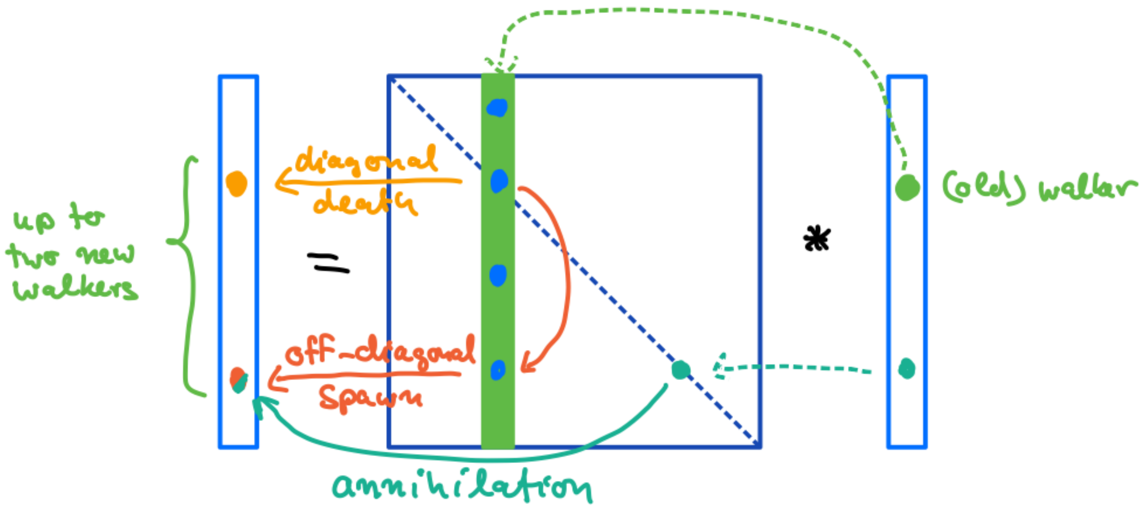
Full Configuration Interaction Quantum Monte Carlo for Ultracold Atoms



Joachim Brand

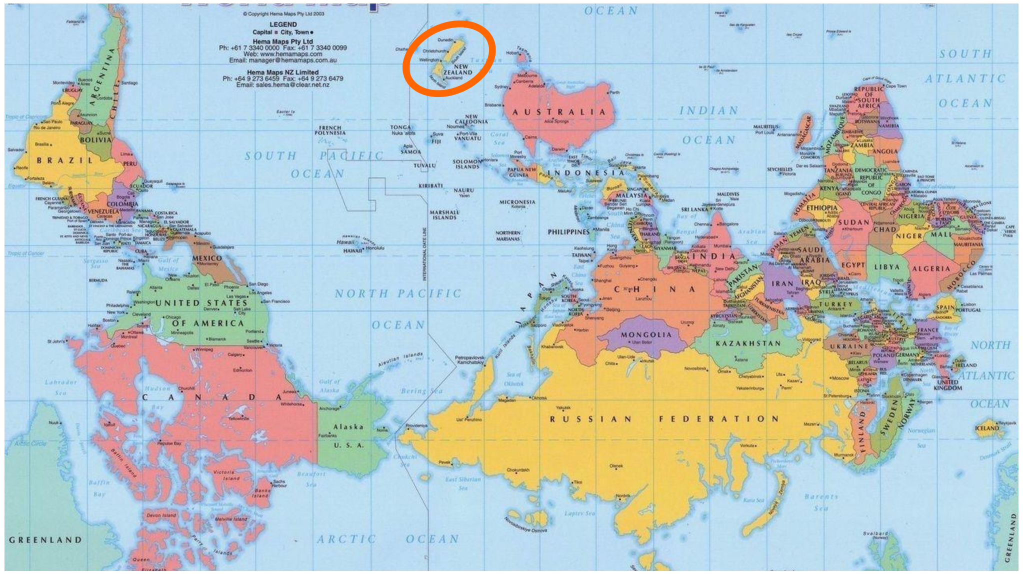
Massey University
COLLEGE OF SCIENCES

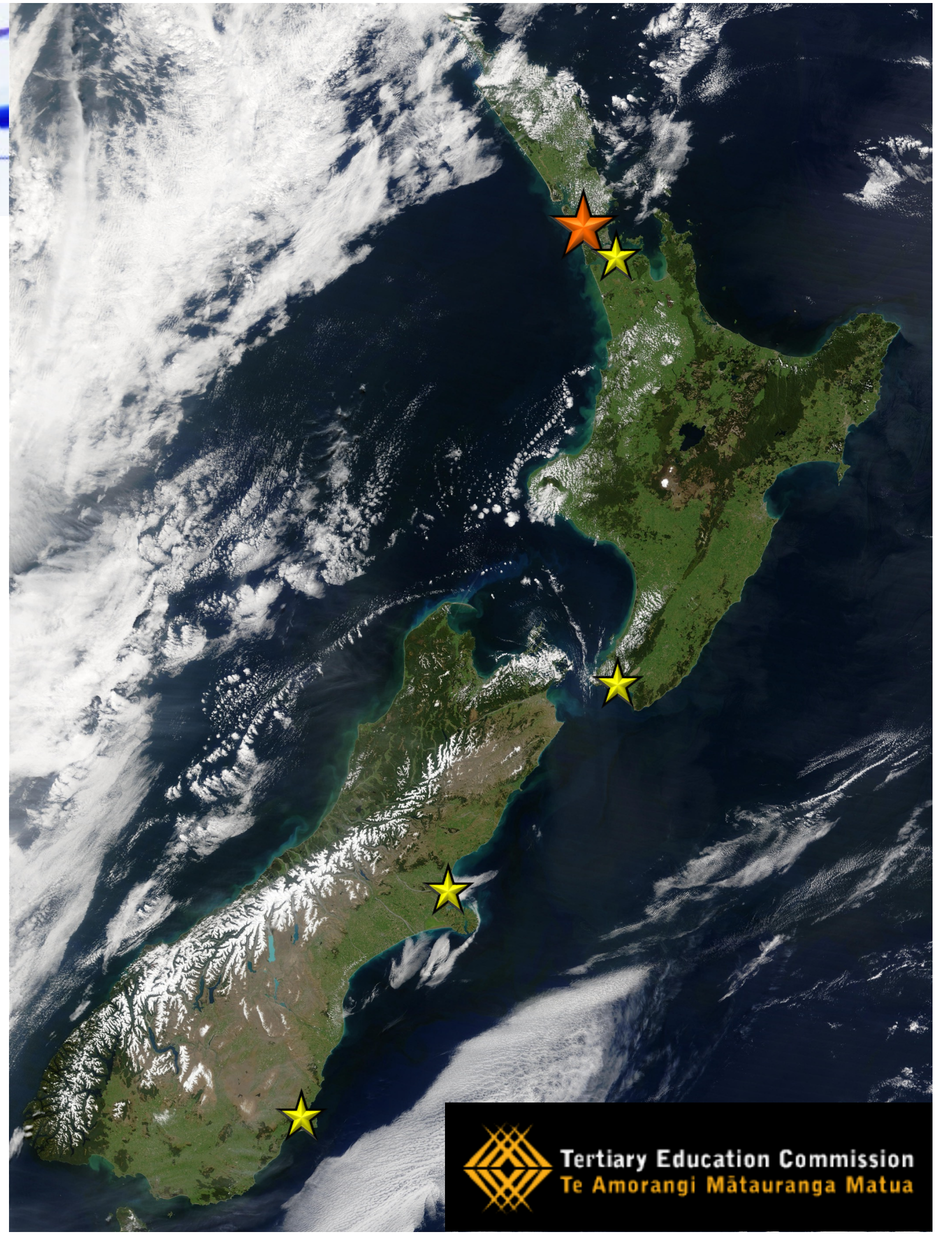
UPC webinar, Barcelona, 22 March 2022

The Dodd-Walls Centre
for Photonics and Quantum Technology

The Dodd-Walls Centre
for Photonic and Quantum Technologies

- Government funded **Centre of Research Excellence** (re-funded through 2028)
- Main areas:
    - Ultra-cold atoms, quantum gases
    - Quantum optics
    - Nonlinear fibre optics
    - Biophotonics





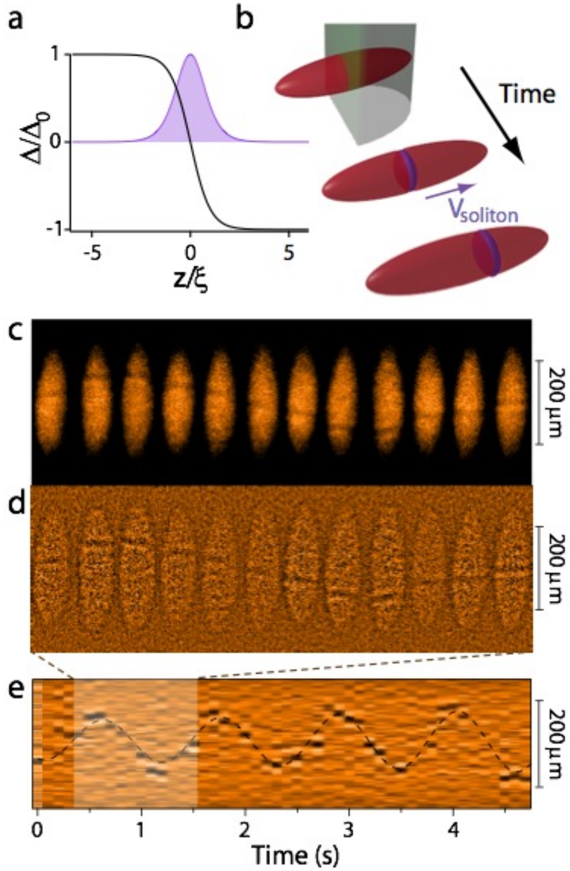
ARTICLE

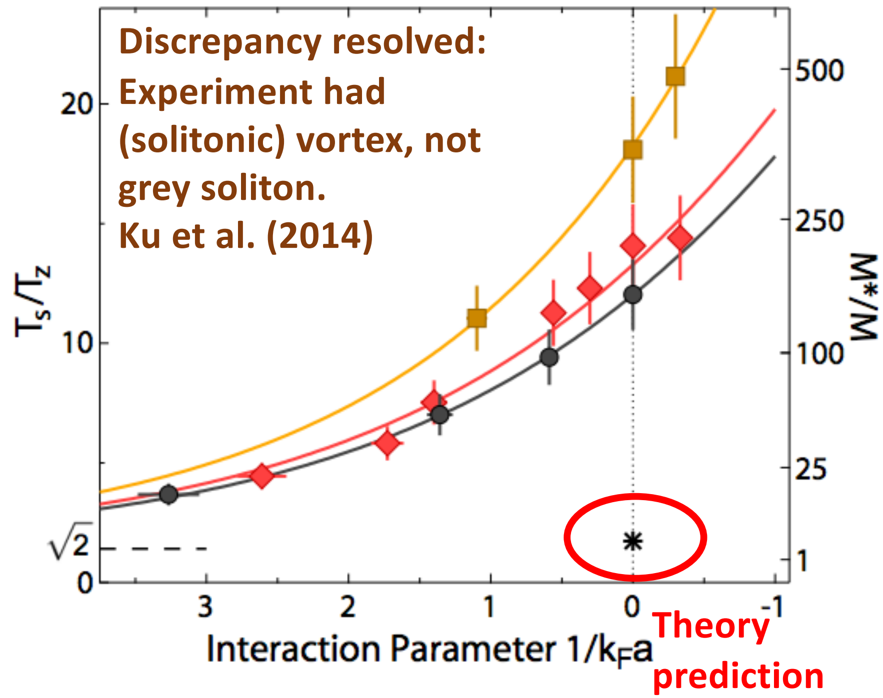
2013

doi:10.1038/nature12338

Heavy solitons in a fermionic superfluid

Tarik Yefsah[1], Ariel T. Sommer[1], Mark J. H. Ku[1], Lawrence W. Cheuk[1], Wenjie Ji[1], Waseem S. Bakr[1] & Martin W. Zwierlein[1]





Theory:
Liao, Brand, PRA (2011)
Scott, *et al.* PRL (2011)

Can we understand soliton phenomena beyond (fermionic) mean-field theory?

