Unbiased Numerics for BCS-BEC Crossover Problem

Part 1. Critical Temperature and Thermodynamics

Part2. Resonant Fermipolaron *(with Nikolay Prokof'ev; preliminary results)*

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Computational resources:

"Heidar" cluster, ETH

Oakridge Cray "Phoenix"

"Mammoth" cluster, U. of Sherbrooke

Santa Barbara, 2007

Diagrammatic Monte Carlo

Take a convergent positive-definite diagrammatic series, say the one for polaron Green's function,

and interpret it as a partition function for an ensemble of graphical objects (diagrams). Introduce a Markov process generating ensemble, and calculate corresponding histograms/averages.

The Markov process can be organized in the form of pairs of complementary updates. In such a pair, A-B, the update A creates a new graphical element with corresponding continuous variable, while the update B removes the element. For example, A creates a new propagator, while B removes it:

Balancing Diagrammatic Markov Process by Metropolis Algorithm

Acceptance ratios for complementary updates A-B

$$R_A\left(\vec{X}\right) = \frac{New\,Diagram}{Old\,Diagram}\,\frac{1}{W\left(\vec{X}\right)}$$

$$R_B\left(\vec{X}\right) = \frac{New\,Diagram}{Old\,Diagram}\,W\left(\vec{X}\right)$$

(Arbitrary) distribution functions for generating particular values of new continuous variables in the update A

Model of Resonant Fermions

No explicit interactions—just the boundary condition:

$$\forall i,j \quad \text{at} \quad \left|\mathbf{r}_{\uparrow i}-\mathbf{r}_{\downarrow j}\right|\to 0: \qquad \Psi\left(\mathbf{r}_{\uparrow 1},...,\mathbf{r}_{\uparrow N},\mathbf{r}_{\downarrow 1},...,\mathbf{r}_{\downarrow N}\right) \to \frac{A}{\left|\mathbf{r}_{\uparrow i}-\mathbf{r}_{\downarrow j}\right|}+B, \qquad \frac{B}{A}=c=\text{const}$$

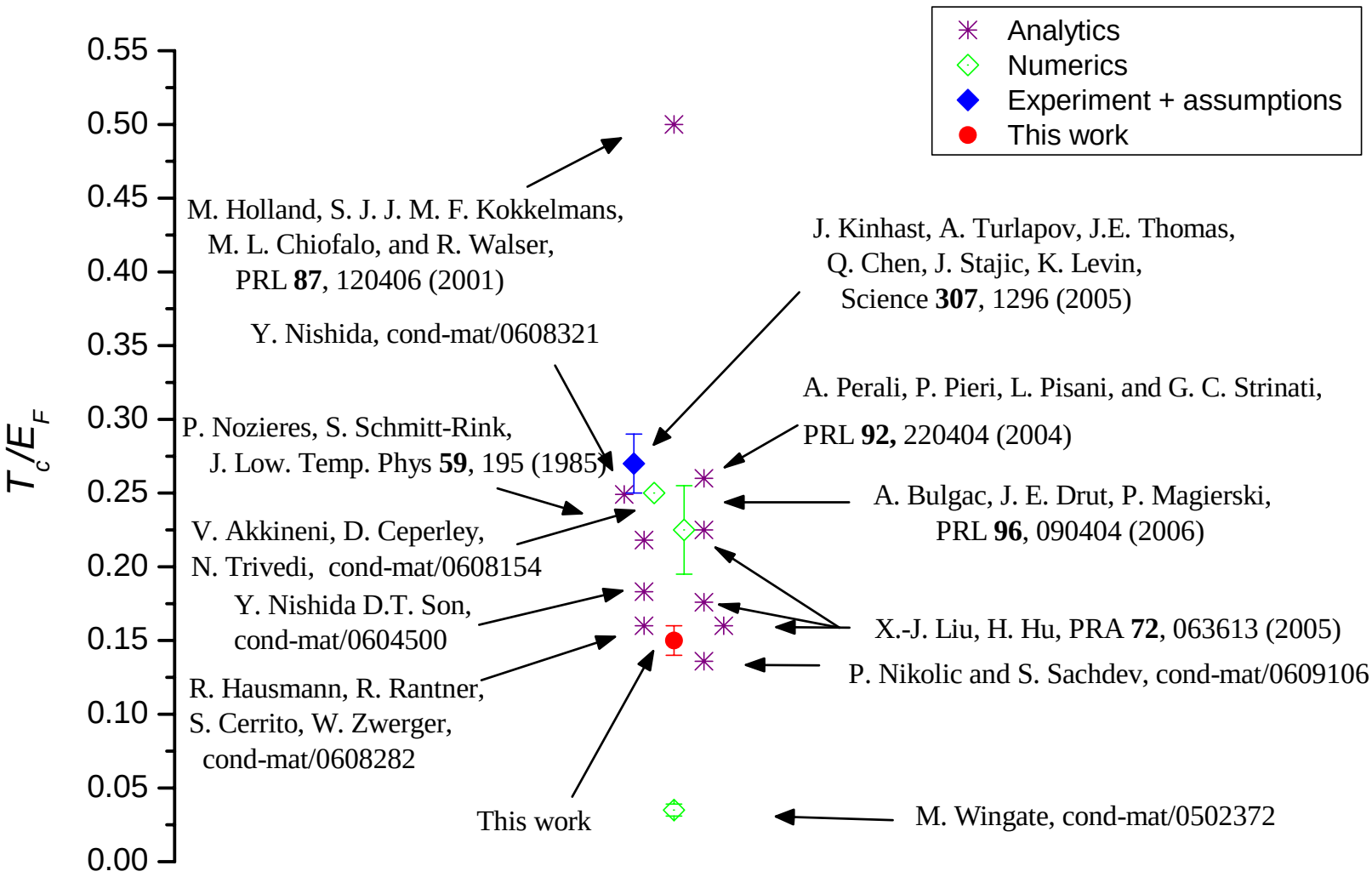
$$c \gg n^{1/3}\sim k_F \quad \Rightarrow \quad \text{BCS regime}$$

$$|c| \ll n^{1/3}\sim k_F \quad \Rightarrow \quad \text{unitarity regime}$$

$$-c \gg n^{1/3}\sim k_F \quad \Rightarrow \quad \text{BEC regime}$$

(In two-body problem, the parameter c defines the s-scattering length.)

