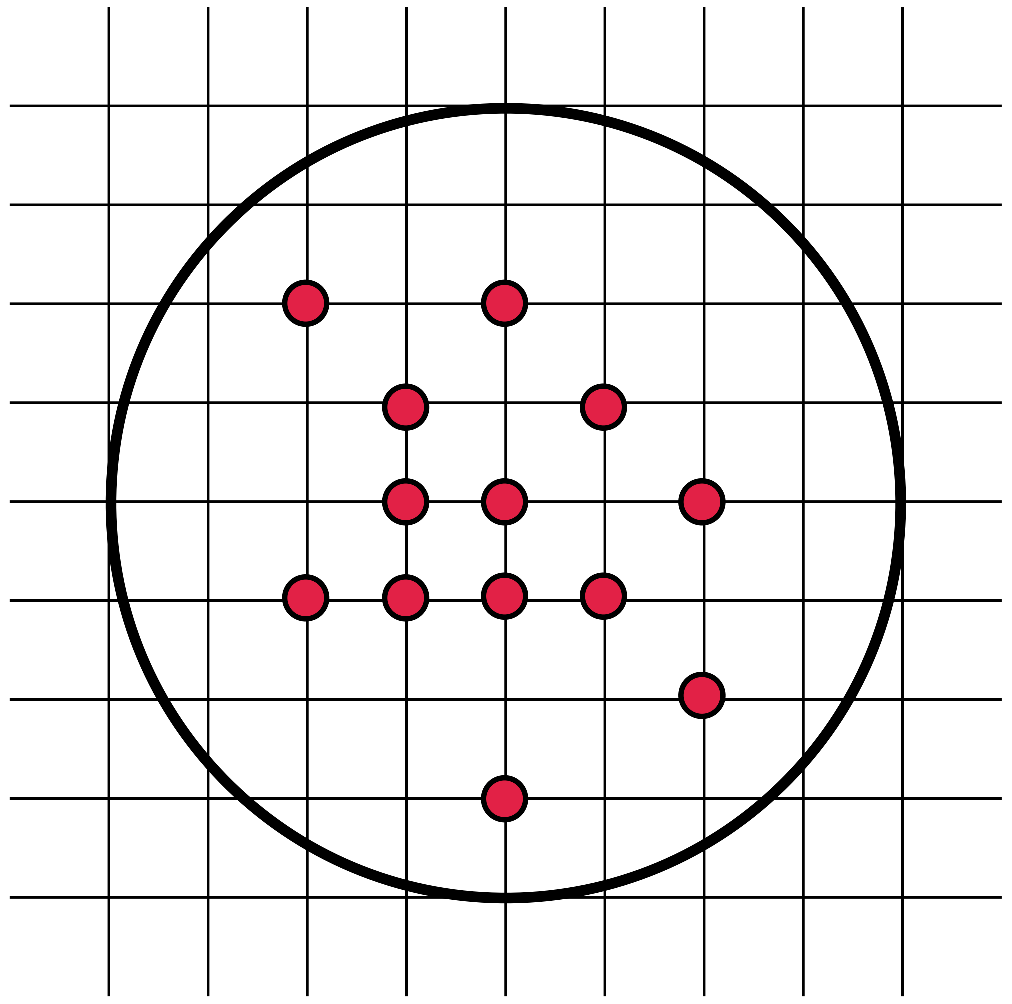
particle number $N \to$ sentence length

momentum grids $M \to$ vocabulary

Except that we are modeling a set of words: no repetition; order does not matter

We use masked casual self-attention Vaswani et al 1706.03762; Alternative solution: Hibat-Allah et al, 2002.02793, Barret et al, 2109.12606

Autoregressive model for $p(\boldsymbol{K})$



$$\binom{49}{13} = 262596783764$$

$$\rho = \sum_{\boldsymbol{K}} p(\boldsymbol{K}) \left| \Psi_{\boldsymbol{K}} \rangle \langle \Psi_{\boldsymbol{K}} \right|$$

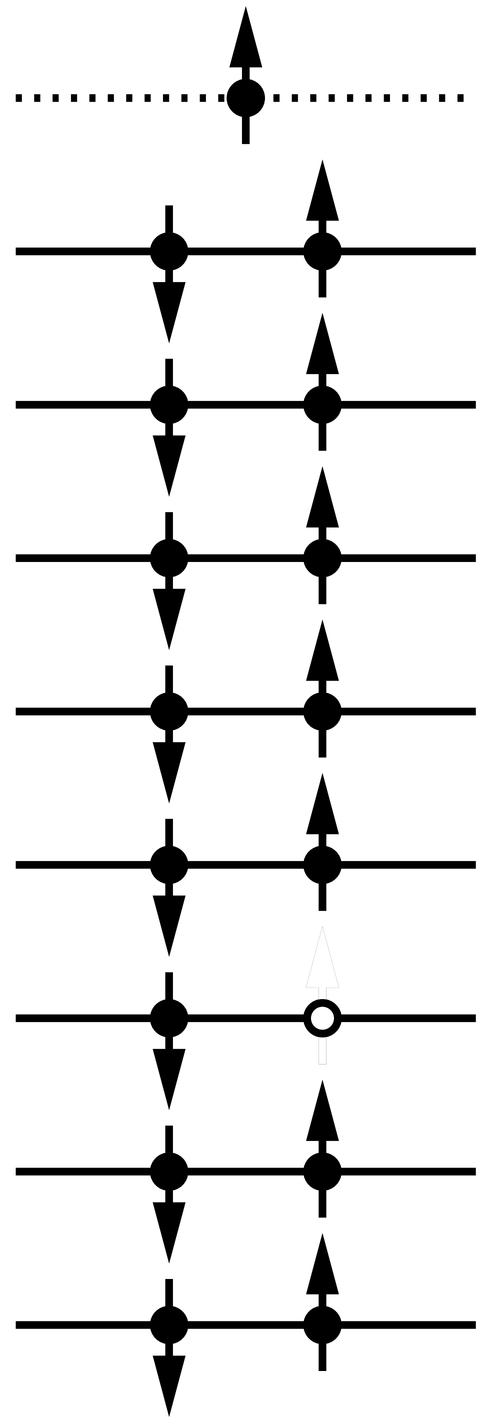
Normalized classical probability for momenta

$$\sum_{\boldsymbol{K}} p(\boldsymbol{K}) = 1$$

Tractable probabilistic model despite of combinatorial large space

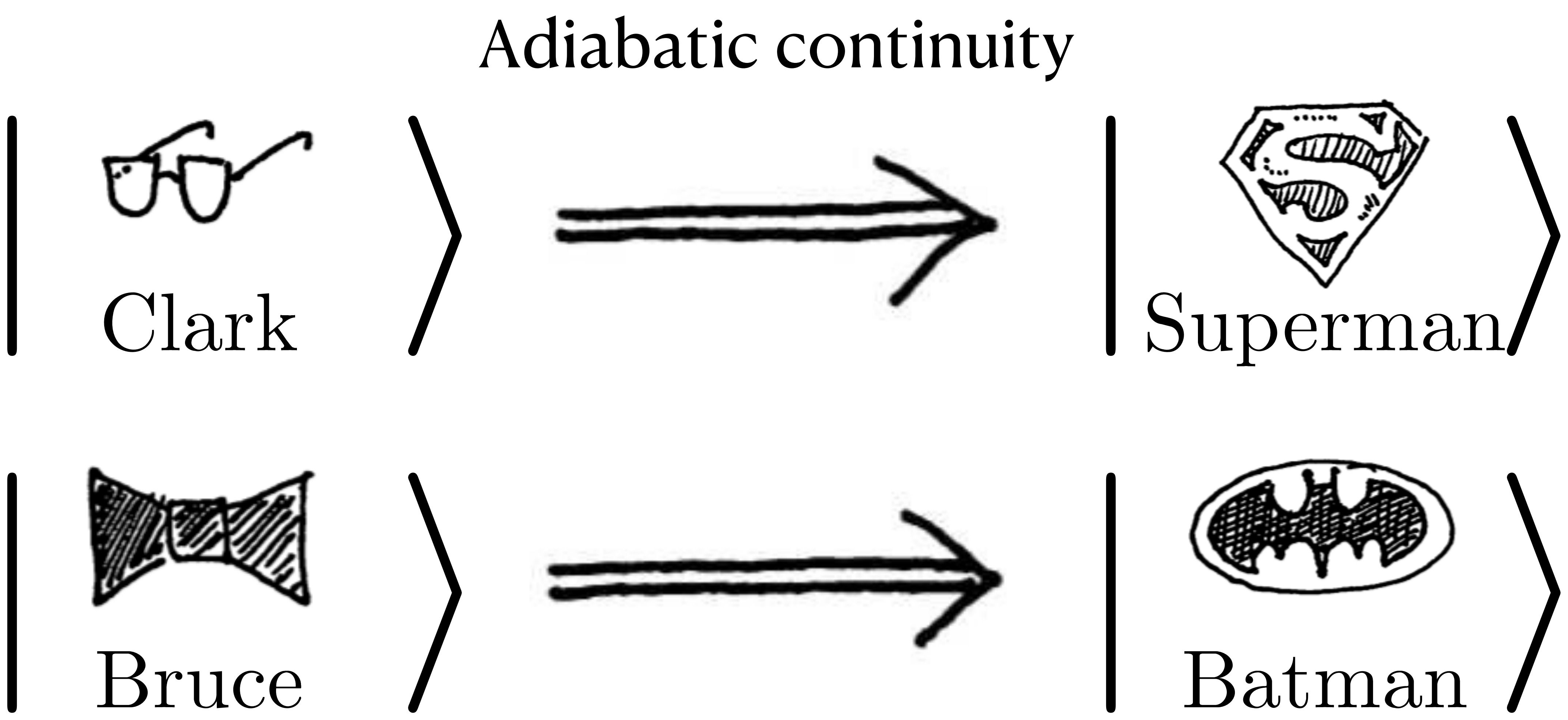
Directly estimate entropy $S = -\,\mathrm{Tr}\rho \ln \rho = -\mathop{\mathbb{E}}_{\boldsymbol{K} \sim p(\boldsymbol{K})} [\ln p(\boldsymbol{K})]$

