Lecture 2

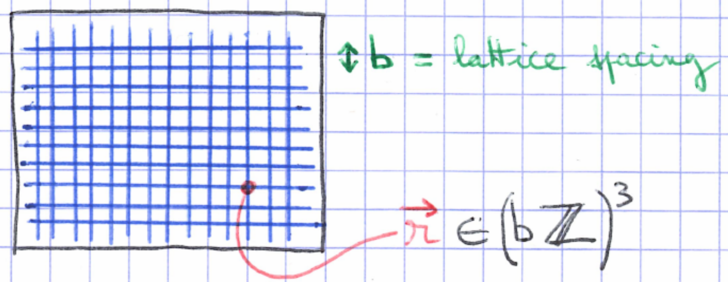
Many-body physics : methods and basic properties

Cubic box, volume $\mathcal{V} = L^3$, periodic boundary conditions.

$$\langle \vec{r} | \vec{k} \rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{\mathcal{V}}} .$$

Chapter 0 Lattice Model

discretize space :



$$\vec{k} \in \left(\frac{2\pi}{L}\mathbb{Z}\right)^3 \cap \mathcal{D} =: \mathcal{D}_L \qquad \mathcal{D} := \left[-\frac{\pi}{b}, \frac{\pi}{b}\right[^3$$

$$-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{\vec{r}_i}\Psi + \sum_{i\leq N_\uparrow<j} V(\vec{r}_i - \vec{r}_j)\Psi = E\Psi$$

V :

$$\boxed{V(\vec{r}_2 - \vec{r}_1) = \frac{g_0}{b^3}\,\delta_{\vec{r}_1,\vec{r}_2}} \qquad \left(\begin{array}{l}\text{on-site :}\\ \text{range} \sim b\end{array}\right)$$

$\Delta_{\vec{r}}$:

$$-\frac{\hbar^2}{2m}\Delta_{\vec{r}}\, e^{i\vec{k}\cdot\vec{r}} := \varepsilon_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}}$$

- Option 1 : $\displaystyle \Delta_{\vec{r}} f(\vec{r}) = \sum_{\alpha=1}^{3}\frac{f(\vec{r}+b\vec{u}_\alpha)+f(\vec{r}-b\vec{u}_\alpha)-2f(\vec{r})}{b^2}$

$$\Rightarrow \quad \varepsilon_{\vec{k}} = -\frac{\hbar^2}{mb^2}\sum_{\alpha=1}^{3}\left[\cos(k_\alpha b) - 1\right]$$

- Option 2 : $\displaystyle \varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$.

Second quantization :

$\hat{\Psi}_\sigma(\vec{r})$ annihilates a particle of spin $\sigma \in \{\uparrow,\downarrow\}$ in state $|\vec{r}\rangle$

$\hat{c}_{\vec{k},\sigma}$ ———————————————— $|\vec{k}\rangle$.

$\hat{n}_\sigma(\vec{r}) = \hat{\Psi}^+_\sigma(\vec{r})\,\hat{\Psi}_\sigma(\vec{r})$. $\hat{n}_{\vec{k},\sigma} = \hat{c}^+_{\vec{k},\sigma}\,\hat{c}_{\vec{k},\sigma}$

$$\hat{H} = \sum_{\sigma\in\{\uparrow,\downarrow\}} \sum_{\vec{k}\in\mathcal{D}_L} \varepsilon_{\vec{k}}\, \hat{n}_{\vec{k},\sigma} + g_0 \sum_{\vec{r}} b^3\, \hat{n}_\uparrow(\vec{r})\,\hat{n}_\downarrow(\vec{r})$$

For option 1 :
$$\hat{H} = -t \sum_{\substack{\vec{r},\vec{r}\,' \\ \|\vec{r}-\vec{r}\,'\|=b}} \hat{\Psi}^+_\sigma(\vec{r})\,\hat{\Psi}_\sigma(\vec{r}\,') + U \sum_{\vec{r}} \hat{n}_\uparrow(\vec{r})\hat{n}_\downarrow(\vec{r}) + 6t\hat{N}$$

$\boxed{t = \frac{\hbar^2}{2mb^2}}$ $\boxed{U = g_0 b^3}$ (Hubbard model)

2-body problem . $\psi(\vec{r})$. $-\frac{\hbar^2}{m}\Delta_{\vec{r}}\psi + V(\vec{r})\psi = E\cdot\psi$

$(L\to\infty)$ Scattering states $\longrightarrow$ a :

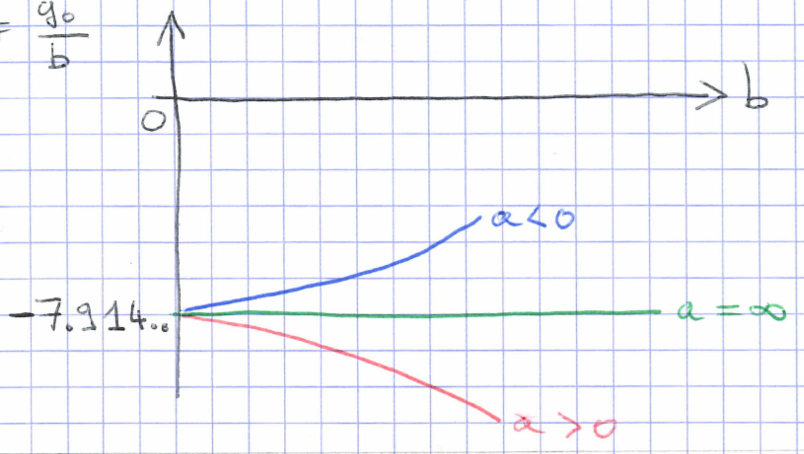
$$\frac{1}{g_0} = \frac{m}{4\pi\hbar^2 a} - I \quad , \quad I = \int_{\mathcal{D}} \frac{d^3k}{(2\pi)^3}\,\frac{1}{2\varepsilon_{\vec{k}}} .$$

Continuum limit [$\Leftrightarrow$ zero-range lim]

$b \to 0$, fixed a .

$$\boxed{I = \#\,\frac{m}{\hbar^2}\cdot\frac{1}{b}} \implies g_0 \underset{b\to 0}{\sim} -\frac{1}{I} = -\#\,\frac{\hbar^2}{m}\,b$$

$\frac{U}{t} = \#\,\frac{g_0}{b}$



filling factor: $n\,b^3 \propto b^3 \xrightarrow[b\to 0]{} 0$.

Chapter 1 — Many-body methods

Part 1: Virial expansion

Unpolarized gas. $(T, n \qquad , a)$

$$\underset{\mu}{\overset{\downarrow}{n}}$$

Grand-canonical: μ.

$$\boxed{\hat{H}\,|\nu\rangle = E_\nu\,|\nu\rangle} \qquad \boxed{\hat{N}\,|\nu\rangle = N_\nu\,|\nu\rangle}.$$

Observable $\hat{Q}$. $\langle\nu|\hat{Q}|\nu\rangle =: Q_\nu$.

$$Q = \langle\hat{Q}\rangle = \frac{\sum_\nu Q_\nu\, e^{-\beta(E_\nu-\mu N_\nu)}}{\sum_\nu e^{-\beta(E_\nu-\mu N_\nu)}} =: \frac{\tilde{Q}}{Z}.$$

$$\boxed{\tilde{Q} = \sum_{N=0}^{\infty} \underbrace{\left(\sum_{\nu/N_\nu=N} Q_\nu\, e^{-\beta E_\nu}\right)}_{\tilde{Q}_N} e^{\beta\mu\cdot N}} \qquad Z = \sum_N Z_N\, e^{\beta\mu\cdot N}$$

$$Q = \sum_{N=0}^{\infty} Q_N\, e^{\beta\mu\cdot N}$$

$\hookrightarrow$ simple combination of $\begin{cases}(\tilde{Q}_0, \cdots, \tilde{Q}_N)\\ (Z_0, \cdots, Z_N)\end{cases}$

$\Rightarrow$ $\leq N$-body problem.

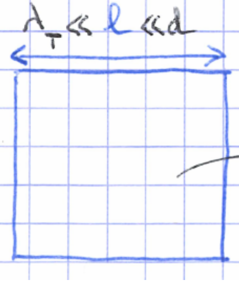
$$Q(\mu, T, a) \underset{\mu\to-\infty}{=} \sum_{N=0}^{\infty} Q_N(T, a)\, e^{\beta\mu N}$$

Can take $\mathcal{V} \to \infty$.

Physical justification: $n\lambda_T^3 \xrightarrow[\beta\mu\to-\infty]{} 0$.

$$e^{\beta\mu} \ll 1 \Rightarrow \lambda_T \ll d.$$

interacting gas $\simeq$ classical ideal gas, except at distances $\lesssim \lambda_T$.



Probability (N particles) $\sim \Big(\underbrace{n\,l^3}_{\ll 1}\Big)^N$

Part 2: Simple variational wavefunctions

$$\min_{\Psi \in \text{Ansatz}} \langle \Psi | \hat{H} | \Psi \rangle \geq E_{\text{exact}} \qquad (T=0)$$

($\hookrightarrow$ lattice model)

$\boxed{\text{BCS}}$ $\quad N_\uparrow = N_\downarrow = M$. $\qquad (N = 2M)$

$$\Psi(\underbrace{\vec{r}_1, \dots, \vec{r}_M}_{\uparrow}, \underbrace{\vec{r}_{M+1}, \dots, \vec{r}_N}_{\downarrow})$$

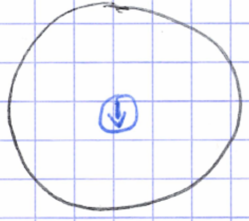
Antisymmetrizing: $\displaystyle (\hat{A}\Psi)(\vec{r}_1, \dots, \vec{r}_N) := \sum_{\substack{P_\uparrow, P_\downarrow \\ \text{permutations} \\ \text{of } \{1,\dots,M\}}} (-1)^{\varepsilon(P_\uparrow)+\varepsilon(P_\downarrow)} \psi(\vec{r}_{P_\uparrow(1)}, \dots, \vec{r}_{P_\uparrow(M)}, \vec{r}_{P_\downarrow(1)}, \dots, \vec{r}_{P_\downarrow(M)})$

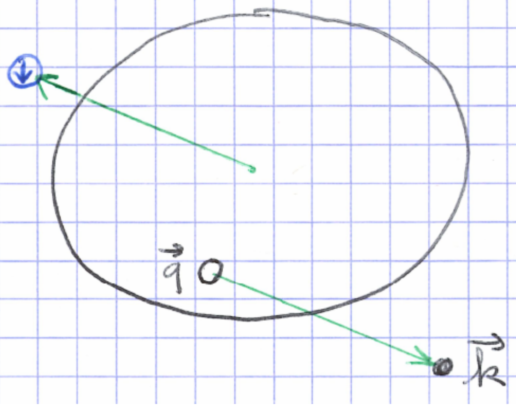
$$\Psi_{BCS} = (\#)\ \hat{A}\tilde{\Psi}, \qquad \tilde{\Psi}(\vec{r}_1, \dots, \vec{r}_N) = \phi(\vec{r}_1 - \vec{r}_{M+1})\phi(\vec{r}_2 - \vec{r}_{M+2}) \cdots \phi(\vec{r}_M - \vec{r}_N)$$

$\boxed{\text{Chevy}}$ $\quad$ Polaron : $\quad N_\downarrow = 1, \quad N_\uparrow \to \infty \quad \left(\text{fixed } \frac{N_\uparrow}{V}\right)$

$$|FS_\uparrow\rangle = \prod_{\substack{\vec{k} \\ k<k_F}} \hat{c}^+_{\vec{k},\uparrow} |0\rangle .$$

$$|\Psi_{\text{Chevy}}\rangle = \underbrace{\alpha_0 \hat{c}^+_{\vec{0},\downarrow} |FS_\uparrow\rangle}_{} + \underbrace{\sum_{\vec{k},\vec{q}} \alpha_{\vec{k},\vec{q}} \hat{c}^+_{\vec{q}-\vec{k},\downarrow} \hat{c}^+_{\vec{k},\uparrow} \hat{c}_{\vec{q},\downarrow} |FS_\uparrow\rangle}_{}$$

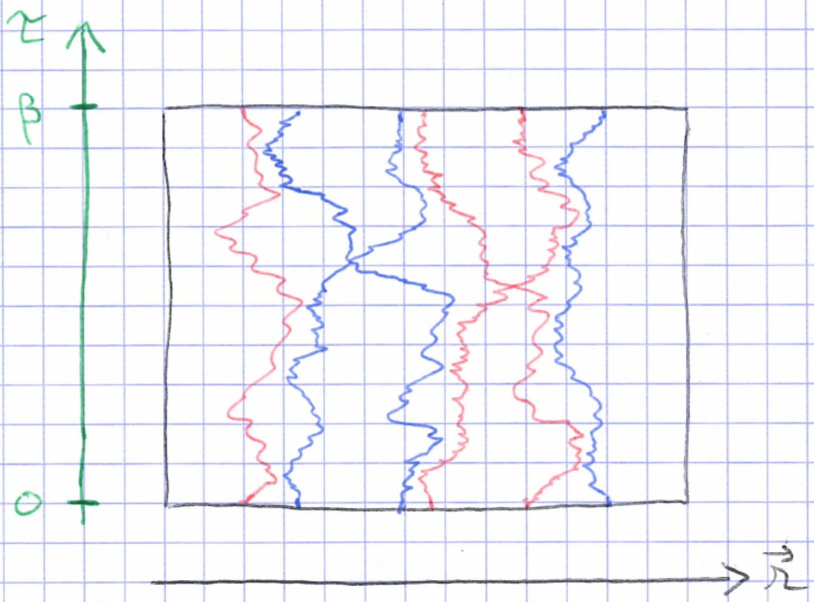




Part 3 : Quantum Monte Carlo (conventional)

$$\boxed{\begin{array}{c}\text{Quantum problem}\\ \vec{r} \in [0,L]^3\end{array}} \xrightarrow[(Z)]{\text{Mapping}} \begin{array}{c}\text{"Classical" problem}\\ (\vec{r}, \underset{\substack{\uparrow\\ \text{imaginary time}}}{\tau}) \in [0,L]^3 \times [0,\beta]\end{array}$$

- Mapping 1 : Path integrals. $\vec{r}_1(\tau), \dots, \vec{r}_N(\tau)$



PIQMC

- Mapping 2 : Auxiliary field $\phi(\vec{r}, \tau)$

AFQMC / Determinant QMC

$$Q = \langle \hat{Q} \rangle = \frac{\sum_{\mathcal{C}} Q(\mathcal{C})\, w(\mathcal{C})}{\sum_{\mathcal{C}} w(\mathcal{C})}$$

→ generically : $w(\mathcal{C})$ can be < 0.

$$\left| \sum_{\mathcal{C}} w(\mathcal{C}) \right| \ll \sum_{\mathcal{C}} |w(\mathcal{C})|$$

$$t_{CPU} \sim \exp(\# \beta \mathcal{V}) .$$

$\boxed{\text{Sign problem}}$ ☹

→ special cases : $w(\mathcal{C}) \geq 0 \, , \, \forall \mathcal{C}$

↳ unpolarized gas + lattice model.