Unitary point critical temperature



Unitarity ($a_{sc} \to \infty$):

$$U_C = -\Pi(0,0)^{-1} = -\left(\int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{2\varepsilon(\mathbf{k})} \right)^{-1}$$

Two ways to "regularize" ultra-violet divergences:

Hubbard model (tight-binding spectrum)

$$\varepsilon(k) = t(6 - 2\cos k_x a - 2\cos k_y a - 2\cos k_z a)$$

$$U_C = -7.915 \times \mathrm{t}$$

Continuous space with momentum cut-off

$$\varepsilon(k) = k^2/2m \quad if \quad k < k_0$$
$$= \infty \quad otherwise$$

$$U_C = -\frac{mk_0}{2\pi^2}$$

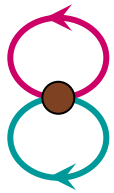
Universality in the low-density limit

$$na^3 \to 0$$
$$nl_0^3 \to 0, \quad l_0 = \pi / k_0$$

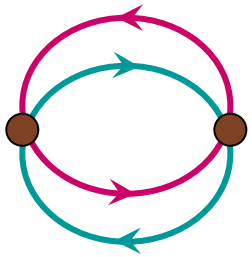
systematic error

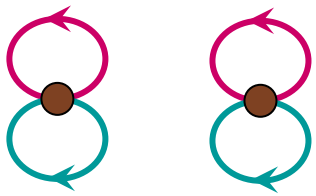
$$\frac{\delta\Gamma}{\Gamma} \propto \frac{n^{1/3}a}{n^{1/3}l_0}$$

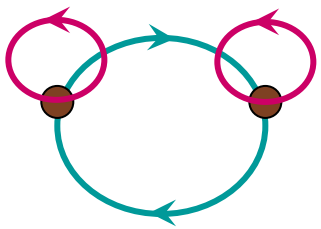
Diagrammatic expansion for the partition function Z

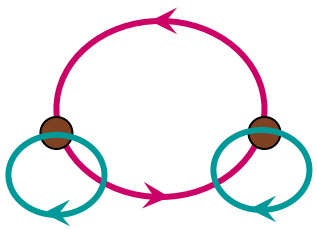


$-U$



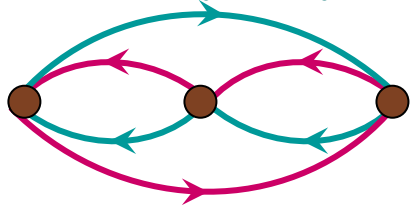






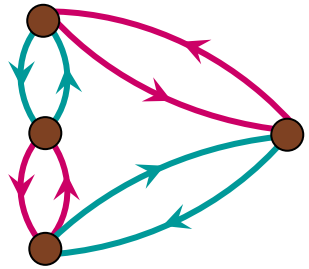
$(-U)^2$

$G_{\uparrow}(r_i - r_j, \tau_i - \tau_j)$



$G_{\downarrow}(r_i - r_j, \tau_i - \tau_j)$

$(-U)^3$



$(-U)^4$

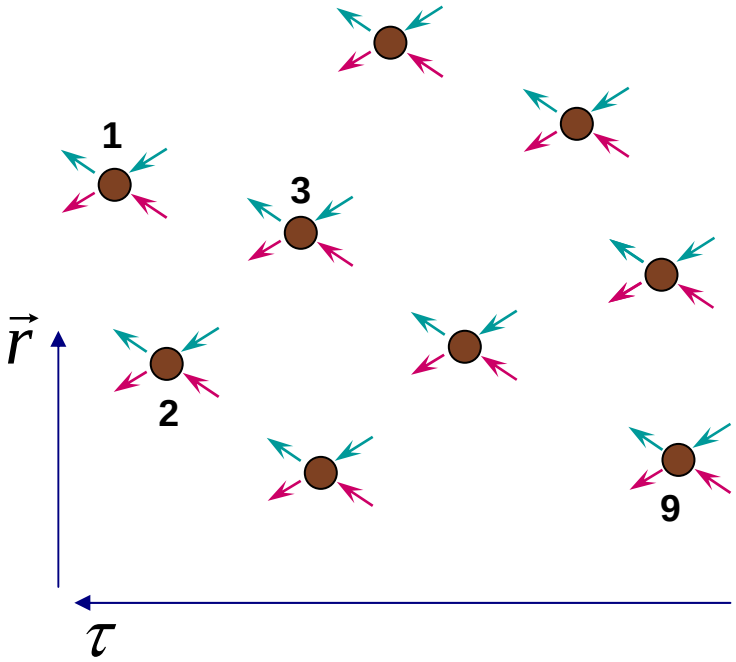
too many to draw all $(p!)^2$ possible topologies …

...but easy to sum all of them!

Determinant representation for diagrams of order p

Rubtsov ' 03

For equal concentrations of components:



The sum of all $(p!)^2$ diagrams for a given vertex configuration $(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2;\ldots;\mathbf{r}_p,\tau_p)$ is a determinant squared

$$\det G_{ij} = \begin{vmatrix} G_{11} & G_{12} & \ldots & G_{1p} \\ G_{21} & G_{22} & \ldots & G_{2p} \\ \ldots & \ldots & \ldots & \ldots \\ G_{p1} & G_{p2} & \ldots & G_{pp} \end{vmatrix}$$

$$Z = \sum_{\xi} D_n(\xi) = \sum_{p} \int \ldots \int (d\vec{r}\,d\tau)^p (-U)^p \det{}^2 G_{\uparrow}(\vec{x}_i, \vec{x}_j)$$