Outline

Full Configuration Interaction Quantum Monte Carlo

Population Control Bias

Transcorrelated Method

Mobile Spin Impurity in 1D Bose Gas

2014 CTCP Massey University group photo with visitors

THE JOURNAL OF CHEMICAL PHYSICS **131**, 054106 (2009)

Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space

George H. Booth,[1] Alex J. W. Thom,[1,2] and Ali Alavi[1,a)]
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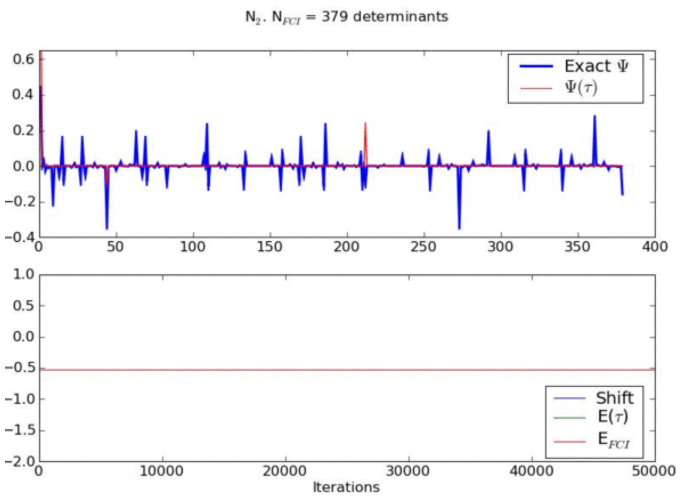
(Received 15 May 2009; accepted 13 July 2009; published online 4 August 2009)

We have developed a new quantum Monte Carlo method for the simulation of correlated many-electron systems in full configuration-interaction (Slater determinant) spaces. The new method is a population dynamics of a set of walkers, and is designed to simulate the underlying imaginary-time Schrödinger equation of the interacting Hamiltonian. The walkers (which carry a positive or negative sign) inhabit Slater determinant space, and evolve according to a simple set of rules which include spawning, death and annihilation processes. We show that this method is



Why a new projector quantum Monte Carlo?

Projector quantum Monte Carlo

- Solve the time-independent Schrödinger equation

$$\hat{H}|\Psi\rangle = E_0|\Psi\rangle$$

- Find stochastic averages for the ground state energy and properties

Existing projector Monte Carlo methods

- Green's function Monte Carlo (GFC: Kalos 1962)
- Diffusion Monte Carlo (DMC: JB Anderson 1975)
- Auxiliary-field quantum Monte Carlo (AFQMC)
- Path integral ground-state Monte Carlo (PIGS)

Why "Full configuration interaction quantum Monte Carlo" (FCIQMC: Booth, Thom, Alavi 2009)?

To get around the fixed-node approximation of DMC.

Full configuration interaction quantum Monte Carlo (FCIQMC)

Major developments

- Integer formulation (Booth, Thom, Alavi 2009)
  First formulation of algorithm
- Initiator rule (Cleland, Booth, Alavi 2010)
  Approximation that softens the sign problem
- Population dynamics with sign problem (Spencer, Blunt, Foulkes 2012)
  Improved understanding of the nature of the sign problem in FCIQMC
- Semistochastic FCIQMC and floating-point coefficients (Petruziello *et al.* 2012)
  Reduces noise and improves efficiency
- Vector compression theory; fast randomized iterations (Lim, Weare 2017)

Our work

- Improved population control (Yang, Pahl, Brand 2020)
- Analysis of population control bias (Brand, Yang, Pahl arXiv:2103.07800)

FCIQMC principles

Representing the Hamiltonian as a matrix, turns the Schrödinger equation into a **generic linear algebra problem**:

$$\mathbf{H}\mathbf{c}_0 = E_0 \mathbf{c}_0$$

FCIQMC iteration equation:

$$\mathbf{c}^{(n+1)} = \mathbf{c}^{(n)} + \delta\tau \left(S^{(n)} \mathbf{1} - \mathbf{H} \right) \mathbf{c}^{(n)}$$

Discretised imaginary time evolution, or power method.

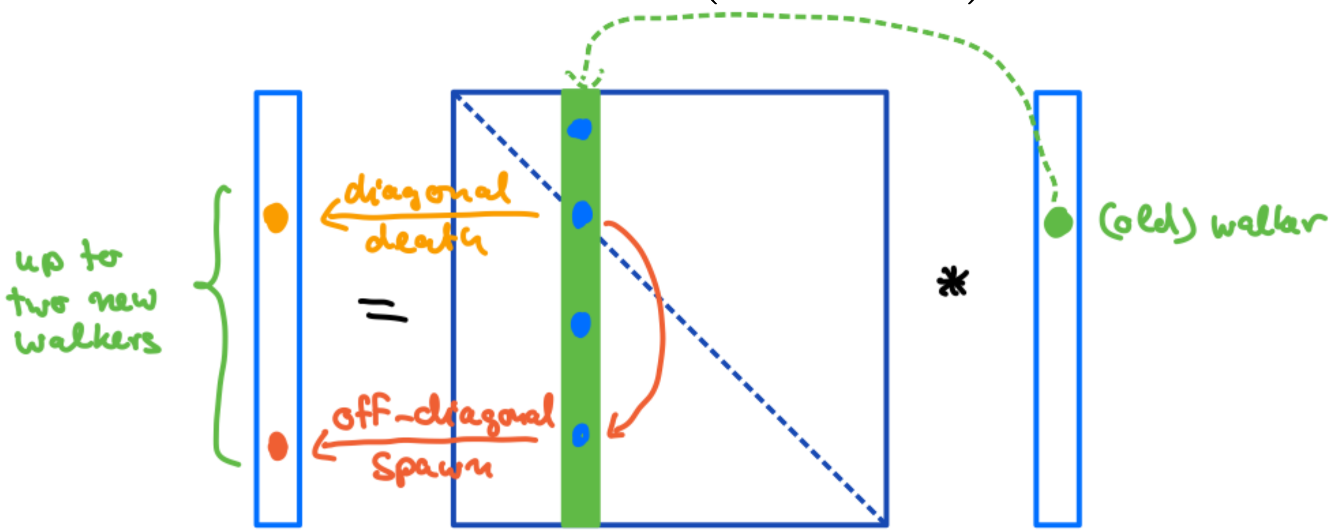
Fixed point (long time limit):

Coefficient vector $\mathbf{c}^{(n)} \to \mathbf{c}_0$

Scalar shift $S^{(n)} \to E_0$

Stochastic sampling procedure

$$\mathbf{c}^{(n+1)} = \mathbf{c}^{(n)} + \delta\tau \left(S^{(n)}\mathbf{1} - \mathbf{H} \right) \mathbf{c}^{(n)}$$

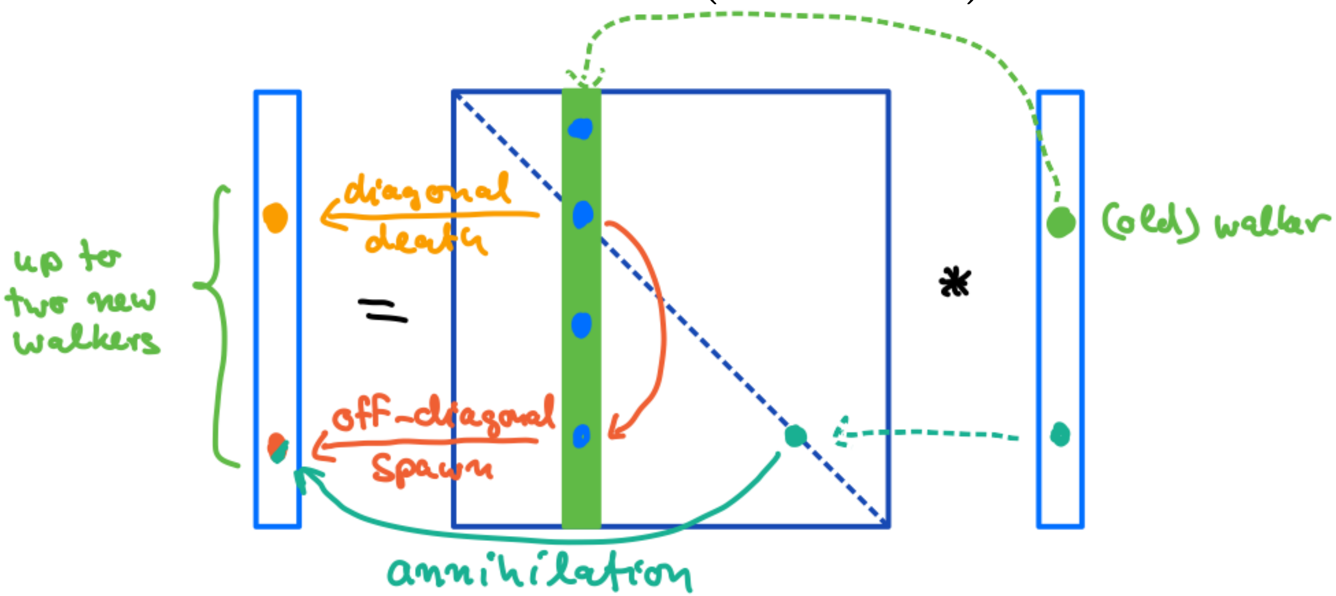


The original formulation uses integer coefficients (walkers without weights).
In every time step, a single walker can spawn 0, 1, or 2 walkers.

