Monte Carlo for Fermi Gases

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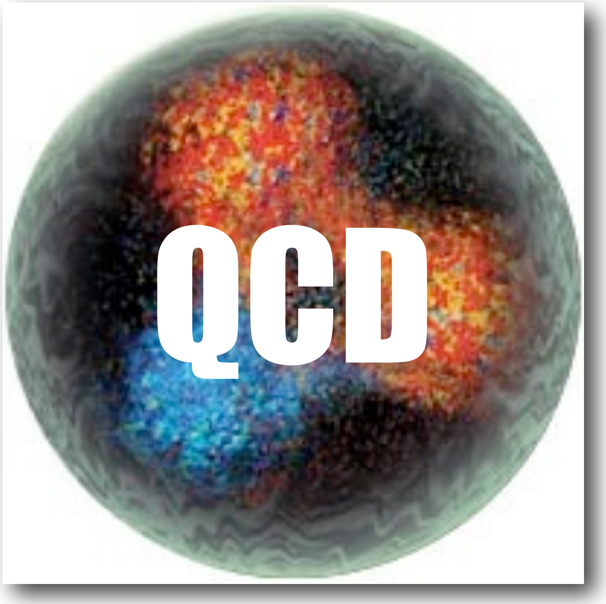
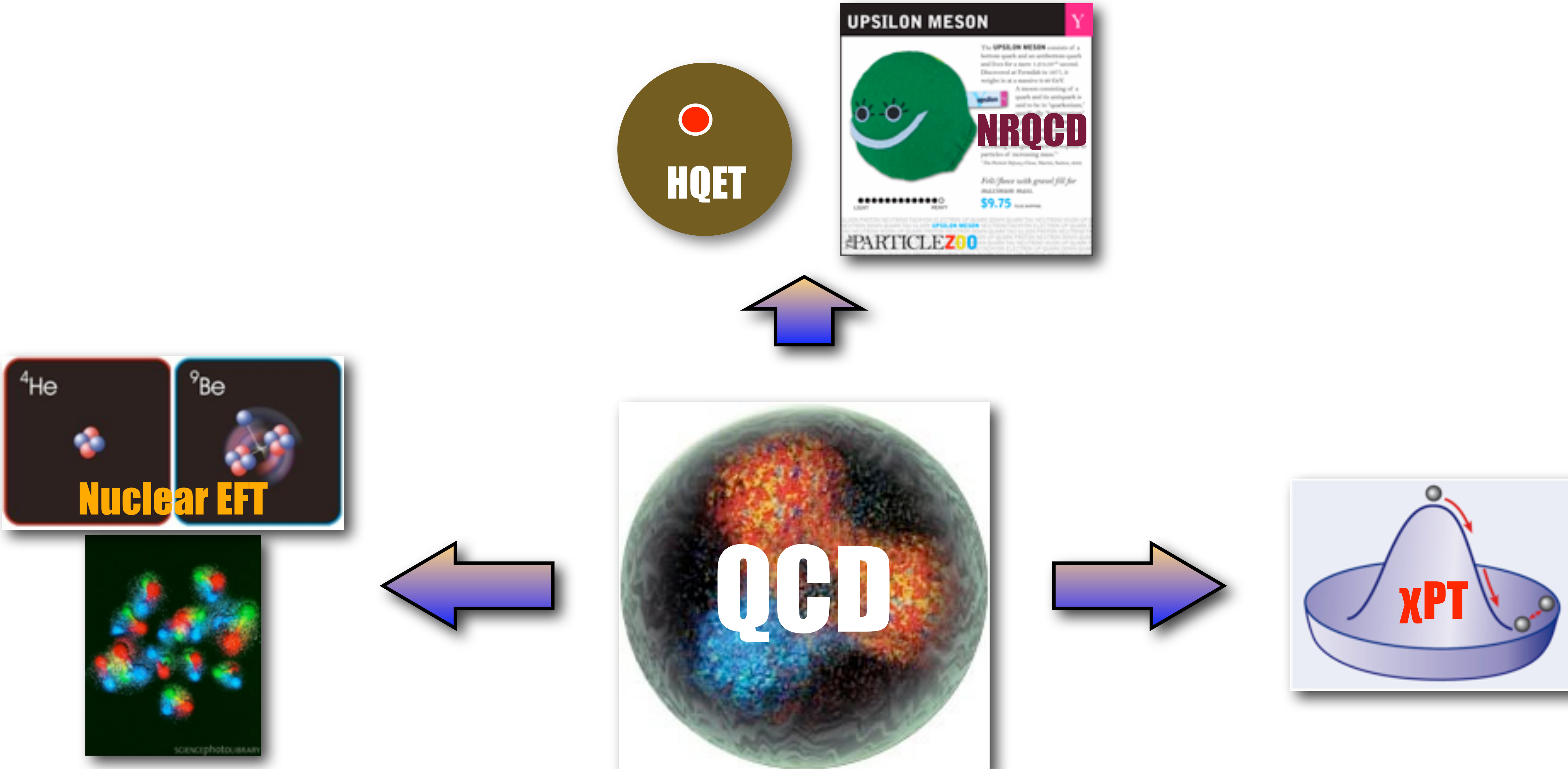
in collaboration with
Olga Goulko (DAMTP)

Strong interactions



Strong interactions



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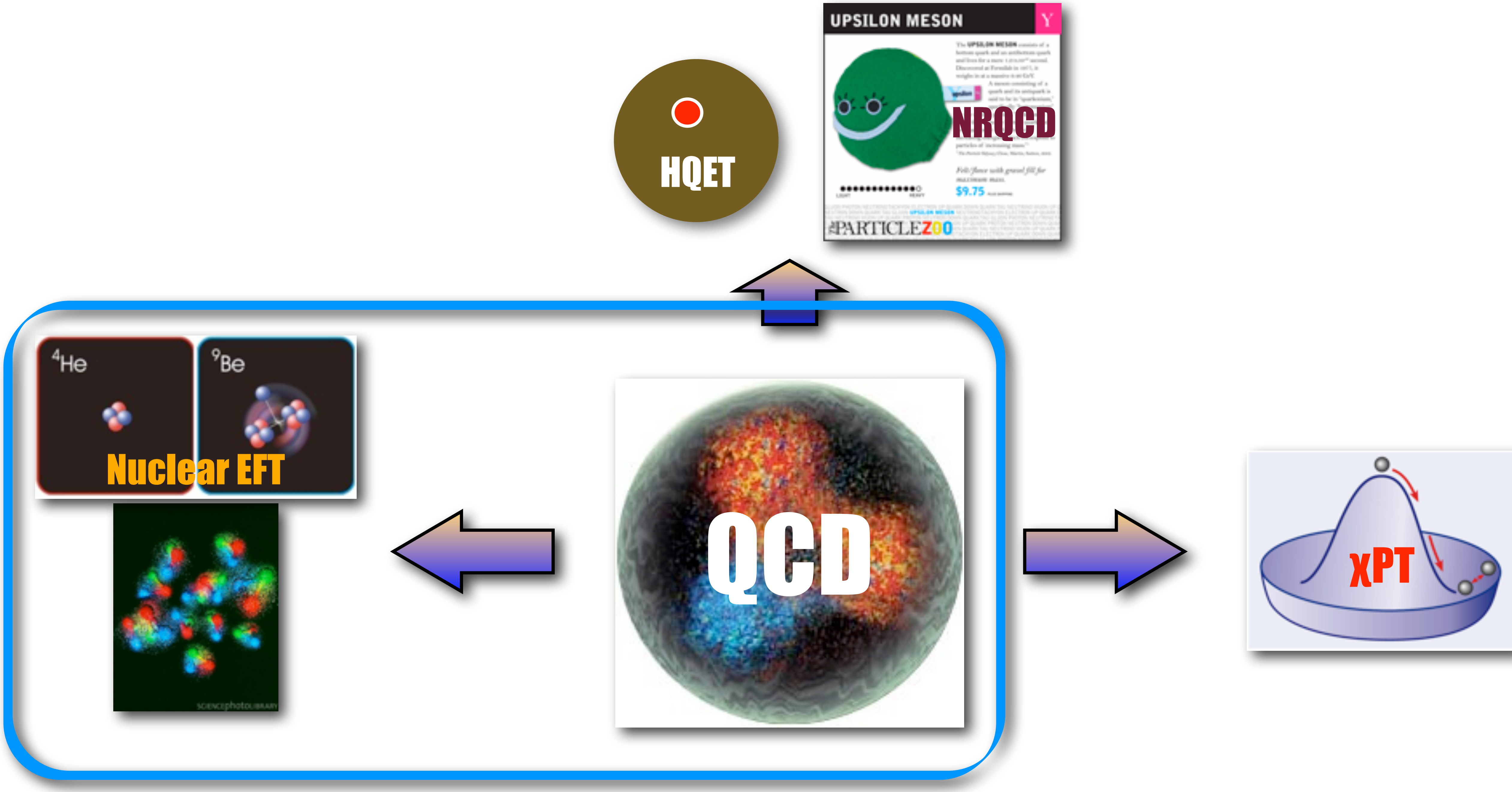
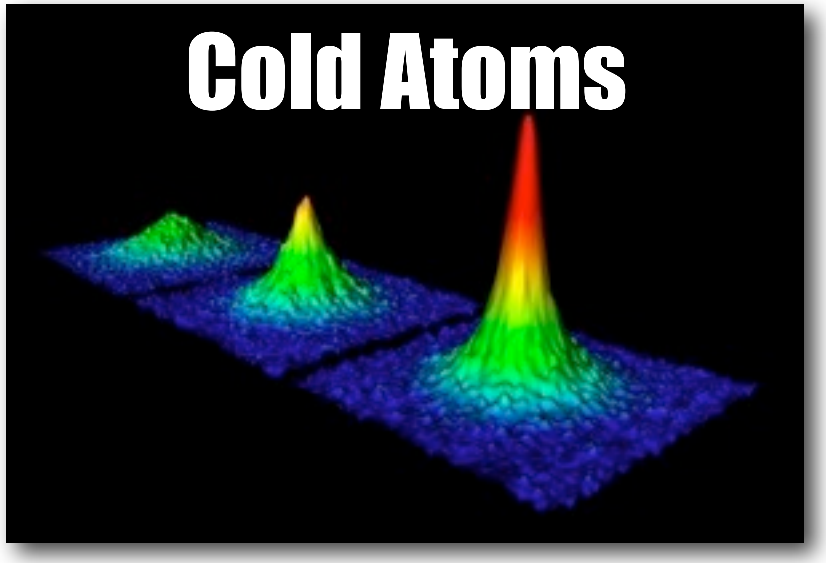