[sign problem = physical ?..]

Approximations to remove sign problem : Fixed-node

$$\mathcal{N}[\Psi] := \left\{ (\vec{r}_1, .., \vec{r}_N) \; / \; \Psi(\vec{r}_1, ..., \vec{r}_N) = 0 \right\}.$$

$$\underset{\{\Psi / \mathcal{N}[\Psi] = \mathcal{N}[\Psi_{\text{Ansatz}}]\}}{\text{Min}} \langle \Psi | \hat{H} | \Psi \rangle$$

$$\text{Ansatz} \longrightarrow \begin{cases} \Psi_{\text{BCS}} & \text{(unpolarized gas in continuous space)} \\ \Psi_{\text{ideal}} & \text{(polarized gas)} \end{cases}$$

Part 4 : Diagrammatic approaches

$$\hat H' := \hat H - \mu_\uparrow \hat N_\uparrow - \mu_\downarrow \hat N_\downarrow .$$

Lattice model : $$\hat H' = \underbrace{\sum_{\vec k,\sigma} (\varepsilon_{\vec k} - \mu_\sigma)\, \hat n_{\vec k,\sigma}}_{\hat H'_0} + g_0 \sum_{\vec r} b^3 \hat n_\uparrow(\vec r)\hat n_\downarrow(\vec r)$$

$$Q(g_0; T, \mu_\uparrow, \mu_\downarrow) = \langle \hat Q \rangle_{H'} \equiv \frac{\mathrm{Tr}[\hat Q\, e^{-\beta \hat H'}]}{\mathrm{Tr}[e^{-\beta \hat H'}]} .$$

E.g. : $\hat Q = \hat n_\uparrow(\vec 0)$. $Q = n_\uparrow$

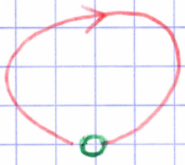
[$n_\sigma(T, \mu_\uparrow, \mu_\downarrow)$ is Eq. of state]

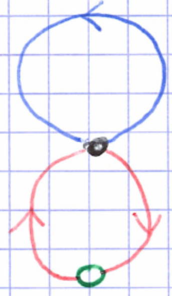
Diagrams for the lattice model

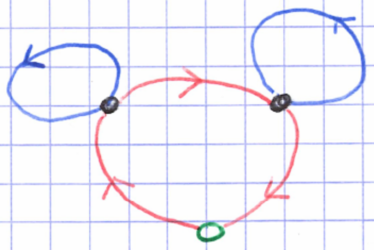
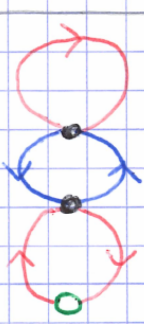
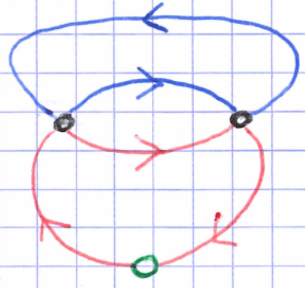
Bare expansion in powers of g_0

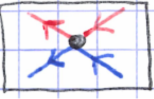
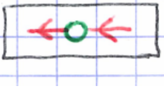
$$Q(g_0) = \sum_{N=0}^{\infty} \underbrace{Q_N\, g_0^N}_{a_N} .$$

For $Q = n_\uparrow$:

$a_0 =$ 

$a_1 =$ 

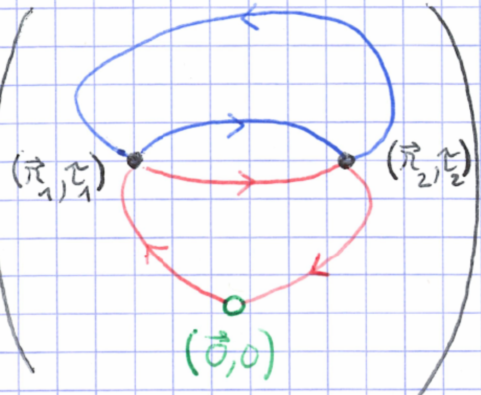
$a_2 =$  +  + 

Rules : • all connected diagrams, with N  and 1 

- Contribution :

Define: $\begin{cases} \hat{\psi}_\sigma(\vec{r},\tau) = e^{\tau H_0'} \hat{\psi}_\sigma(\vec{r}) e^{-\tau H_0'} \\ \hat{\psi}^{+}_\sigma(\text{---}) = \text{---}\ \hat{\psi}^{+}_\sigma(\vec{r})\ \text{---} \end{cases}$ | $G_{0,\sigma}(\vec{r},\tau) = \begin{cases} -\left\langle \hat{\psi}_\sigma(\vec{r},\tau)\hat{\psi}^{+}_\sigma(\vec{0},0)\right\rangle_{H_0'}, & \tau > 0 \\ +\left\langle \hat{\psi}^{+}_\sigma(\vec{0},0)\hat{\psi}_\sigma(\vec{r},\tau)\right\rangle_{H_0'}, & \tau < 0 \end{cases}$

Contribution $\left(\right.$



$\left. \right)$ $= (-1)^{N_\ell} (-g_0)^2 \sum_{\vec{r}_1} b^3 \int_0^\beta d\tau_1 \sum_{\vec{r}_2} \int_0^\beta d\tau_2$

$G_{0\uparrow}(\vec{r}_1,\tau_1)\, G_{0\uparrow}(\vec{r}_2-\vec{r}_1,\tau_2-\tau_1)\, G_{0\uparrow}(-\vec{r}_2,-\tau_2)$

$G_{0\downarrow}(\vec{r}_2-\vec{r}_1,\tau_2-\tau_1)\, G_{0\downarrow}(\vec{r}_1-\vec{r}_2,\tau_1-\tau_2)$

$\boxed{N_\ell = \#\ \text{internal closed loops} = 1}$

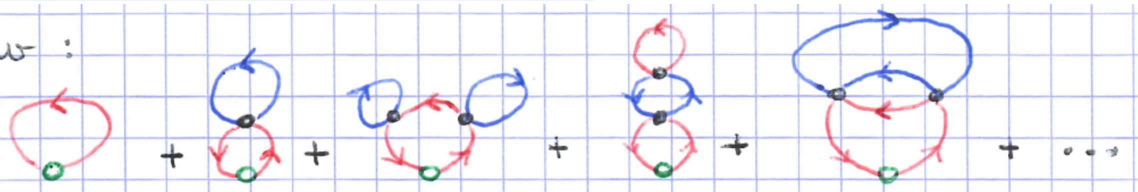
Can take $\mathcal{V} \longrightarrow \infty$ (at fixed μ_σ)

$\sum_{\vec{r}_i \in \text{infinite lattice}}$ converge, because $\begin{cases} \bullet \text{ diagrams are connected} \\ \bullet\ G_0(\vec{r},\tau) \xrightarrow[r\to\infty \text{ (quickly)}]{} 0 \end{cases}$

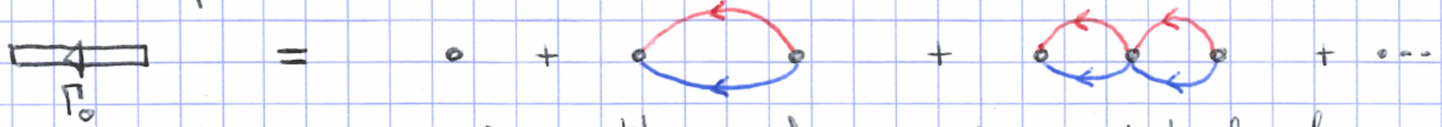
Diagrams for the Zero-Range Model

We saw :

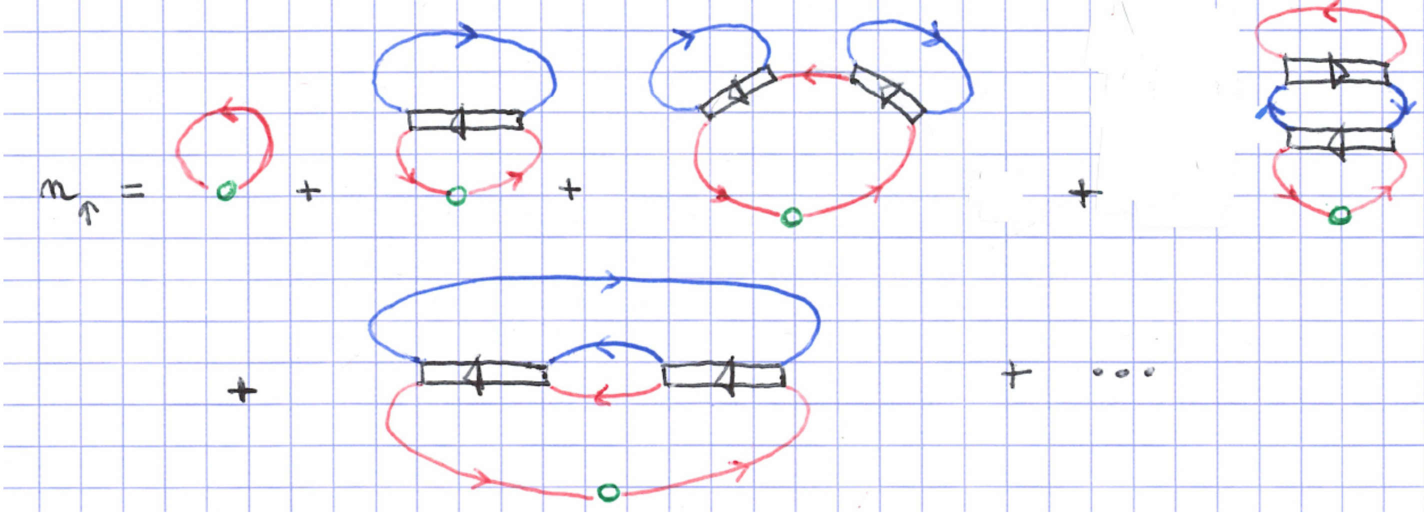
$n_\uparrow$ =



Let us define :



Then we express $n_\uparrow$ using the vertex  instead of ●



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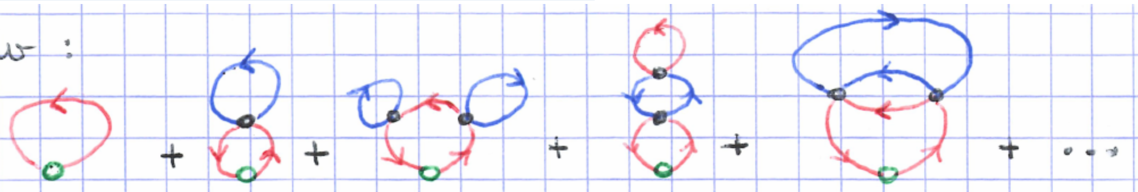
$n_\uparrow =$ 

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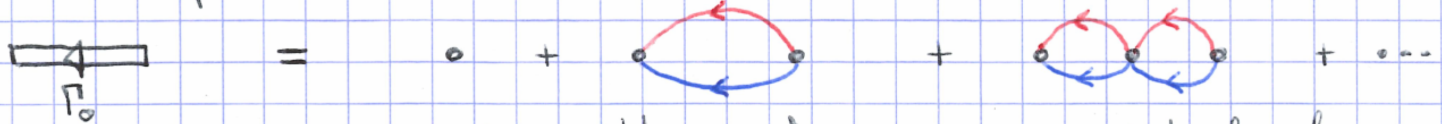

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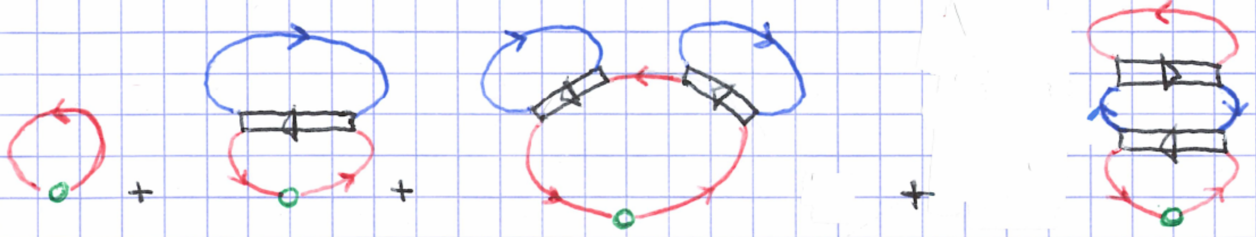
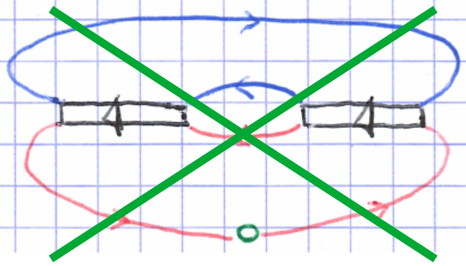
$n_\uparrow =$ 

