Short-range correlations and entropy in ultracold atomic Fermi gases

Phys. Rev. A **80**, 023615 (2009)

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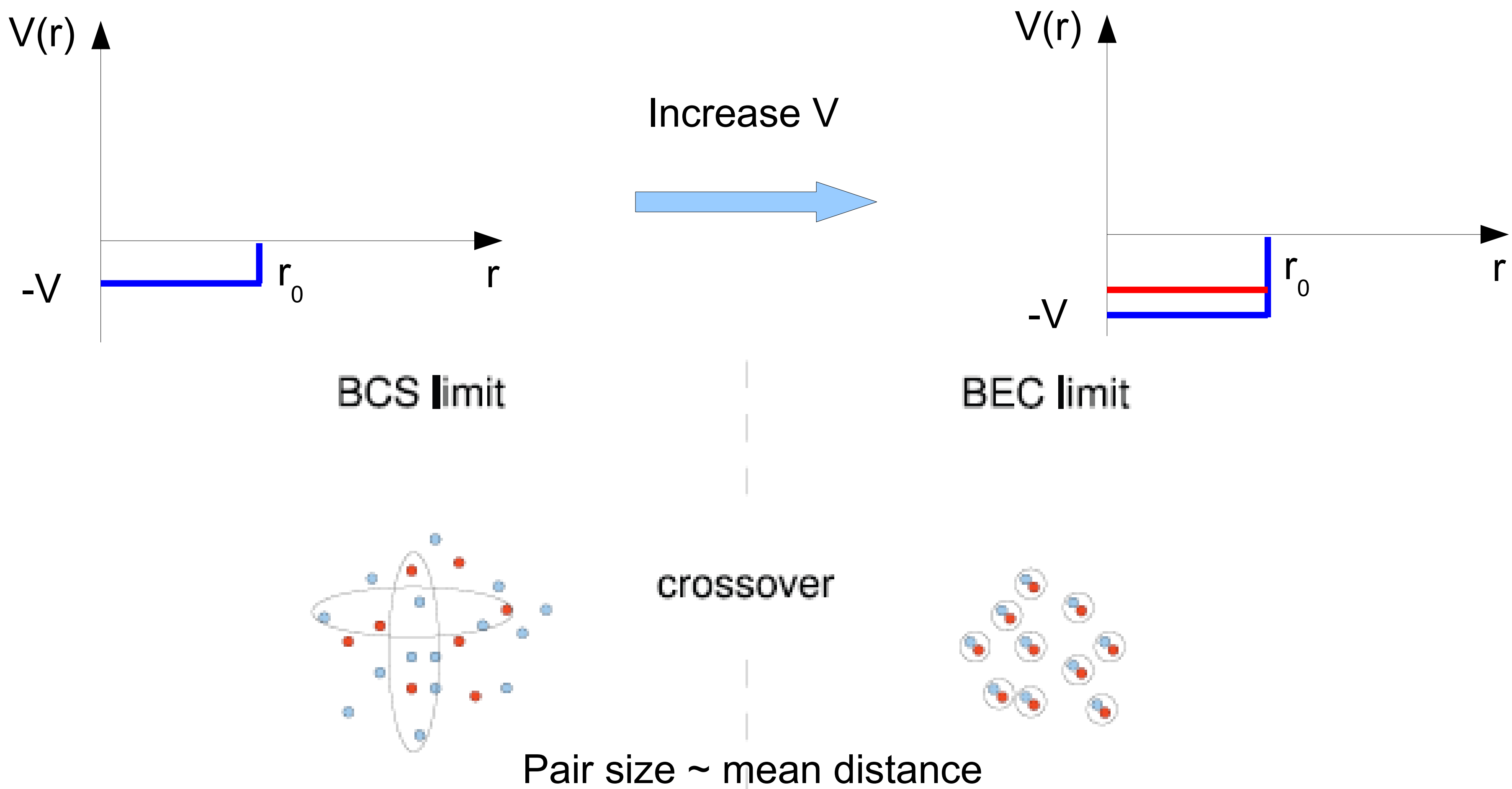
Institute for Nuclear Theory, April 6, 2011

BEC-BCS crossover

D. M. Eagles, Phys. Rev. 186, 456 (1969)
A.J. Leggett, in Modern Trends in the Theory of Condensed Matter, edited by A. Pekalski and R. Przystawa, (Springer-Verlag, Berlin, 1980)
P. Nozeries and S Schmitt-Rink, J. of Low. Temp. Phys. 59, 195 (1985)
C. A. R. Sá de Melo, Mohit Randeria, and Jan R. Engelbrecht, PRL 71, 3202 (1993)

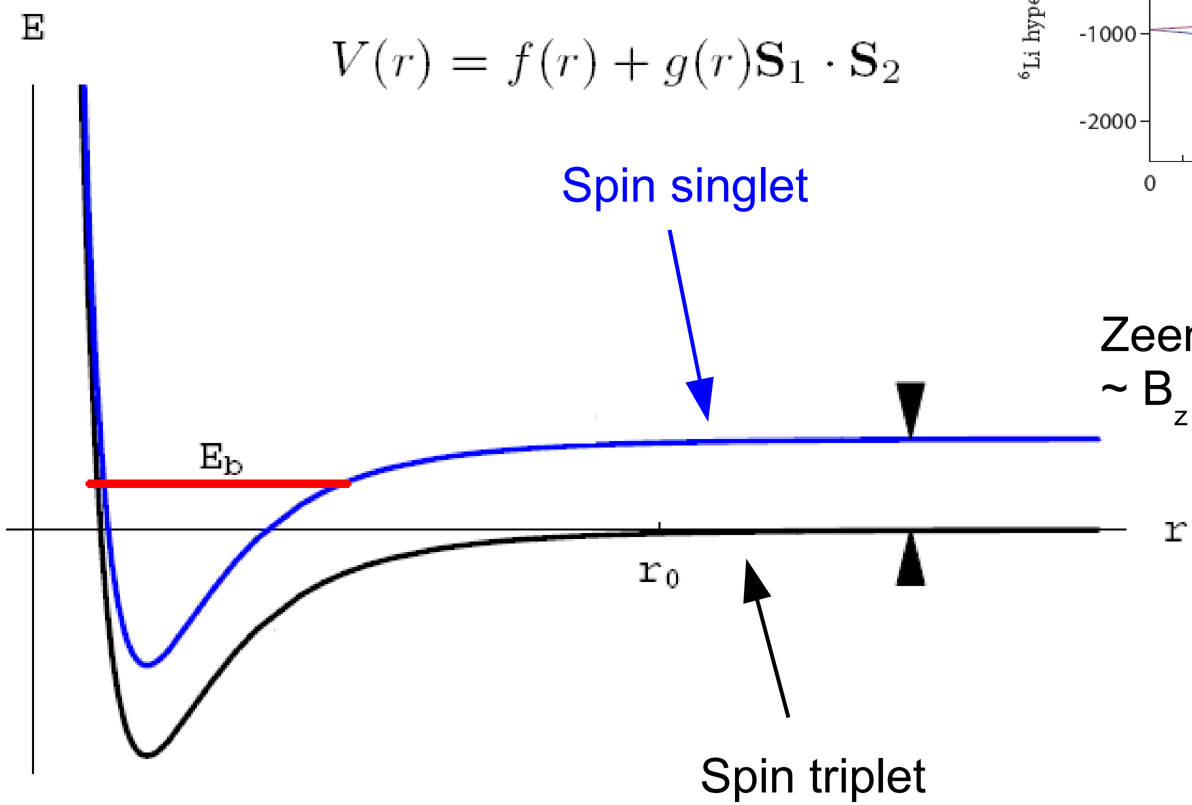
In a two component fermion gas with attractive interactions