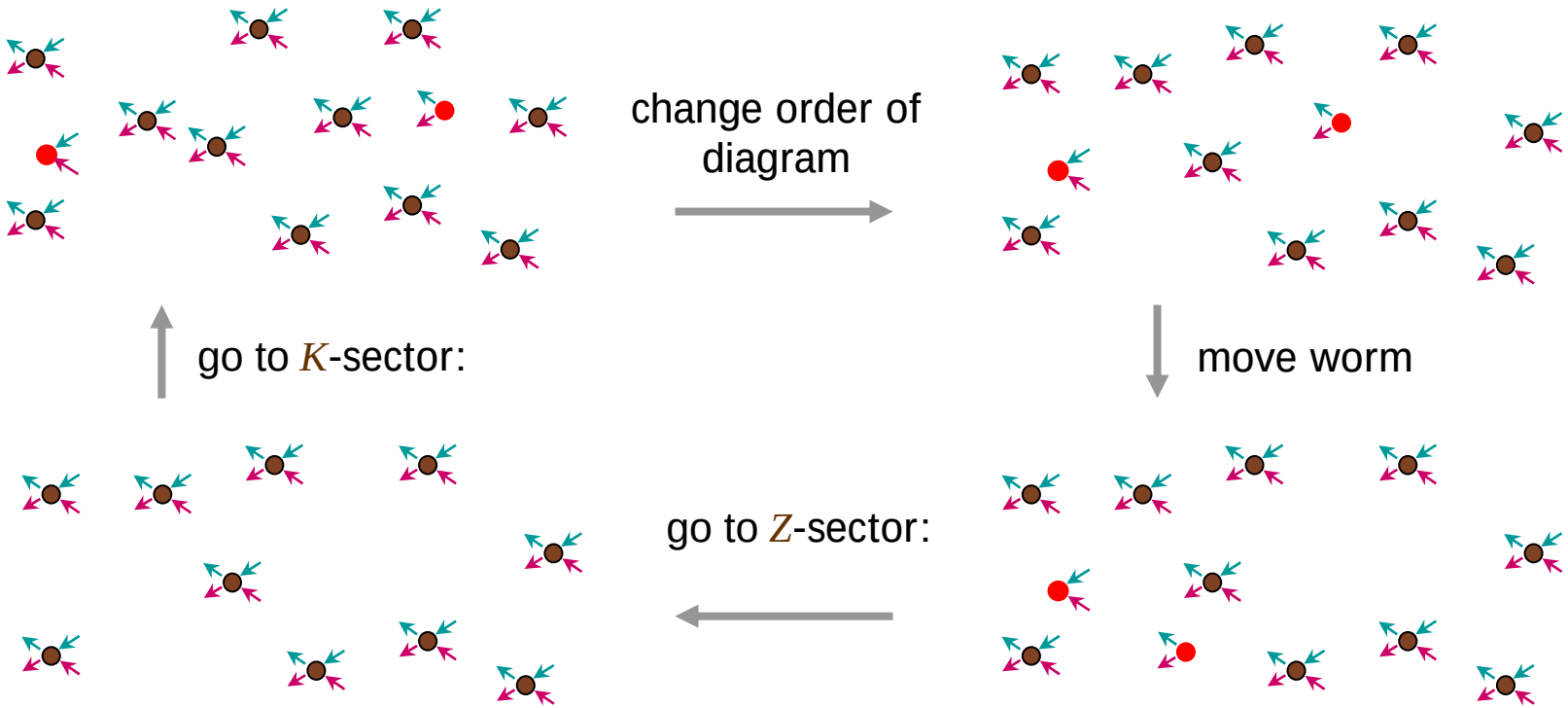
Monte Carlo Scheme: Worm Algorithm

Worm algorithm = extended configuration space of $K \cup Z$

$$K(\mathbf{r}_2 - \mathbf{r}_1, \tau_2 - \tau_1) = \left\langle \mathrm{T}_\tau \; \Psi^+_\downarrow(\mathbf{r}_2, \tau_2)\Psi^+_\uparrow(\mathbf{r}_2, \tau_2) \; \Psi_\uparrow(\mathbf{r}_1, \tau_1)\Psi_\downarrow(\mathbf{r}_1, \tau_1) \right\rangle$$

+ all updates are through the pair operators exclusively!

Prokof'ev, Svistunov, and Tupitsyn '98



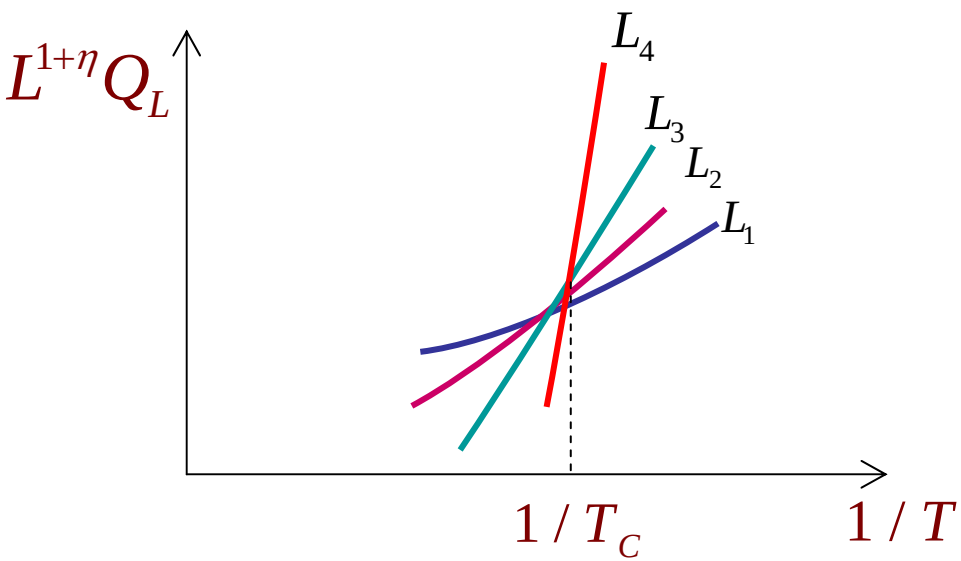
Critical point from finite-size scaling of

$$Q = \frac{1}{V\beta}\int_{-\beta}^{\beta} d\tau \int d\mathbf{r}\, K(\mathbf{r},\tau) \sim \mathrm{n}_0$$ ← pair condensate density

$$t = \left|\frac{T - T_C}{T_C}\right| << 1: \qquad Q_L L^{1+\eta} = f(tL^{1/\nu_\xi}) \times (1 + c/L^{\omega} + \ldots)$$