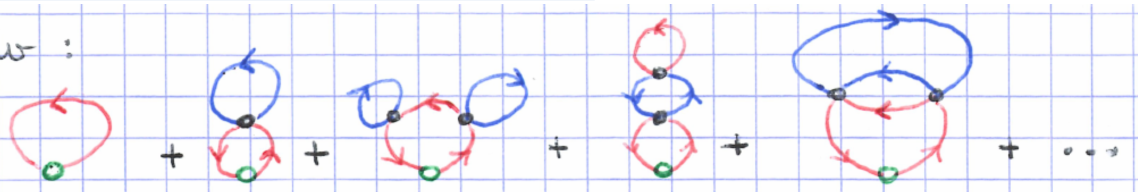
\+  + . . .

forbidden
(avoid double-counting)

Diagrams for the Zero-Range Model

We saw:

$n_\uparrow$ =



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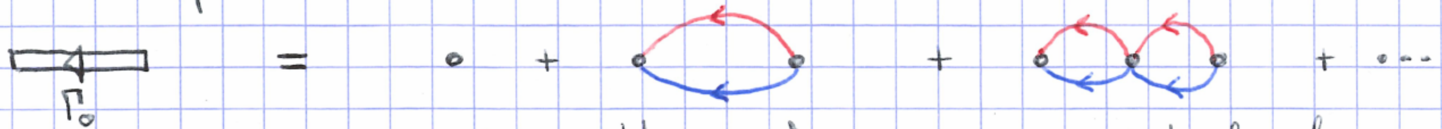

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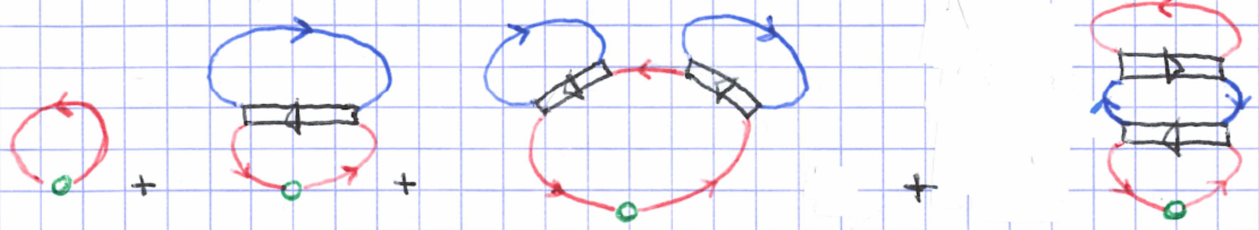
$n_\uparrow$ =



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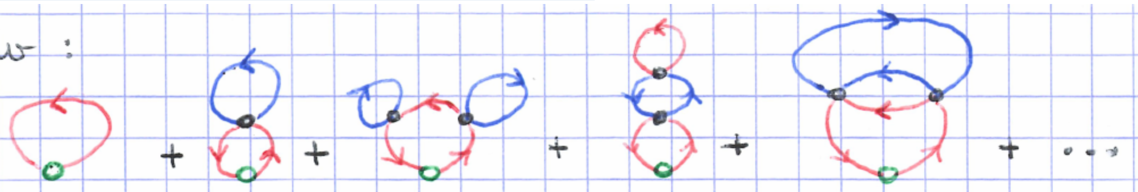

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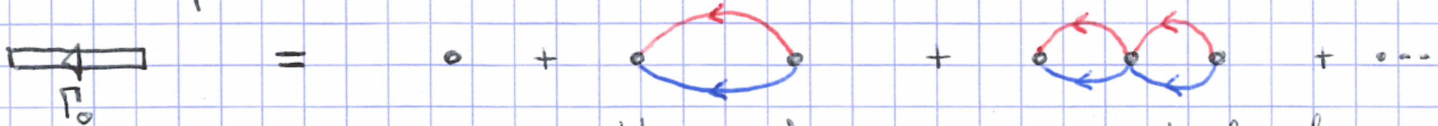

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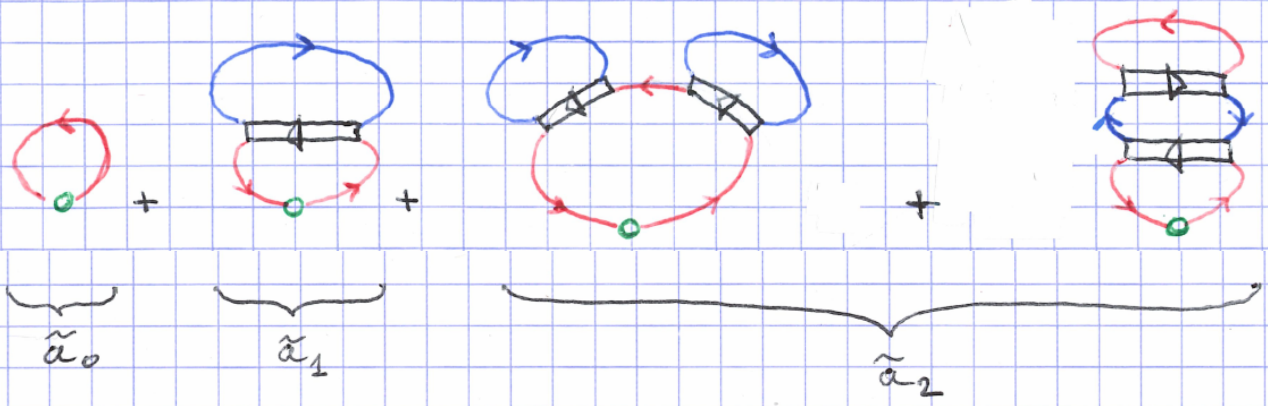

$$n_\uparrow = \sum_{N=0}^{\infty} \underbrace{\tilde{a}_N}_{\longrightarrow N \ \Gamma_0\text{-vertices}}$$

Continuum limit : $\Gamma_0 \longrightarrow$ Finite limit

$\tilde{a}_N \longrightarrow$ ______________

☺

$n_\uparrow \simeq \tilde{a}_0 + \tilde{a}_1$ Nozières — Schmitt-Rink

Sum all $\tilde{a}_N$?

Diagrammatic MC : $\tilde{a}_N$, $N \leq N_m = 9$.

Problem : $\sum_{N=0}^{N_m} \tilde{a}_N$ diverges for $N_m \to \infty$.

$$|\tilde{a}_N| \sim (N!)^{1/5}$$

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Solution :

$$\sum_{N=0}^{\infty} \tilde{a}_N$$

we need to give a meaning to this sum

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$$|\tilde{a}_N| \sim (N!)^{1/5}$$

Solution :

$$f(z) \underset{z \to 0}{=} \sum_{N=0}^{\infty} \tilde{a}_N \, z^N$$

$$\Big\downarrow \text{ Unique .}$$

$f(z)$ constructed so that $f(1) = n_\uparrow$

$$\begin{array}{c} f(z) \\ \shortparallel \\ \langle n_\uparrow \rangle_{S(z)} \\ (T > T_c) \end{array}$$

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$\big\downarrow$ Unique . (conformal Borel transformation)

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$(T > T_c)$

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$\downarrow$ Unique. (conformal Borel transformation)

$f(z)$ constructed so that $f(1) = m_\uparrow$

$$f(z) = \langle m_\uparrow \rangle_{S(z)}$$

$(T > T_c)$

NB: For polaron problem:

- Very efficient algorithm $\Rightarrow$ can reach $N_m = 30$
- Series divergence is much slower, $\tilde{a}_N \underset{N\to\infty}{\sim} (-A)^N$ with $A \simeq 1.1$

$\Rightarrow$ resummable by simple conformal transformation

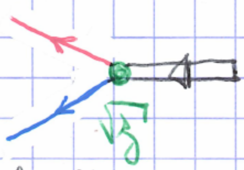
[Rossi *et al.*, PRB **101**, 045134 (2020)]

Appendix A : Construction of $f(z)$

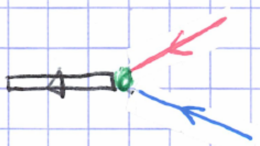
Introduce a model defined by an action $S^{(z)}$ (z is a formal parameter):

$$S^{(z)}[\underbrace{\varphi_\uparrow , \varphi_\downarrow}_{\substack{\text{fermionic}\\ \text{fields}\\ \text{(Grassmann)}}} , \underbrace{\eta}_{\substack{\text{bosonic}\\ \text{field}\\ \text{(complex)}}}]$$

- $S^{(0)}$ such that $\begin{cases} G_{0,\sigma}(\vec{r},\tau) = -\langle \varphi_\sigma(\vec{r},\tau)\bar{\varphi}_\sigma(\vec{0},0)\rangle_{S^{(0)}} \\ \Gamma_0(\vec{r},\tau) = -\langle \eta(\vec{r},\tau)\bar{\eta}(\vec{0},0)\rangle_{S^{(0)}} \end{cases}$
- interaction :



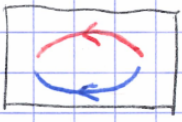
and



- + term to avoid double-counting

$$S^{(z)}[\varphi_\uparrow,\varphi_\downarrow,\eta] = -\int d^3r \int_0^\beta d\tau \Big[\sum_{\sigma=\uparrow,\downarrow} \bar{\varphi}_\sigma G_{0,\sigma}^{-1}\varphi_\sigma + \bar{\eta}\Gamma_0^{-1}\eta$$
$$- z\,\bar{\eta}\,\Pi_0\,\eta + \sqrt{z}\,(\bar{\eta}\,\varphi_\downarrow\varphi_\uparrow + \bar{\varphi}_\uparrow\bar{\varphi}_\downarrow\,\eta)\Big](\vec{r},\tau),$$

$\Pi_0 := G_{0\uparrow}G_{0\downarrow} =$



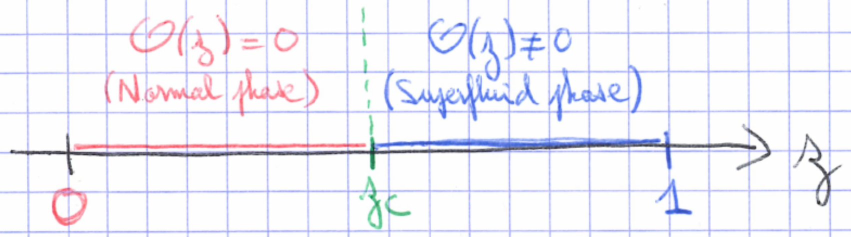
[Rossi et. al., PRB $\underline{93}$, 161102(R) (2016) ;
Rossi et al., PRL $\underline{121}$, 130405 (2018)]

Appendix B : Extension to superfluid phase

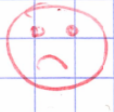
Let $\mathcal{O}(z) := \langle \psi_\downarrow \psi_\uparrow \rangle_{S(z)}$.

$\mathcal{O}(1) \neq 0$. Thus :

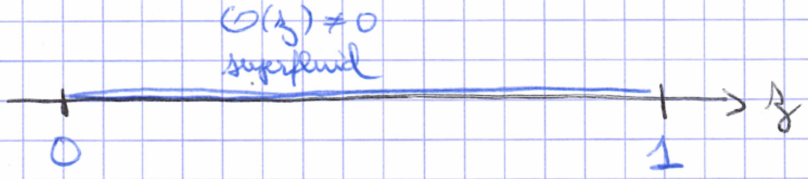
→ if $S^{(0)}$ does not break $U(1)$ (i.e., conserves N)
then : $\mathcal{O}(0) = 0$ (given that $S^{(0)}$ is quadratic).



⇒ a phase transition as a function of z, at $z_c < 1$



→ Solution : take $S^{(0)}$ which breaks $U(1)$,
e.g. $S^{(0)} = S_{BCS}$. Then, $\mathcal{O}(0) \neq 0$



The resulting diagrams contain "anomalous" propagators :

$$\begin{cases} \langle \psi_\uparrow(\vec{r},\tau)\, \psi_\downarrow(\vec{0},0) \rangle_{S^{(0)}} \\ \langle \psi^+_\downarrow(\vec{r},\tau)\, \psi^+_\uparrow(\vec{0},0) \rangle_{S^{(0)}} \end{cases}$$

Diagrammatic MC for the attractive Hubbard model in the superfluid phase : [Spada et al., arXiv:2103.12038]

Appendix C : Determinant Diagrammatic Monte Carlo

(a.k.a. Continuous-Time INTeraction expansion)

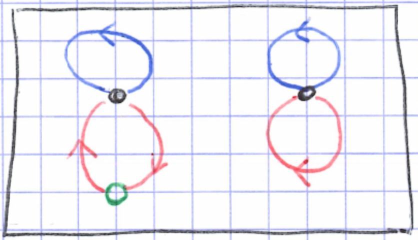
$$Q = \frac{A}{Z}$$ Separately expand in powers of g_0

(instead of expanding Q as above).

$$\Rightarrow \quad A = \sum_{N=0}^{\infty} A_N \, g_0^{\,N} , \qquad Z = \sum_{N=0}^{\infty} Z_N \, g_0^{\,N} .$$

Now, disconnected diagrams are allowed.

E.g. A_2 contains the disconnected diagram :



$$\xrightarrow[v \to \infty]{} \infty$$

$\Rightarrow$ need to work with finite system.

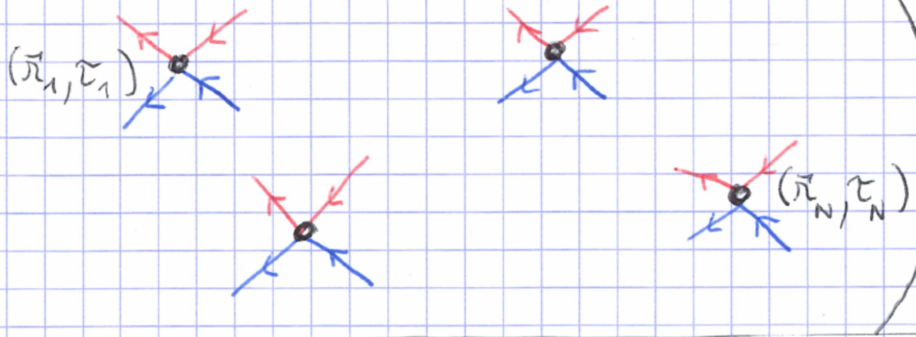
(This is actually a "conventional" QMC method, as discussed in Part 3)

Also, each diagram $\longrightarrow 0$ in the continuum limit $b \to 0$.