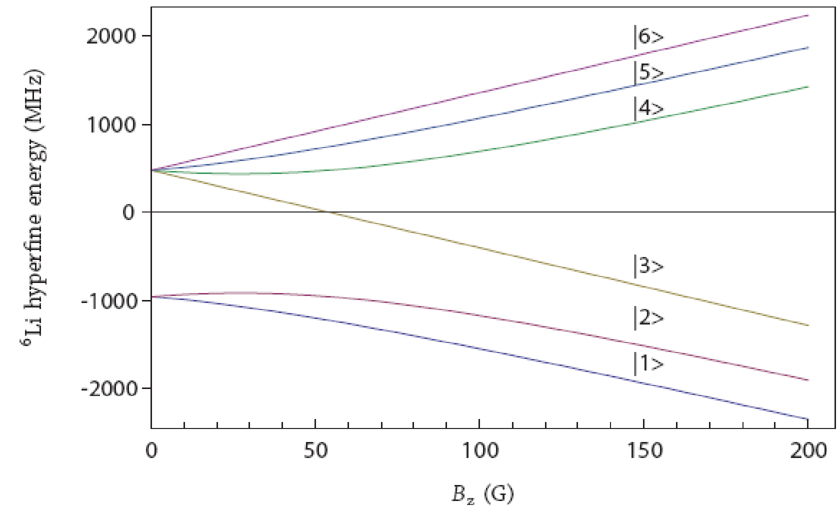


Feshbach resonances

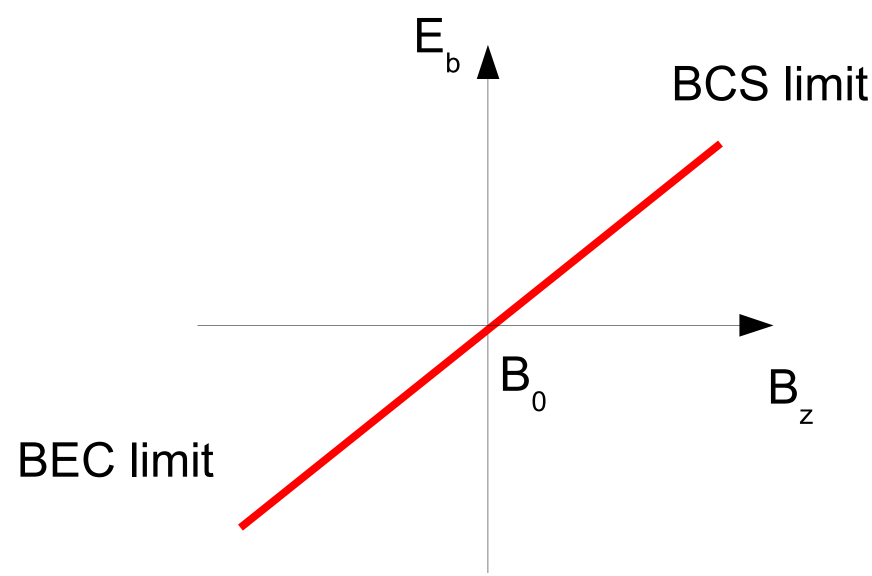
The interaction couples scattering in multiple channels.

$$V(r) = f(r) + g(r)\mathbf{S}_1 \cdot \mathbf{S}_2$$





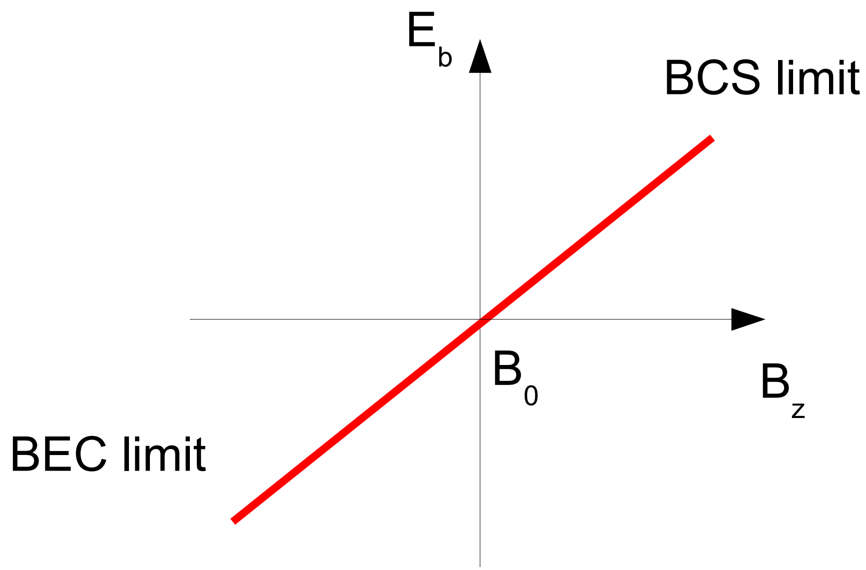
Zeeman energy difference
$\sim B_z \Delta S_z$