Neural canonical transformations



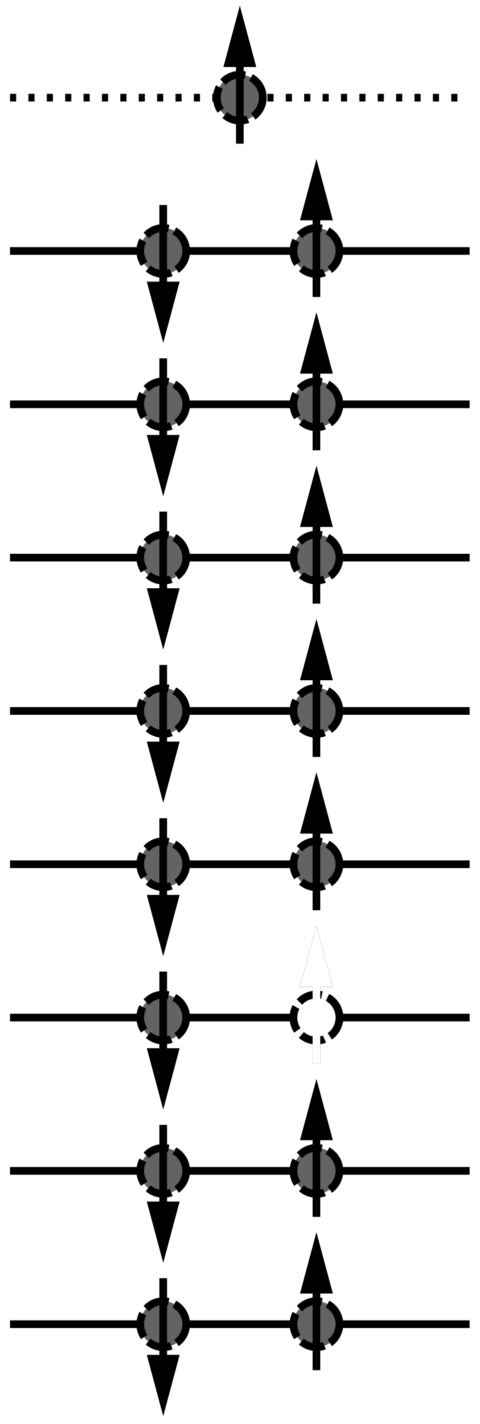
Momentum distribution

$p(\boldsymbol{K})$



Transformation of electron coordinates

$\zeta \leftrightarrow \boldsymbol{R}$



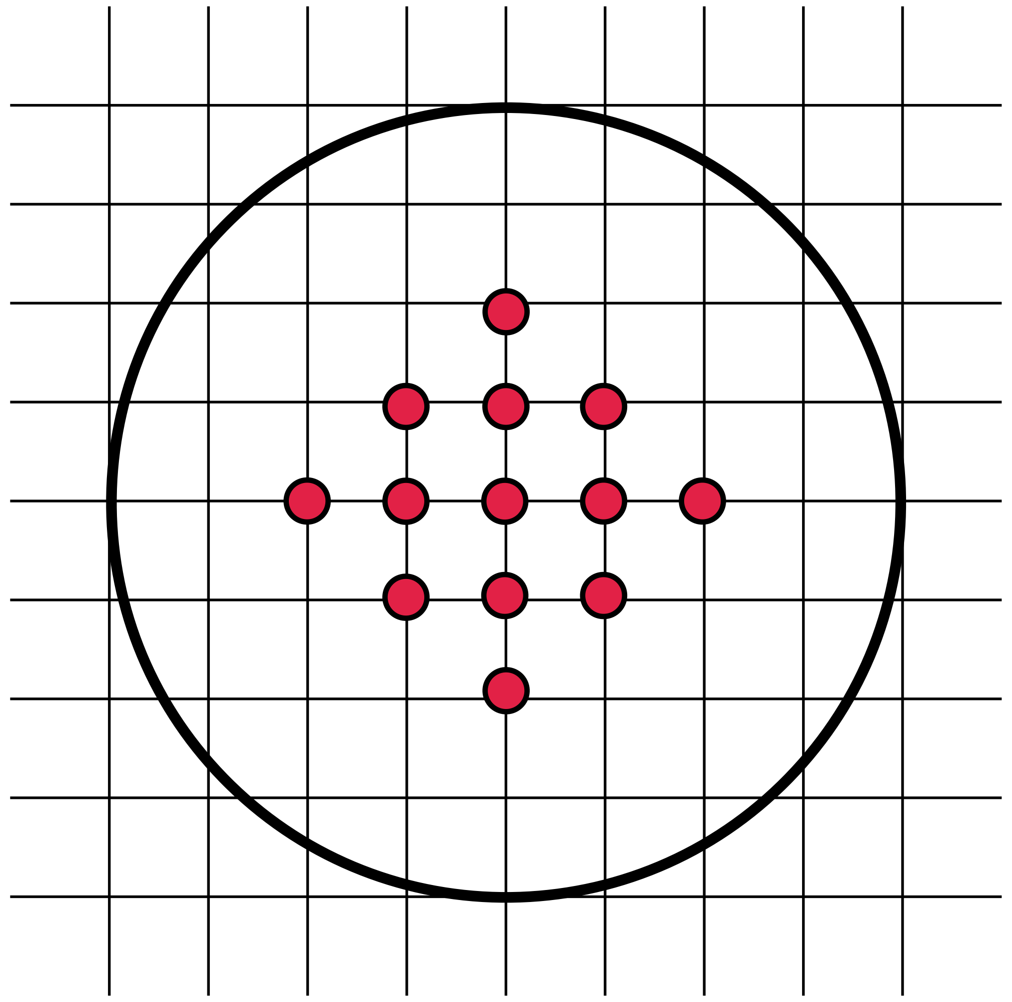
Interacting density matrix

ρ

Variational optimization over an ensemble of unitarily transformed states

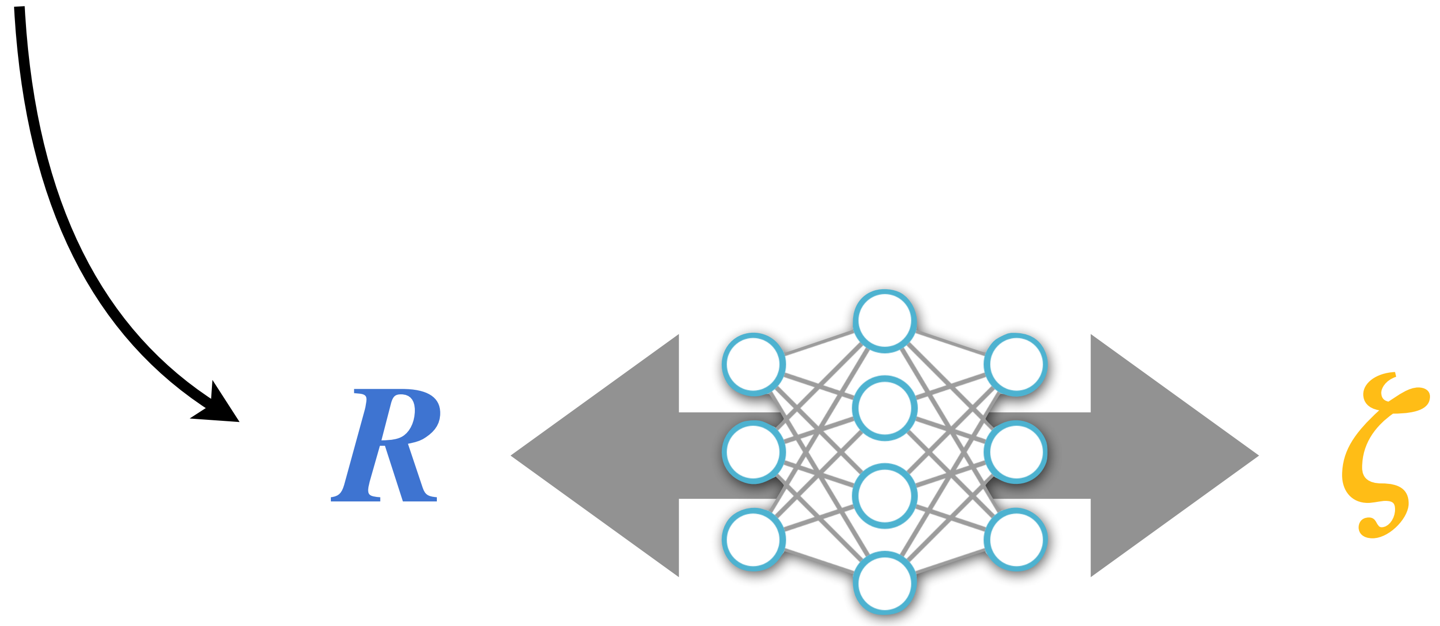
Limiting case 1: Interacting electrons at T=0

$K = \{k_i\}$



$p(K) = 1$ for the closed shell momentum configuration

$$E = \mathop{\mathbb{E}}_{R \sim |\Psi_K(R)|^2} \left[\frac{\langle R | H | \Psi_K \rangle}{\langle R | \Psi_K \rangle} \right]$$

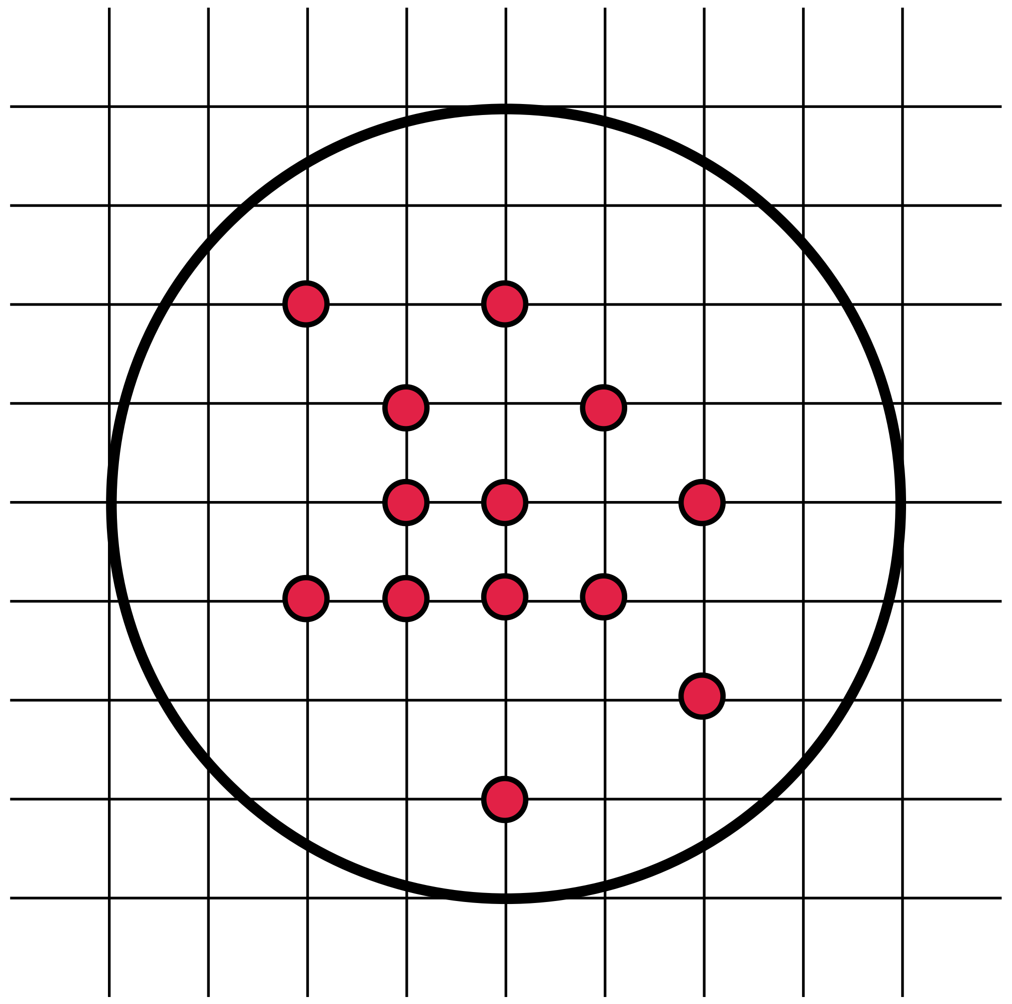


Reduces to ground state variational Monte Carlo with a single normalizing flow wavefunction

Limiting case 2: Noninteracting electrons at T>0

$$F = \mathop{\mathbb{E}}_{K \sim p(\boldsymbol{K})} \left[\frac{1}{\beta} \ln p(\boldsymbol{K}) + \sum_{i=1}^{N} \frac{\hbar^2 \boldsymbol{k}_i^2}{2m} \right]$$

$\boldsymbol{K} = \{\boldsymbol{k}_i\}$



A classical statistical mechanics problem:
Noninteracting fermions in canonical ensemble

(Not as trivial as you might think) Borrmann & Franke, J. Chem. Phys. 1993

Distribute fermions within the momentum cutoff to minimize free-energy

General case: double expectation

$$F = \mathop{\mathbb{E}}_{\boldsymbol{K}\sim p(\boldsymbol{K})} \left[\frac{1}{\beta} \ln p(\boldsymbol{K}) + \mathop{\mathbb{E}}_{\boldsymbol{R}\sim \left|\langle \boldsymbol{R} | \Psi_{\boldsymbol{K}} \rangle\right|^2} \left[\frac{\langle \boldsymbol{R} | H | \Psi_{\boldsymbol{K}} \rangle}{\langle \boldsymbol{R} | \Psi_{\boldsymbol{K}} \rangle} \right] \right]$$