But :
- The series always converges
- For $\mu_\uparrow = \mu_\downarrow$: efficient sign-free algorithm
  - $\Rightarrow$ one can reach very high orders (several 10^3)

Contribution to Z_N :

$$\sum_{\substack{\text{all}\\ \text{connections}}} \Bigg($$



$$\Bigg) = \prod_{\sigma=\uparrow,\downarrow} \det \underbrace{\mathcal{G}^{(\sigma)}}_{\downarrow \; N^3 \text{ operations}} ,$$

$$\mathcal{G}^{(\sigma)}_{ij} := G_{0,\sigma}(\vec{r}_i - \vec{r}_j, \tau_i - \tau_j).$$

[Burovski et al., PRL 96, 160402 (2006)] [also : Rubtsov, arXiv: 0302228 ; PRB 72, 035122]

Chapter 2

Many-body physics: some basic properties

Part 1: Unpolarized unitary gas

Equation of state

$T = 0$ $\xi \simeq 0.37$

Experiments:

- MIT + correction(Heidelberg) [Ku *et al.*, Science **335**, 563 (2012); Zürn *et al.*, PRL **110**, 135301 (2013)]:

  $$\xi = 0.370(5)_{\mathrm{stat}}(8)_{\mathrm{sys}}$$

- USTC [Li *et al.*, Science **375**, 528 (2022)]:

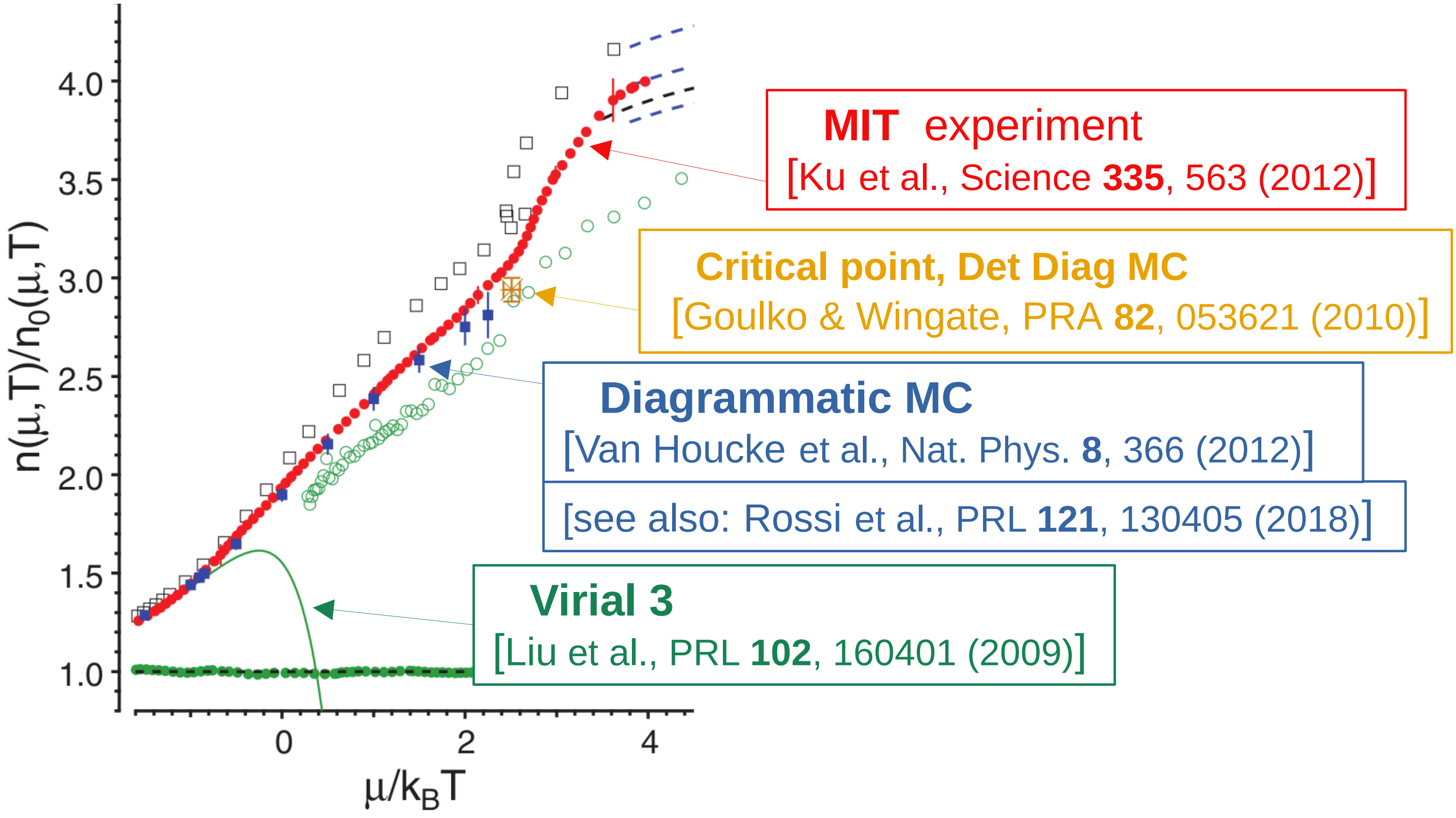
  $$\xi = 0.367(9)$$

AFQMC [Carlson *et al.*, PRA **84**, 061602(R) (2011)]: $\xi = 0.372(5)$

Variational calculations: BCS ansatz: $\xi < 0.59$

Fixed-node QMC: $\xi < 0.38$ [Forbes *et al.*, PRL **106**, 235303 (2011)]

Finite T



MIT experiment
[Ku et al., Science **335**, 563 (2012)]

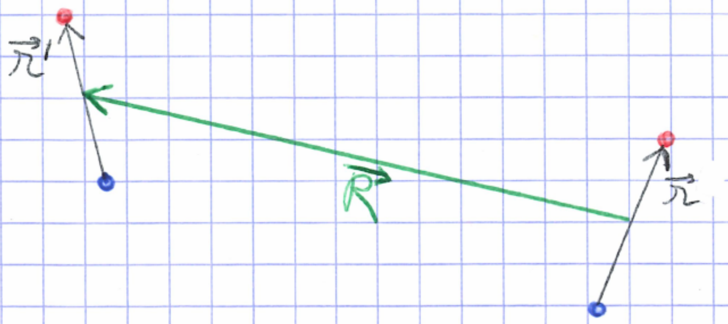
Critical point, Det Diag MC
[Goulko & Wingate, PRA **82**, 053621 (2010)]

Diagrammatic MC
[Van Houcke et al., Nat. Phys. **8**, 366 (2012)]

[see also: Rossi et al., PRL **121**, 130405 (2018)]

Virial 3
[Liu et al., PRL **102**, 160401 (2009)]

Long - range order



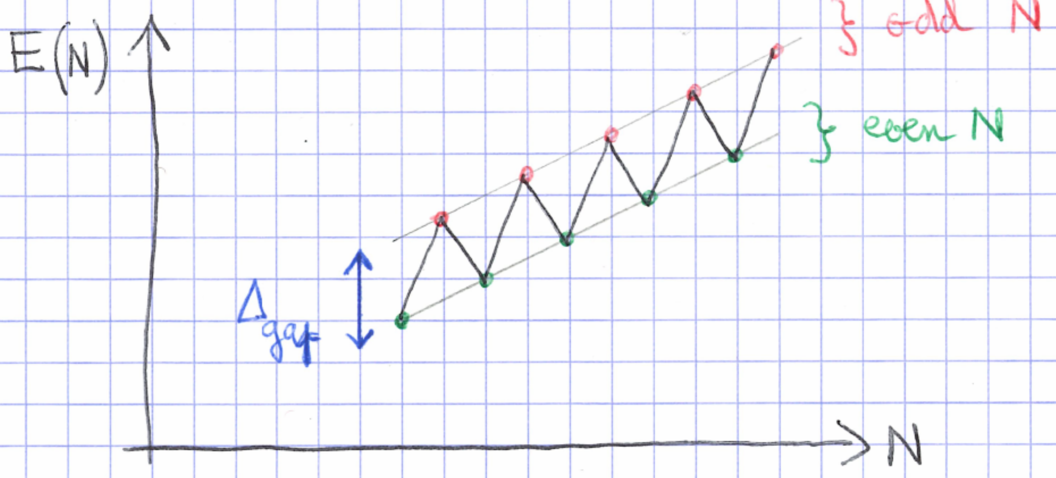
$$\left\langle \hat\Psi^+_\uparrow\left(\vec R + \frac{\vec r'}{2}\right) \hat\Psi^+_\downarrow\left(\vec R - \frac{\vec r'}{2}\right) \hat\Psi_\downarrow\left(-\frac{\vec r}{2}\right) \hat\Psi_\uparrow\left(\frac{\vec r}{2}\right) \right\rangle$$

$$\xrightarrow[R\to\infty]{} \left(\frac{m}{4\pi\hbar^2}\right)^2 |\Delta|^2 \;\phi_p(r')\; \underbrace{\phi_p(r)}_{\text{Pair wavefunction.}}$$

order parameter

$$\underset{r\to 0}{\sim} \frac{1}{r}$$

Pairing gap



$$\Delta_{gap} = \lim_{M\to\infty}\left[\frac{E(2M+1)+E(2M-1)}{2} - E(2M)\right]$$

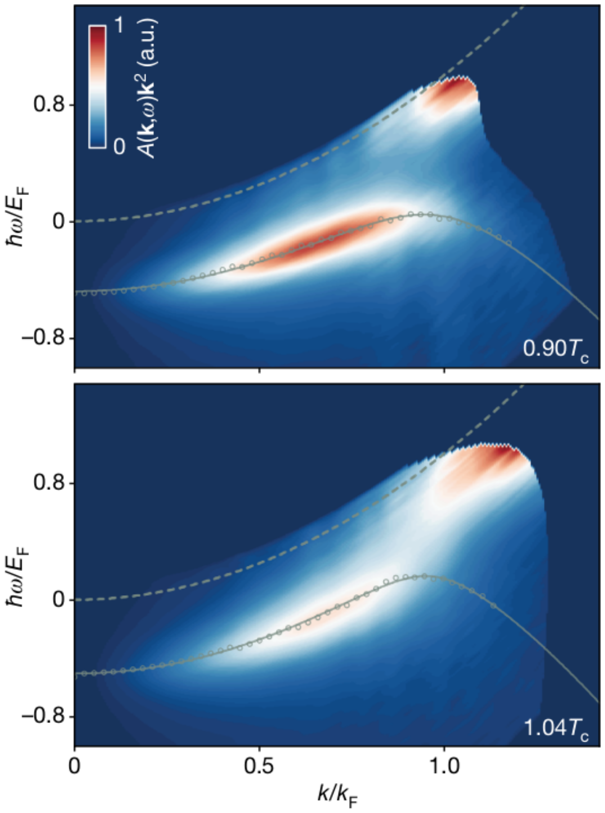
"cost for breaking a pair"

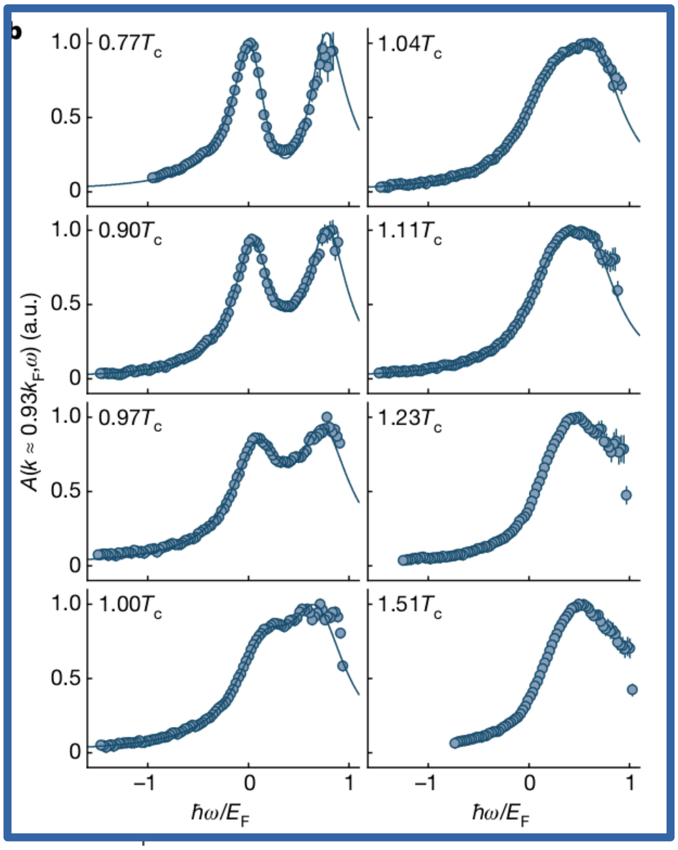
$\boxed{\Delta_{gap} \neq \Delta}$ (except for BCS theory, in regime $\mu > 0$)

	Fixed-node QMC [Carlson & Reddy, PRL <u>100</u>, 150403 (2008)]	Experiments	
		MIT [Schirotzek et al, PRL <u>101</u>, 140403 (2008)]	Swinburne [Hoinka et al., Nat. Phys. <u>13</u>, 943 (2017)]
$\frac{\Delta_{gap}}{\varepsilon_F}$	0.45(5)	0.44(3)	0.47(3)