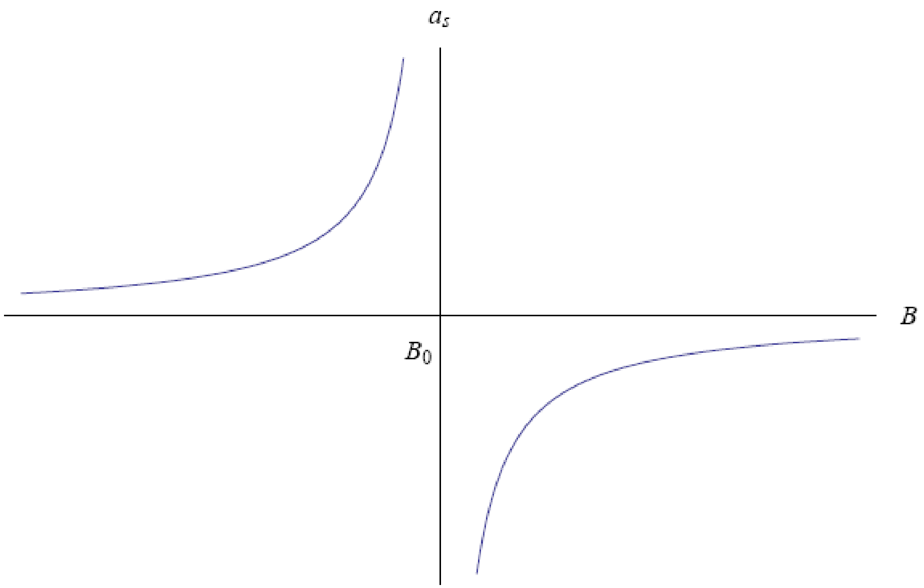


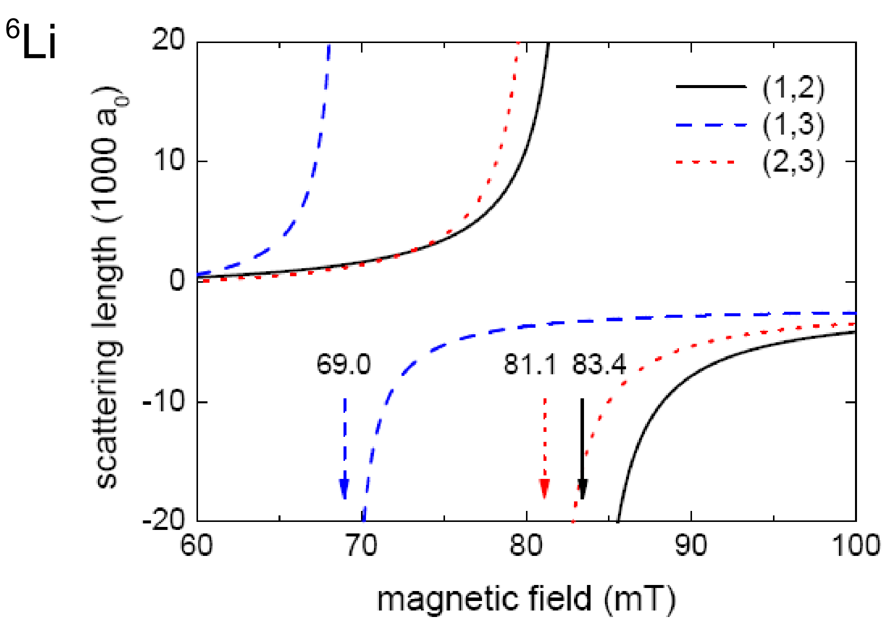
e.g., I. Bloch, J. Dalibard, and W. Zwerger
Rev. Mod. Phys. 80, 885 (2008)

Feshbach resonances

The s-wave scattering length tells the effective scattering in one channel.







Strongly interacting regime

$$|n^{1/3}a| >> 1$$

Challenging for microscopic theories

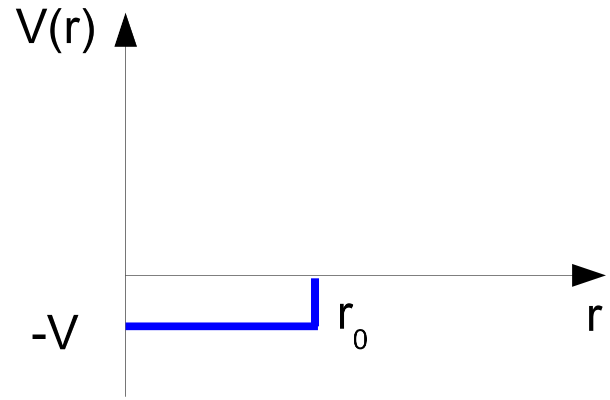
M. Bartenstein et al, Phys. Rev. Lett. 94, 103201 (2005)

Correlations at short distances

In a gas consisting of particles of species |i> and |j> interacting with a potential with range r_0, in the dilute limit r_0<<d (mean distance between particles), the correlation functions have the asymptotic form

$$\langle \psi_i^+(\vec{r})\psi_j^+(0)\psi_j(0)\psi_i(\vec{r})\rangle \sim C_{ij}\underline{(1/r-1/a_{ij})^2}$$

Jastrow factor



r_0<<d

in the regime r_0<<r<<d

Where a_ij is the s-wave scattering length characterizing the low energy scattering between |i> and |j>.

The Jastrow factor comes from solving the zero-energy Schrodinger equation of the relative coordinates at short distances

$$\langle \psi_i^+(\vec{r})\psi_i^+(0)\psi_i(0)\psi_i(\vec{r})\rangle \sim \chi_{ij}^2(r)/r^2$$

$$\left(-\frac{1}{m}\frac{d^2}{dr^2}+V_{ij}(r)\right)\chi_{ij}(r)=0$$

for $r_0 \ll r \ll d$

$$\chi_{ij}(r)\sim 1-r/a_{ij}$$

Determined by two-body physics

Correlation strength & free energy

The correlation strength (contact) is determined by non-trivial many-body physics

$$C_{ij}(a_{ij}, n_i, n_j, T)$$

The contact encapsulates essential thermodynamic inforamtion

$$C = -\frac{m}{4\pi}\frac{\partial(F/V)}{\partial a^{-1}}$$

S. Tan, Ann. of Phys. 323, 2952 (2008); S. Tan, *ibid* 323, 2971 (2008).
S. Zhang and A.J. Legget, Phys. Rev. A 79, 023601 (2009).
E. Braaten and L. Platter, Phys. Rev. Lett. 100 205301 (2008).

The hamiltonian

$$H = \sum_{\sigma=1}^{2}\int d\vec{r}\,\psi_\sigma^{+}(\vec{r})\left(-\frac{\nabla^2}{2\mathrm{m}}\right)\psi_\sigma(\vec{r}) + \int d\vec{r}\int d\vec{r}\,'\,V(|\vec{r}-\vec{r}\,'|)\,\psi_1^{+}(\vec{r})\psi_2^{+}(\vec{r}\,')\psi_2(\vec{r}\,')\psi_1(\vec{r})$$

Let us $V(r) \to \lambda V(r)$ $\quad a \to a_\lambda$ We will take λ=1 at the end.

$$\frac{\partial(F_\lambda/V)}{\partial a_\lambda^{-1}} = \frac{\partial(F_\lambda/V)}{\partial\lambda}\frac{\partial\lambda}{\partial a_\lambda^{-1}}$$

$$1 - r/a_\lambda$$

$$= \int d\vec{r}\,V(r)\langle\psi_1^{+}(\vec{r})\psi_2^{+}(0)\psi_2(0)\psi_1(\vec{r})\rangle\frac{\partial\lambda}{\partial a_\lambda^{-1}} = C_\lambda\int_0^\infty dr\,V(r)\chi_\lambda^2(r)\frac{\partial\lambda}{\partial a_\lambda^{-1}}$$