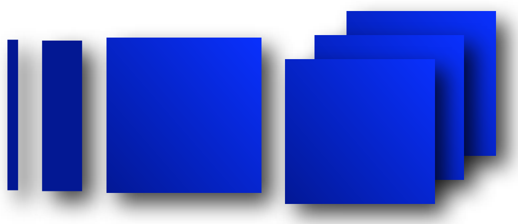
Monte Carlo calculations

Tunable universes



Tunable universes

Dimensionality



Coupling

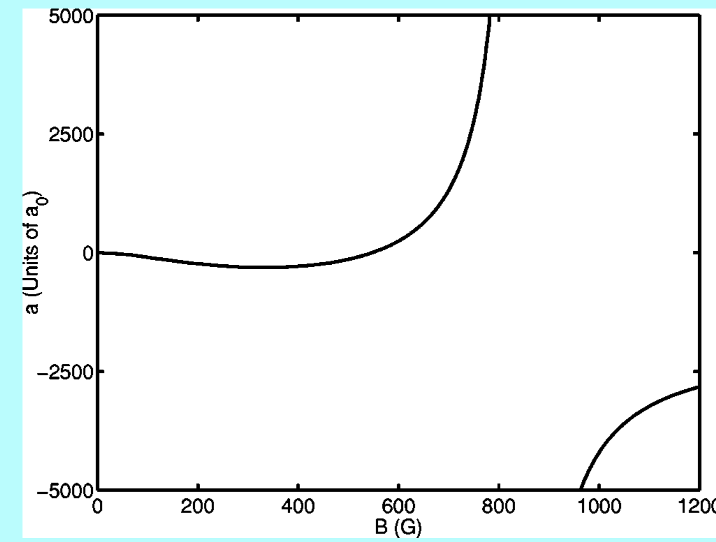
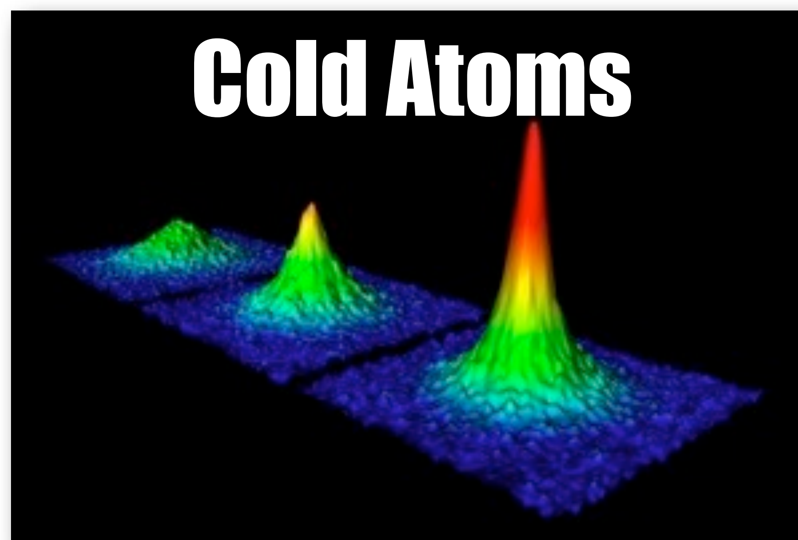
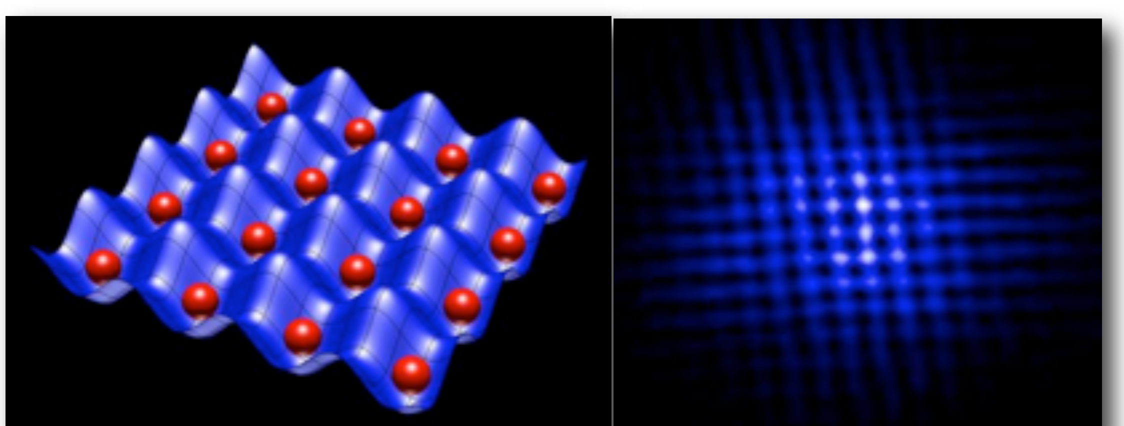


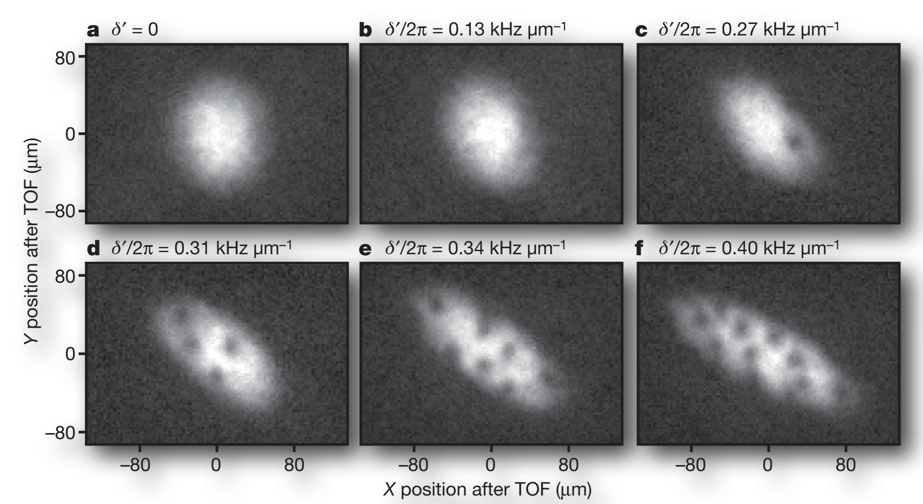
FIG. 1. Scattering length as a function of magnetic field, for the $(f, m_f) = (1/2, -1/2)$ and $(1/2, 1/2)$ mixed spin channel of ^{6}Li.