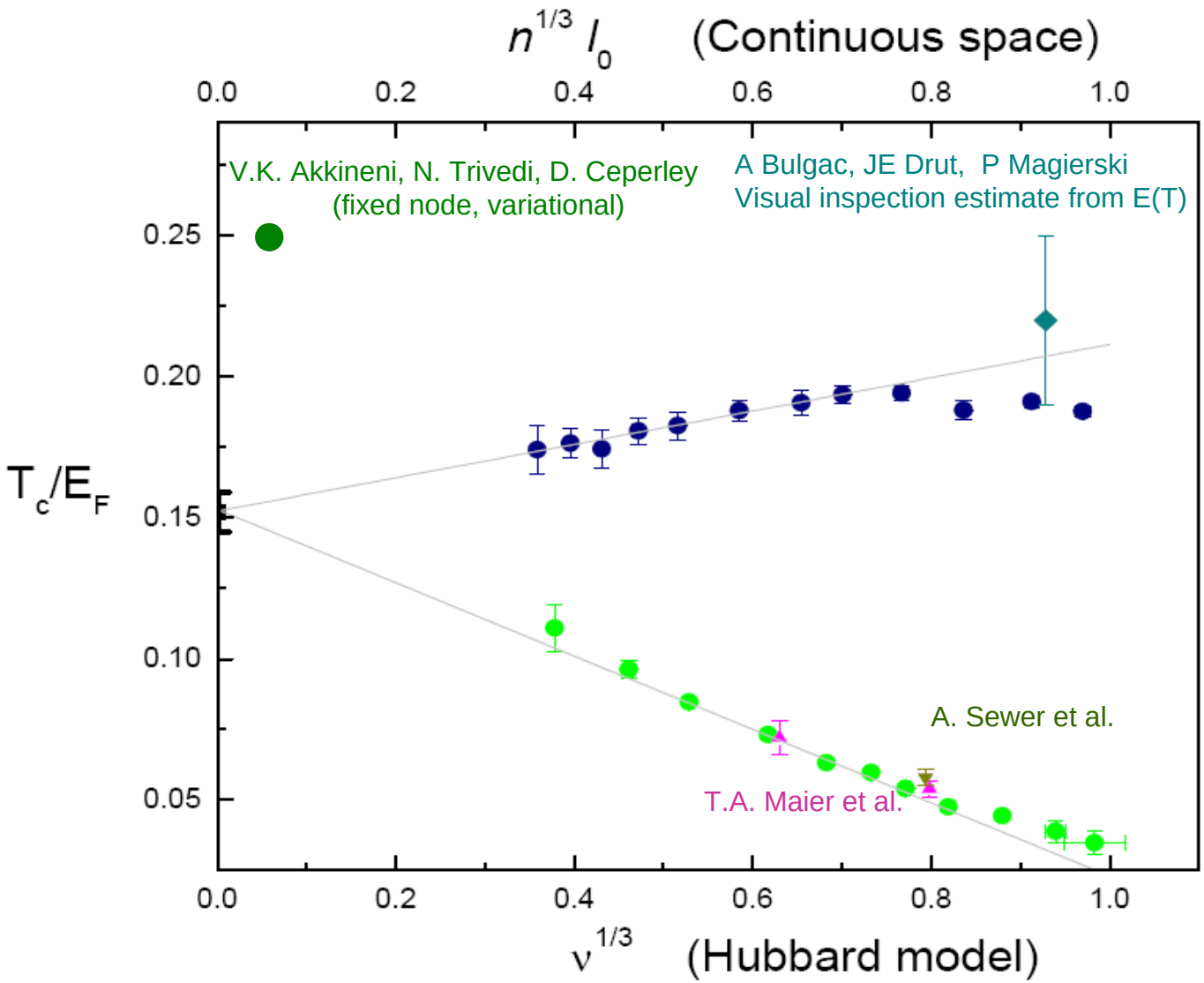
(3D XY-universality class)