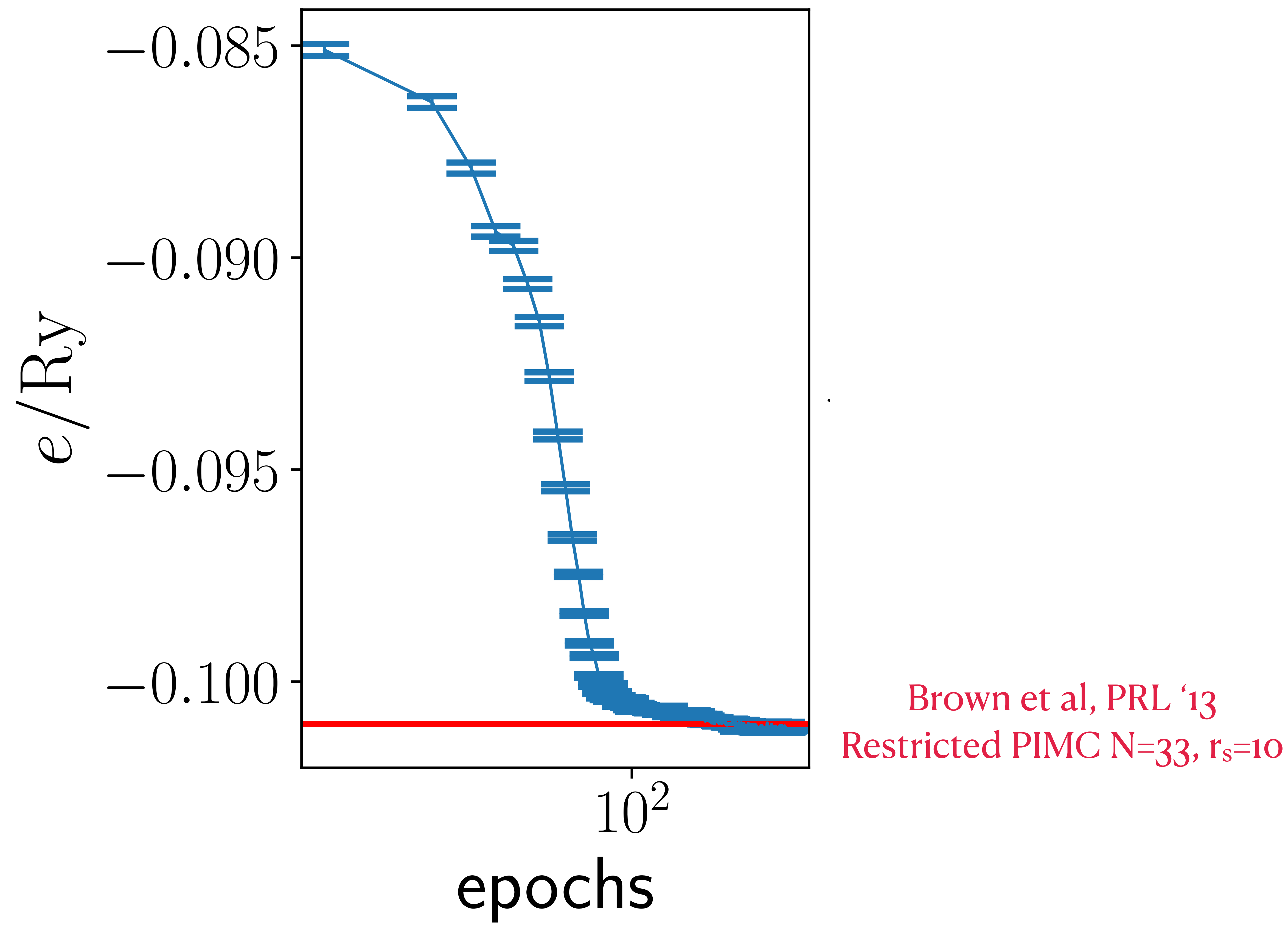
Boltzmann distribution

Born rule

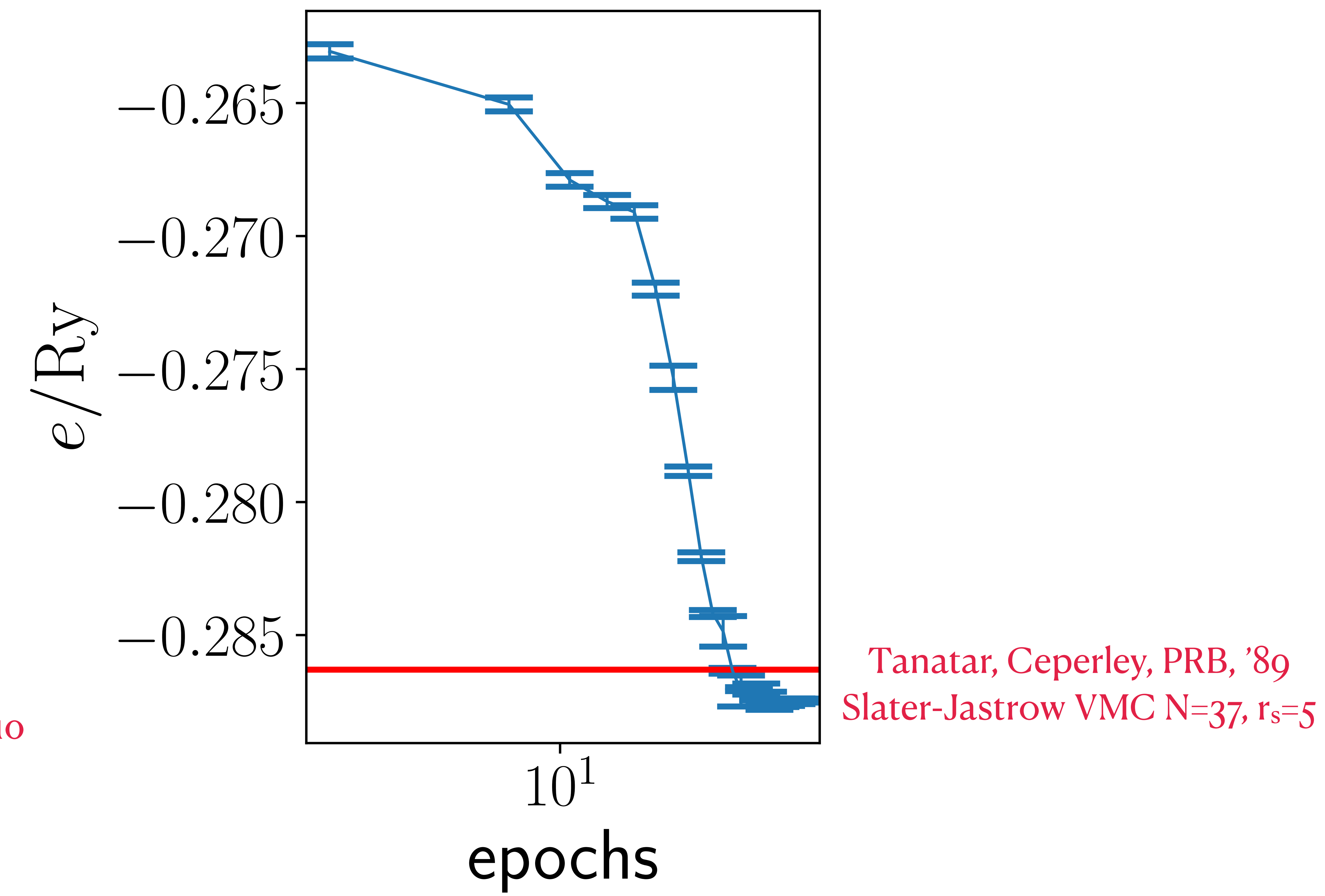
Jointly optimize $|\Psi_{\boldsymbol{K}}\rangle$ and $p(\boldsymbol{K})$ to minimize the variational free-energy