Lattice models



Gauge fields



Approaches

- ✤ Design your own universe
- ✤ Atomic simulations of CM, Nuclear, HE phenomena
- ✤ Role of nonperturbative calculations
    - ✦ Bridge the gap
    - ✦ "Fundamental constants" (e.g. unitary Fermi gas)
    - ✦ Discover a solution to fermion algorithm problem

Conundrum

- ✤ Nonperturbative problems solvable numerically
- ✤ Efficient algorithms for bosonic systems
- ✤ Fermions matter since matter's fermionic
- ✤ Why is life so difficult? ➙
- ✤ Is there a general solution waiting to be discovered?

Lattice Monte Carlo in a nutshell

Gluonic expectation values

$$\begin{aligned}\langle \Theta \rangle &= \frac{1}{Z}\int [d\psi][d\bar{\psi}][dU]\,\Theta[U]\,e^{-S_g[U]-\bar{\psi}Q[U]\psi} \\ &= \frac{1}{Z}\int [dU]\,\Theta[U]\,\det Q[U]\,e^{-S_g[U]}\end{aligned}$$

Fermionic expectation values

$$\langle \bar{\psi}\Gamma\psi \rangle = \int [dU]\,\frac{\delta}{\delta\bar{\zeta}}\Gamma\frac{\delta}{\delta\zeta}\,e^{-\bar{\zeta}Q^{-1}[U]\zeta}\,\det Q[U]e^{-S_g[U]}\Big|_{\zeta,\bar{\zeta}\to 0}$$

Lattice Monte Carlo in a nutshell

Gluonic expectation values

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Probability weight

Fermionic expectation values

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Determinant in probability weight difficult

1) Requires nonlocal updating; 2) Matrix becomes singular

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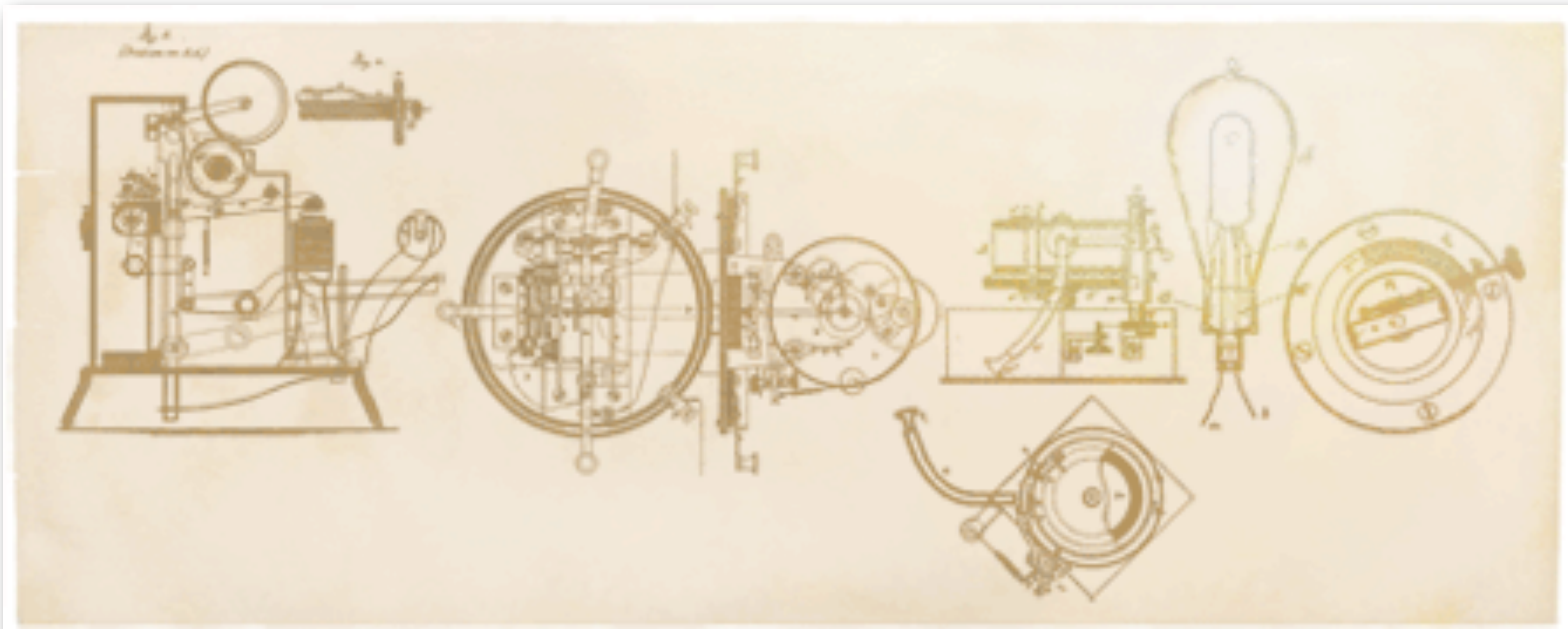
Yesterday's Google Doodle



"Genius is 1% inspiration and 99% perspiration"

-- Thomas Edison (born 11 February 1847)

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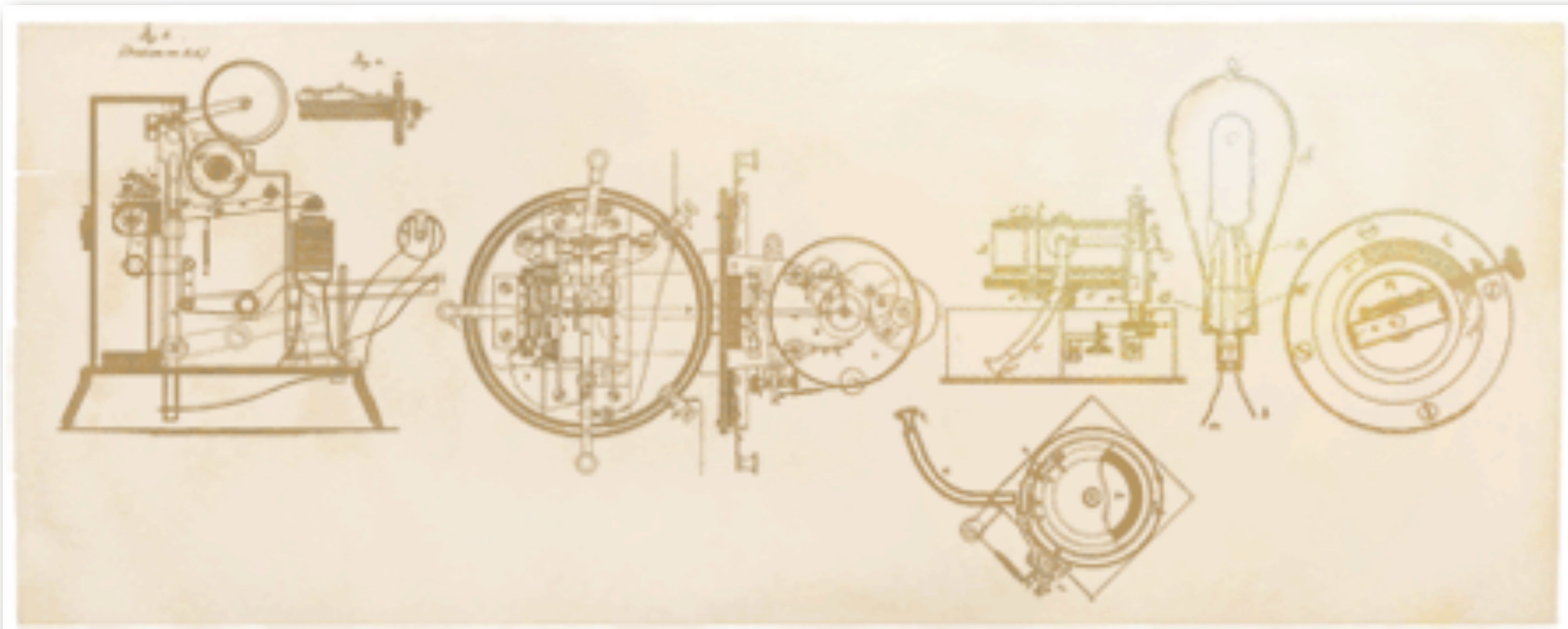

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"All work and no play makes Jack a dull boy."