$$\eta \approx 0.0380, \quad \nu_\xi = 0.6715, \quad \omega = 0.80$$

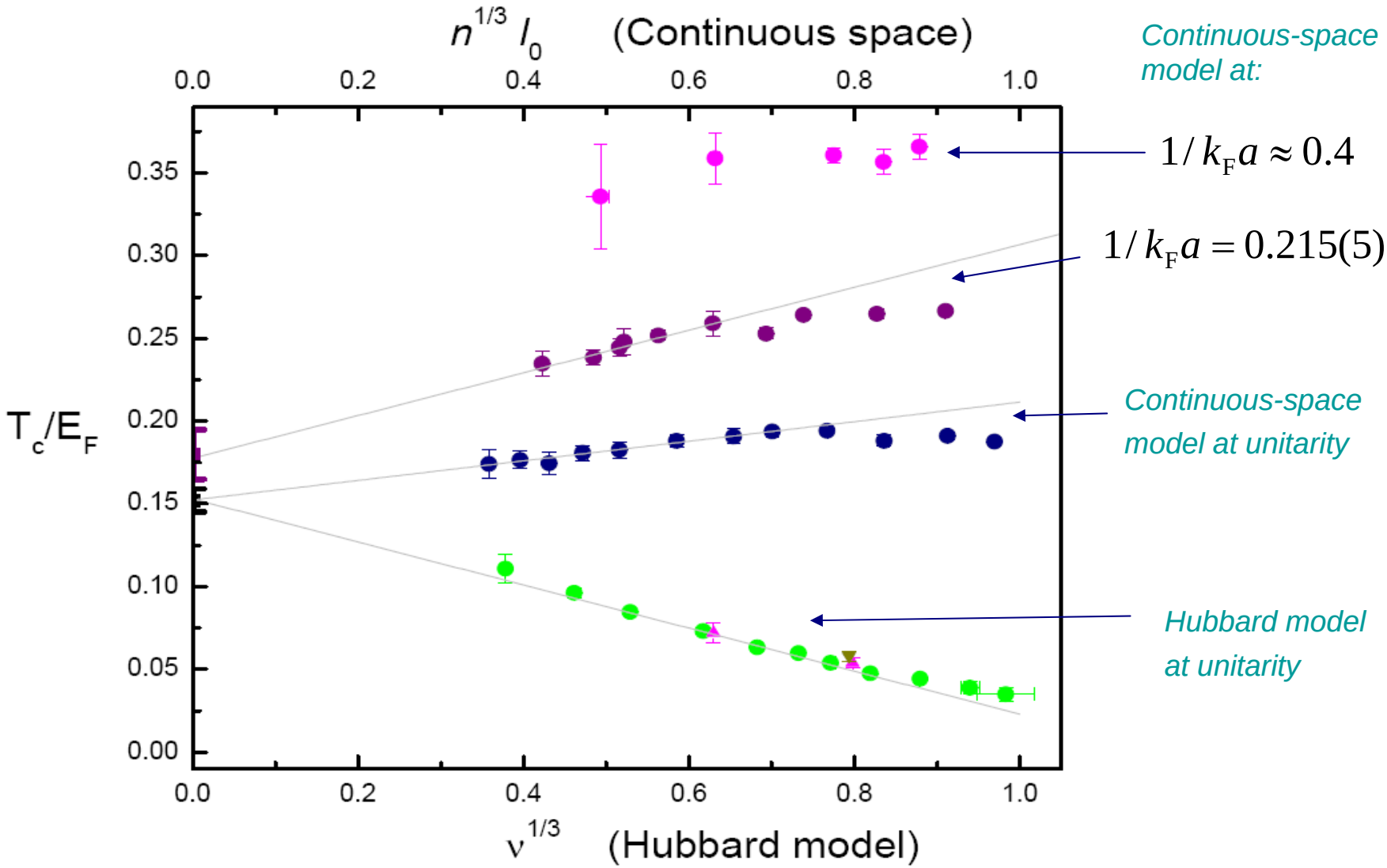


$$|T_C(L) - T_C(\infty)| \sim 1/\mathrm{L}^{\omega+1/\nu_\xi} \sim L^{-2.3}$$

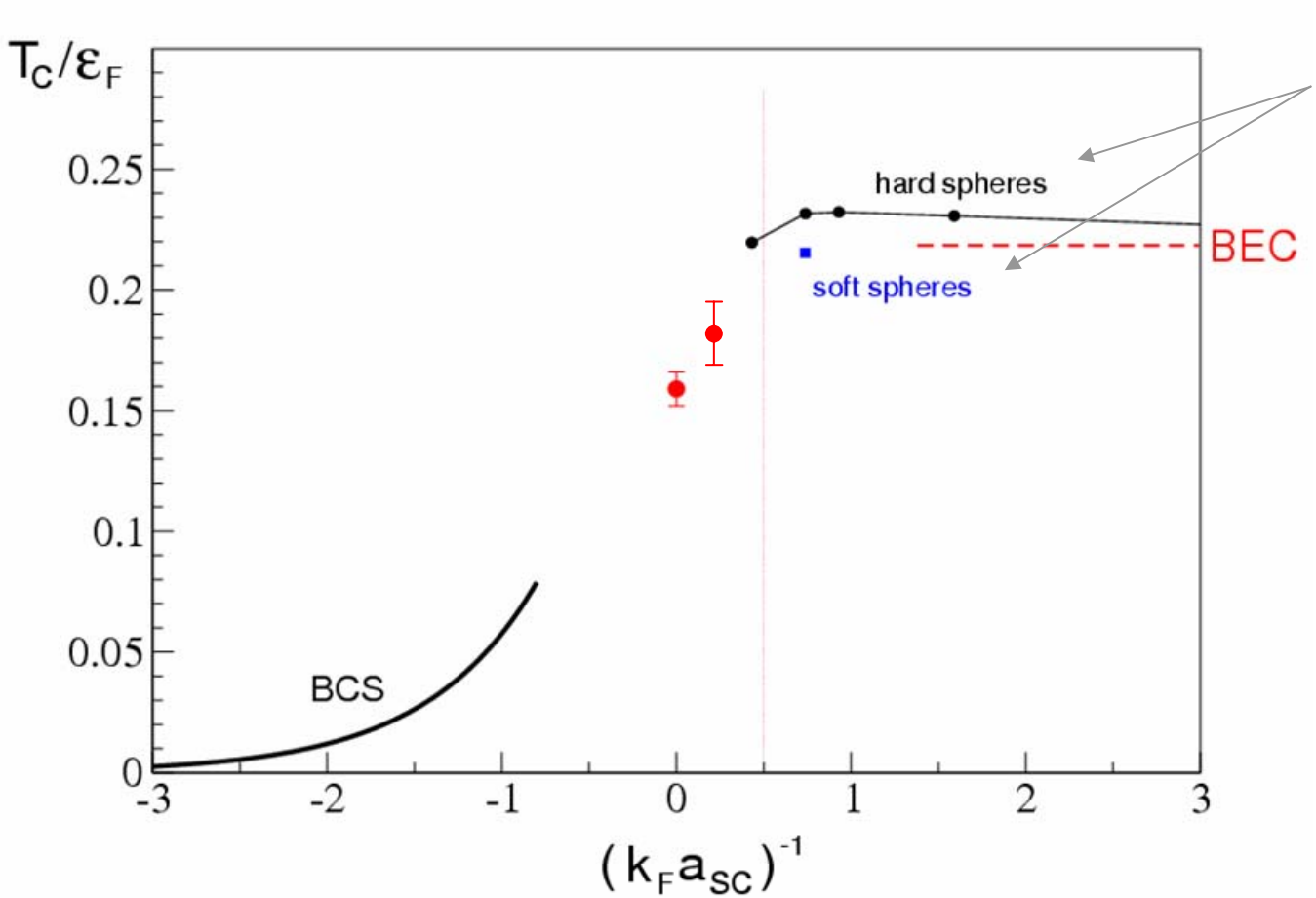
T_c at unitary point



$$T_c / E_F = 0.152(7)$$


$n^{1/3}\,l_0$ (Continuous space)
0.0
0.2
0.4
0.6
0.8
1.0
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
T_c/E_F
$\nu^{1/3}$ (Hubbard model)
Continuous-space model at:
$1/k_F a \approx 0.4$
$1/k_F a = 0.215(5)$
Continuous-space model at unitarity
Hubbard model at unitarity

The crossover curve (in progress ...)