Correlation strength & free energy

$$\int_0^{r_c} dr\,\chi_{\lambda'}(r)\left(-\frac{1}{m}\frac{d^2}{dr^2}+\lambda V(r)\right)\chi_\lambda(r)=0 \qquad r_0 \ll r_c \ll n^{-1/3}$$

$$-\frac{1}{m}(\chi_{\lambda'}\chi_\lambda{}'-\chi_{\lambda'}{}'\chi_\lambda)_0^{r_c}+\int_0^{r_c} dr\left[\left(-\frac{1}{m}\frac{d^2}{dr^2}+\lambda V(r)\right)\chi_{\lambda'}(r)\right]\chi_\lambda(r)=0$$

$$\left(-\frac{1}{m}\frac{d^2}{dr^2}+\lambda' V(r)\right)\chi_{\lambda'}(r)=0 \qquad \chi_\lambda(0)=0 \qquad \chi_\lambda(r)=1-r/a_\lambda,\ @\, r\sim r_c$$

$$1/a_\lambda-1/a_{\lambda'}=-m(\lambda'-\lambda)\int_0^\infty dr\,V(r)\chi_\lambda(r)\chi_{\lambda'}(r)$$

In the limit $\lambda\to\lambda'$

$$\int_0^\infty dr\,V(r)\chi_\lambda^2(r)\frac{\partial\lambda}{\partial a_\lambda^{-1}}=-\frac{1}{m}$$

Taking $\lambda=1$

$$\boxed{C=-\frac{m}{4\pi}\frac{\partial(F/V)}{\partial a^{-1}}}$$

Correlation strength at zero temperature

The ground state energy per particle

$$\frac{E_{gnd}}{2\mathrm{N}}=\frac{3}{5}(1+\beta(\xi))E_F \qquad E_F=k_F^2/2\mathrm{m},\, n=k_F^3/6\pi^2,\, \xi=-1/k_F a$$

The contact

$$C(T=0)=\frac{k_F^4}{40\pi^3}\frac{\partial\beta}{\partial\xi}$$

In the BEC limit, $a\rightarrow 0^+$, fermions form bosonic molecules with bound energy $E_b=-1/ma^2$

$$\frac{E}{2\mathrm{N}}=\frac{E_b}{2}+\frac{\pi}{6}E_F k_F a_m\left(1+\frac{128}{15\sqrt{6\pi^3}}(k_F a_m)^{3/2}+\ldots\right) \qquad C=\frac{n}{2\pi a}$$

the scattering length between molecules

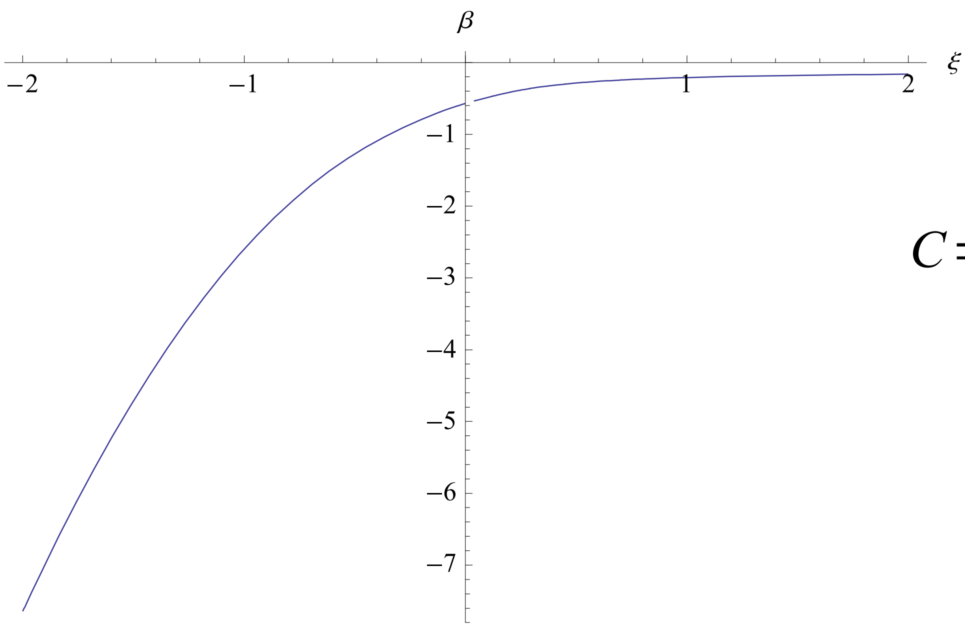
In the BCS limit, $a\rightarrow 0^-$, BCS pairing is exponentially small

$$\frac{E}{2\mathrm{N}}=E_F\left[\frac{3}{5}+\frac{2}{3\pi}k_F a+\frac{4(11-2\log 2)}{35\pi^2}(k_{Fa})^2+\ldots\right] \qquad C=a^2n^2$$

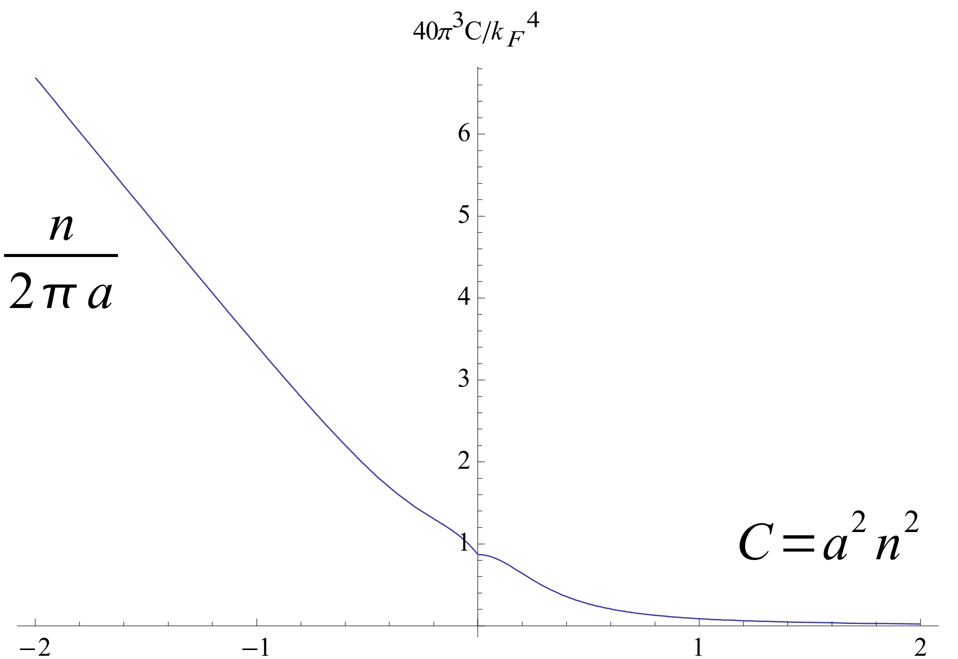
Correlation strength @ T=0

Generally, β can be calculated by quantum Monte Carlo simualtion

G.E. Astrakharchik, J. Boronat, J. Casulleras, and S. Giorgini, Phys. Rev. Lett. 93, 200404 (2004).



$$C = \frac{n}{2\pi a}$$



In the BEC limit, $a \to 0^+$, fermions form bosonic molecules with bound energy $E_b = -1/ma^2$

In the BCS limit, $a \to 0^-$, BCS pairing is exponentially small; the leading interaction energy is the Hartree mean field energy.