Modern formulations use floating point coefficients, and stochastic vector compression.

Stochastic sampling procedure

$$\mathbf{c}^{(n+1)} = \mathbf{c}^{(n)} + \delta\tau \left(S^{(n)} \mathbf{1} - \mathbf{H} \right) \mathbf{c}^{(n)}$$



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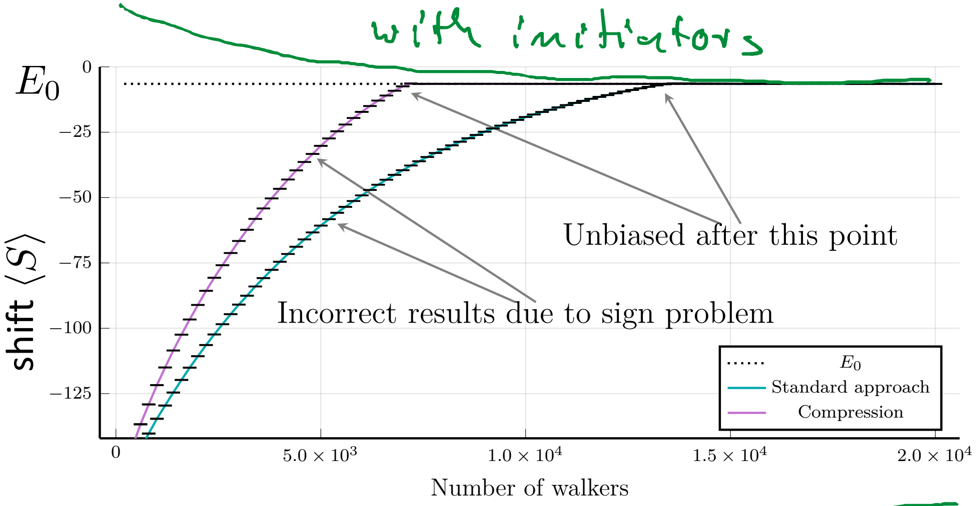
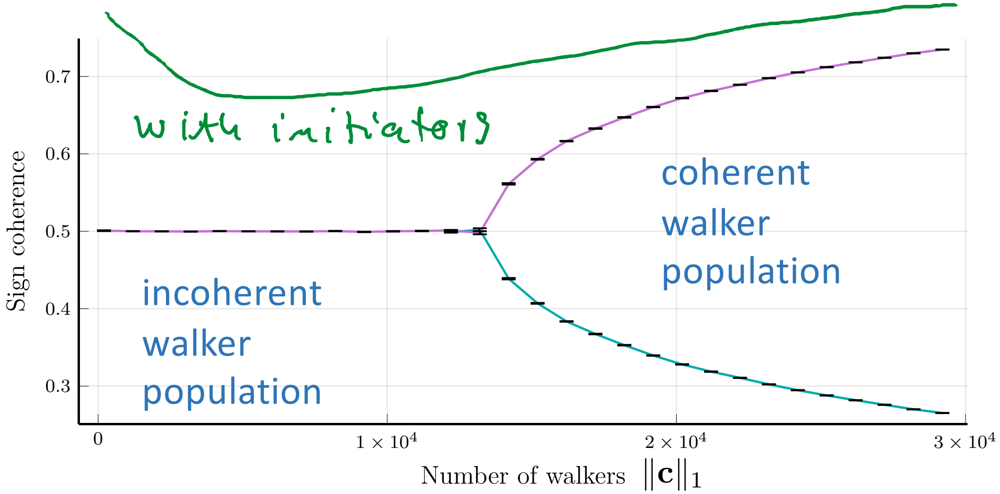
Modern formulations use floating point coefficients, and stochastic vector compression.

The sign problem as a critical phenomenon

- The Monte Carlo sign problem appears as a phase transition in FCIQMC
- Algorithmic changes can lower the number of walkers where the phase transition occurs.
- Interesting connections to phase transitions and critical phenomena in complex networks remain to be explored.
- The **initiator rule** restores coherence: Only configurations with above threshold population may spawn to unoccupied configurations

Shepherd *et al.* arXiv:1209.4023
Čufar, Pahl, Brand (to be published)
Cleland *et al.* 2010

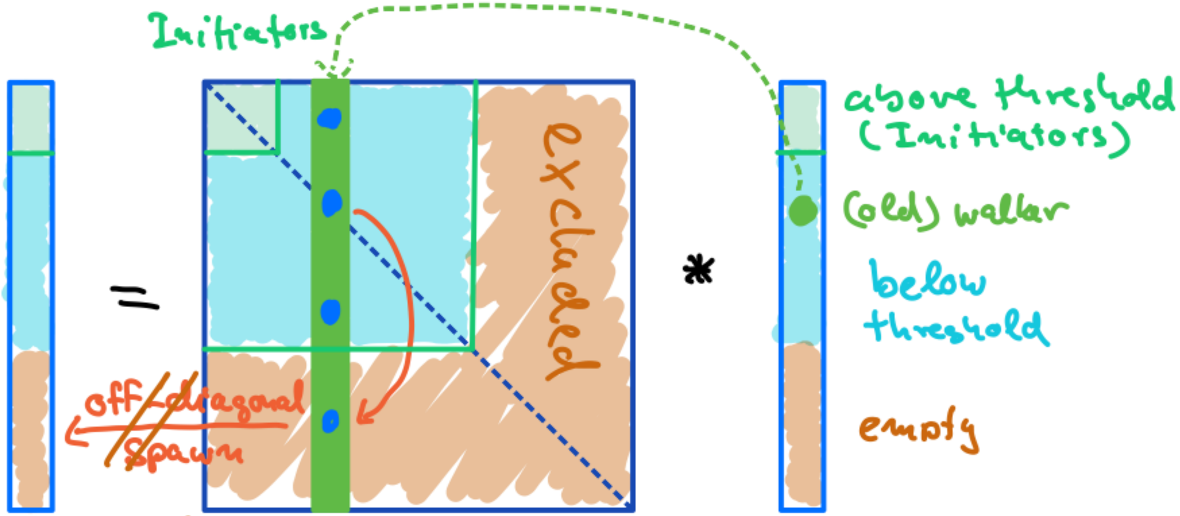




Stochastic sampling with initiator rule

$$\mathbf{c}^{(n+1)} = \mathbf{c}^{(n)} + \delta\tau \left(S^{(n)} \mathbf{1} - \mathbf{H} \right) \mathbf{c}^{(n)}$$

- The **initiator rule** restores coherence: Only configurations with above threshold population may spawn to unoccupied configurations



not allowed by initiator rule if spawn leads to unoccupied configuration

Completing the story: Population control

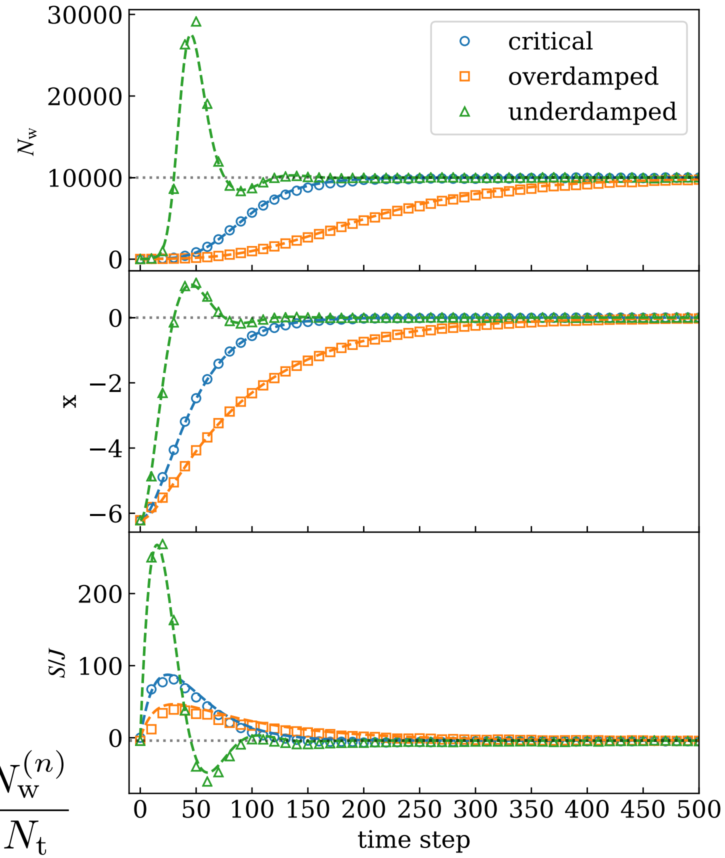
It is necessary to control the growth of the number of walkers: $N_{\mathrm{w}}^{(n)} = \|\mathbf{c}^{(n)}\|_1 = \sum_j |c_j^{(n)}|$

$$\mathbf{c}^{(n+1)} = \mathbf{c}^{(n)} + \delta\tau \left(S^{(n)}\mathbb{1} - \mathbf{H}\right)\mathbf{c}^{(n)}$$

$$S^{(n+1)} = S^{(n)} - \frac{\zeta}{\delta\tau}\ln\frac{N_{\mathrm{w}}^{(n+1)}}{N_{\mathrm{w}}^{(n)}} - \frac{\xi}{\delta\tau}\ln\frac{N_{\mathrm{w}}^{(n+1)}}{N_{\mathrm{t}}}$$

damping term opposes change in walker number

restoring force enforces target walker number
Yang, Pahl, Brand (2020)



The population dynamics maps to a damped harmonic oscillator for $x = \ln\frac{N_{\mathrm{w}}^{(n)}}{N_{\mathrm{t}}}$

Yang, Pahl, Brand, J. Chem. Phys. **153**, 174103 (2020)

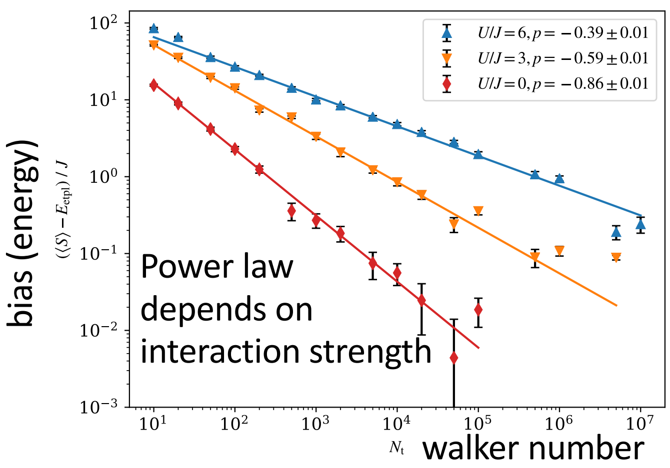
Kalos 1969
Hetherington 1984
Nightingale, Blöte 1986
Umrigar, Nightingale, Runge 1993
Vigor *et al.* 2015