Bosonic systems

(Prokof'ev, *et al.)*

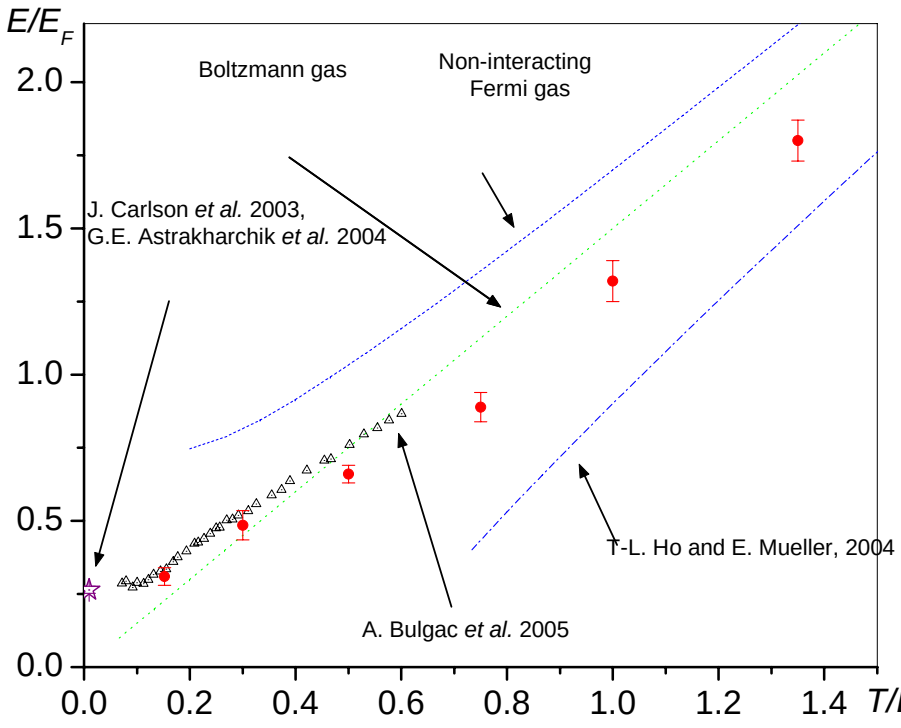
BCS: $T_c/E_F \propto e^{-\pi/2k_F|a|}$

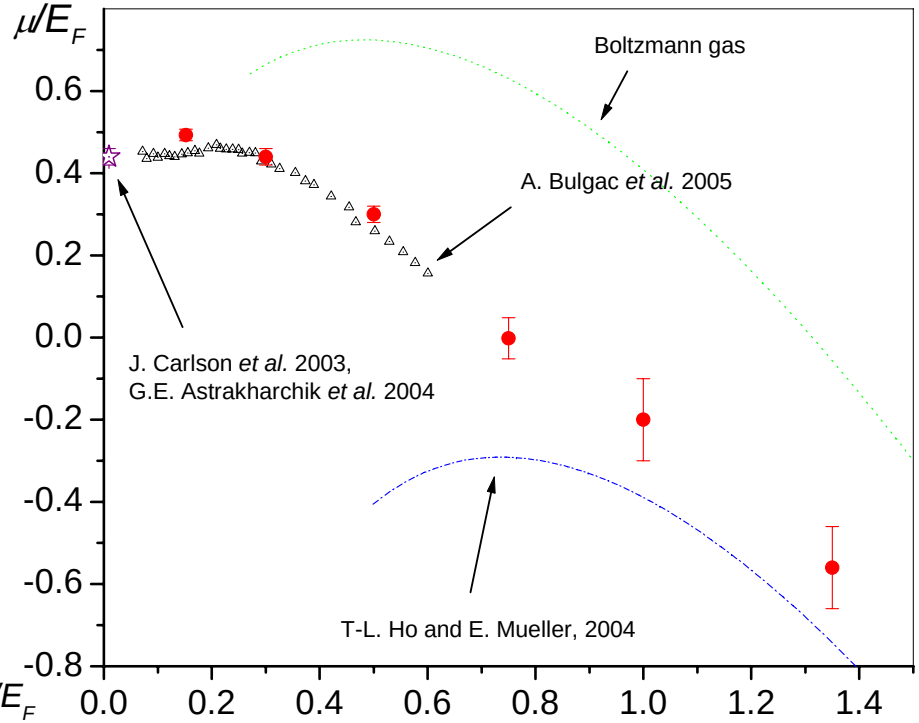
BEC: $T_c/E_F \approx 0.218 + c \times k_F a, \quad c > 0$

Thermodynamics at the unitary point

At unitarity, thermodynamics is self-similar: $PV = 2E/3$

$$S/N = (5E/3 - \mu N)/NT$$





Can be used for e.g. thermometry of dilute ultracold gases

Summary for Part 1.