How does C(T) vary with T ?

By thermodynamic identity

$$\frac{\partial C}{\partial T} = -\frac{m}{4\pi}\frac{\partial}{\partial a^{-1}}\frac{\partial(F/V)}{\partial T} = \frac{m}{4\pi}\frac{\partial(S/V)}{\partial a^{-1}}$$

C is related to the isentropes in the T-a plane.

In the limit $T \to 0,$ in the superfluid phase, phonons are the only gapless excitations

$$S \approx S_{phonon} = \frac{2\pi^2}{45} V\left(\frac{T}{v_s}\right)^3$$

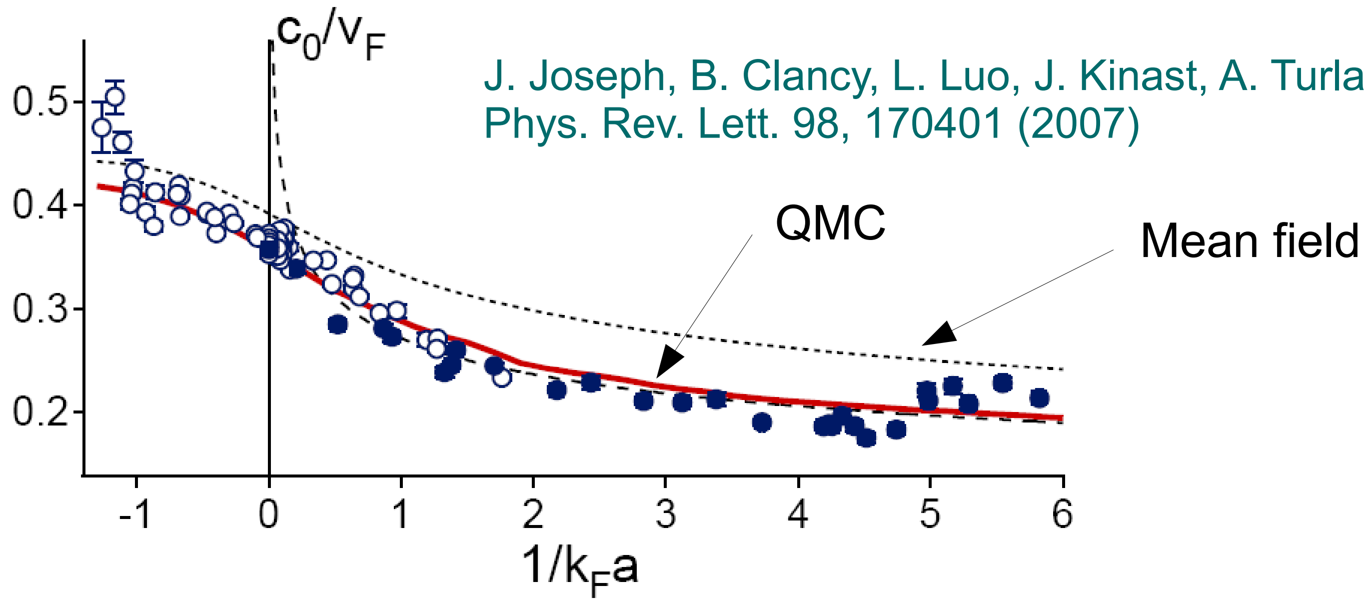
The sound velocity v_s can be calculated by the formula

$$m v_s^2 = n\frac{\partial \mu}{\partial n}$$

@ T=0

$$\mu = \frac{\partial E}{\partial N} = E_F\left(1+\beta-\frac{1}{5}\beta'\xi\right) \qquad \left(\frac{v_s}{k_F/\sqrt{3m}}\right)^2 = 1+\beta-\frac{3}{5}\beta'\xi+\frac{1}{10}\beta''\xi^2$$

Correlation strength in the low T limit



J. Joseph, B. Clancy, L. Luo, J. Kinast, A. Turlapov, and J. E. Thomas
Phys. Rev. Lett. 98, 170401 (2007)

$$\frac{\partial v_s}{\partial a^{-1}} < 0 \qquad \frac{\partial S_{phonon}}{\partial a^{-1}} = -\frac{3 S_{phonon}}{v_s} \frac{\partial v_s}{\partial a^{-1}} > 0$$

$$\boxed{\delta C = C(T) - C(0) = -\frac{\pi m}{120} \left(\frac{T}{v_s} \right)^4 \frac{\partial v_s}{\partial a^{-1}} > 0}$$

Phonon enhanced correlations

Correlation strength in the low T limit

At higher temperatures, pairs are dissociated by thermal energy; fermionic excitations reduce C.

$$\frac{\partial C}{\partial T} = \frac{m}{4\pi} \frac{\partial (S/V)}{\partial a^{-1}}$$

Within the BCS mean field approach,

$$\frac{\delta (S_f/V)}{\delta a^{-1}} = \frac{1}{V} \sum_k \frac{\delta S_f}{\delta f_k} \frac{\delta f_k}{\delta \Delta} \frac{\delta \Delta}{\delta a^{-1}}$$

Since

$$\frac{\delta F}{\delta f_k} = 0, \frac{\delta S_f}{\delta f_k} = \frac{E_k}{T}$$

$$\frac{\delta f_k}{\delta \Delta} < 0, \frac{\delta \Delta}{\delta a^{-1}} > 0$$

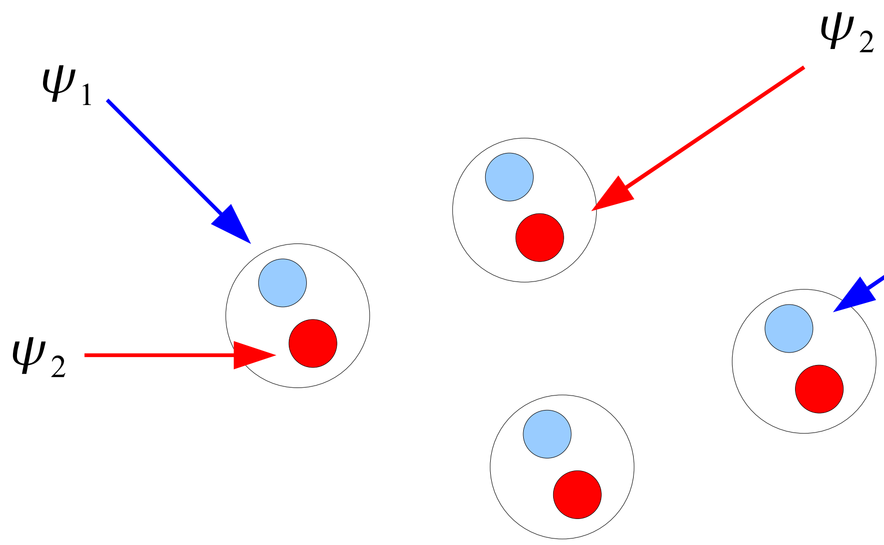
Thus

$$\frac{\delta (S_f/V)}{\delta a^{-1}} < 0$$

Illustration of phonon enhanced correlations in the BEC limit

$$\lim_{r\to 0}\langle \psi_1^+(\vec{r})\psi_2^+(0)\psi_2(0)\psi_1(\vec{r})\rangle$$

measures the probability of fermions staying close to each other.