A caveat: Population Control Bias

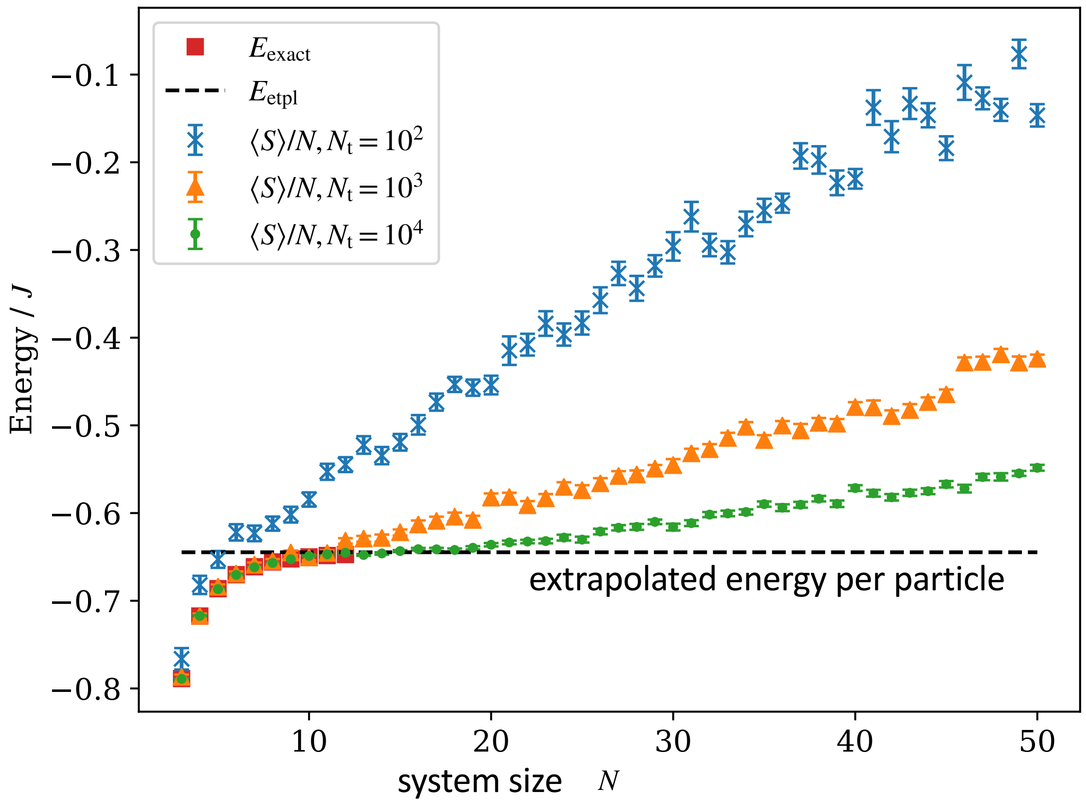
$$H = -J \sum_{\langle i,j,\rangle} \hat{a}_i^\dagger \hat{a}_j + U \sum_i \hat{n}_i(\hat{n}_i - 1)$$

Bose Hubbard model in real space

- Sign problem is absent (stoquastic Hamiltonian)
- Bias grows with system size
- Non-universal scaling with walker number



Mott insulator U/J = 6, N/M=1



Brand, Yang, Pahl, arXiv:2103.07800

A scalar model of population control

Consider time a continuous variable and write a **stochastic differential equation** for the walker number $N_W(t)$ and the shift $S(t)$:

exact energy

noise strength

Wiener noise

$$dN_\mathrm{w} = \left[S(t) - \tilde{E}\right] N_\mathrm{w}(t)\, dt - \mu N_\mathrm{w}(t)\, d\check{W}(t)$$

$$dS = -\frac{\zeta}{\delta\tau} d\ln N_w(t) - \frac{\xi}{\delta\tau^2} \ln\frac{N_w(t)}{N_\mathrm{t}}\, dt$$

A variable transformation and use of **Itô's lemma** allows us to identify the **population control bias:**

population control bias

$$x(t) = \ln\frac{N_\mathrm{w}(t)}{N_\mathrm{t}} \Longrightarrow dx = \left[S(t) - \tilde{E} - \frac{1}{2}\mu^2\right] dt - \mu\, d\check{W}(t) \Longrightarrow \langle S\rangle = \tilde{E} + \frac{1}{2}\mu^2$$

$$dS = -\frac{\zeta}{\delta\tau}\, dx - \frac{\xi}{\delta\tau^2} x(t)\, dt$$

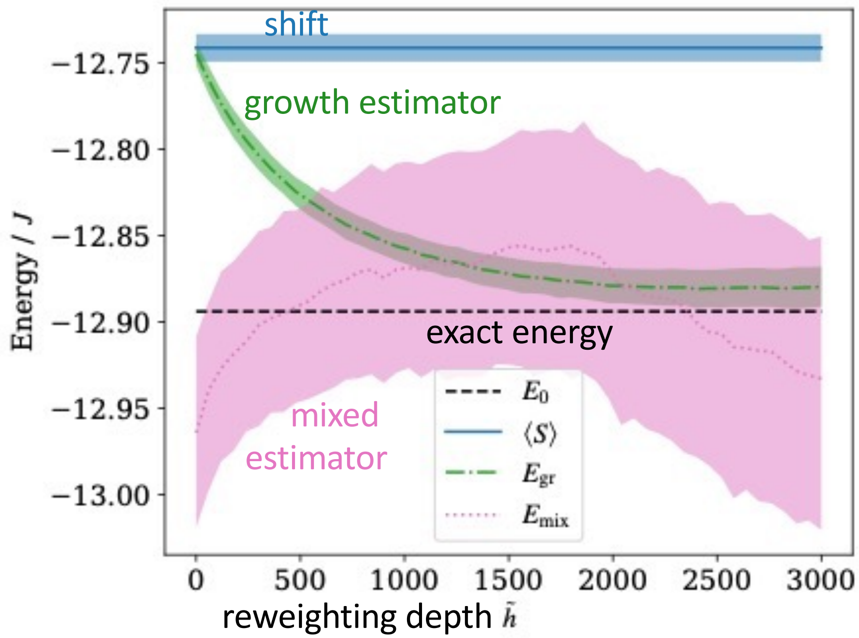
noisy damped harmonic oscillator

Brand, Yang, Pahl, arXiv:2103.07800

How to avoid the population control bias?

- Large walker numbers
- Importance sampling (but can worsen sign problem)
- Unbiased estimators via reweighting
  - Nightingale, Blöte (1986)
  - Umrigar, Nightingale, Runge (1993)
- Combination of importance sampling and reweighting
  - Ghanem, Lieberman, Alavi (2021)

Reweighting procedure



Brand, Yang, Pahl, arXiv:2103.07800

Outline

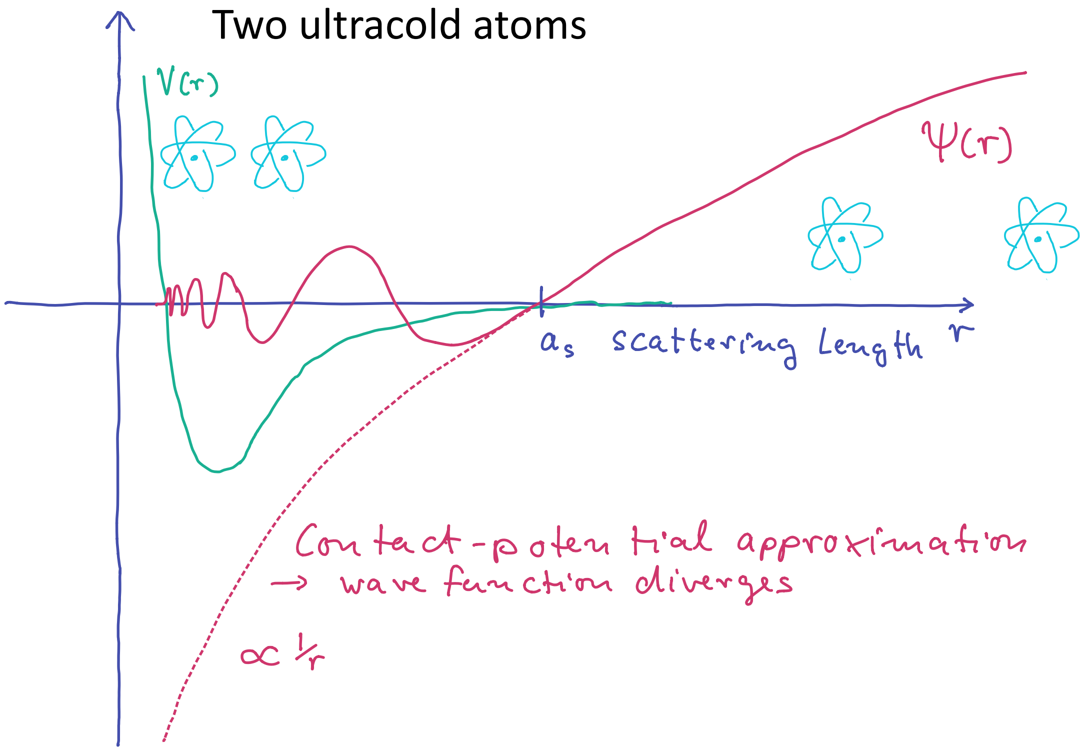
Full Configuration Interaction Quantum Monte Carlo

Population Control Bias

Transcorrelated Method

Mobile Spin Impurity in 1D Bose Gas

Transcorrelated Method:
How to deal with the wave function cusp?



Short-range interactions lead to divergent wave functions

Can be avoided with transcorrelated (similarity) transformation

Basis set expansion converges much faster

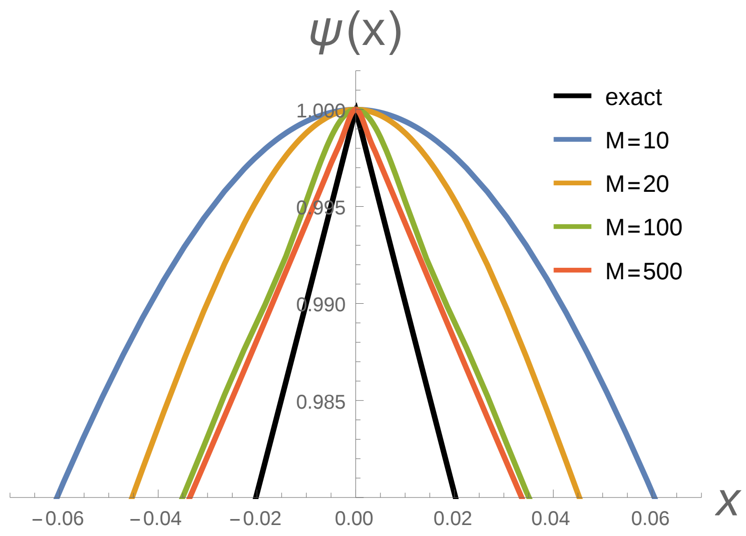
Jeszenszki, Luo, Alavi, Brand, Phys. Rev. A (2018); Phys. Rev. Research (2020)

Pseudopotential Hamiltonian (1D)

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2} + \sum_{j=1}^{N} V(x_j) - \frac{2\hbar^2}{ma}\sum_{\langle i,j\rangle}\delta(x_i - x_j)$$

The delta potential produces cusp in wave function (Bethe-Peierls boundary condition)

Approximating the cusp with a product of *M* plane waves.