Benchmarks on spin-polarized electron gases

3D electron gas T/T_F=0.0625

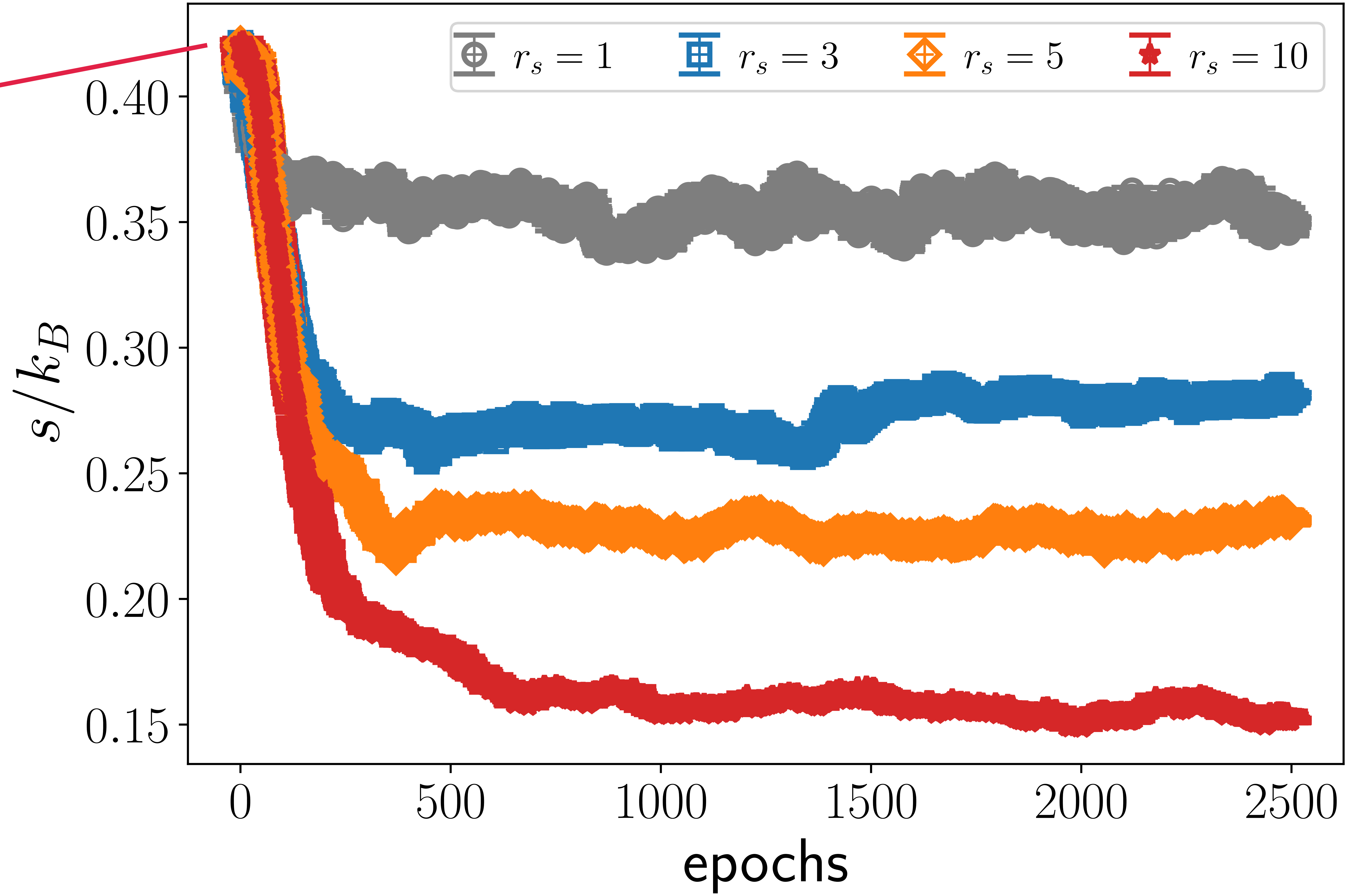


2D electron gas T=0



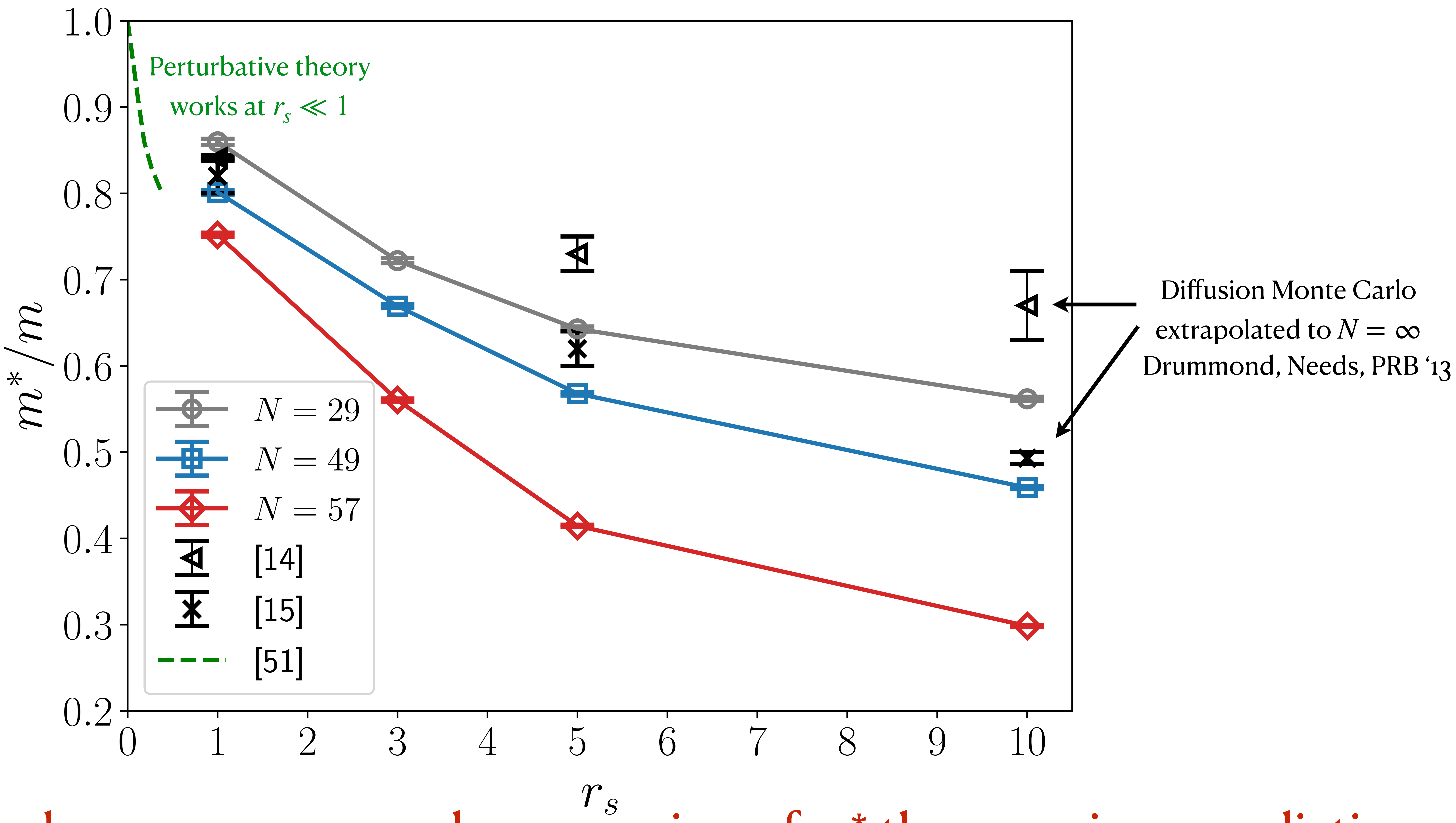
37 spin-polarized electrons @ T/T$_F$=0.15