Phonons assist molecues to stay close to each other.

The pair structure of the molecules is rigid since $|E_b| \gg T$

Illustration of phonon enhanced correlations in the BEC limit

The same low temperature physics is described by the boson model

$$H_m = \int d\vec{r}\, \phi^+(\vec{r}) \left(-\frac{\nabla^2}{2\mathrm{M}} \right) \phi(\vec{r}) + \frac{1}{2} \int d\vec{r} \int d\vec{r}\,' V_m(|\vec{r} - \vec{r}\,'|) \phi^+(\vec{r}) \phi^+(\vec{r}\,') \phi(\vec{r}\,') \phi(\vec{r})$$

Characterized by a_m

The boson correlation function has the similar asymptotic form

$$\lim_{r\to 0} \langle \phi^+(\vec{r}) \phi^+(0) \phi(0) \phi(\vec{r}) \rangle \sim C_m (1/r - 1/a_m)^2$$

$$C_m = -\frac{M}{2\pi} \frac{\partial (F_m / V)}{\partial a_m^{-1}} \qquad M = 2m$$

Since the thermal induced variation $\delta F = \delta F_m$

$$\delta C = -\frac{m}{4\pi} \frac{\partial(\delta F / V)}{\partial a^{-1}} = -\frac{m}{4\pi} \frac{\partial(\delta F_m / V)}{\partial a_m^{-1}} \frac{\partial a_m^{-1}}{\partial a^{-1}} = \frac{m}{2M} \frac{\partial a_m^{-1}}{\partial a^{-1}} \delta C_m$$

Bogoliubov approximation in the BEC limit

Let us assume the contact pseudopotential

$$V_m(r) = U_0 \delta(\vec{r}), U_0 = 4\pi a_m / M$$

Divide the field operator into the condensate and fluctuation parts

$$\phi(\vec{r}) = \phi_0 + \delta\phi(\vec{r})$$

To the second order of the fluctuaions,

$$\lim_{r\to 0} \langle \phi^+(\vec{r}) \phi^+(0) \phi(0) \phi(\vec{r}) \rangle = n_0^2 + 2\mathrm{n}_0 (2\langle \delta\phi^+ \delta\phi \rangle + \langle \delta\phi^+(\vec{r}) \delta\phi^+(0) \rangle) + \ldots$$

Phonon operators

$$\langle \delta\phi^+ \delta\phi \rangle = \frac{1}{V} \sum_k [v_k^2 + (u_k^2 + v_k^2) \langle \alpha_k^+ \alpha_k \rangle]$$

$$\lim_{r\to 0} \langle \delta\phi^+(\vec{r}) \delta\phi^+(0) \rangle = -\frac{n_0 a_m}{r} - \frac{1}{V} \sum_k \left(u_k v_k - \frac{U_0 n_0}{k^2} \right) - \frac{2}{V} \sum_k u_k v_k \langle \alpha_k^+ \alpha_k \rangle$$

$$v_k^2 = (\xi_k / E_k - 1)/2, u_k^2 = (\xi_k / E_k + 1)/2, \xi_k = k^2 / 2M + U_0 n_0$$

Bogoliubov approximation in the BEC limit

To calculate δC_m,

we only need to focus on the temperature variance of r-independent part of

$$\lim_{r\to 0}\langle \phi^+(\vec{r})\phi^+(0)\phi(0)\phi(\vec{r})\rangle \sim C_m(1/r-1/a_m)^2$$

which is

$$\frac{\delta C_m}{a_m^2}=\frac{2n}{V}\sum_k (u_k^2+v_k^2-2u_k v_k)\langle \alpha_k^+\alpha_k\rangle=\frac{\pi^2}{30}nT^4 v_s^{-4}$$

$$v_s^2=U_0 n_0/M^2$$

$$\boxed{\delta C=-\frac{\pi m}{120}\left(\frac{T}{v_s}\right)^4\frac{\partial v_s}{\partial a^{-1}}}$$

agrees with the general phonon argument

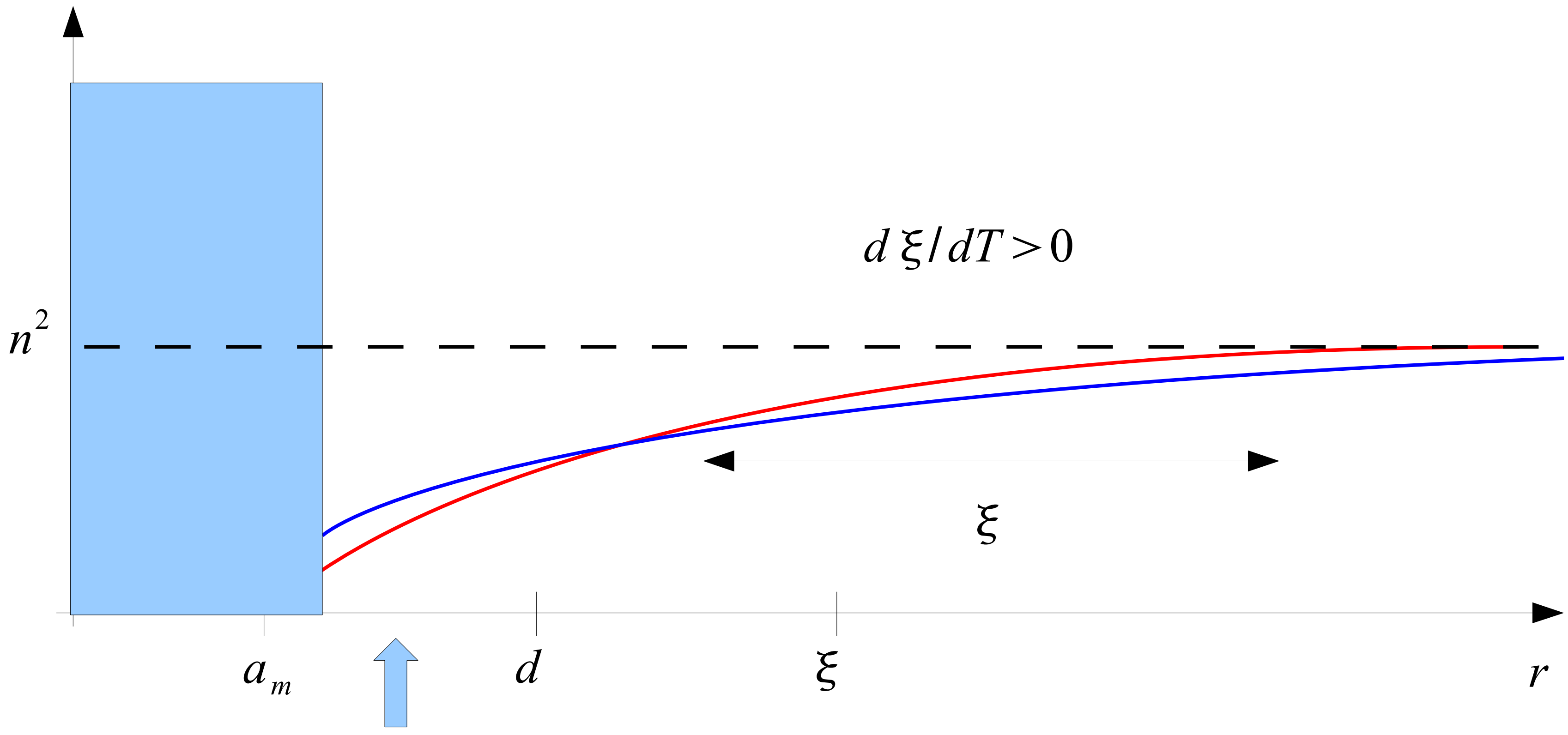
Physical picture of phonon enhanced correlation strength