Slow convergence

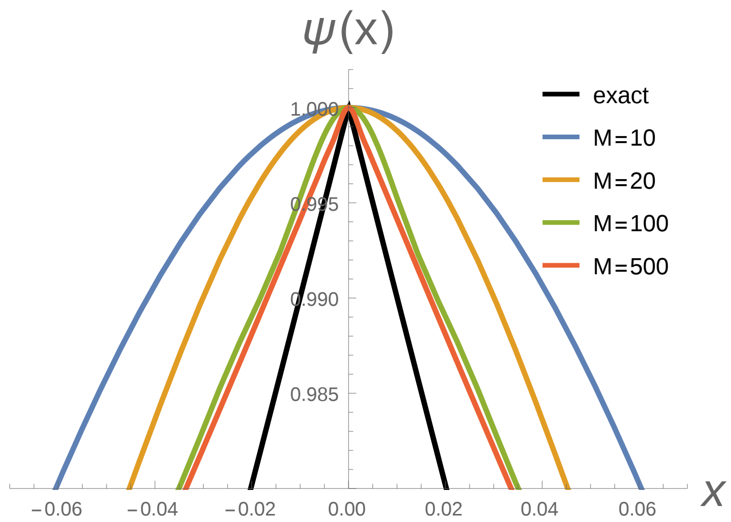
Compute the ground state energy for spin-1/2 fermions by exact diagonalisation expansion, i.e. in a basis of Slater determinants (Fock states) from *M* orbitals.

Harmonic oscillator basis (Grining et al. *NJP* (2015)):
$$E - E_{\text{exact}} \sim \frac{1}{\sqrt{M}}$$

Plane wave basis:
$$E - E_{\text{exact}} \sim \frac{1}{M}$$

Renormalised coupling constant:
$$E - E_{\text{exact}} \sim \frac{1}{M^2}$$

Transcorrelated:
$$E - E_{\text{exact}} \sim \frac{1}{M^3}$$



Jeszenszki, Luo, Alavi, Brand, Phys. Rev. A (2018)

Transcorrelated approach

$$\Psi(x_1, \ldots, x_N) = e^{\tau}\Phi(x_1, \ldots, x_N)$$

$$\tau = \sum_{ij} u(|x_i - x_j|)$$

e^{τ} - Jastrow factor – short-range correlation, the cusp

Φ - smooth function – carries long-range correlations

$$H\Psi = E\Psi$$

$$e^{-\tau}He^{\tau}\Phi = E\Phi$$

Similarity transformation yields *transcorrelated* Hamiltonian with identical spectrum

$$\tilde{H} = e^{-\tau}He^{\tau}$$

Boys, Handy (1969)
Luo, Alavi (2018)

The transcorrelated Hamiltonian

Has a simple explicit form:

$$\tilde{H} = e^{-\tau} H e^{\tau}$$
$$= H - \frac{\hbar^2}{m} \sum_i \left[\frac{1}{2} \partial_{ii}\tau + \partial_i \tau \partial_i + \frac{1}{2} (\partial_i \tau)^2 \right]$$

Can also be conveniently written in 2nd quantisation.

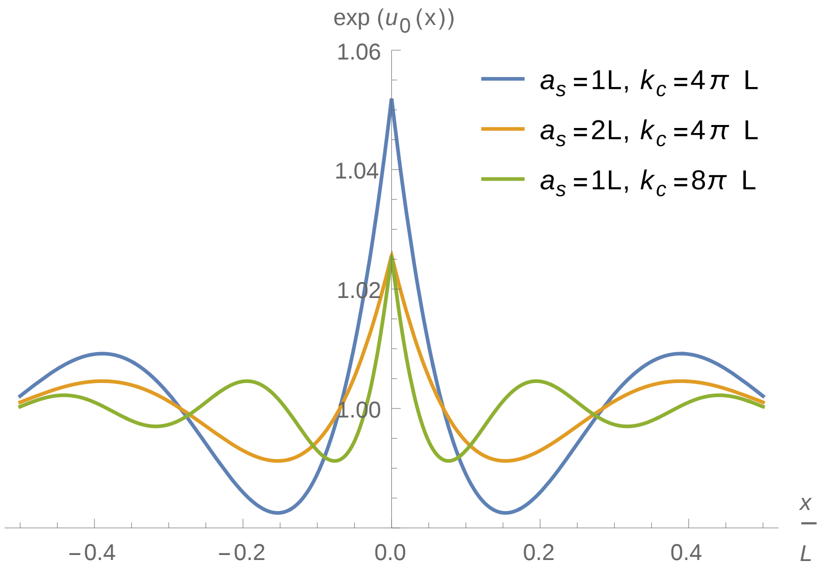
- It is not hermitian (but real eigenvalues)
- Is less singular (delta function is removed)
- Has 2-body and 3-body terms (can be approximated or neglected in dilute limit)

The correlation factor

$$\Psi(x_1,\ldots,x_N) = e^{\tau}\Phi(x_1,\ldots,x_N) \qquad \tau = \sum_{ij} u(|x_i - x_j|)$$

For Ψ to satisfy Bethe-Peierls boundary conditions, *u* also needs to have a cusp. We choose it to have a simple Fourier transform:

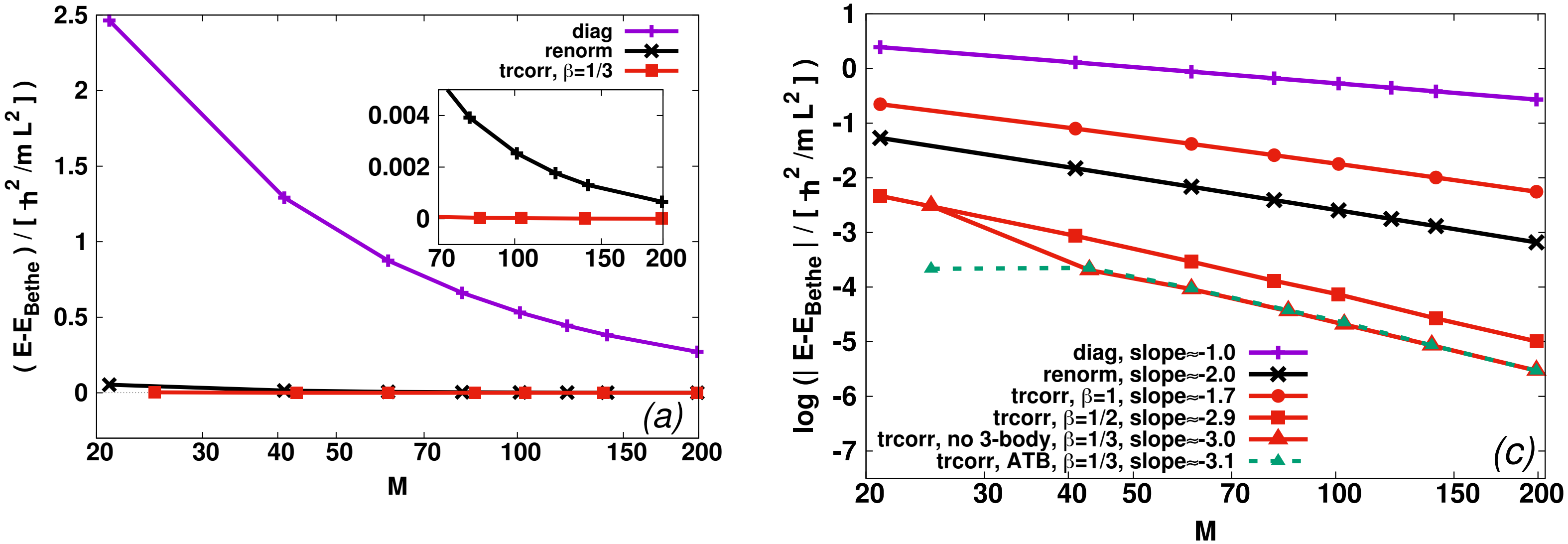
$$\tilde{u}(k) = \begin{cases} \frac{2}{ak^2} & \text{if } |k| \geq k_c \ , \\ 0 & \text{if } |k| < k_c \ , \end{cases}$$



Jeszenszki, Luo, Alavi, Brand, Phys. Rev. A (2018)

Energy convergence in a truncated Fock basis (plane waves)

Three particles with attractive interactions (a=10L)
Spin-1/2 fermions, $N_\uparrow = 2$, $N_\downarrow = 1$



$$\tilde{u}(k) = \begin{cases} \frac{2}{ak^2} & \text{if } |k| \geq k_c \ , \\ 0 & \text{if } |k| < k_c \ , \end{cases} \qquad k_c = \beta k_{\max} = \beta \frac{\pi}{L} M$$

Jeszenszki, Luo, Alavi, Brand, Phys. Rev. A (2018)