Spectral function

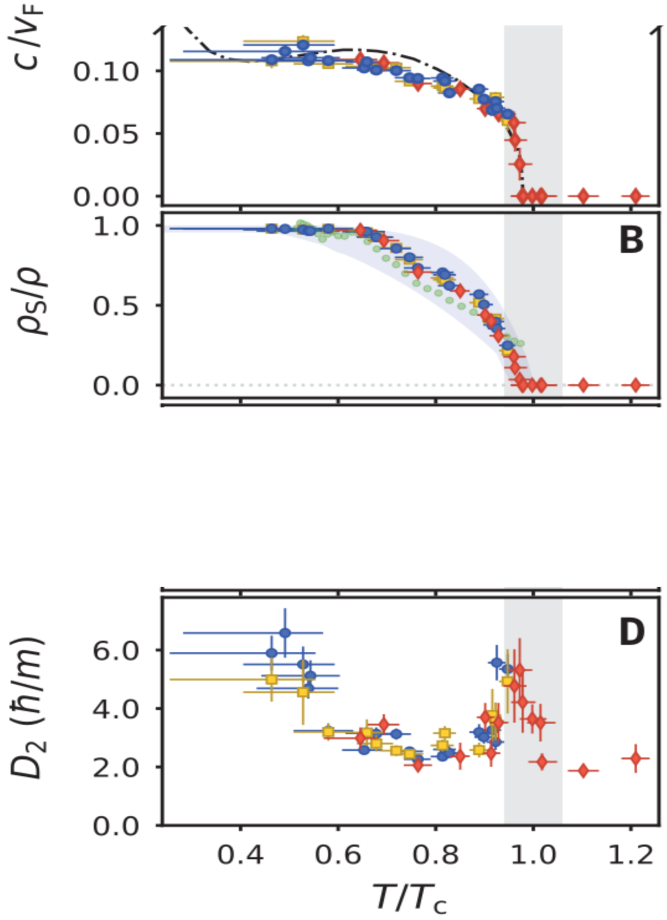
USTC [Li et al., Nature **626,** 288 (2024)]



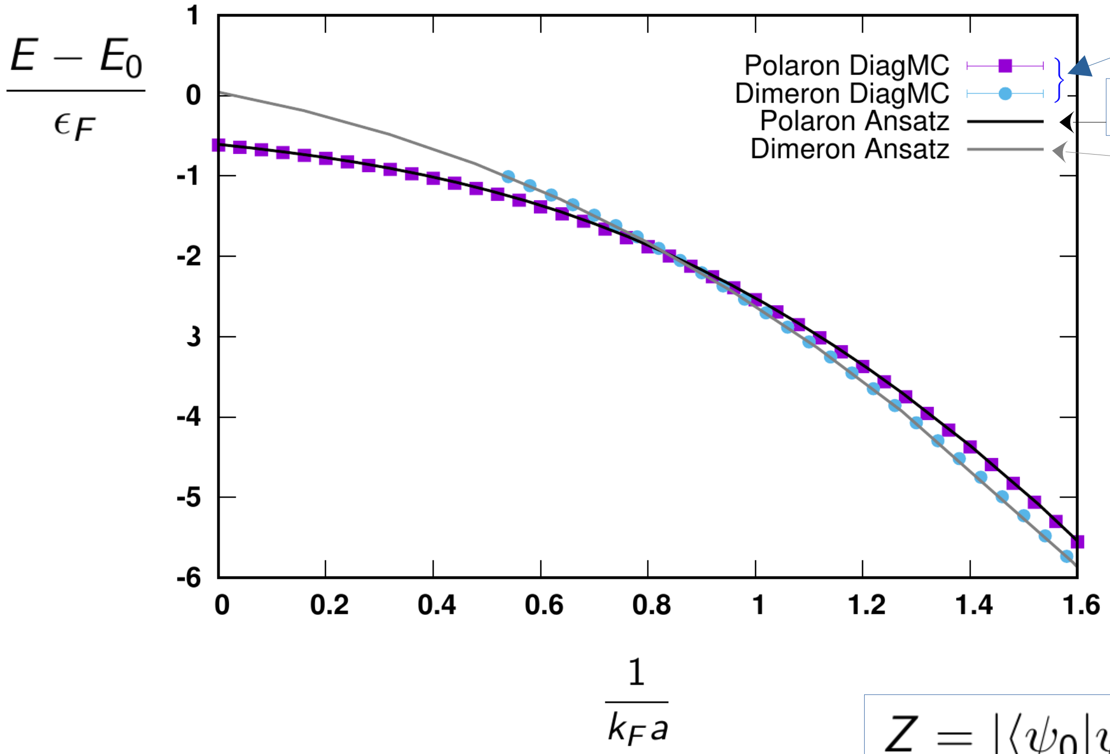


Second sound

MIT [Yan et al., Science **383**, 629 (2024)]



Part 2: Fermi polaron



[Vlietinck et al., PRB **87**, 115133 (2013) ; Prokof'ev & Svistunov, PRB **77**, 020408(R) (2008)]

[Chevy, PRA **74**, 063628 (2006)]

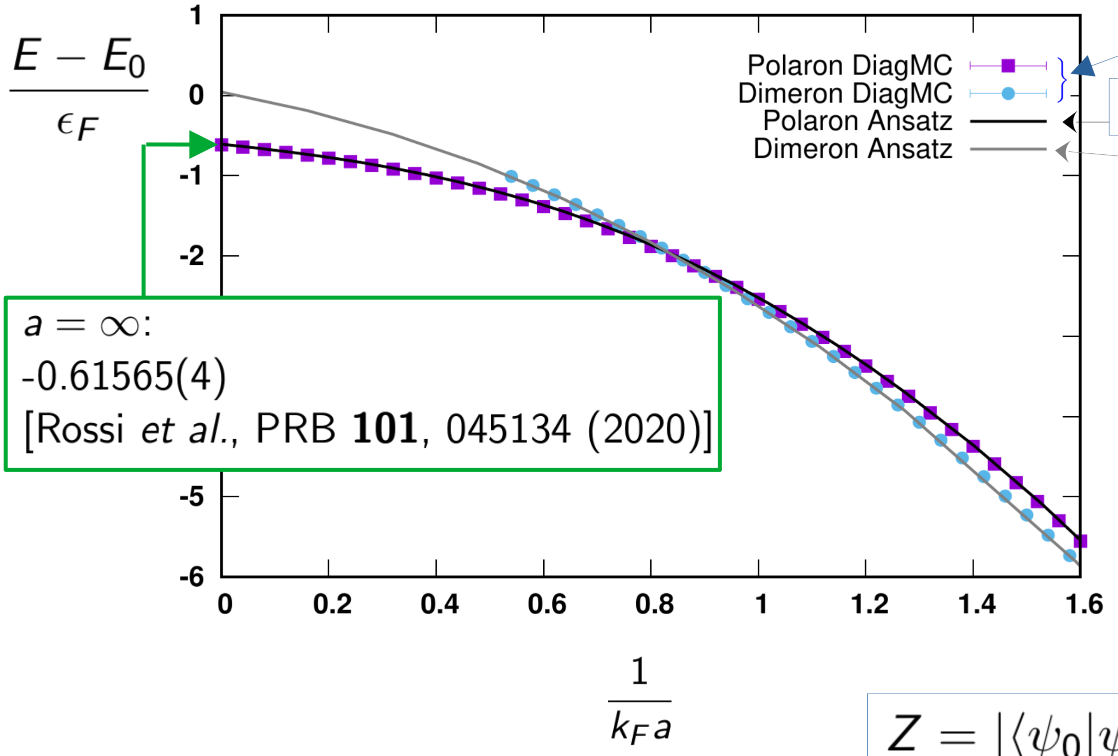
[Punk et al., PRA **80**, 053605 (2009)]

non-interacting: $\boxed{|\psi_0\rangle = c^{\dagger}_{\vec{0},\downarrow}\,|\mathrm{FS}_{\uparrow}\rangle}$ $\boxed{E_0}$

$$Z = |\langle\psi_0|\psi\rangle|^2 \neq 0\,, \quad \text{polaron}$$

$$= 0\,, \quad \text{dimeron}$$

Part 2: Fermi polaron



$a = \infty$:
-0.61565(4)
[Rossi *et al.*, PRB **101**, 045134 (2020)]

[Vlietinck et al.,
PRB **87**, 115133 (2013) ;
Prokof'ev & Svistunov,
PRB **77**, 020408(R) (2008)]

[Chevy, PRA **74**, 063628 (2006)]

[Punk et al.,
PRA **80**, 053605 (2009)]

non-interacting: $|\psi_0\rangle = c^\dagger_{\vec{0},\downarrow}\,|\mathrm{FS}_\uparrow\rangle$ $\boxed{E_0}$

$$Z = |\langle\psi_0|\psi\rangle|^2 \neq 0\,, \quad \text{polaron}$$
$$= 0\,, \quad \text{dimeron}$$

Part 3: Polarized gas

SF – normal phase transition : 1st order at low T

exp: MIT [Shin et al., Nature **451**, 689 (2008)]
ENS [Nascimbène et al., Nature **463**, 1057 (2010) ;
Navon et al., Science **328**, 729 (2010)]

fixed-node QMC [Pilati & Giorgini, PRL **100**, 030401 (2008)]

unconventional SF phases:

p-wave

FFLO

Lecture 3

2-body and 3-body contacts

Lecture 3

2-body and 3-body contacts

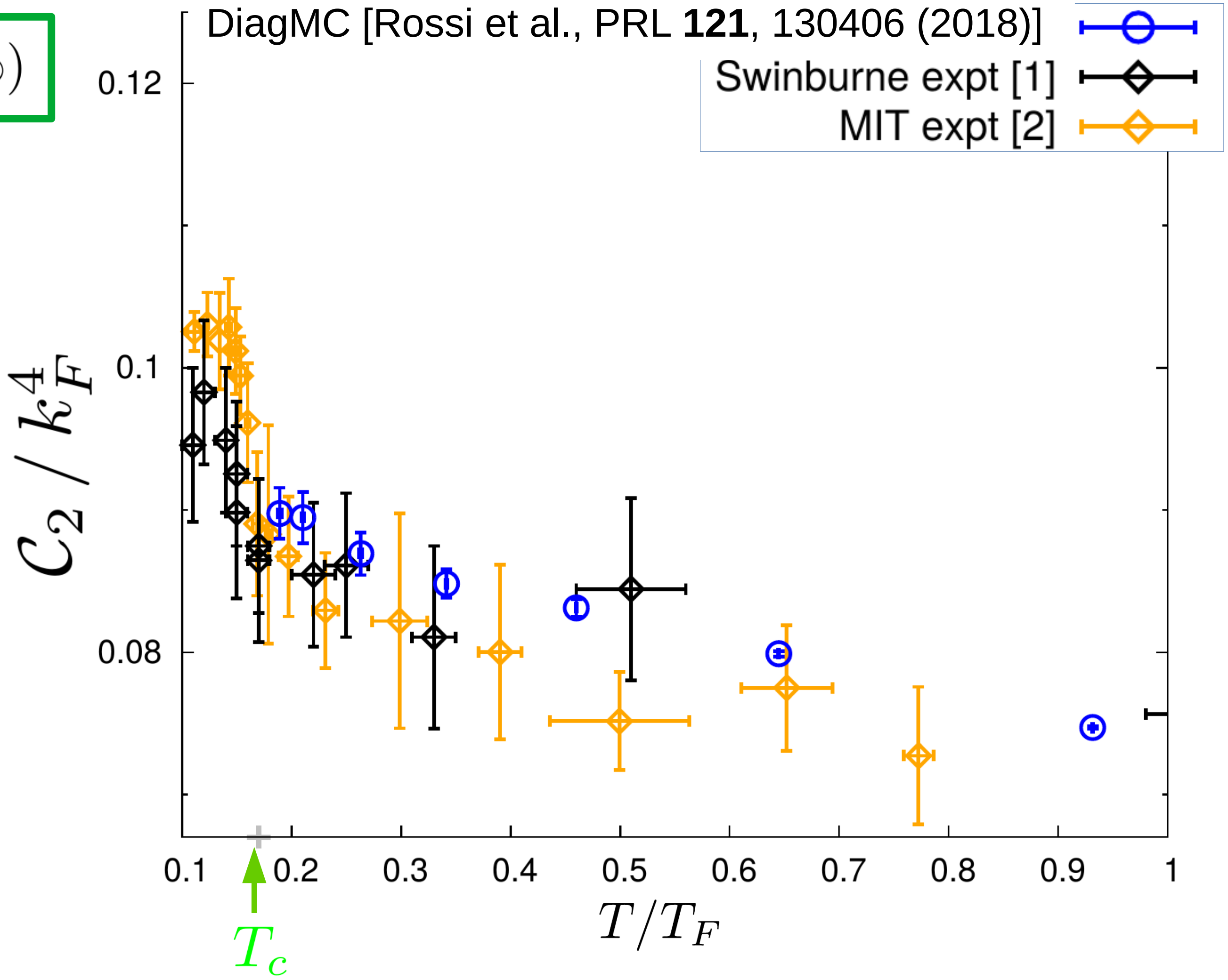
- S. Tan, Ann. Phys. **323**, 2952 (2008); Ann. Phys. **323**, 2971 (2008)
- with Y. Castin: Lect. Notes Phys. **836**, 127 (2012); PRA **86**, 013626 (2012)
- with X. Leyronas: C. R. Phys. **25**, 179 (2024)

Tan’s two-body contact

$$\langle\, \hat{n}_\uparrow(\mathbf{r})\, \hat{n}_\downarrow(\mathbf{0})\, \rangle \underset{r\to 0}{\sim} \frac{\mathcal{C}_2}{(4\pi\, r)^2}$$

$$n_\sigma(k) \underset{k\to\infty}{\sim} \frac{\mathcal{C}_2}{k^4} \qquad (\sigma = \uparrow, \downarrow)$$