In the number conversed state,

$$\int d\vec{r}\langle\phi^+(\vec{r})\phi^+(0)\phi(0)\phi(\vec{r})\rangle=(N-1)n \qquad \text{normalized}$$

For repulsive bosons $a_m \sim r_0$ $\quad a_m \ll d \ll \xi$

$\langle\phi^+(\vec{r})\phi^+(0)\phi(0)\phi(\vec{r})\rangle$



$C_m(1/r-1/a_m)^2$

Thermal energy overcomes the repulsive interactions.

Correlation strength in high T limit

Calculate the partition function

$$Z = Tr\, e^{-\beta(H-\mu_1 N_1-\mu_2 N_2)}$$

within the Virial expansion.

L. D. Landau and E. M. Lifshitz, *Statistical Physics I* (Pergamon Press, Oxford, 1980)

To the second order in the fugacity $z_i = e^{\beta\mu}$

$$\ln(Z/Z_0) = 2^{3/2} V z_1 z_2 b_2/\lambda^3$$

$$b_2 = \sum_i e^{\beta|E_b^i|} + \int_0^\infty \frac{dk}{\pi} \frac{d\delta(k)}{dk} e^{-\beta k^2/m}$$

Bound states due to V(r)

the s-wave phase shift
for the scattering states

the thermal wavelength $\lambda = \sqrt{2\pi\beta/m}$

E. Beth and G. E. Uhlenbeck, Physica (Amsterdam) 4, 915 (1937)

Correlation strength in high T limit

In the BEC-BCS crossover regime, we consider the only relevant bound state with

$$E_b = -1/ma^2$$

For the scattering continuum

$$k \cot\delta(k) = -\frac{1}{a}$$

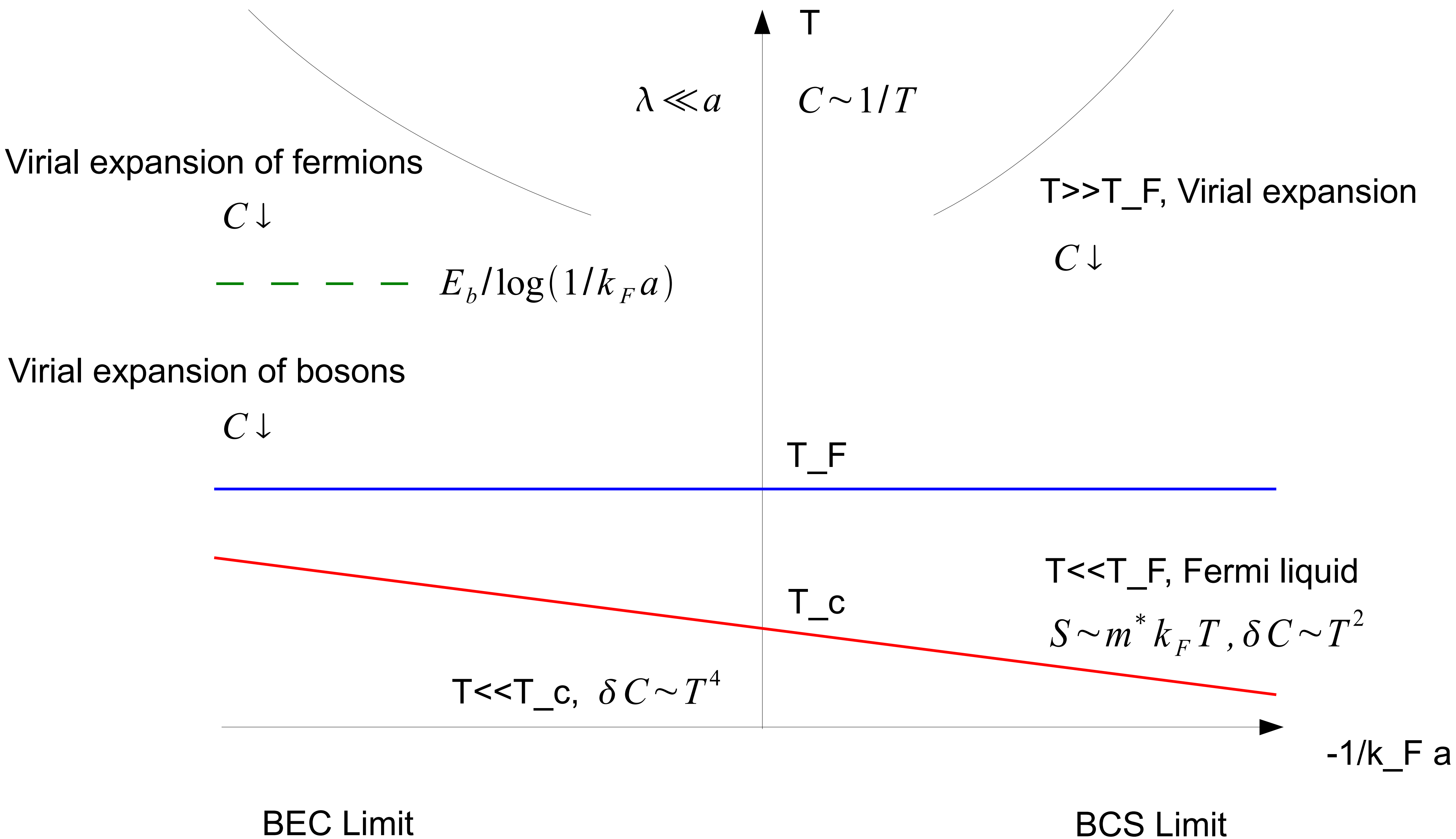
$$b_2(\lambda/a) = \left(\frac{1}{2} - \frac{1}{\sqrt{\pi}} \int_0^{\lambda/\sqrt{2\pi}a} e^{-t^2} dt \right) e^{\lambda^2/2\pi a^2}$$