-- Jack Nicholson, as he loses his sanity in *The Shining*

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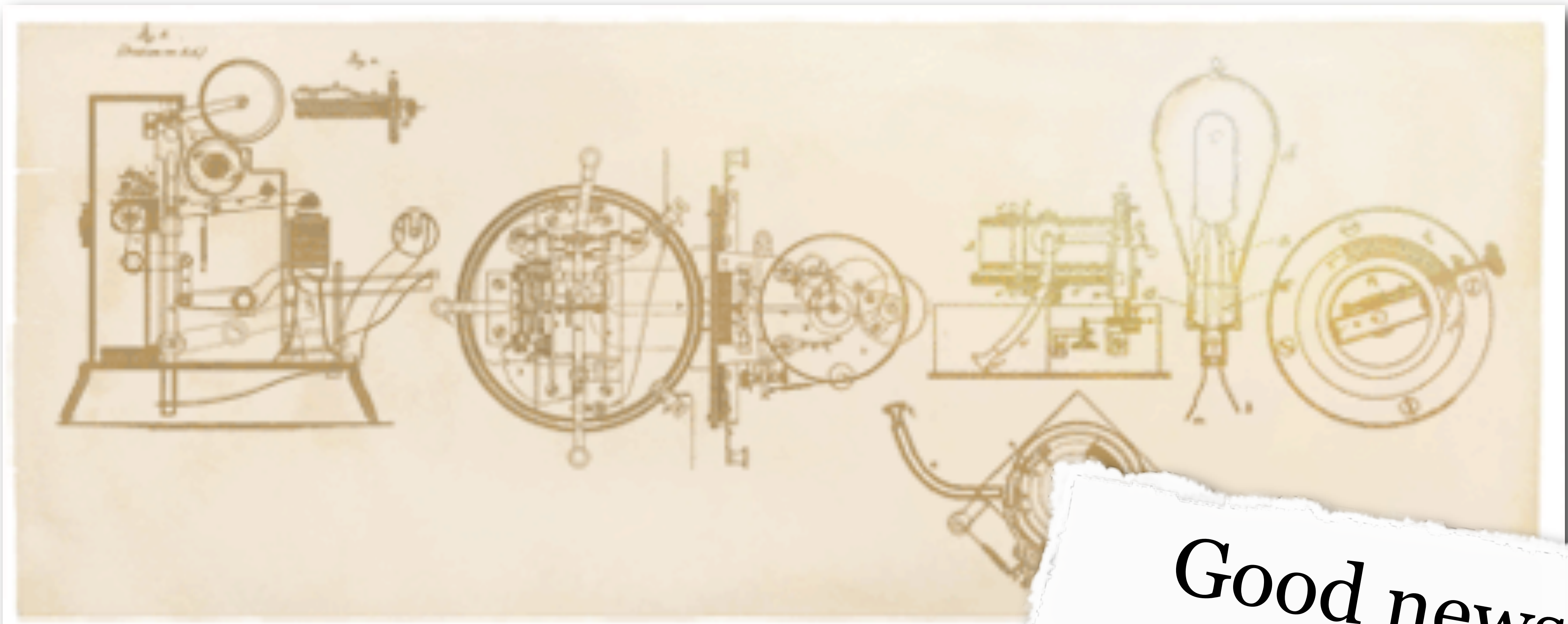

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Good news:

1) Jack was a novelist

2) Jack didn’t attend stimulating workshops

Outline

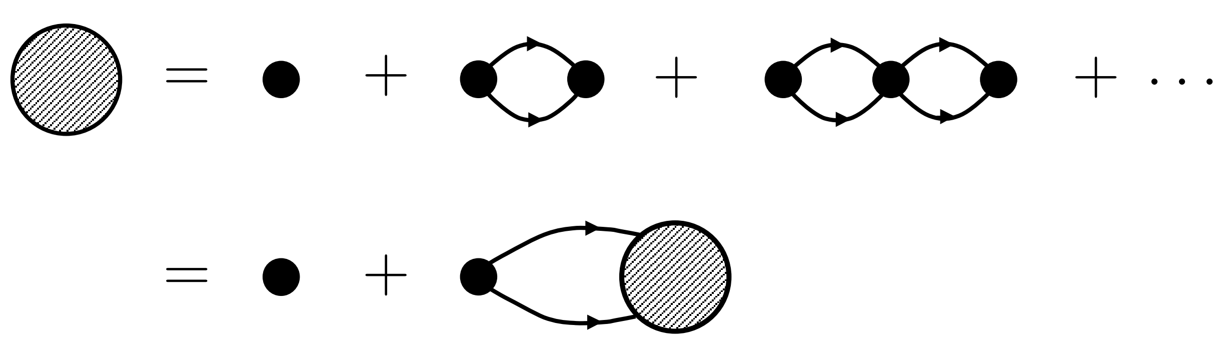
- “Unitary Fermi Gas” (2-component gas of nonrelativistic fermions interacting with divergent scattering length, in 3 dimensions, *i.e.* at the BEC-BCS crossover)
- Diagrammatic Determinant Monte Carlo
- Results for critical temperature, contact density
- Outlook
- Note J. Carlson’s talk after coffee

Dilute Fermi Gas

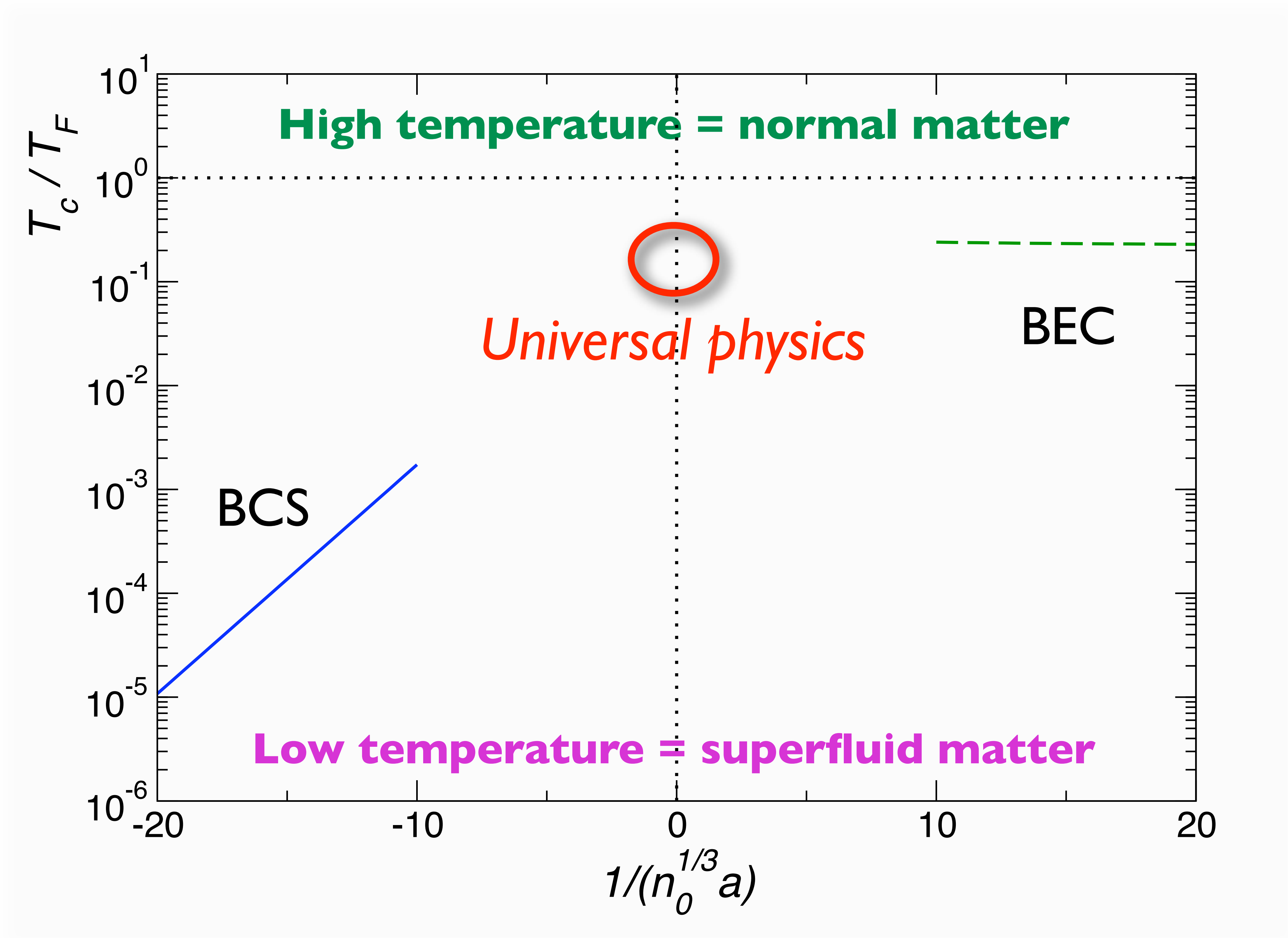
- Physical interactions: Van der Waals, short range r_{VdW}
- Dilute, $(V/n)^{1/3} \gg r_{\mathrm{VdW}}$, implies details of potential are negligible