Outline

Full Configuration Interaction Quantum Monte Carlo

Population Control Bias

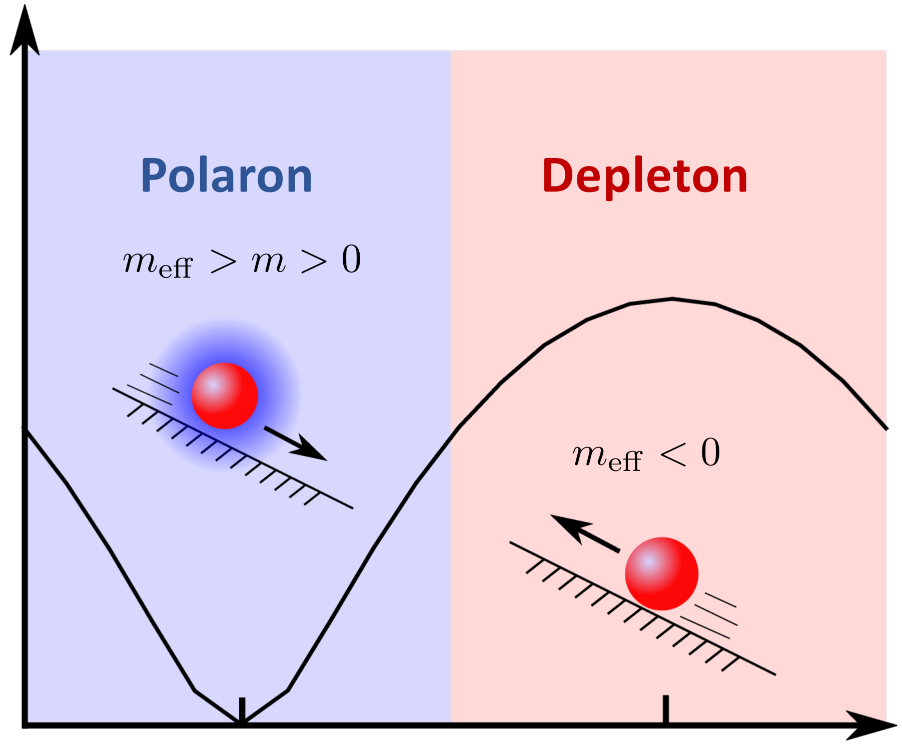
Transcorrelated Method

Mobile Spin Impurity in 1D Bose Gas

Spin impurity of a one-dimensional Bose gas

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + g_{\mathrm{BB}}\sum_{i<j}\delta(x_i - x_j) \quad \text{Bose gas}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_{\mathrm{I}}^2} + g_{\mathrm{IB}}\sum_{i}\delta(x_i - x_{\mathrm{I}}) \quad \text{Impurity}$$



Spin impurity in a 1D Bose gas

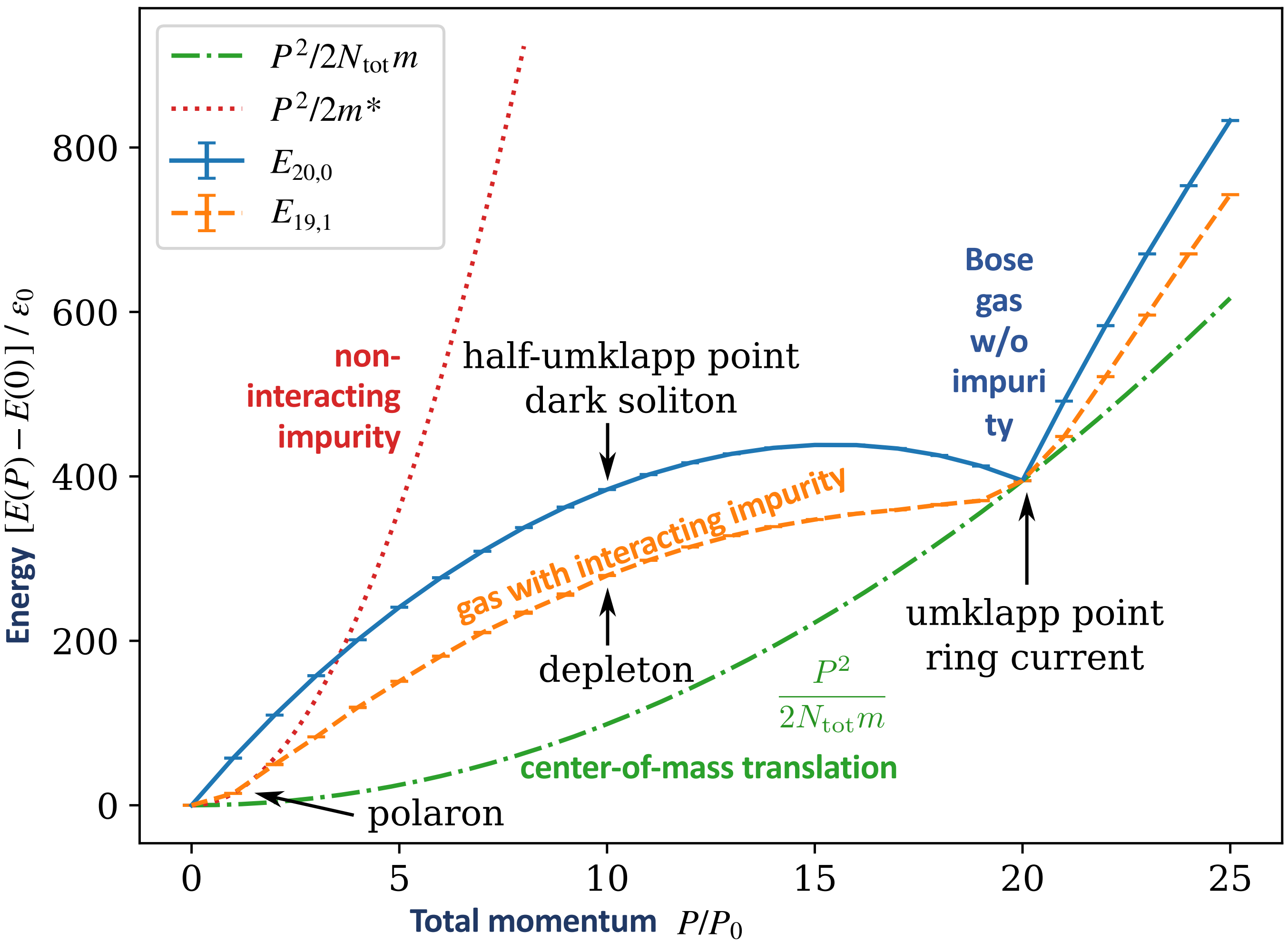
Finite system with N=20 particles and periodic boundary conditions (quantum ring)

Bose gas

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + g_{\mathrm{BB}}\sum_{i<j}\delta(x_i - x_j)$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_{\mathrm{I}}^2} + g_{\mathrm{IB}}\sum_{i}\delta(x_i - x_{\mathrm{I}})$$

Impurity

Yrast excitation spectrum for N=20 particles

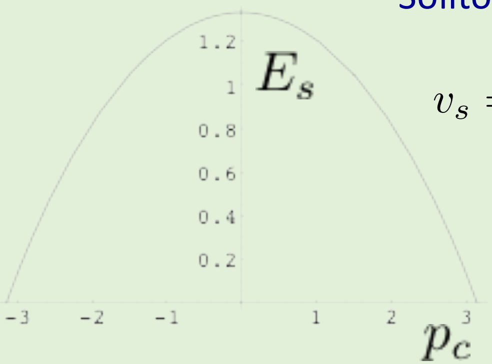


1D Bose gas without impurity:
What connects dark solitons to yrast dispersion?

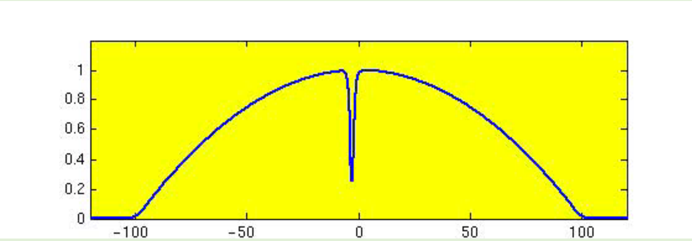
Mean field theory (Gross Pitaevskii)

Dark/grey solitons are known as time-dependent solutions of the Gross-Pitaevskii mean field theory

Soliton velocity:

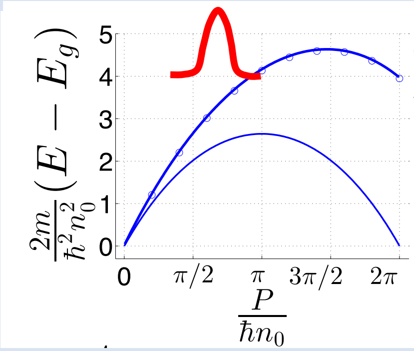


$$v_s = \frac{dE_s}{dp_c}$$



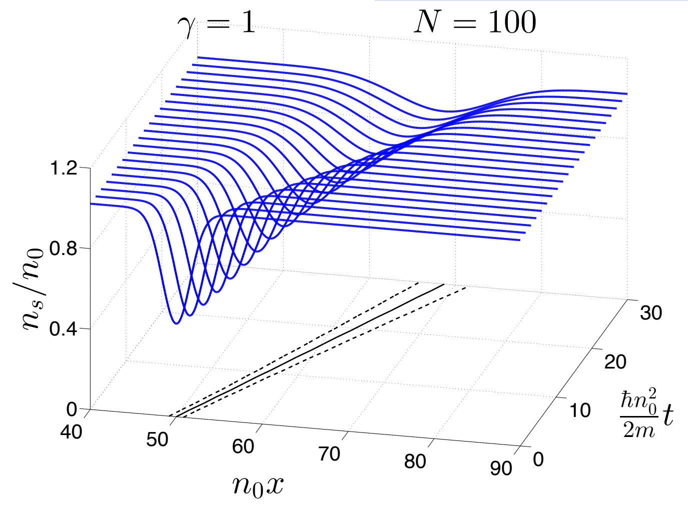
Movie credits: Nick Parker

Full quantum theory / Lieb-Liniger model



Circles: finite system (ring), *N* = 10, γ=1

Thermodynamic limit, *N* = ∞, γ=1



Exact time evolution of a "wave packet" of yrast states

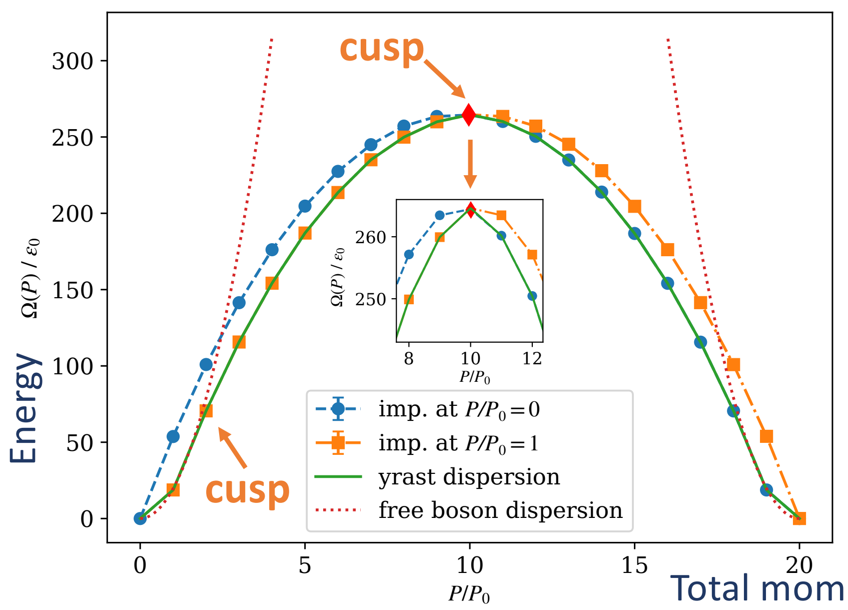
See also:
Kanamoto, Carr, Ueda 2010
Astrakharchik, Pitaevskii 2012
Fialko, Delattre, Brand, Kolovsky 2012
Sato et al. 2012
Syrwiv, Sacha 2015