Starting point:
Ideal gas entropy s_0



$$\frac{m^*}{m} = \frac{s}{s_0}$$

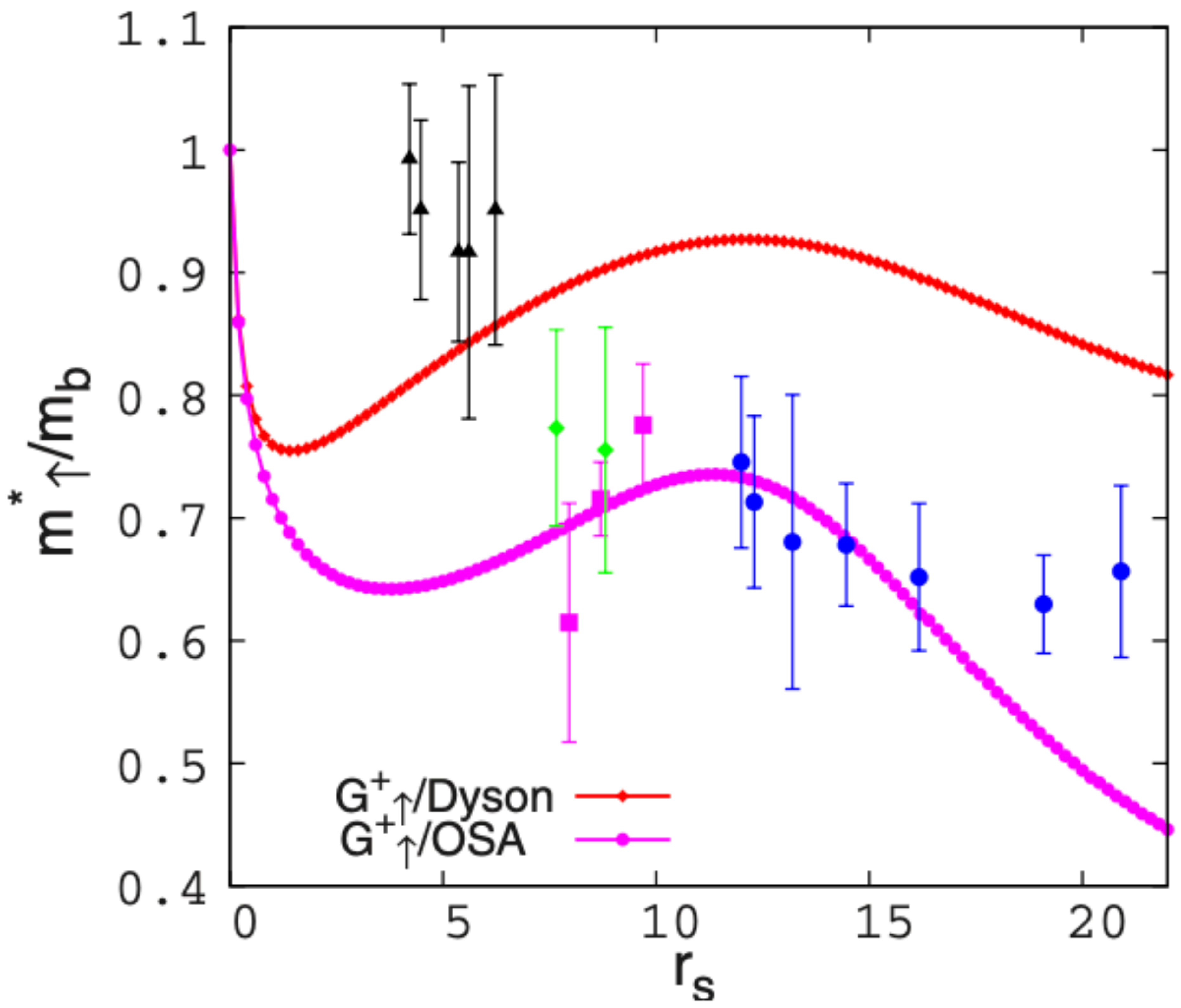
Effective mass of spin-polarized 2DEG



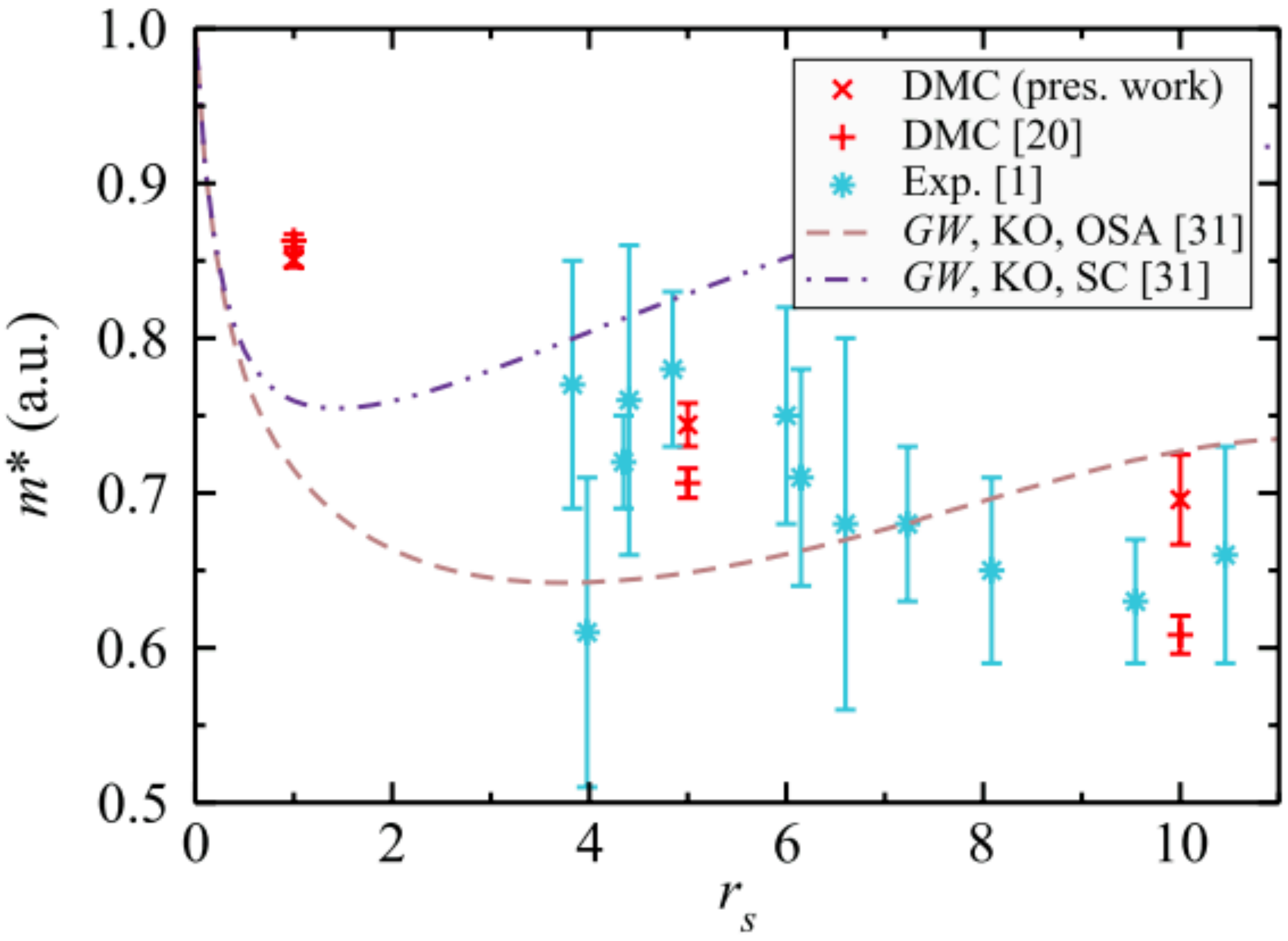
We've found more pronounced suppression of m* than previous predictions

Experiments on spin-polarized 2DEG

Asgari et al, PRB '09



Drommond, Needs, PRB'13



Quantum oscillation experiments
Padmanabhan et al, PRL '08
Gokmen et al, PRB '09

Entropy measurement of 2DEG

ARTICLE

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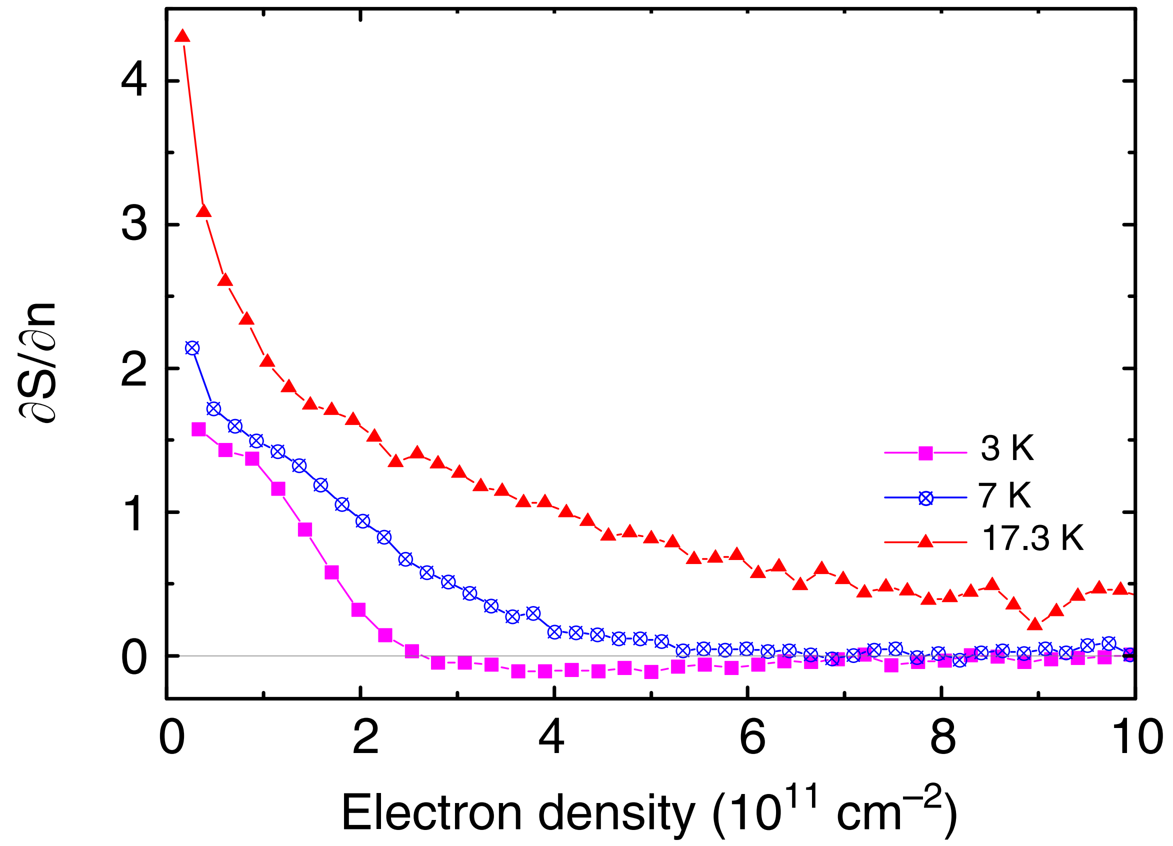
DOI: 10.1038/ncomms8298