$$\mathcal{H} = -\frac{1}{2m}\sum_{\sigma}\bar{\psi}_{\sigma}\nabla^{2}\psi_{\sigma} - \frac{g^{2}}{2}\left(\bar{\psi}_{1}\bar{\psi}_{2}\psi_{2}\psi_{1}\right)$$

- 2-body scattering calculation matches coupling to physical scattering length



Phase diagram

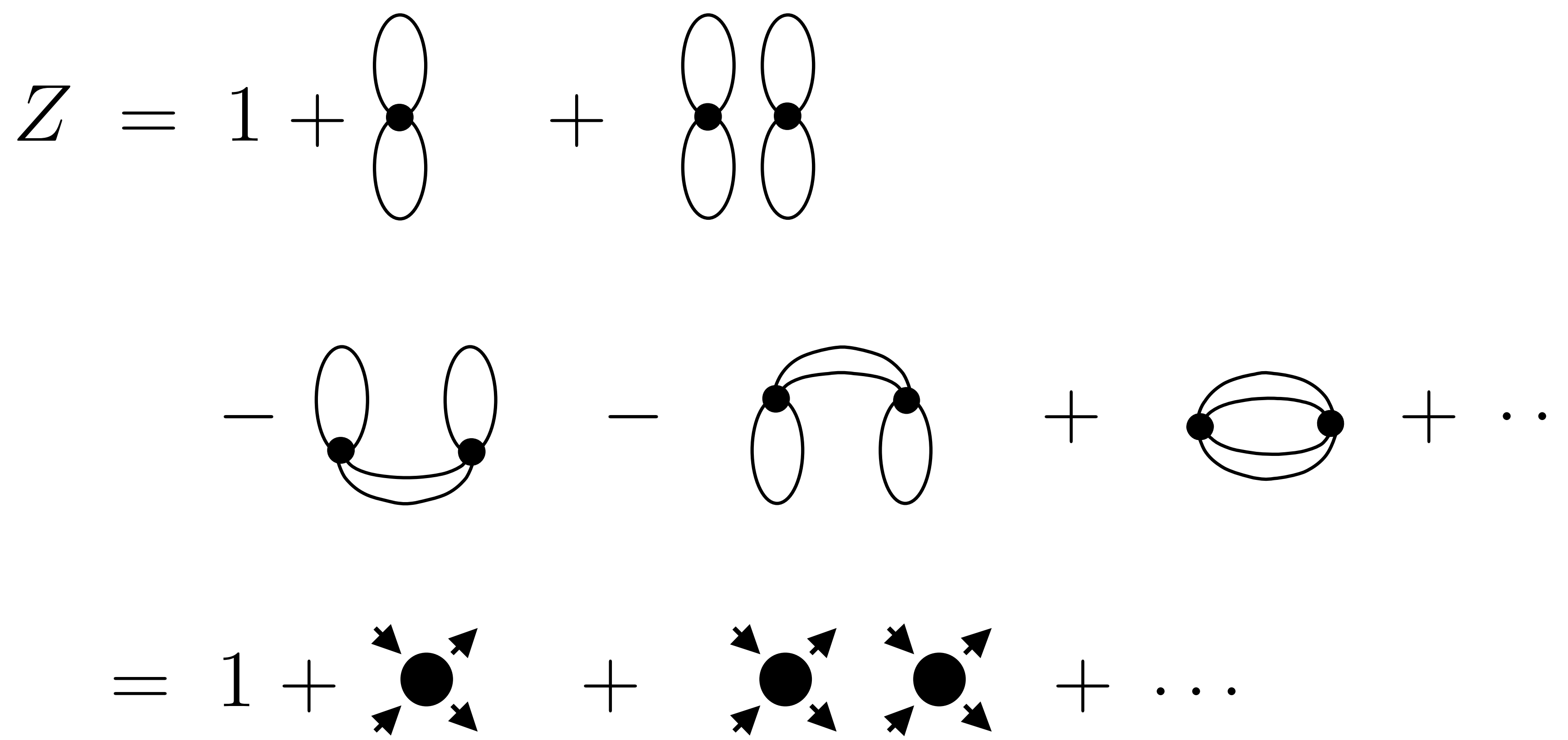


Diagrammatic Determinant M.C.

- Rubtsov, Savkin, Lichtenstein: sampling of diagrams, fast updates using ratio of determinants
- Burovski, Prokof'ev, Svistunov, Troyer: worm-type updates, full scale calculation of T_c in continuum limit
- Goulko: new update, reducing autocorrelations, sign-quenched method for spin-polarized gas

Diagrammatic expansion

$$\boldsymbol{Z} = \mathbf{Tr}\ \mathbf{exp}\left[-\boldsymbol{\beta}(\hat{\boldsymbol{H}} - \boldsymbol{\mu}\hat{\boldsymbol{N}})\right]$$