- Determinant Diagrammatic Monte Carlo: a novel systematic-error-free numeric method for fermions on a lattice and in continuous space

- Critical temperature & thermodynamics at unitarity $T_c/E_F = 0.152(7)$

- Critical temperature across the BEC-BCS crossover (in progress)

- Solved the attractive Fermi-Hubbard model at unitarity for all fillings

Part2. Resonant Fermipolaron

with Nikolay Prokof'ev

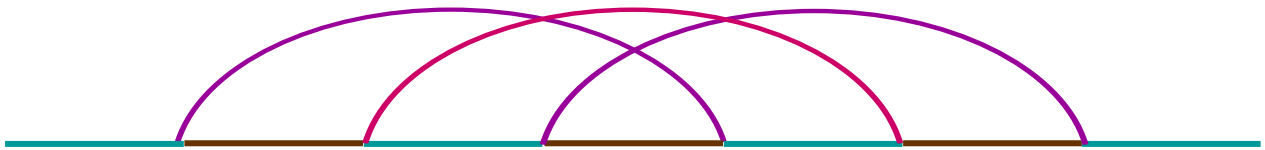
Diagram elements:

$G_{\uparrow}\left(k > k_F\right)$

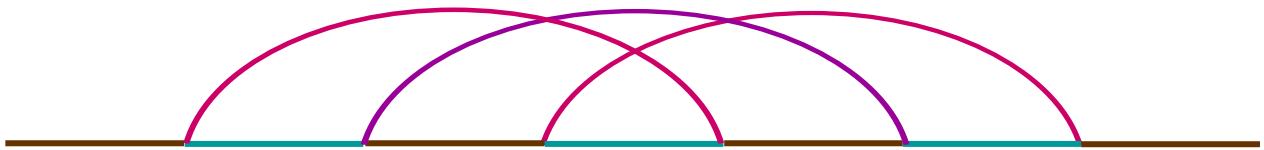
$G_{\downarrow}^{(0)}$

$G_{\uparrow}\left(k < k_F\right)$

Γ



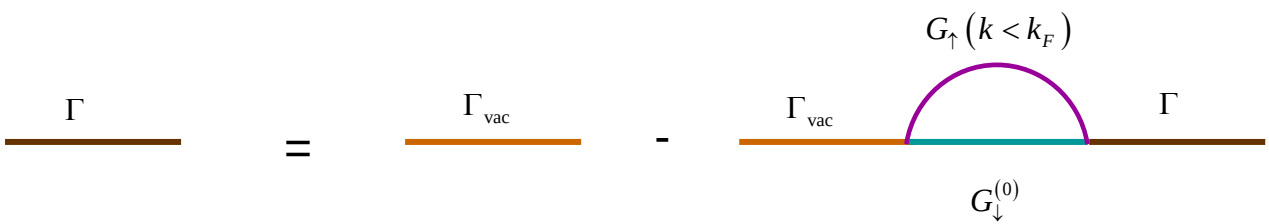
a polaron diagram



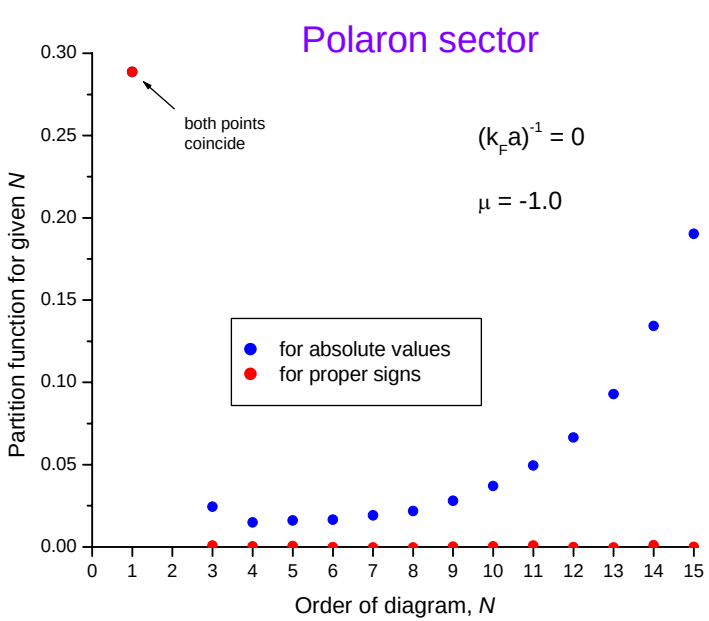
a molecule diagram

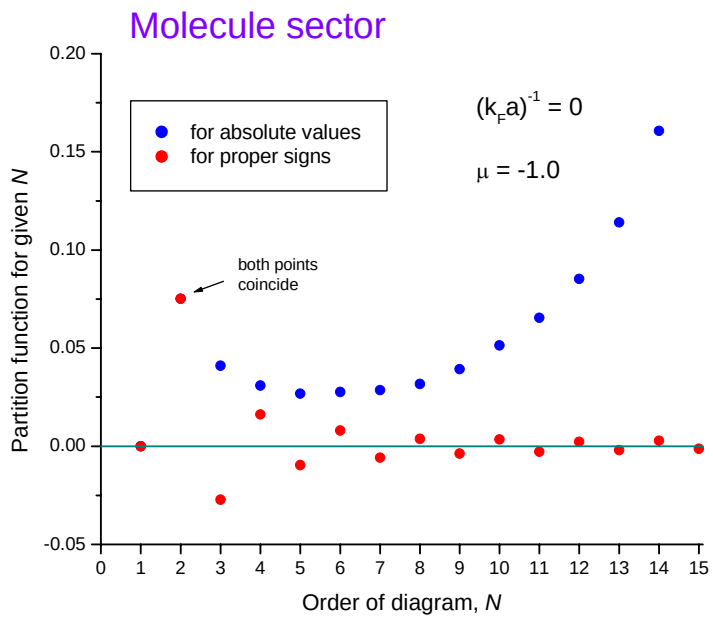
T-Matrix by Bold-Line Diagrammatic Monte Carlo

Evaluating T-matrix in imaginary-time representation forms a separate problem because we have not got an analytic expression. We obtain T-matrix numerically by recently developed Bold-Line Diagrammatic Monte Carlo (BLDM) (arXiv:cond-mat/0702555)*. The BLDM technique allows one to simulate a function expressed diagrammatically through itself. In our case, the equation to be solved by BLDM is as follows:*



Convergence of the diagrammatic series





Fermionic sign is crucial for convergence !