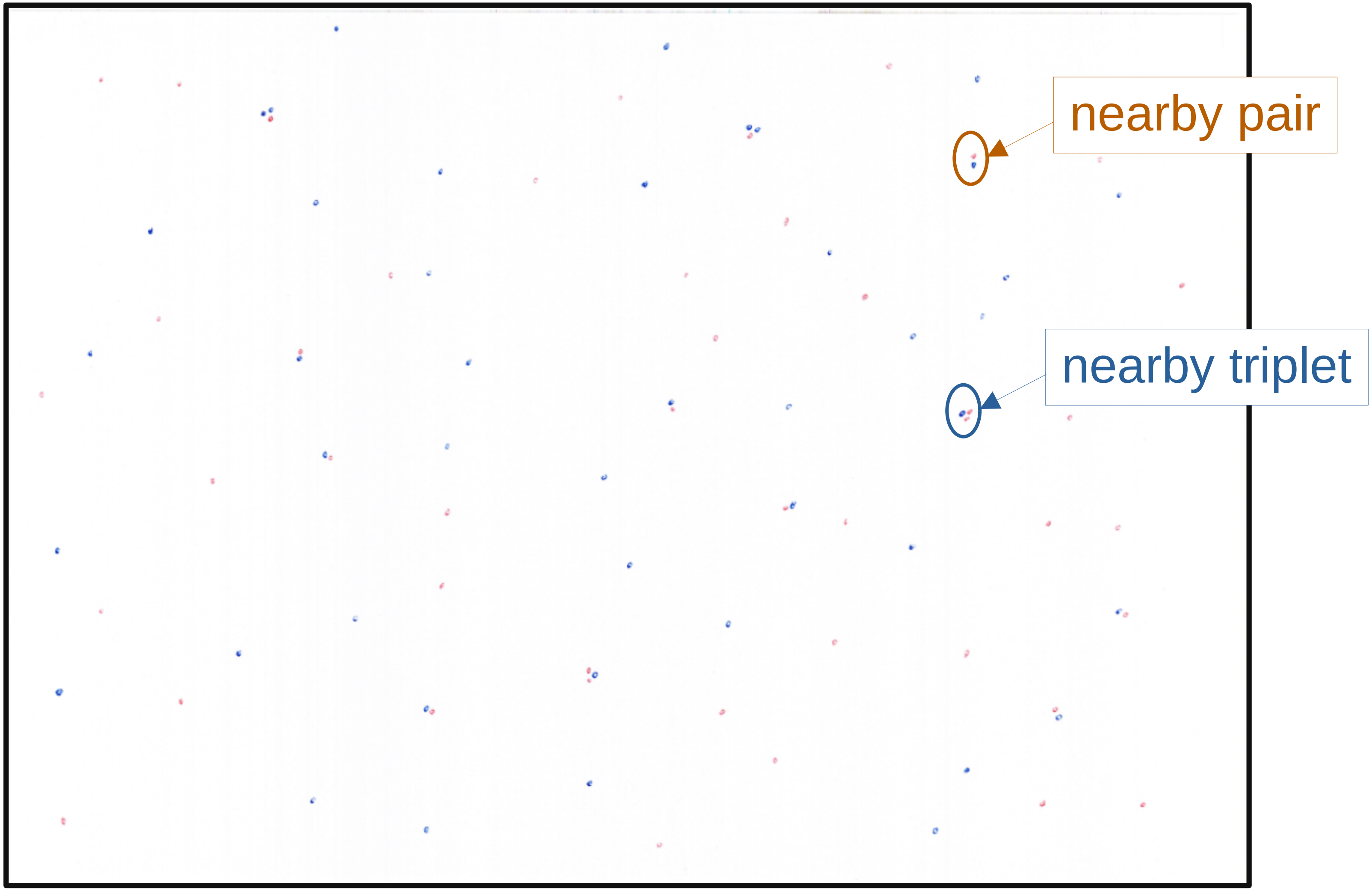
unitary Fermi gas $\quad (a_2 = \infty)$



[1] **Carcy, Hoinka, Lingham, Dyke, Kuhn, Hu, Vale, PRL 2019**
[2] **Mukherjee, Patel, Yan, Fletcher, Struck, Zwierlein, PRL 2019**

NUMBER OF NEARBY PAIRS & TRIPLETS

Gedankenexperiment: Measure positions of $|\uparrow\rangle$ and $|\downarrow\rangle$ atoms



nearby pair

nearby triplet

NUMBER OF NEARBY PAIRS & TRIPLETS

$$\boxed{N_2(\epsilon) := \text{number of pairs separated by } r < \epsilon}$$

$$\left[\text{ without interactions: } \quad N_2^{(0)}(\epsilon) \;\propto\; \epsilon^3 \quad \right]$$

$$\boxed{N_2(\epsilon) \underset{\epsilon\to 0}{\sim} C_2 \, \frac{\epsilon}{4\pi}}$$

[Tan 2008]

NUMBER OF NEARBY PAIRS & TRIPLETS

(CC): $\psi \propto 1/r$ for $r \to 0$

$\Downarrow$

$N_2(\epsilon) :=$ number of pairs separated by $r < \epsilon$

$$\left[\text{ without interactions: } \quad N_2^{(0)}(\epsilon) \propto \epsilon^3 \right]$$

$$\boxed{N_2(\epsilon) \underset{\epsilon \to 0}{\sim} C_2 \frac{\epsilon}{4\pi}}$$

[Tan 2008]

NUMBER OF NEARBY PAIRS & TRIPLETS

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[Tan 2008]

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[Tan 2008]

$$\left[\text{ without interactions: } \quad N_2^{(0)}(\epsilon) \, \propto \, \epsilon^3 \quad \right]$$

$$N_3(\epsilon) := \text{number of triplets of hyperradius } R < \epsilon$$

$$R := \sqrt{\frac{2}{3} \left(r_{ij}^2 + r_{ik}^2 + r_{jk}^2 \right)}$$

NUMBER OF NEARBY PAIRS & TRIPLETS

$N_2(\epsilon) :=$ number of pairs separated by $r < \epsilon$

$$\left[\text{ without interactions: } \quad N_2^{(0)}(\epsilon) \, \propto \, \epsilon^3 \quad \right]$$

$$\boxed{N_2(\epsilon) \underset{\epsilon \to 0}{\sim} C_2 \, \frac{\epsilon}{4\pi}}$$

[Tan 2008]

$N_3(\epsilon) :=$ number of triplets of hyperradius $R < \epsilon$

NUMBER OF NEARBY PAIRS & TRIPLETS

$N_2(\epsilon) :=$ number of pairs separated by $r < \epsilon$

$$\left[\text{ without interactions: } \quad N_2^{(0)}(\epsilon) \propto \epsilon^3 \right]$$

$$\boxed{N_2(\epsilon) \underset{\epsilon\to 0}{\sim} C_2 \frac{\epsilon}{4\pi}}$$

[Tan 2008]

$N_3(\epsilon) :=$ number of triplets of hyperradius $R < \epsilon$

$$\boxed{N_3(\epsilon) \underset{\epsilon\to 0}{\sim} C_3 \, \epsilon^{2s+2}}$$

$$C_3 = \underbrace{C_{2,1}}_{\uparrow\uparrow\downarrow} + \underbrace{C_{1,2}}_{\uparrow\downarrow\downarrow}$$

$s = s(2,1)$
$= 1.7727\ldots$

$$\Uparrow$$

short-range scaling law: $\psi \propto R^{s-2}$ for $R \to 0$

NUMBER OF NEARBY PAIRS & TRIPLETS

$N_2(\epsilon) :=$ number of pairs separated by $r < \epsilon$

$$\left[\ \text{without interactions:}\quad N_2^{(0)}(\epsilon)\ \propto\ \epsilon^3\ \right]$$

$$\boxed{N_2(\epsilon)\ \underset{\epsilon\to 0}{\sim}\ C_2\,\frac{\epsilon}{4\pi}}$$

[Tan 2008]

$N_3(\epsilon) :=$ number of triplets of hyperradius $R < \epsilon$

$$\boxed{N_3(\epsilon)\ \underset{\epsilon\to 0}{\sim}\ C_3\ \epsilon^{\boxed{2s+2}}}$$

$$C_3 = \underbrace{C_{2,1}}_{\uparrow\uparrow\downarrow} + \underbrace{C_{1,2}}_{\uparrow\downarrow\downarrow}$$

$$\boxed{\begin{aligned} s &= s(2,1)\\ &= 1.7727\ldots \end{aligned}}$$

$$\boxed{= 5.54545\ldots}$$

without interactions:

$$N^{(0)}_{3,\ \text{fermions}}(\epsilon)\ \propto\ \epsilon^8$$

$$N^{(0)}_{3,\ \text{distinguishable}}(\epsilon)\ \propto\ \epsilon^6$$

NUMBER OF NEARBY PAIRS & TRIPLETS

$N_2(\epsilon) :=$ number of pairs separated by $r < \epsilon$

$$\left[\text{ without interactions: } N_2^{(0)}(\epsilon) \propto \epsilon^3 \right]$$

$$\boxed{N_2(\epsilon) \underset{\epsilon\to 0}{\sim} C_2 \frac{\epsilon}{4\pi}}$$

[Tan 2008]

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$$\boxed{N_3(\epsilon) \underset{\epsilon\to 0}{\sim} C_3\, \epsilon^{\boxed{2s+2}}}$$

$$C_3 = \underbrace{C_{2,1}}_{\uparrow\uparrow\downarrow} + \underbrace{C_{1,2}}_{\uparrow\downarrow\downarrow}$$

$s = s(2,1)$
$= 1.7727\dots$

$= 5.54545\dots$

without interactions:

$$N^{(0)}_{3,\text{ fermions}}(\epsilon) \propto \epsilon^8$$

$$N^{(0)}_{3,\text{ distinguishable}}(\epsilon) \propto \epsilon^6$$

BCS ansatz:

$$N_{3,\,\text{BCS}}(\epsilon) \propto \epsilon^4$$

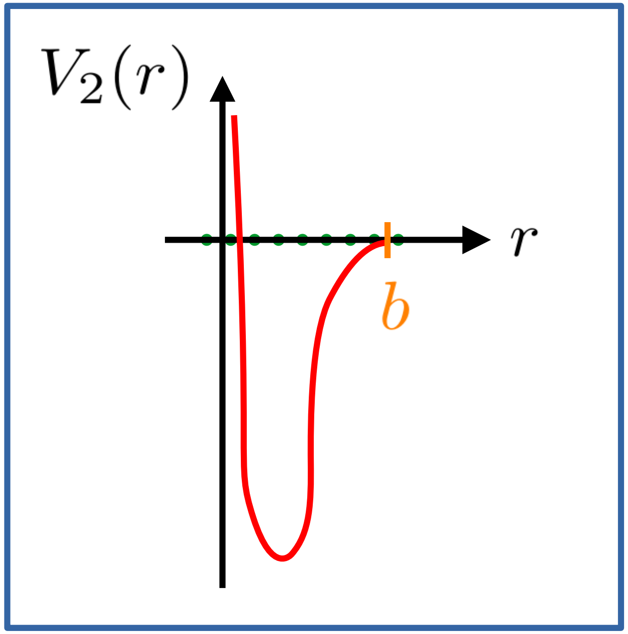
(wrong)

THREE-BODY LOSS RATE

a_3 defined by:

$$\Psi_{\mathsf{m}}(\mathbf{R}) \simeq \left(R^s - \frac{a_3}{R^s}\right)\frac{1}{R^2}\,\phi_{\mathsf{m}}(\boldsymbol{\Omega})$$

in the region $\{b \ll r_{ij} \ll |a_2|,\ \forall i < j\}$



THREE-BODY LOSS RATE

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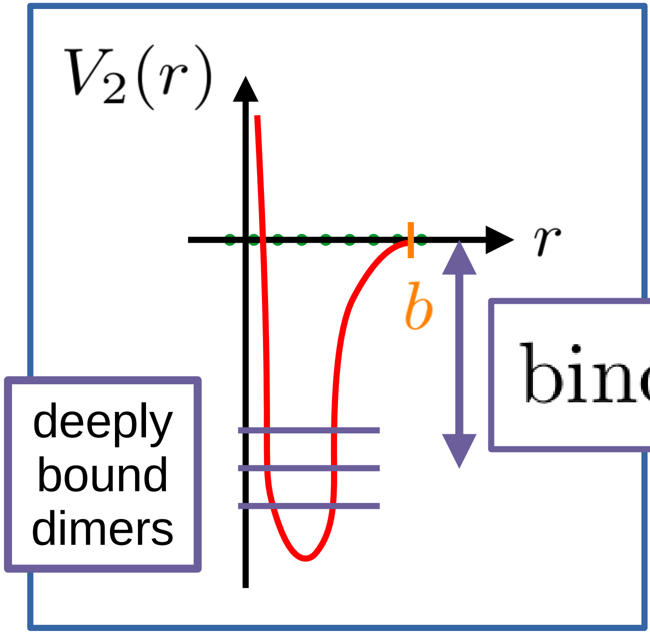
in the region $\{b \ll r_{ij} \ll |a_2|, \ \forall i < j\}$



deeply bound dimers

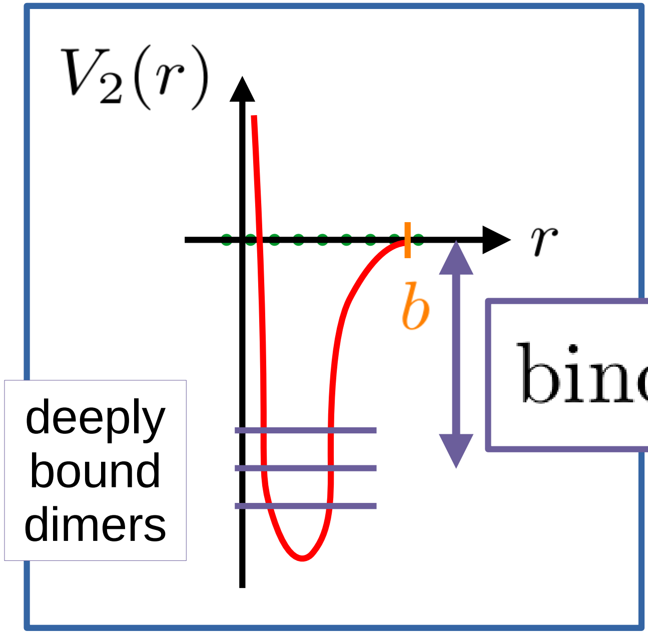
binding energy $\sim \dfrac{\hbar^2}{mb^2}$