Shamailov, Brand Phys. Rev. A (2019)

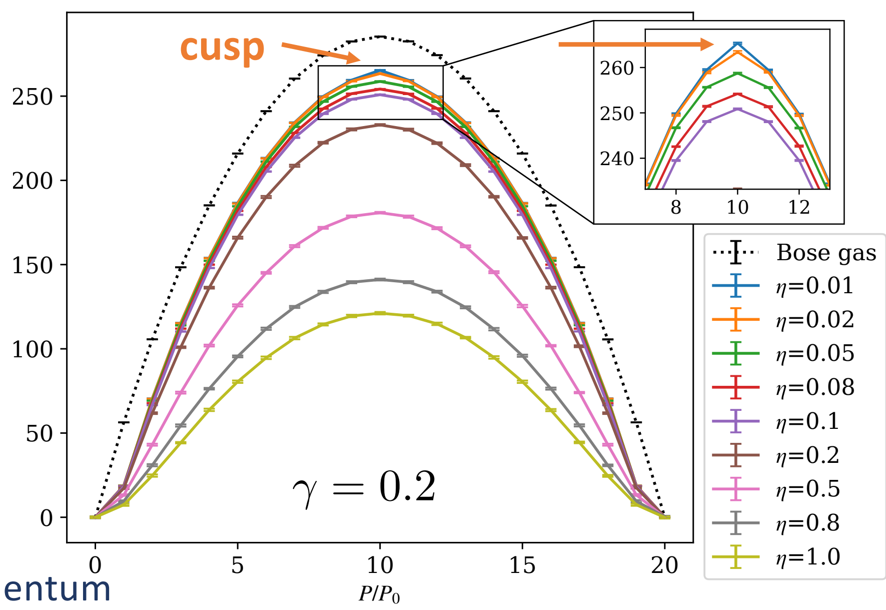
Bose gas with impurity: Yrast dispersion

Subtract centre-of-mass kinetic energy: $\Omega(P) = E(P) - E(0) - \dfrac{P^2}{2N_{\text{tot}} m}$

Non-interacting impurity



Interacting impurity



Total momentum

$$\gamma = \frac{m g_{\mathrm{BB}}}{\hbar^2 n}$$

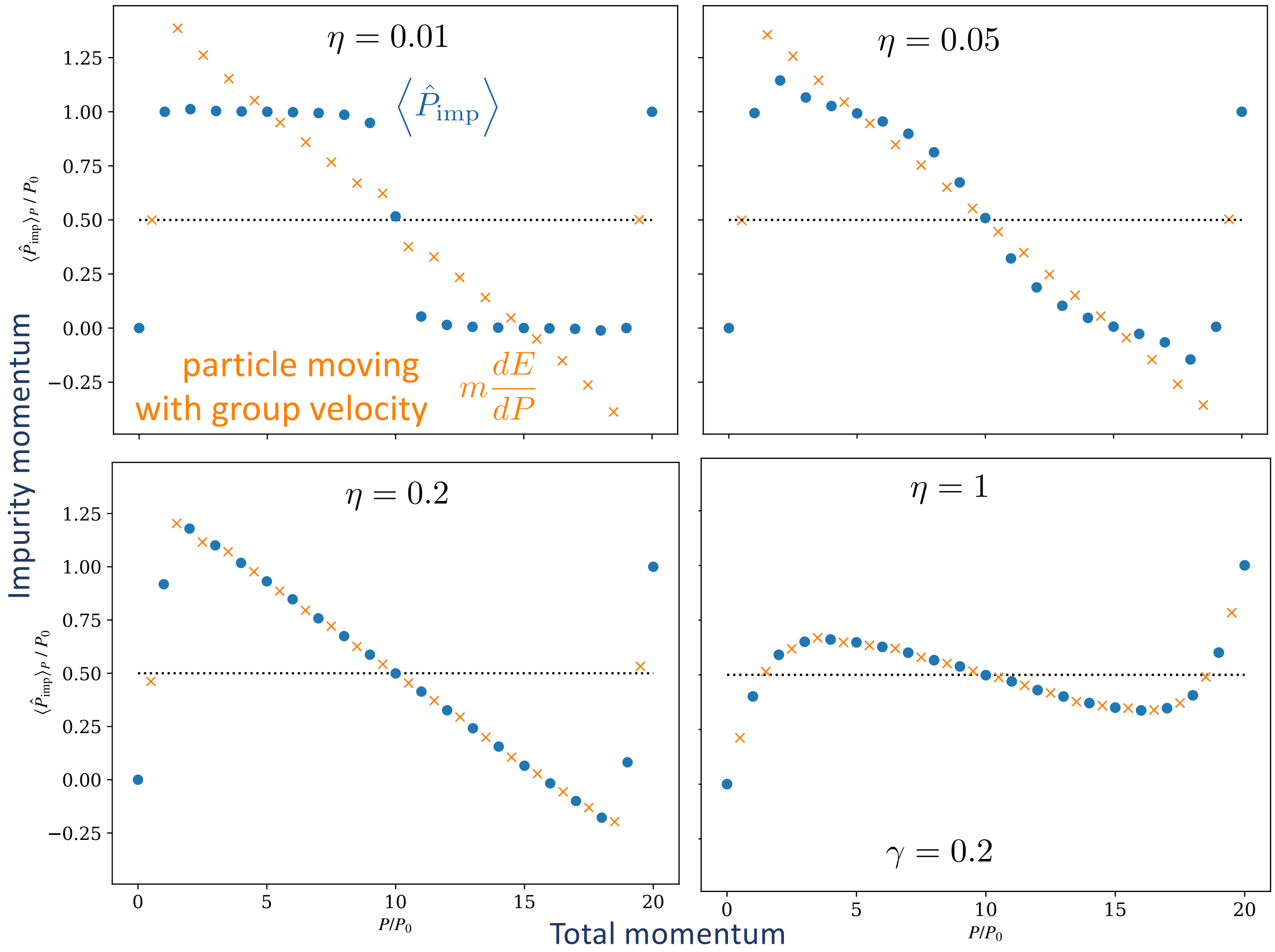
$$\eta = \frac{m g_{\mathrm{IB}}}{\hbar^2 n}$$

Soliton and impurity motion synchronises for sufficiently strong interactions

According to Hellman-Feynman theorem (thermodynamic limit):

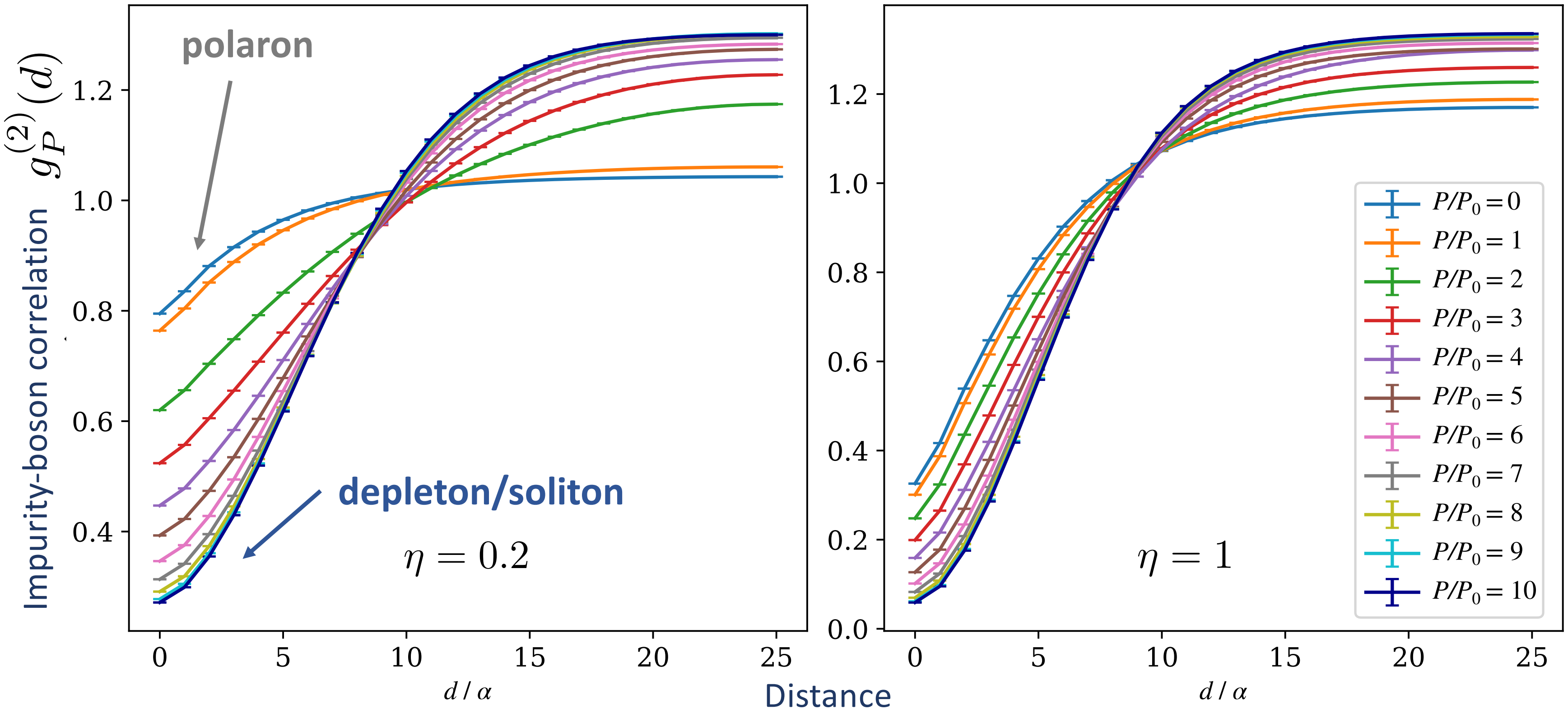
$$\left\langle \hat{P}_{\mathrm{imp}} \right\rangle = m\frac{dE}{dP}$$

Knap *et al.* (2014)