Strongly correlated two-dimensional plasma explored from entropy measurements

A.Y. Kuntsevich[1,2], Y.V. Tupikov[3], V.M. Pudalov[1,2] & I.S. Burmistrov[2,4]

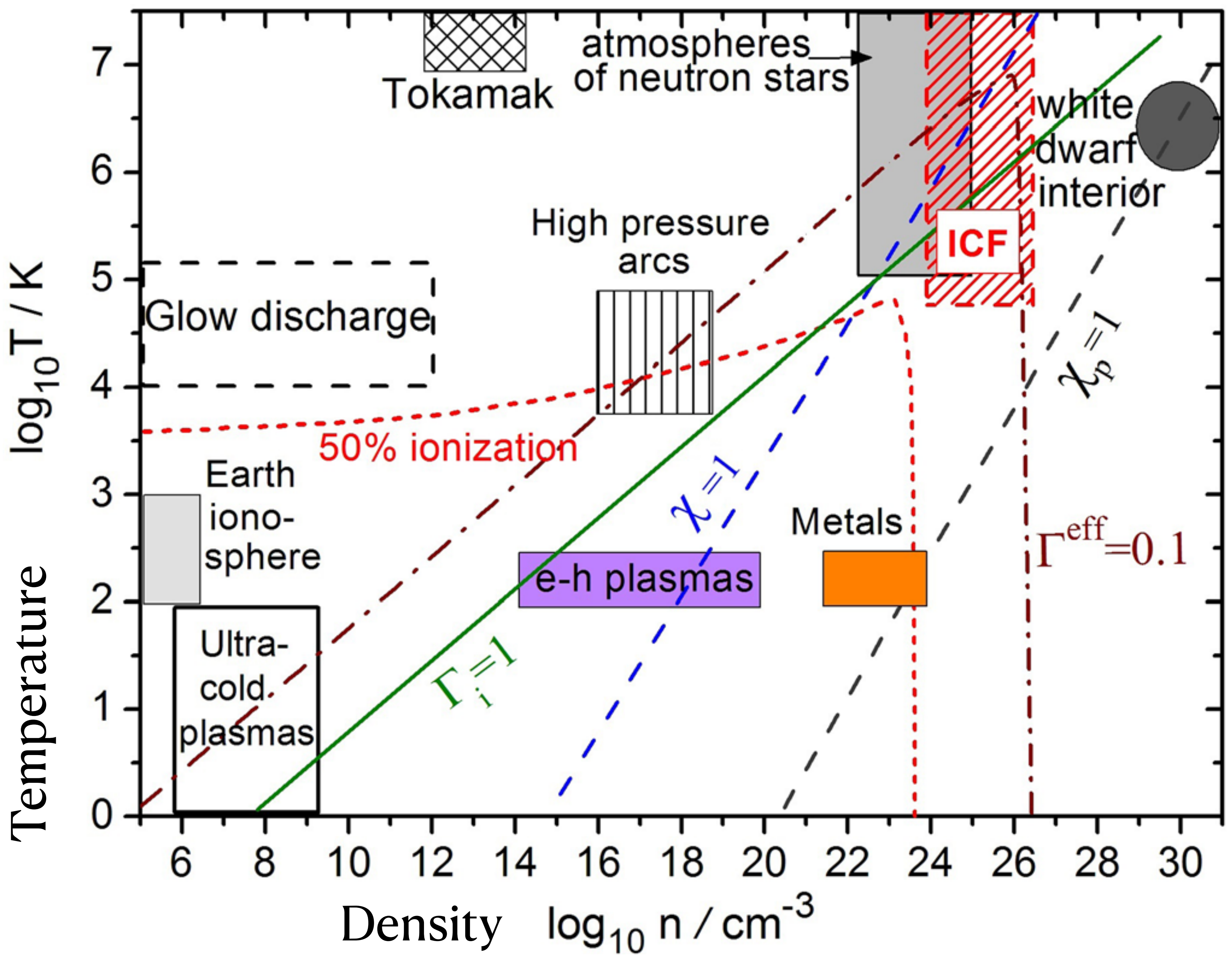
Maxwell relation $$\left(\frac{\partial S}{\partial n}\right)_T = -\left(\frac{\partial \mu}{\partial T}\right)_n$$



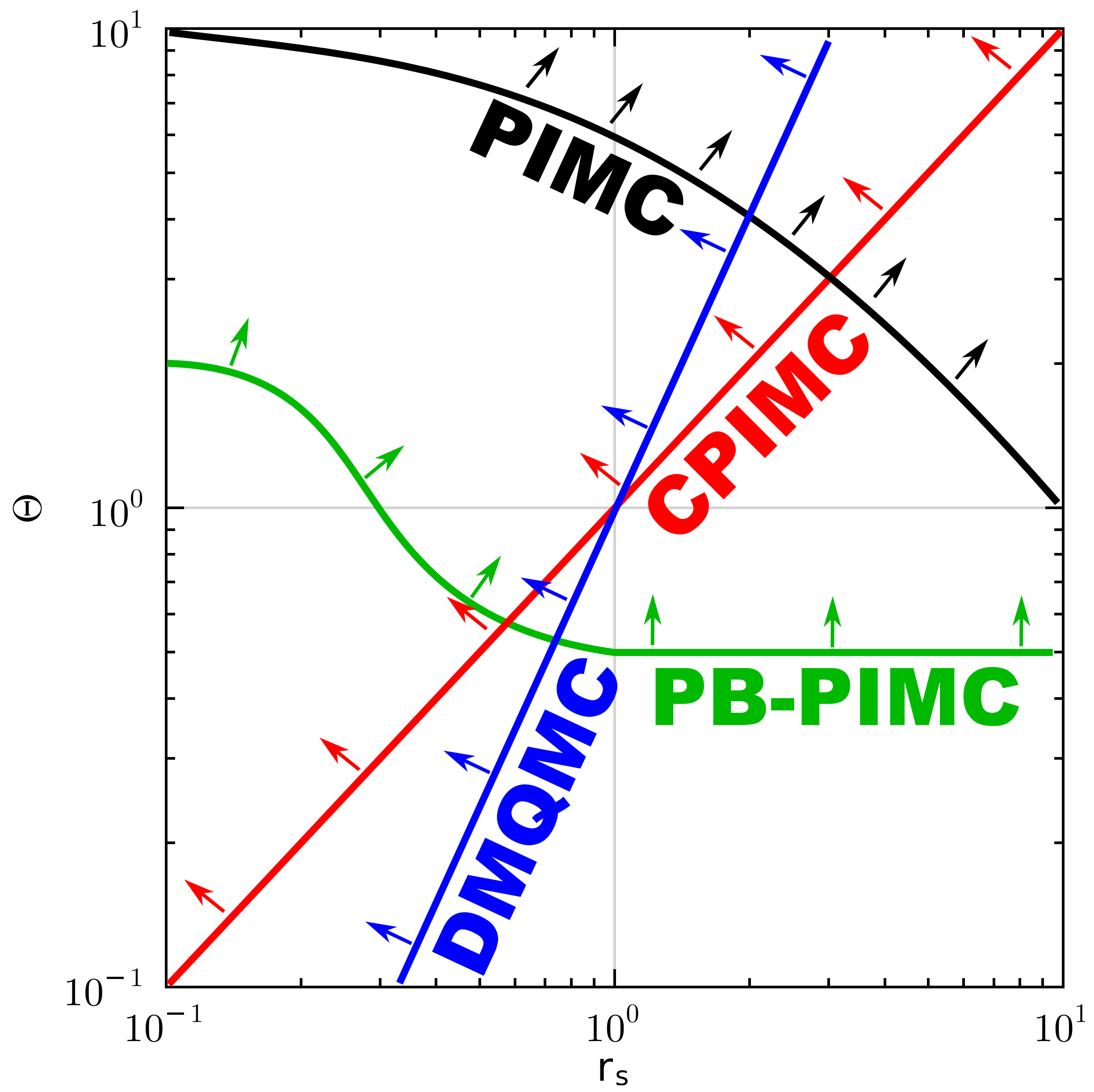
It would be interesting to directly compare calculated entropy with experiment