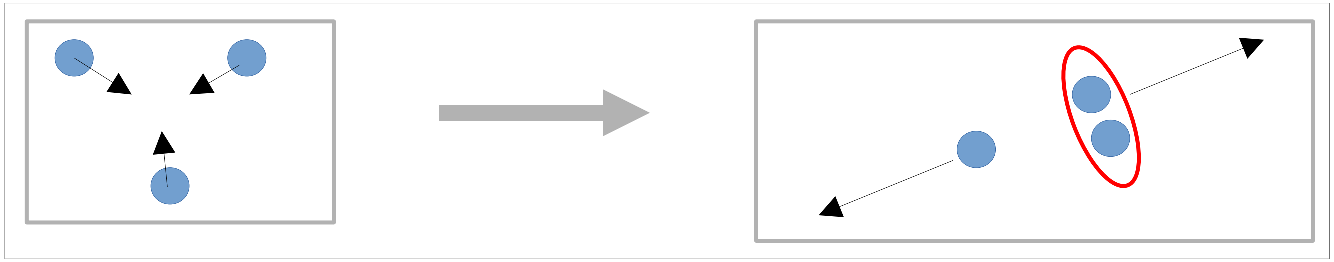
THREE-BODY LOSS RATE

a_3 defined by:

$$\Psi_{\mathrm{m}}(\mathbf{R}) \simeq \left(R^s - \frac{a_3}{R^s}\right)\frac{1}{R^2}\,\phi_{\mathrm{m}}(\boldsymbol{\Omega})$$

in the region $\{b \ll r_{ij} \ll |a_2|,\ \forall i < j\}$





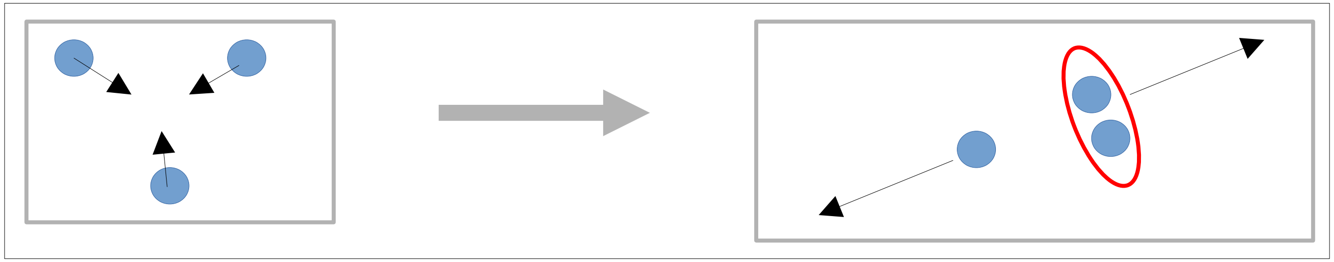
binding energy $\sim \dfrac{\hbar^2}{mb^2}$

THREE-BODY LOSS RATE

a_3 defined by:

$$\Psi_{\mathsf{m}}(\mathbf{R}) \simeq \left(R^s - \frac{a_3}{R^s}\right) \frac{1}{R^2} \, \phi_{\mathsf{m}}(\boldsymbol{\Omega})$$

in the region $\{b \ll r_{ij} \ll |a_2|, \; \forall i < j\}$



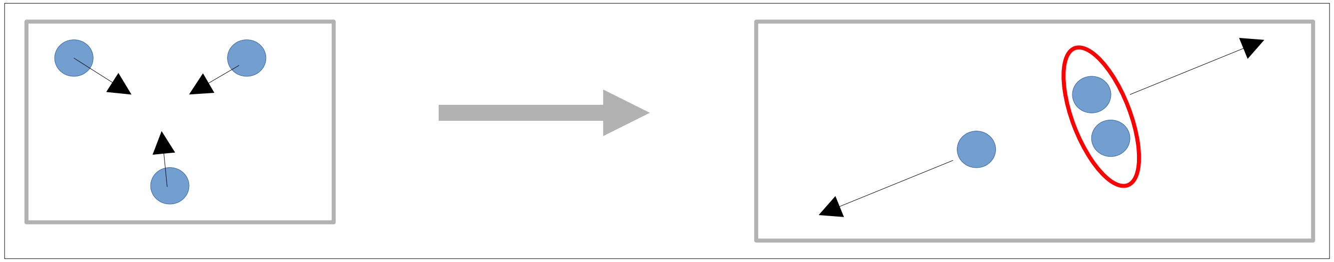
$$\frac{dN}{dt} = -3\,\Gamma_3$$

THREE-BODY LOSS RATE

a_3 defined by:

$$\Psi_{\mathrm{m}}(\mathbf{R}) \simeq \left(R^s - \frac{a_3}{R^s}\right)\frac{1}{R^2}\,\phi_{\mathrm{m}}(\boldsymbol{\Omega})$$

in the region $\{b \ll r_{ij} \ll |a_2|,\ \forall i < j\}$



$$\frac{dN}{dt} = -3\,\Gamma_3$$

$$\Gamma_3 \simeq -\frac{\hbar}{m}\,8s(s+1)\,C_3\,\mathrm{Im}\,a_3$$

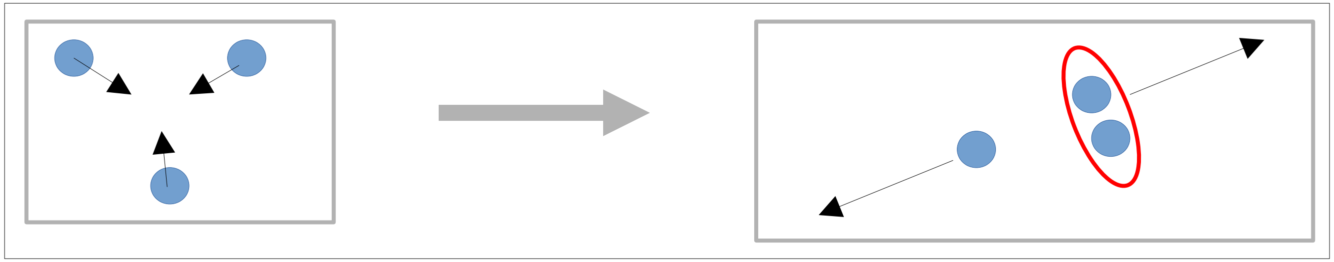
[FW & X. Leyronas, C. R. Phys. **25**, 179 (2024)]

THREE-BODY LOSS RATE

a_3 defined by:

$$\Psi_{\mathsf{m}}(\mathbf{R}) \simeq \left(R^s - \frac{a_3}{R^s}\right)\frac{1}{R^2}\,\phi_{\mathsf{m}}(\mathbf{\Omega})$$

in the region $\{b \ll r_{ij} \ll |a_2|,\ \forall i<j\}$



$$\frac{dN}{dt} = -3\,\Gamma_3$$

$$\Gamma_3 \simeq -\frac{\hbar}{m}\,8s(s+1)\,C_3\,\mathrm{Im}\,a_3$$

order of magnitude:

$$a_3 \sim b^{2s}$$

$$\Rightarrow \frac{-\dot{N}/N}{\epsilon_F/\hbar} \sim (k_F b)^{2s} \ll 1$$

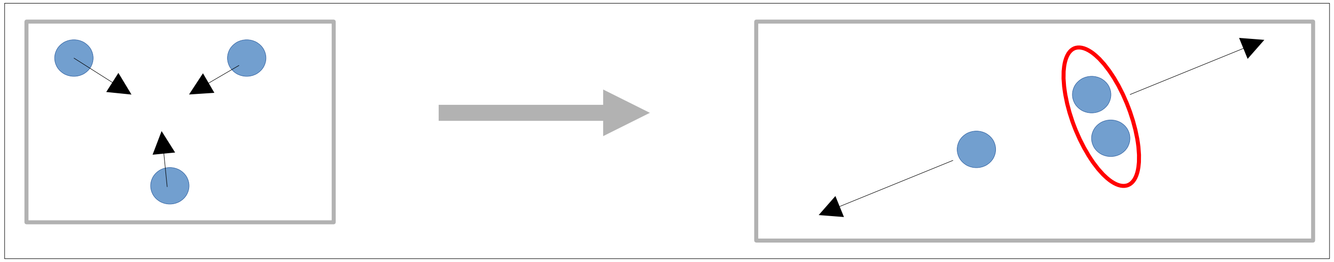
[Petrov *et al.*, PRL 93, 090404 (2004)]

THREE-BODY LOSS RATE

a_3 defined by:

$$\Psi_{\mathsf{m}}(\mathbf{R}) \simeq \left(R^s - \frac{a_3}{R^s}\right)\frac{1}{R^2}\,\phi_{\mathsf{m}}(\boldsymbol{\Omega})$$

in the region $\{b \ll r_{ij} \ll |a_2|,\ \forall i < j\}$



$$\frac{dN}{dt} = -3\,\Gamma_3$$

$$\Gamma_3 \simeq -\frac{\hbar}{m}\,8s(s+1)\,C_3\,\mathrm{Im}\,a_3$$

order of magnitude:

$$a_3 \sim b^{2s}$$

$$C_3|_{\mathrm{finite-range}} \simeq C_3|_{\mathrm{zero-range}}$$

Derivation : $\mathbf{X} := (\mathbf{r}_1, \ldots, \mathbf{r}_N)$

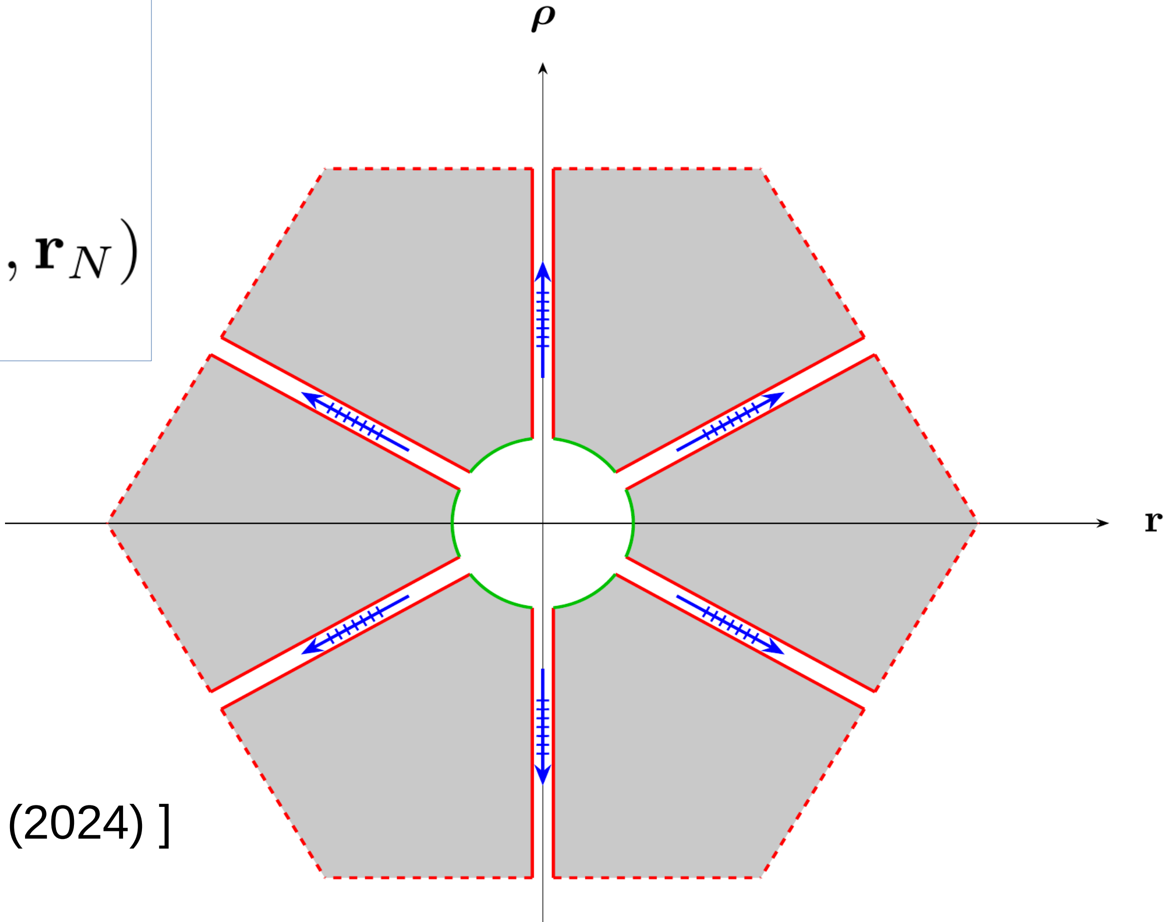
$$\text{Gamov state: } \begin{cases} H\,\psi(\mathbf{X}) = E\,\psi(\mathbf{X}), \quad E \in \mathbb{C} \\ \psi(\mathbf{X}) \underset{\infty}{\simeq} \text{outgoing (atom + deep-dimer) wave} \end{cases}$$

$$\Gamma_3 = \int_{\mathcal{S}_3} \mathbf{d^{3N-1}S} \cdot \frac{\hbar}{m} \,\mathrm{Im}\,(\psi^* \boldsymbol{\nabla}_{\mathbf{X}}\,\psi)$$

$$\psi(\mathbf{X}) \underset{\mathbf{X}\in\mathcal{S}_3}{\simeq} \left(R^s - \frac{a_3}{R^s}\right) \frac{1}{R^2} \times \sum_{\mathsf{m}=-1}^{+1} \phi_{\mathsf{m}}(\boldsymbol{\Omega})\; B_{\mathsf{m}}(\mathbf{C}; \mathbf{r}_4, \ldots, \mathbf{r}_N)$$

$$\boxed{\Gamma_3 \simeq -\frac{\hbar}{m}\, 8s(s+1)\, C_3 \;\mathrm{Im}\, a_3}$$

[FW & X. Leyronas, C. R. Phys. **25**, 179 (2024)]



C_3 in non-degenerate limit

[X. Leyronas & FW,
in preparation]