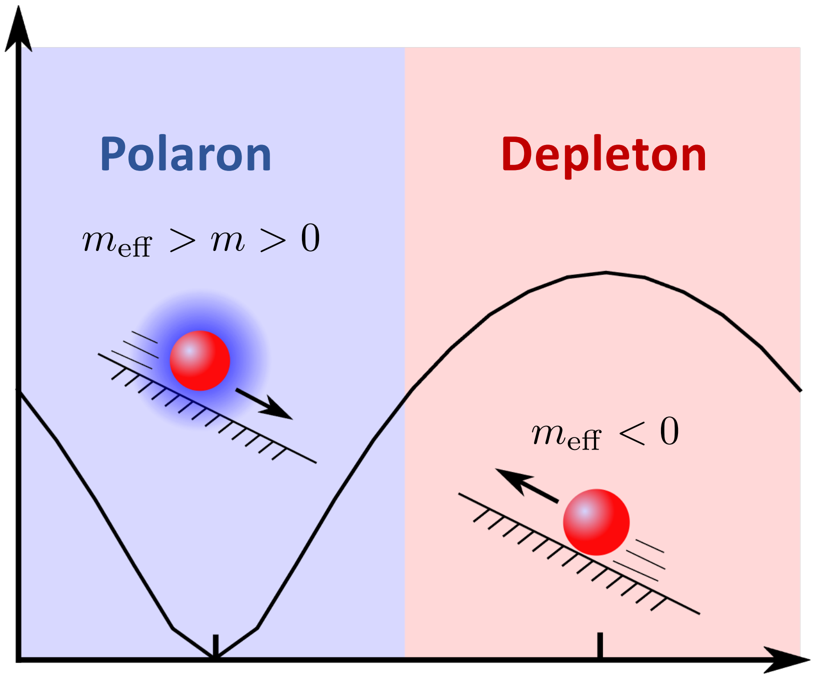


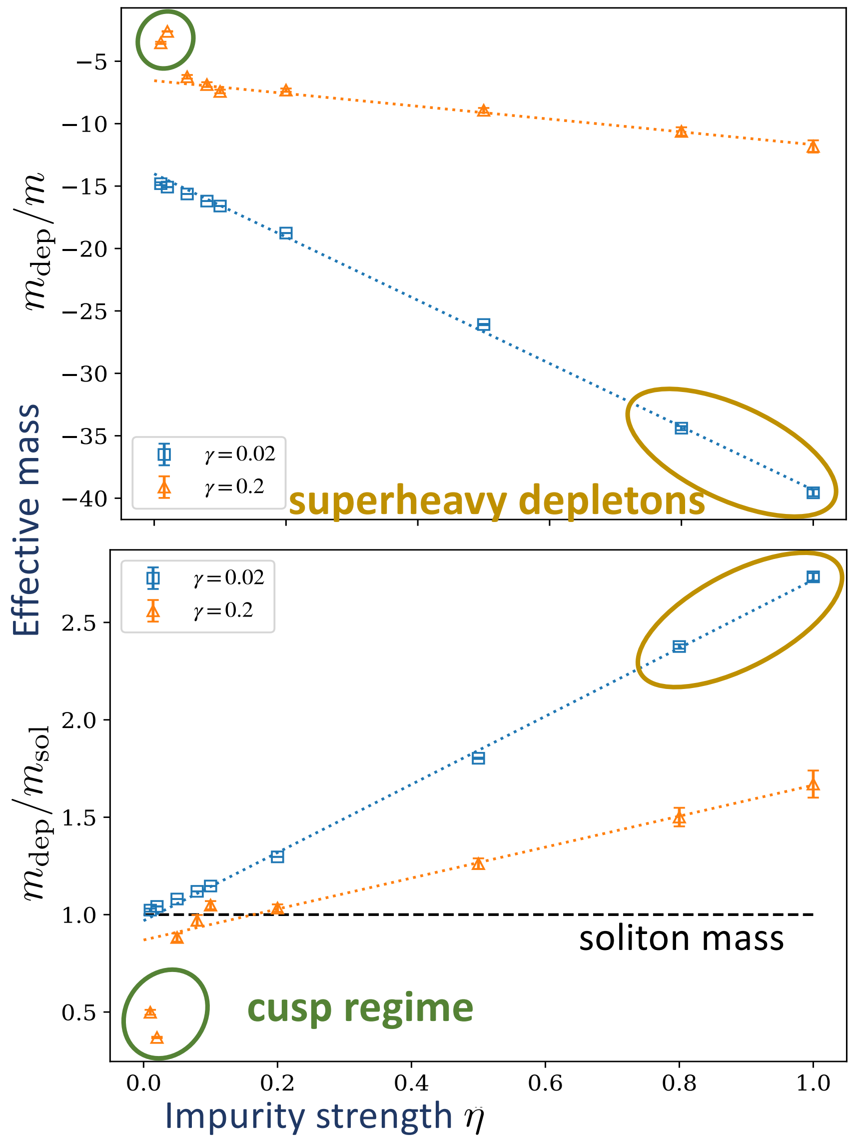
Impurity-boson correlation function

$$g_P^{(2)}(d) = \frac{L}{N}\int_0^L \langle \Psi_P|\hat{\psi}^\dagger(x+d)\hat{\psi}^\dagger_{\mathrm{imp}}(x)\hat{\psi}_{\mathrm{imp}}(x)\hat{\psi}(x+d)|\Psi_P\rangle \, \mathrm{d}x$$



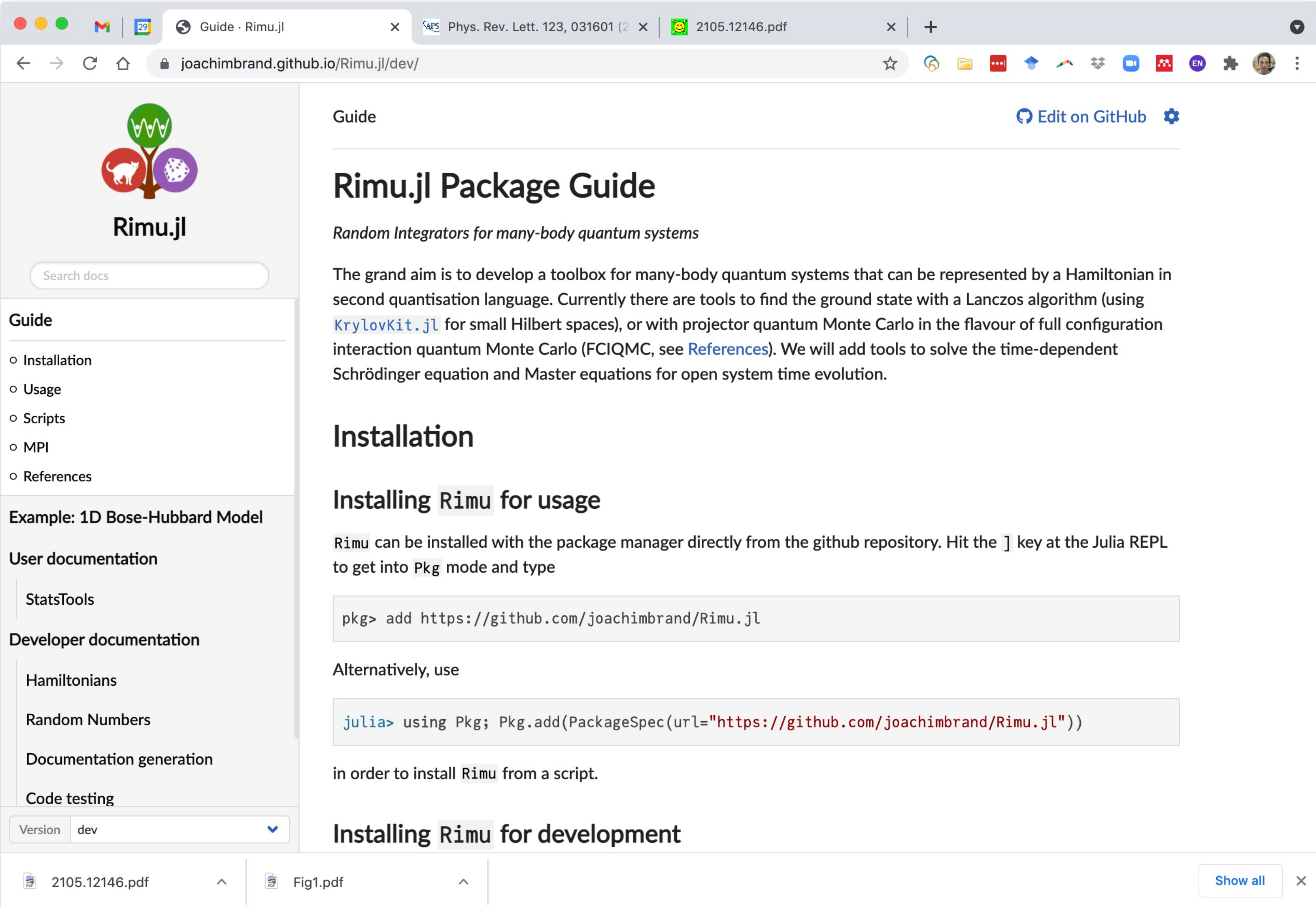
Depleton effective mass





Summary / Takeaways

- FCIQMC allows us to treat arbitrary (matrix) Hamiltonian
  Hence, it allows us to find yrast spectrum (lowest energy states of momentum-conserving Hamiltonian)
- The transcorrelated method makes for an efficient finite matrix representation of quantum particles interacting with short-range interactions



Open-source package
Developed since 2016

So far:

- Bosons, fermions
- Hubbard, Transcorrelated
- Exact diagonalization
- FCIQMC

Future:

- Time evolution
- Spinor gases, mixtures
- Open quantum systems
- Spin-orbit coupling

Thanks

Massey:

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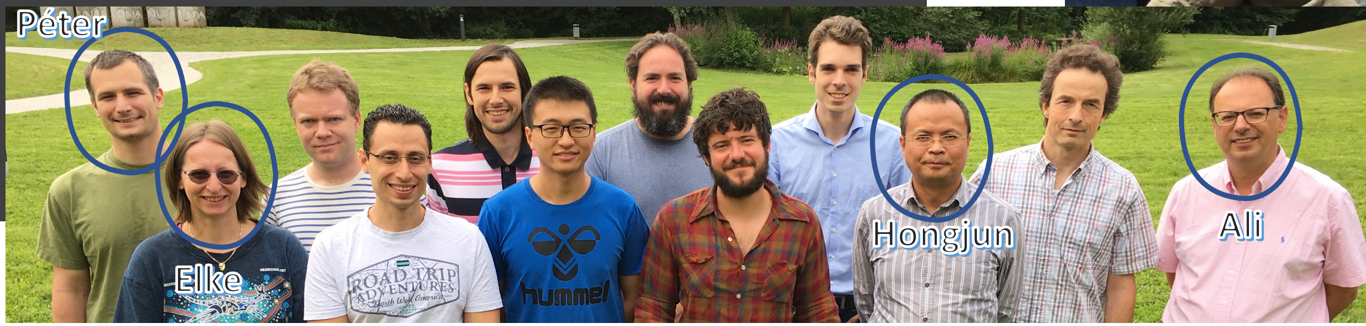
- Chris Bradly
- Péter Jeszenzki
- Ulrich Ebling
- Sophie Shamailov

- Auckland:
  - Elke Pahl
- Stuttgart:
  - Ali Alvi
  - Hongjun Luo



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