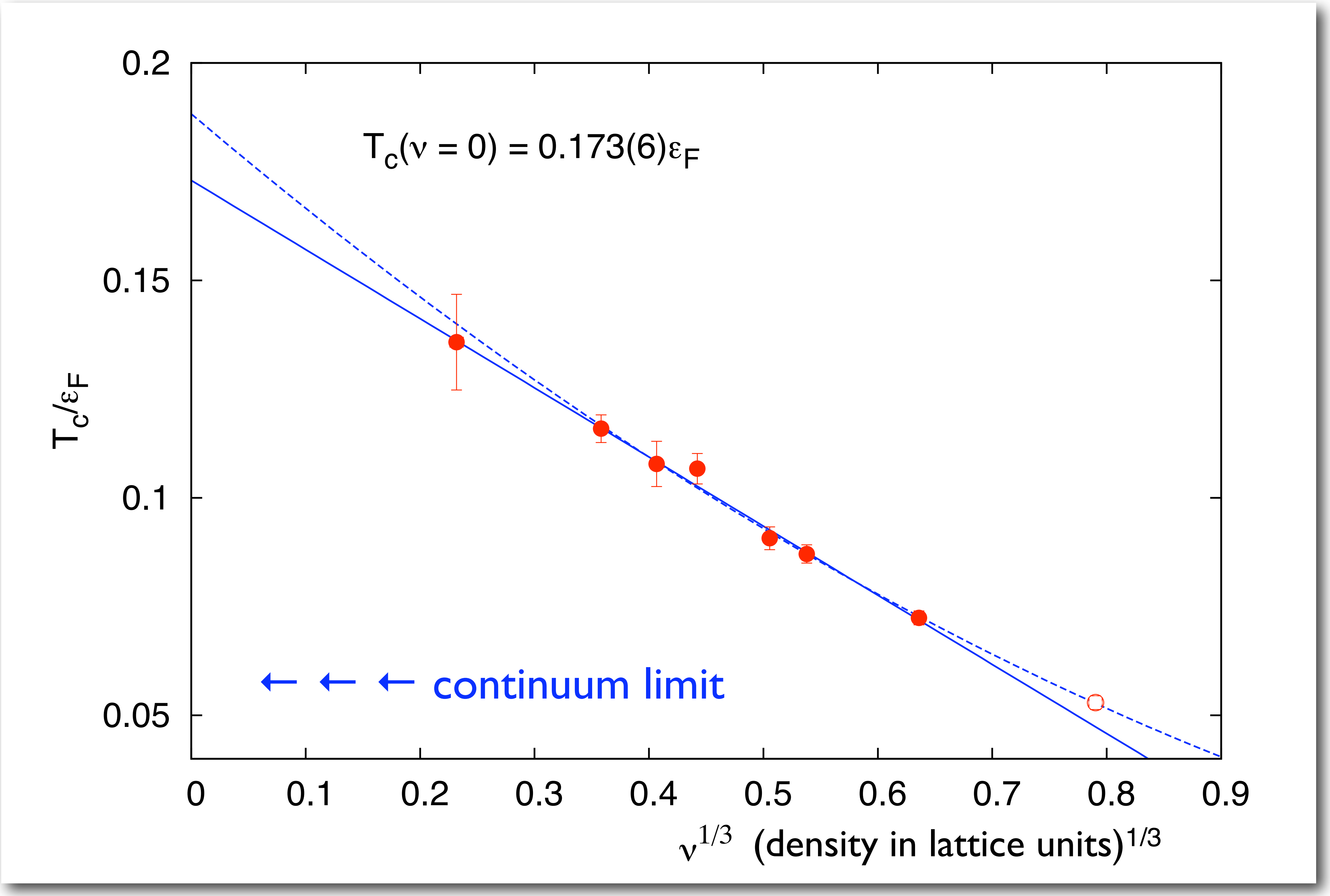


$$Z = \sum_{p=0}^{\infty} (-U)^p \sum_{\mathcal{S}_p} \det \mathbf{A}^{\uparrow}(\mathcal{S}_p) \det \mathbf{A}^{\downarrow}(\mathcal{S}_p)$$

Coupling large. Do not truncate! Sample using Monte Carlo.

Results

T_c, equal spin populations



Goulko & Wingate, Phys. Rev. A **83**, 053621 (2010)

Monte Carlo results for T_c/T_F

DDMC	Burovski, Prokof'ev, Svistunov, Troyer	0.152(7)
	Burovski, Kozik, Prokof'ev, Svistunov, Troyer	0.152(9)
	Bulgac, Drut, Magierski	0.15(1)
	Abe, Seki	0.189(12)
DDMC	Goulko, Wingate	0.173(6)

Finite size scaling (order parameter)

Integrated pairing-correlation function

$$R(L,T) = \left[f_0 + f_1 (T - T_c) L^{1/\nu_\xi} + \ldots\right] \left(1 + cL^{-\omega}\right)$$

Calculation of corrected crossing on 2 lattices sizes: L_i, L_j

$$R(L_i, T_{ij}) = R(L_j, T_{ij}) \quad \Rightarrow \quad T_{ij} - T_c = \kappa\, g(L_i, L_j)$$

with

$$g(L_i, L_j) = \frac{(L_j/L_i)^{\omega} - 1}{L_j^{\omega}(L_j^{1/\nu_\xi} - L_i^{1/\nu_\xi}) + cL_j^{1/\nu_\xi}[1 - (L_i/L_j)^{-\omega+1/\nu_\xi}]}$$

We find this method sometimes ambiguous

Instead we peform a global fit to 4 parameters. Robust.

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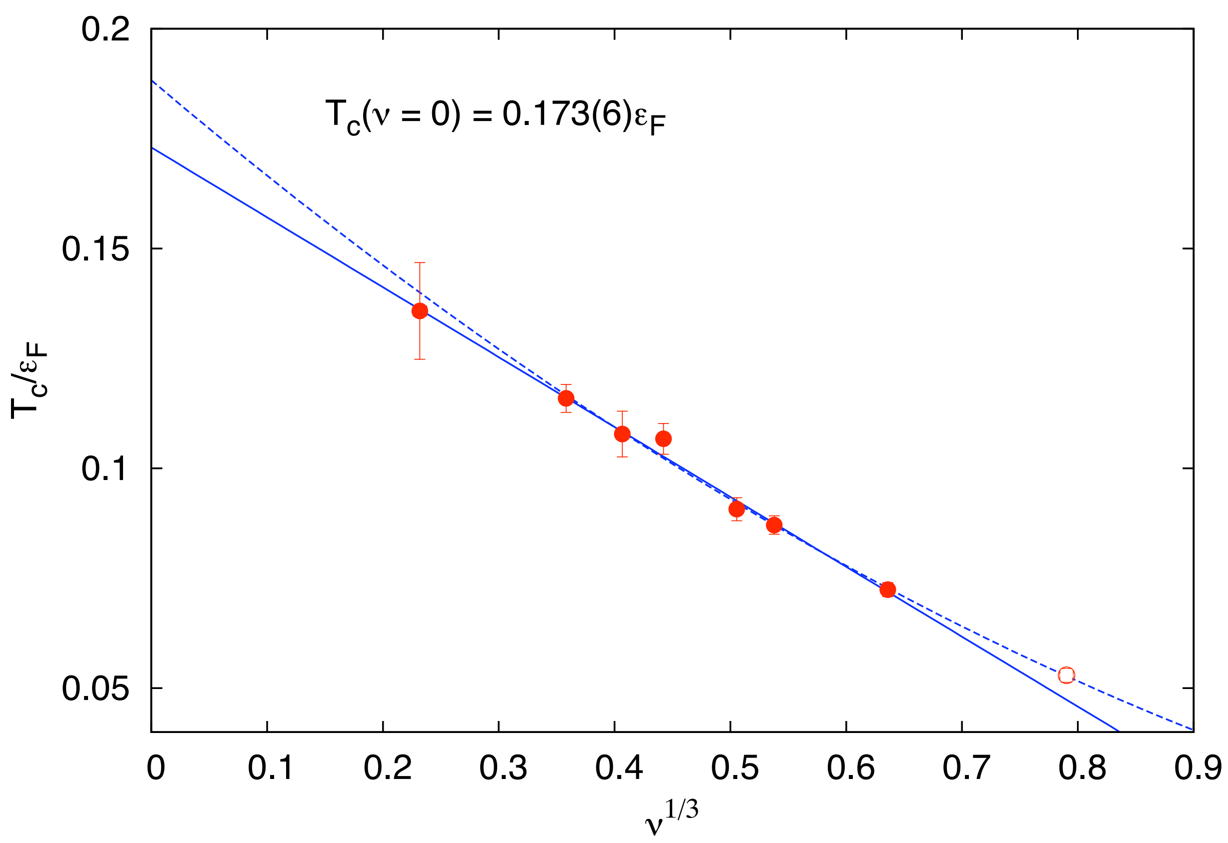
neglect?

We find this method sometimes ambiguous

Instead we peform a global fit to 4 parameters. Robust.