Future: ab-initio study of quantum matters at finite temperature

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_{I,i}\frac{Z_I e^2}{|R_I - r_i|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|r_i - r_j|} - \sum_I \frac{\hbar^2}{2m_I}\nabla_I^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J e^2}{|R_I - R_J|}$$



Bonitz et al, Phys. Plasmas '20



Dornheim et al, Phys. Plasmas '17

Why now ?

Variational free-energy is a fundamental principle for $T>0$ quantum systems

However, it was under exploited for solving practical problems (mostly due to intractable entropy for nontrivial density matrices)

Now, it is has became possible by integrating recent advances in generative machine learning

FAQs

Where are data ?

There is no training dataset. Data are self-generated from the model.

How do we know it is correct ?

Variational principle: lower free-energy is better.

Do I understand the "black box" model ?

a) I don't care (as long as it is sufficiently accurate).

b) $\ln p(\boldsymbol{K})$ contains the Landau energy functional

$$E[\delta n_k] = E_0 + \sum_k \epsilon_k \delta n_k + \frac{1}{2}\sum_{k,k'} f_{k,k'} \delta n_k \delta n_{k'}$$

$\zeta \leftrightarrow \boldsymbol{R}$ illustrates adiabatic continuity.

A tensor network/quantum computing approach

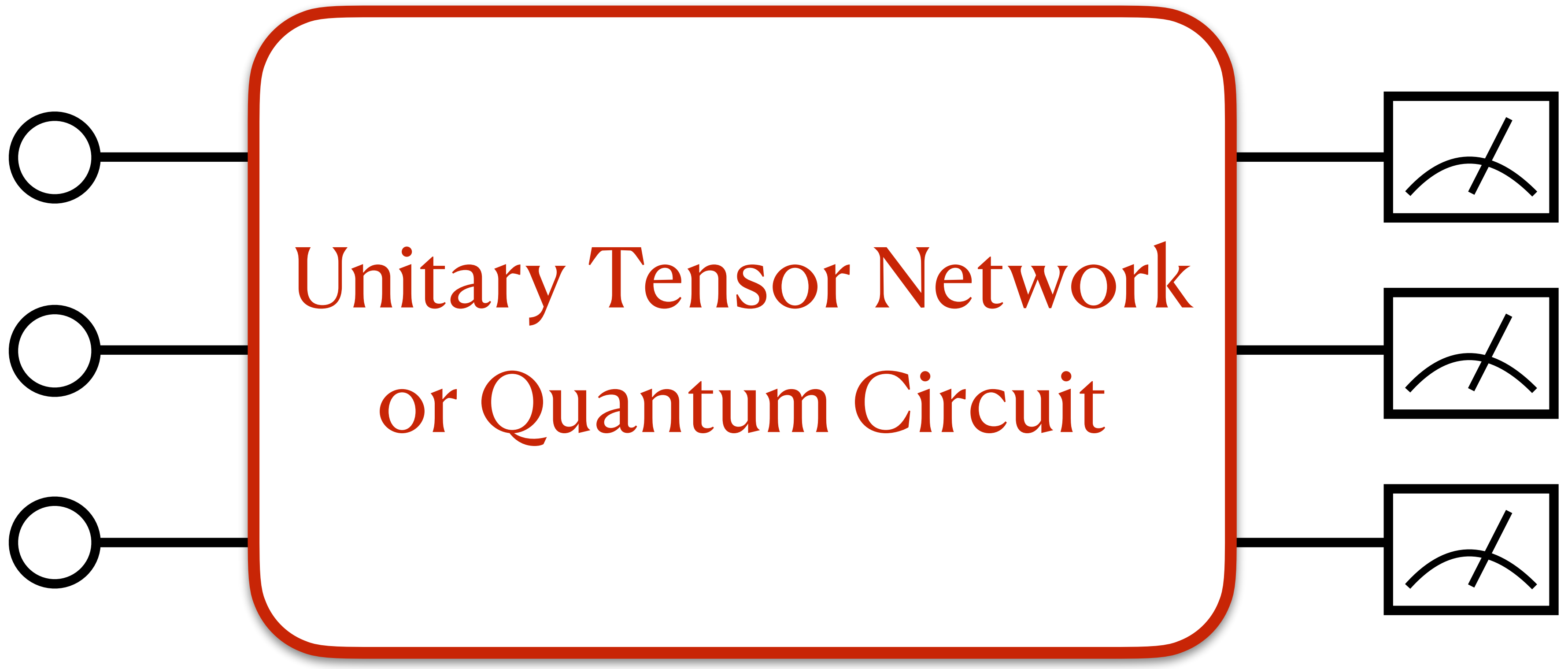
Martyn et al 1812.01015

Verdon et al 1910.02071

Autoregressive net + Q circuit, Liu et al, 1912.11381

Experiment, Guo et al, 2107.06234

$x \sim p(x)$



$$\rho = \sum_x p(x) U |x\rangle\langle x| U^\dagger$$

$$F = \frac{1}{\beta}\mathrm{Tr}(\rho \ln \rho) + \mathrm{Tr}(H\rho) \geq -\frac{1}{\beta}\ln Z$$

Variational optimize classically tractable unitary tensor networks, or, quantum circuits

Summary

m*: new ML-powered method, new results on 2DEG and more

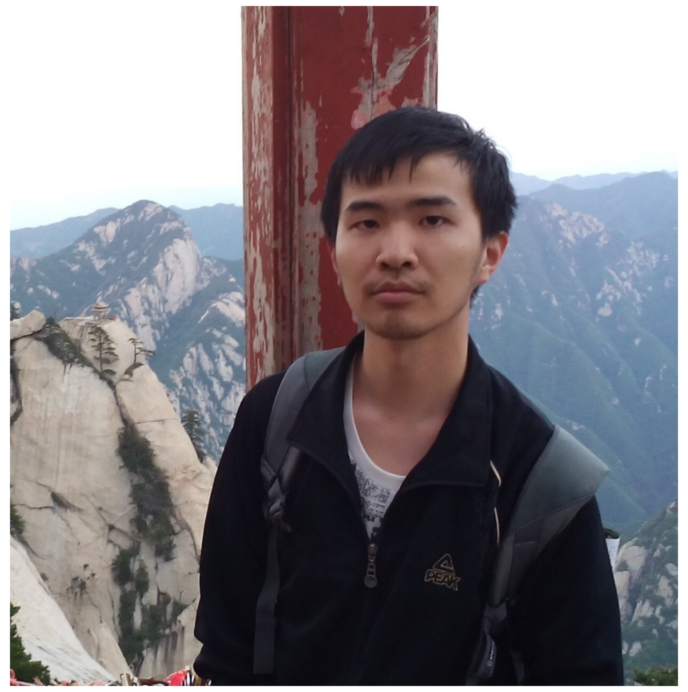
More quantities: Landau fermi parameters and spectral functions

Beyond electron gases: warm dense matter, hydrogen plasma, ultracold fermi gases, thermal density functionals...

Thank you!

2105.08644
2201.03156

github/fermiflow



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