Extracting the Energy

From asymptotic behavior of the Green's function:

$$G_{\downarrow}(\mathbf{p},\tau) \rightarrow Z\,\mathrm{e}^{-E\tau} \quad \text{at} \quad \tau \rightarrow \infty$$

From self-energy:

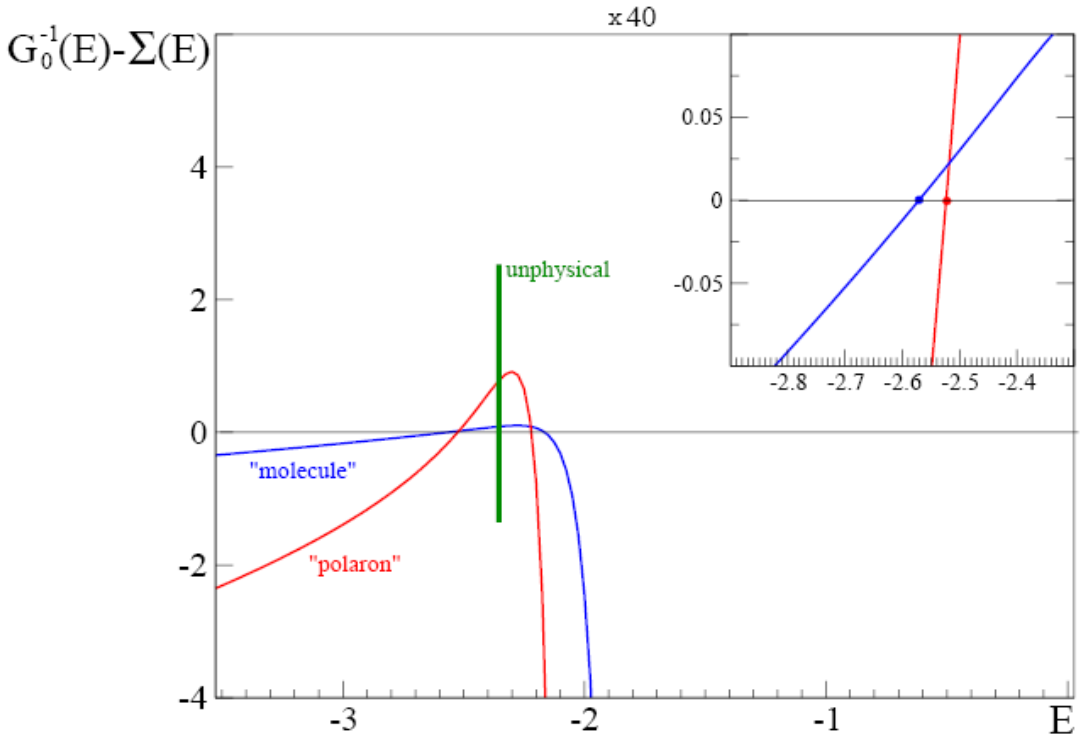
$$\left[G_{\downarrow}^{(0)}(\mathbf{p},\omega = E)\right]^{-1} - \int_0^{\infty} \Sigma(\mathbf{p},\tau)\mathrm{e}^{E\tau} d\tau = 0$$

Most efficient !

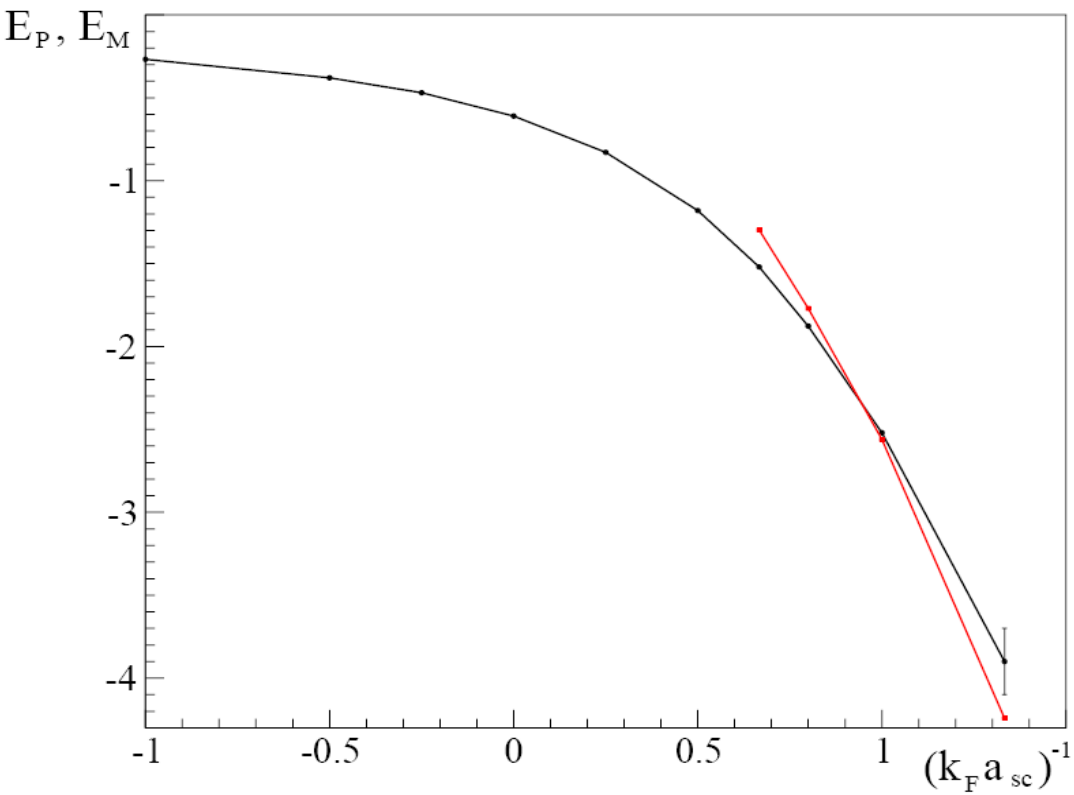
known quantity

The integral is directly sampled from diagrammatic Monte Carlo simulation of self-energy.

$k_F a = 1.0$


x 40
$G_0^{-1}(E)-\Sigma(E)$
4
2
0
-2
-4
-3
-2
-1
E
unphysical
"molecule"
"polaron"
0.05
0
-0.05
-2.8
-2.7
-2.6
-2.5
-2.4

$$\left(k_F a\right)_{\text{molecule}} \approx 1.0$$



Conclusion for Part 2.

- It works!

- $\left(k_F a\right)_{\text{molecule}} \approx 1.0$