Toward improvement



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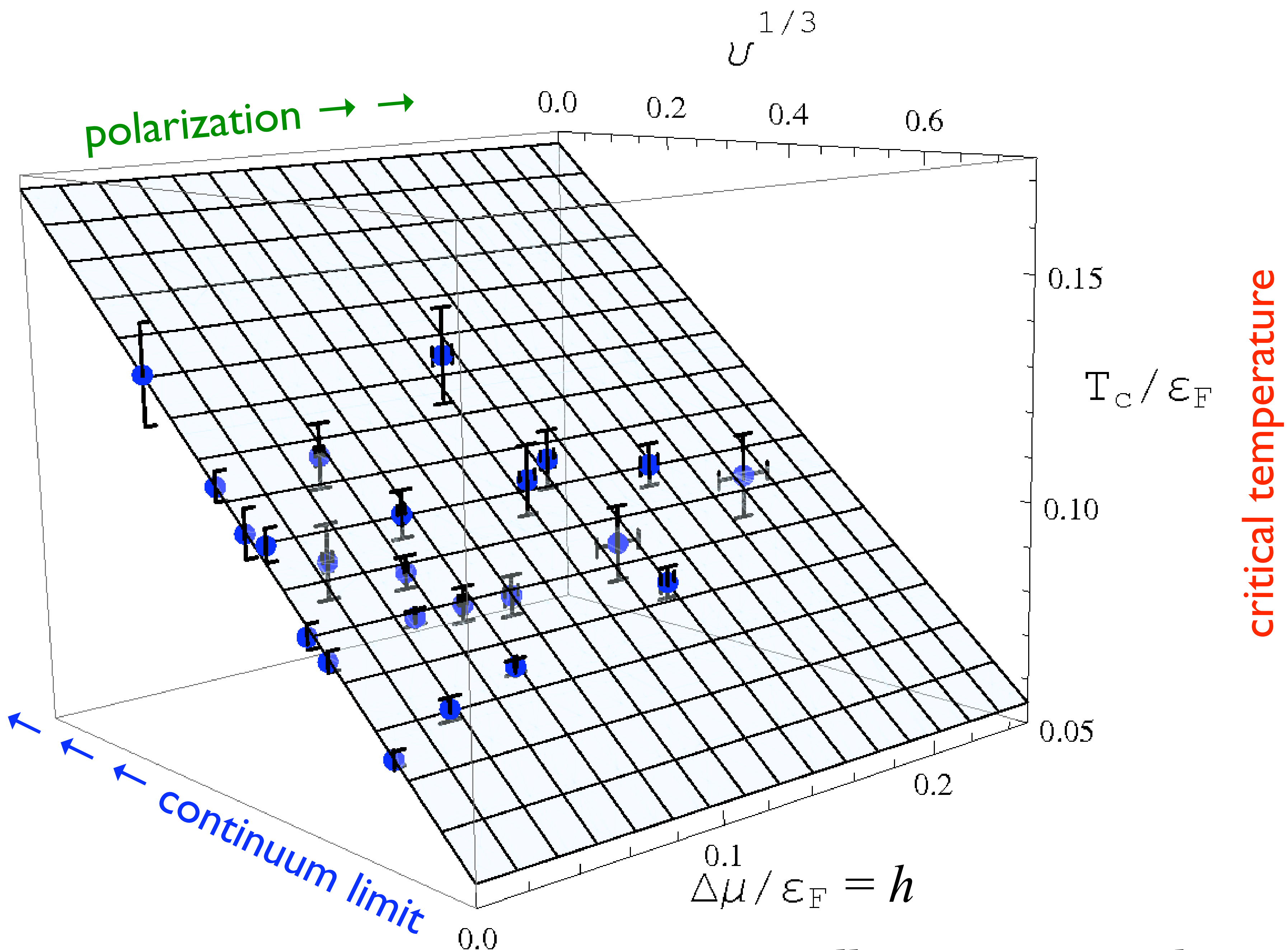
- Large lattice artifacts (large slope)
- Lee & Thompson proposal to improve scaling

Spin imbalanced gas

- $\mu_1 \neq \mu_2$ yields sign problem (no longer $\det^2$)
- Absorb sign into observable, rather than weight ("sign-quenched" method)
- Doomed to fail eventually, but can explore small polarizations

T_c with slight spin imbalance

$$T_c(\nu, h) = 0.171(5) + 0.07(11)h^2 - 0.155(8)\nu^{1/3}$$



Goulko & Wingate, Phys. Rev. A **83**, 053621 (2010)

How imbalanced?

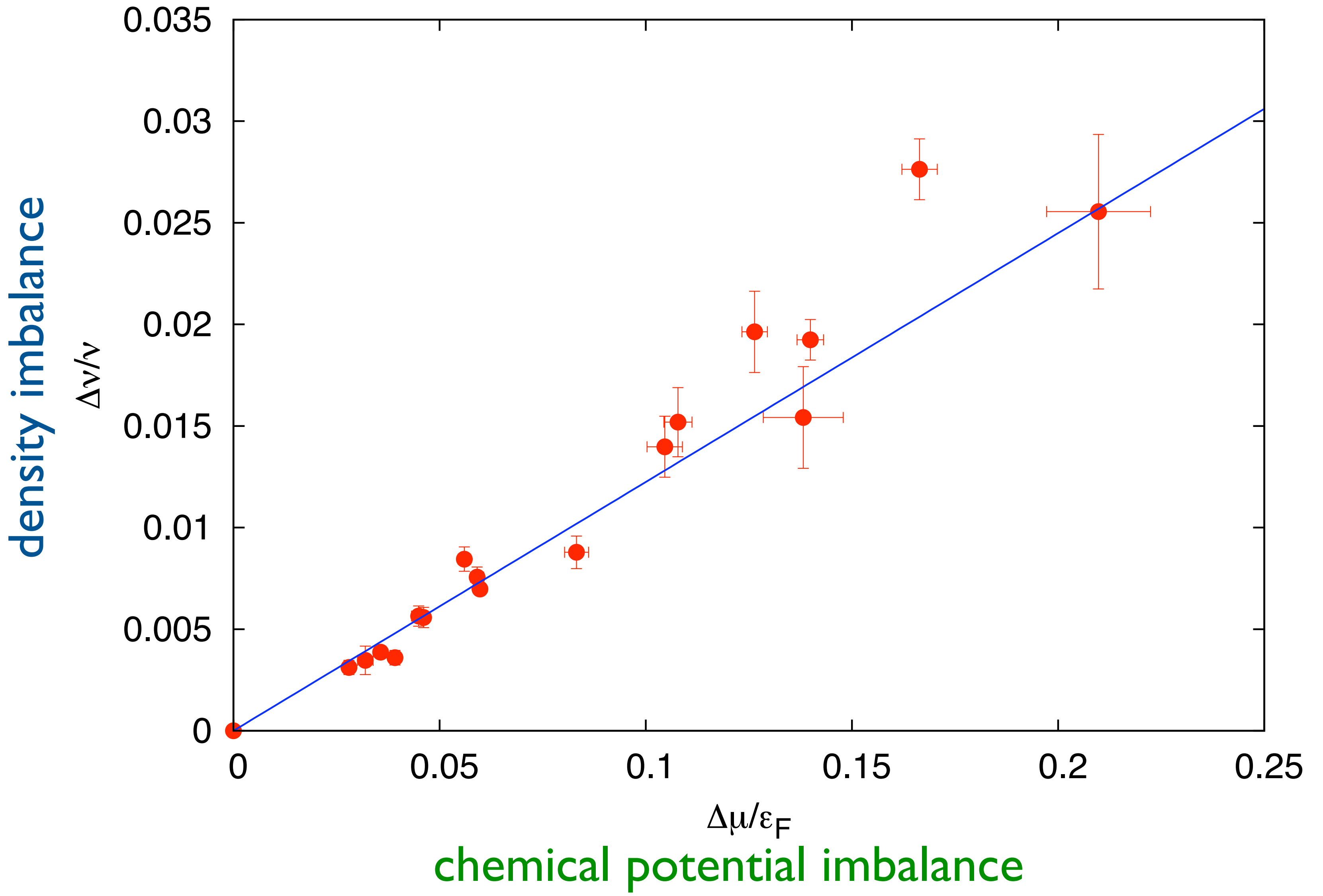


FIG. 10. (Color online) Relation between the chemical potential difference and the relative density difference at T_c.