C_3 in non-degenerate limit

unitary Fermi gas $(a_2 = \infty)$

$$\mathcal{C}_3 := \frac{C_3}{\text{Volume}}$$

Virial expansion
solution of 3-body problem

→

$$\mathcal{C}_3 \simeq n^3 \left(\frac{\hbar^2}{mk_B T}\right)^{2-s} \times 4.5552892\ldots$$

$$\mathcal{C}_3 = \zeta_3\left(\frac{T}{T_F}\right) n^{\frac{2s+5}{3}}$$

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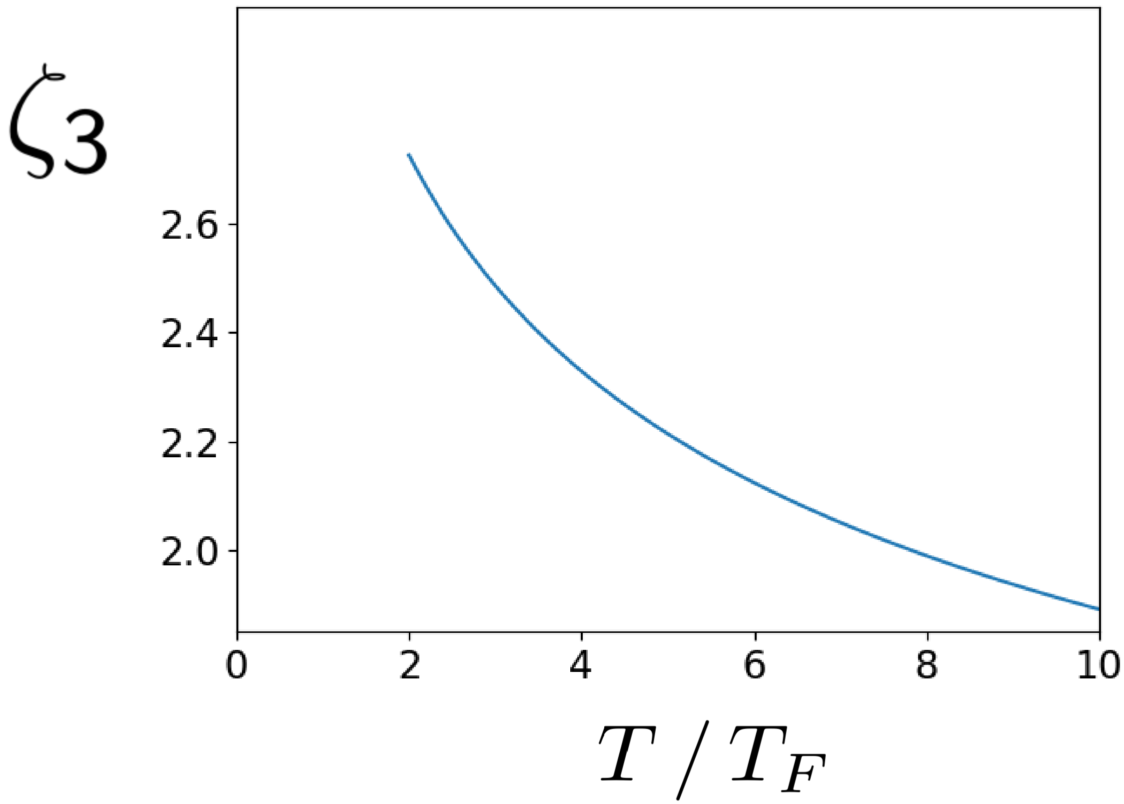

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$$\zeta_3 \propto \frac{1}{(T/T_F)^{2-s}}$$
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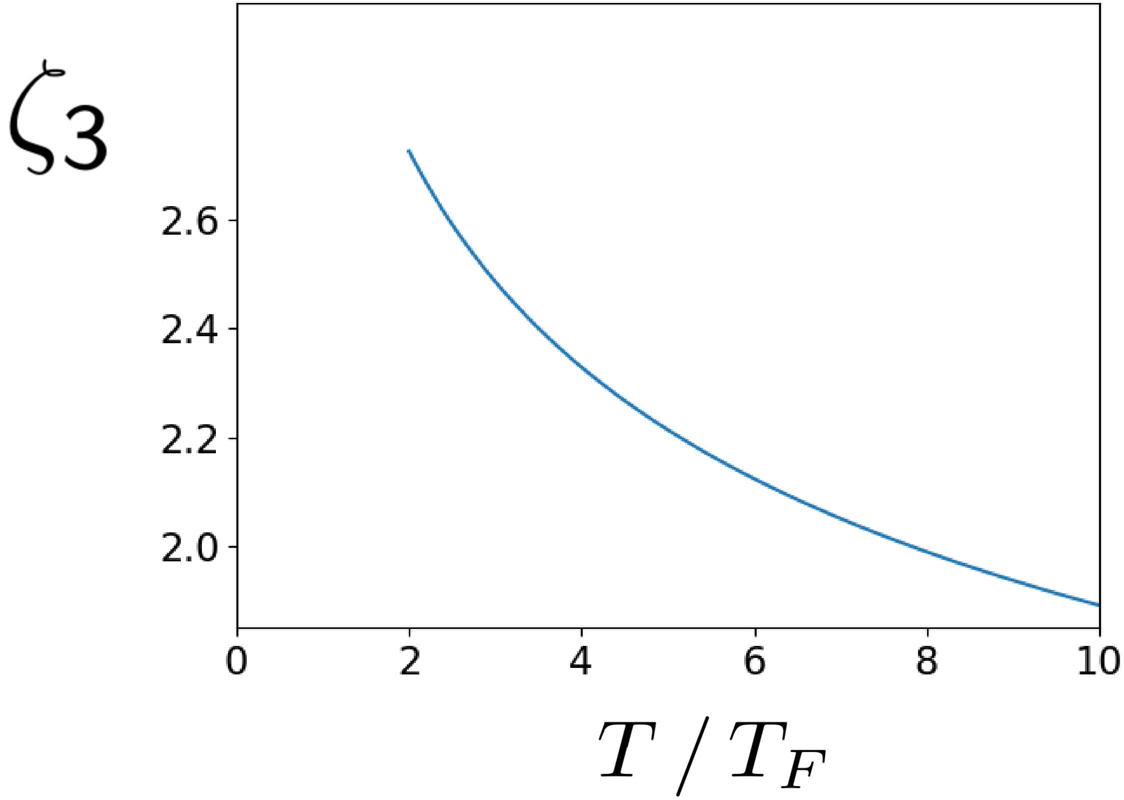

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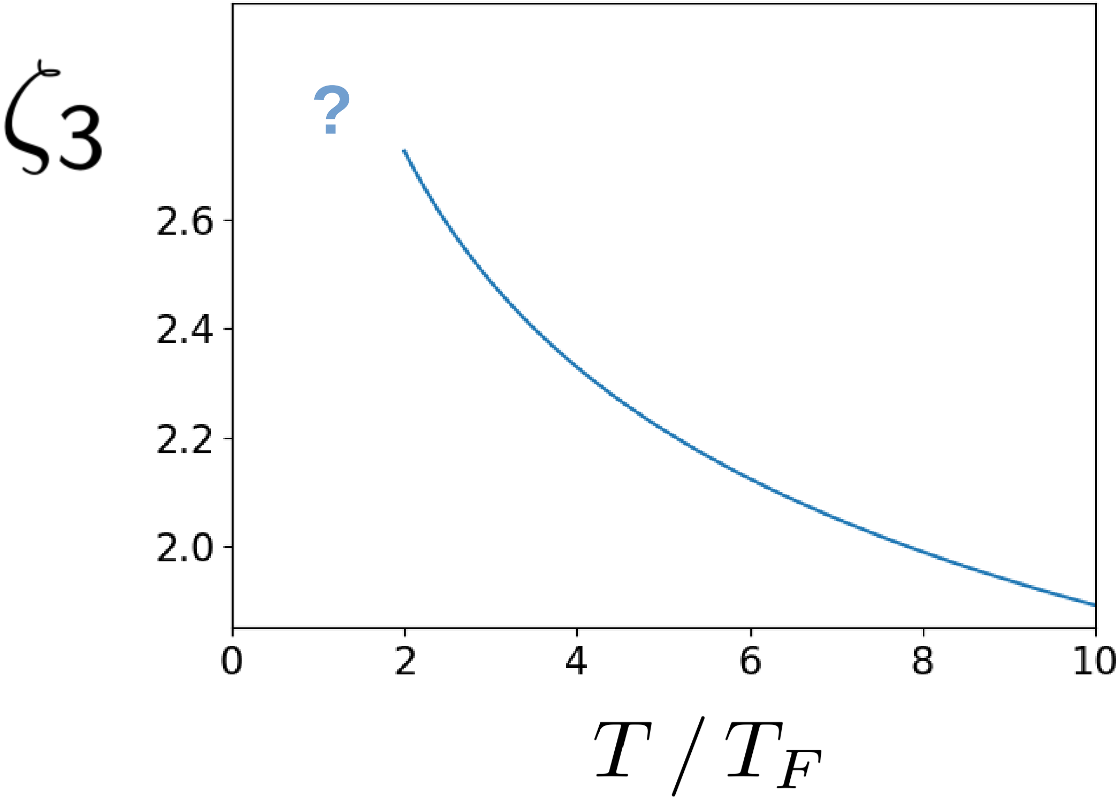

C_3 for the degenerate unitary gas

article in preparation

with

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Doerte **Blume**
Oklahoma

Generalization

$$a_3^{(\uparrow\uparrow\downarrow)} \neq a_3^{(\uparrow\downarrow\downarrow)}$$

$$\Gamma_3 = \Gamma_3^{(\uparrow\uparrow\downarrow)} + \Gamma_3^{(\uparrow\downarrow\downarrow)}$$

$$\begin{cases} \Gamma_3^{(\uparrow\uparrow\downarrow)} = -\dfrac{\hbar}{m}\, 8s(s+1)\, C_3^{(\uparrow\uparrow\downarrow)}\, \mathrm{Im}\, a_3^{(\uparrow\uparrow\downarrow)} \\ \Gamma_3^{(\uparrow\downarrow\downarrow)} = -\dfrac{\hbar}{m}\, 8s(s+1)\, C_3^{(\uparrow\downarrow\downarrow)}\, \mathrm{Im}\, a_3^{(\uparrow\downarrow\downarrow)} \end{cases}$$

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Determination of $\mathrm{Im}\, a_3^{(\uparrow\uparrow\downarrow)}$

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3 atoms ($\uparrow\uparrow\downarrow$), harmonic trap ($\omega_{\mathrm{rad}}/\omega_z = 6.773$), $a_2 = \infty$, ground state

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C_3 for the unitary gas

unpolarized

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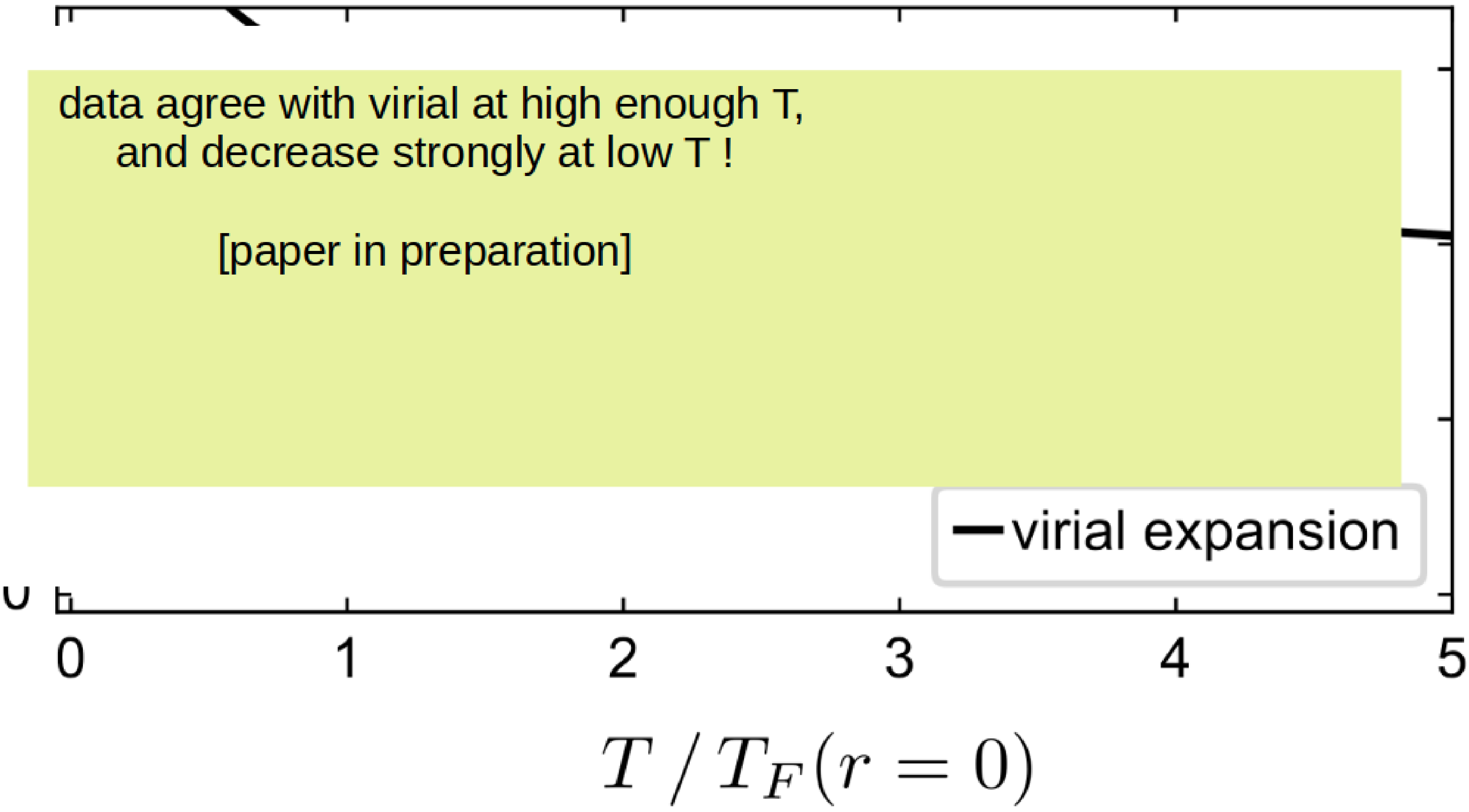

data agree with virial at high enough T,
and decrease strongly at low T !

[paper in preparation]