Contact

To be discussed by next speaker(s)
Intoduced by Tan; OPE: Braaten & Platter; Review: Braaten, arXiv:1008.2922

Small (compared to a) separations

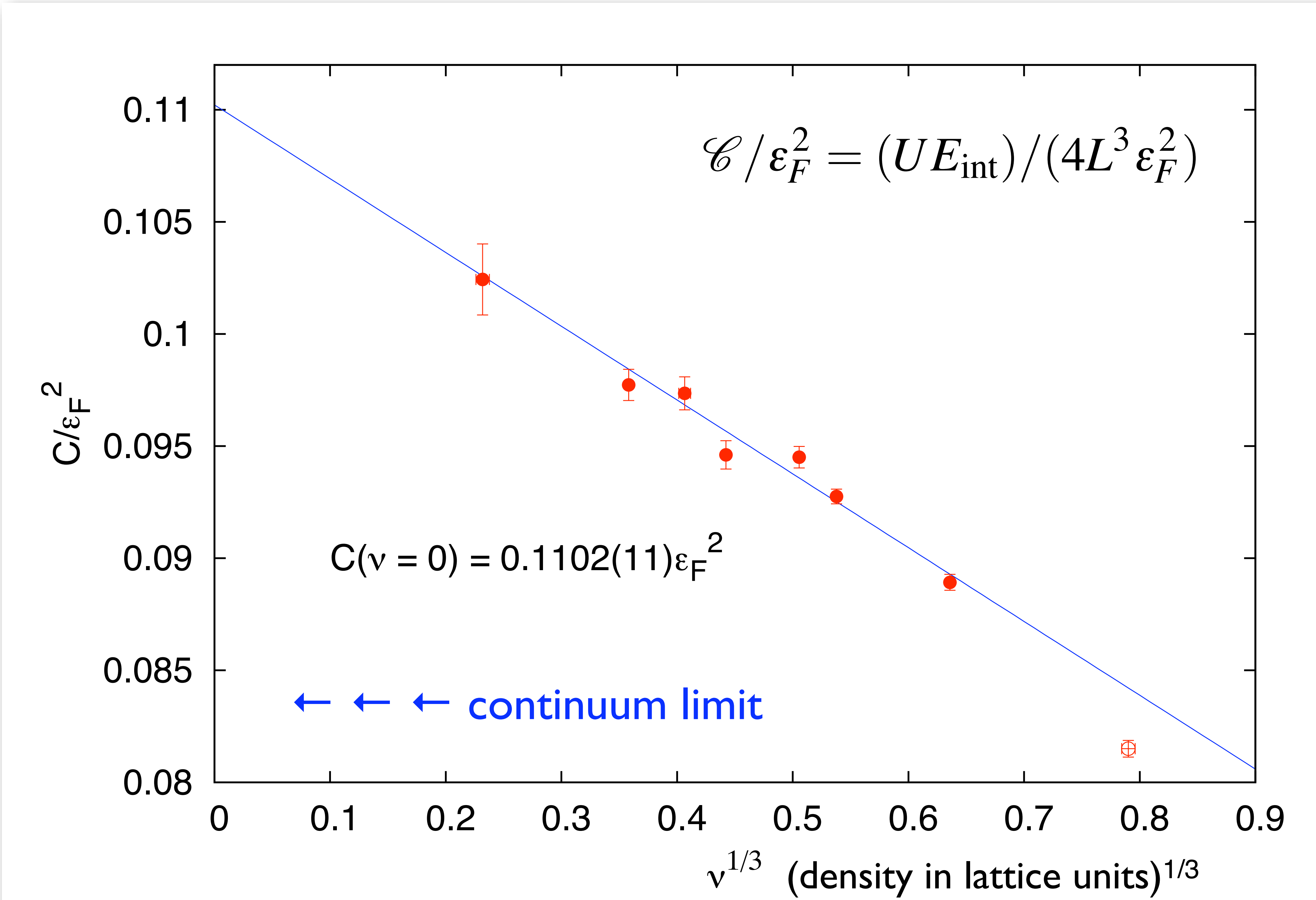
$$\langle n_1(\boldsymbol{R}+\boldsymbol{r}_1)\ n_2(\boldsymbol{R}+\boldsymbol{r}_2)\rangle \longrightarrow \frac{1}{16\pi^2|\boldsymbol{r}_1-\boldsymbol{r}_2|^2}\mathcal{C}(\boldsymbol{R}).$$

Number of pairs in small sphere (radius s)

$$N_{\rm pair}(\boldsymbol{R},s) \longrightarrow \frac{s^4}{4}\mathcal{C}(\boldsymbol{R}).$$

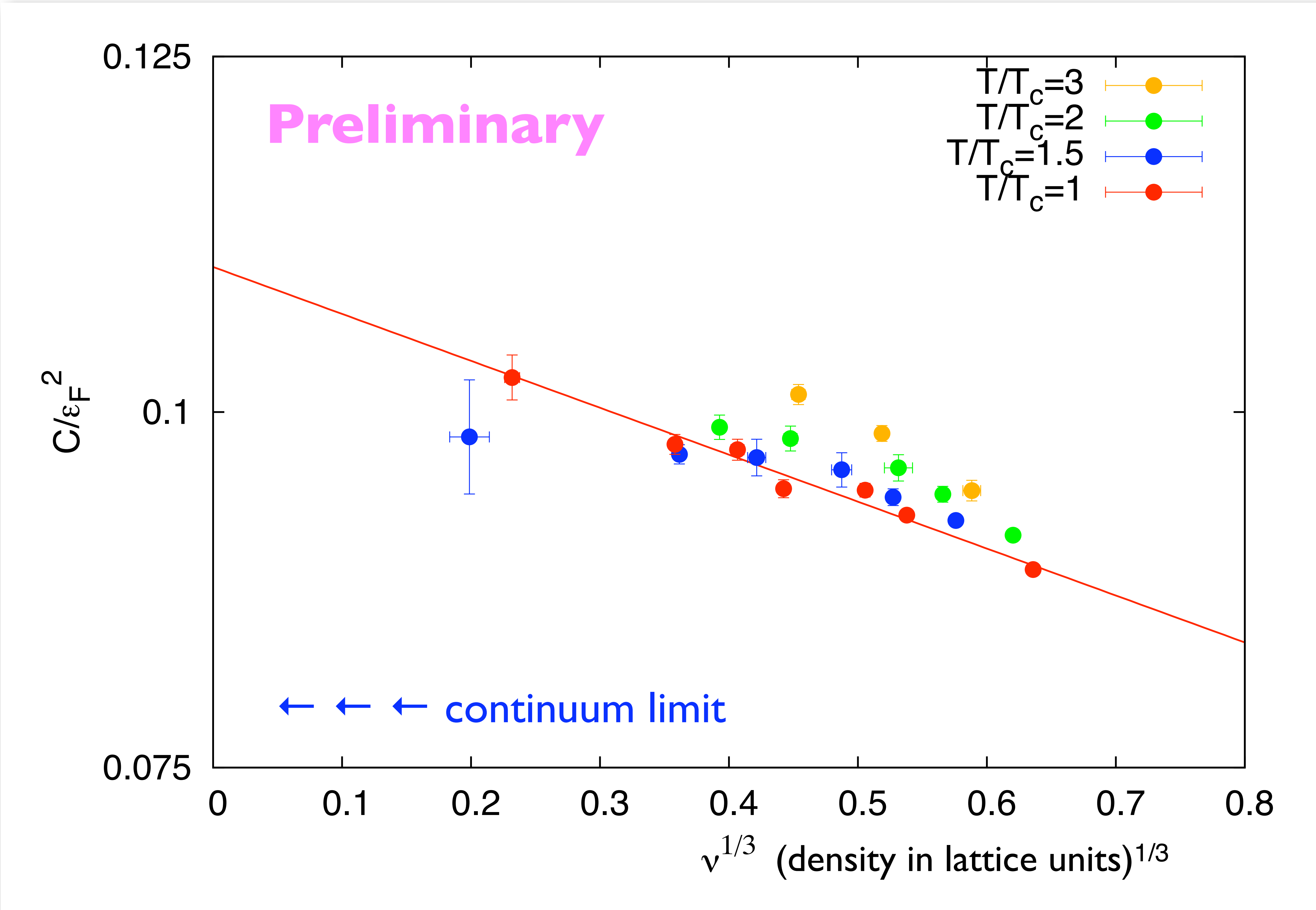
Is the single long distance quantity in several relations

Contact density at T_c



Goulko & Wingate, arXiv:1011.0312

Contact density, *T* dependence



Outlook

- DDMC very efficient for small volumes
- Scales like (number lattice points)^2
- Pseudofermion methods (briefly ➙)
- Go beyond balanced unitary Fermi gas (lower dimensions, gauge fields)

Pseudofermion Monte Carlo

$$\mathcal{Z} = \int \mathcal{D}\phi \, \mathcal{D}\zeta \, \exp\left[-\left(\int \zeta^\dagger \widetilde{\mathcal{A}}^{-1} \zeta + \frac{1}{2}\phi^2\right)\right]$$

- HMC: Molecular dynamics + accept/reject step
- Naively scales like the number of lattice points
- Requires inversion of sparse matrix
- But matrix becomes singular in physical limit

Chen & Kaplan, Wingate, Lee & Schaefer, Lee *et al.*, Drut *et al.*

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