T.-L. Ho and E. J. Mueller, Phys. Rev. Lett. **92**, 160404 (2004)

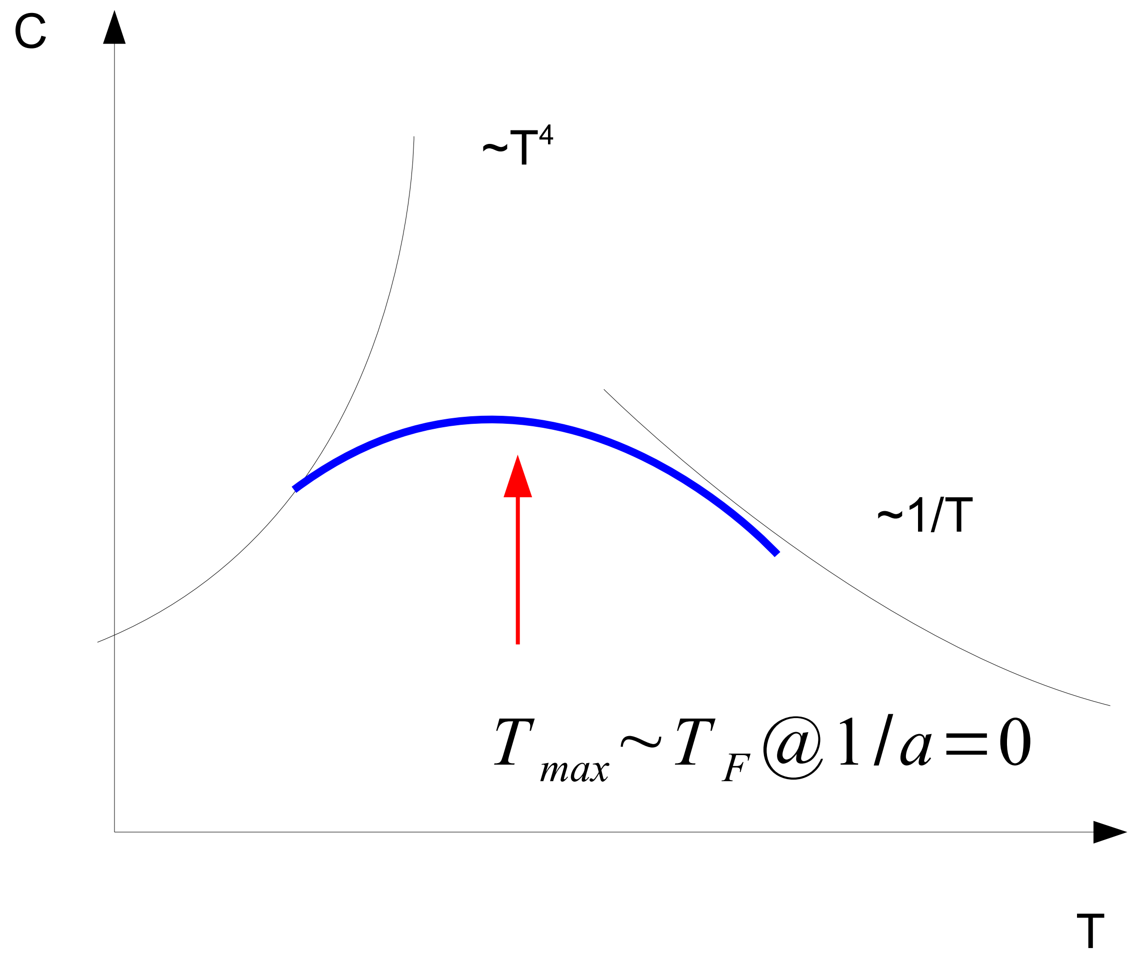
$$C = \frac{m}{4\pi\beta V} \frac{\partial \log Z}{\partial a^{-1}} = \sqrt{2} n_1 n_2 \lambda^2 \frac{\partial b_2(\lambda/a)}{\partial(\lambda/a)} \rightarrow \frac{2n^2}{mT}$$

for $\lambda/a \rightarrow 0, \quad \frac{\partial b_2(\lambda/a)}{\partial(\lambda/a)} = \frac{1}{\sqrt{2}\pi}$

Correlation strength at finite T



Maximum of the correlation strength at finite T



$$T_{max} \sim T_F @ 1/a = 0$$

Correlation strength and isentropes

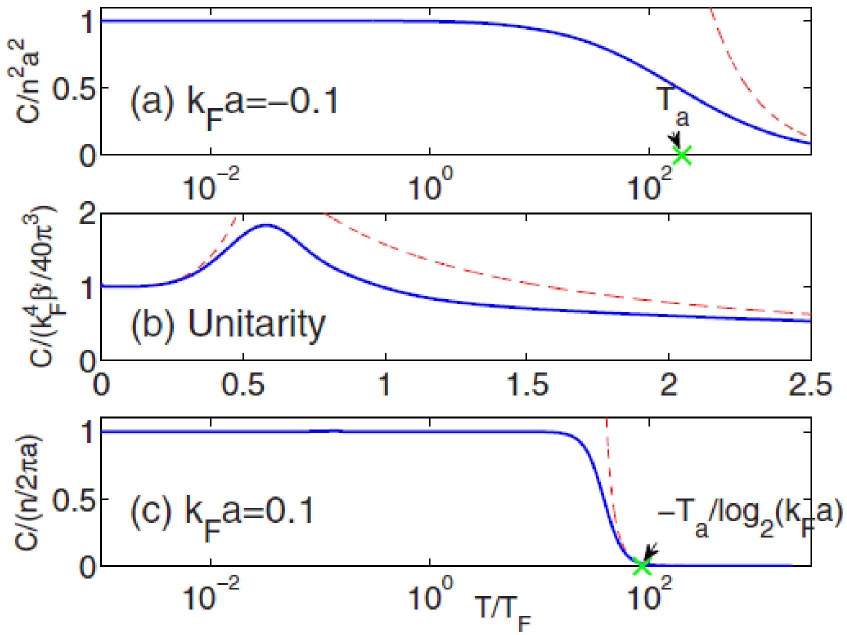


FIG. 1. (Color online) The correlation strength $C(T)$ in the (a) BCS, (b) unitary, and (c) BEC limits. The dashed lines at high T are the virial results, and the dashed line at low T in (b) is from Eq. (17). The solid lines are qualitative interpolations between the increasing low T results and the decreasing high T results. The maximum in $C(T)$ for $T=T_{\max}$ is prominent in the strong-coupling limit, but in the BCS and BEC limits are too small to be visible here.

T_max~T_F prominent around unitarity

Correlation strength and isentropes

$$\frac{\partial C}{\partial T} = \frac{m}{4\pi} \frac{\partial (S/V)}{\partial a^{-1}}$$

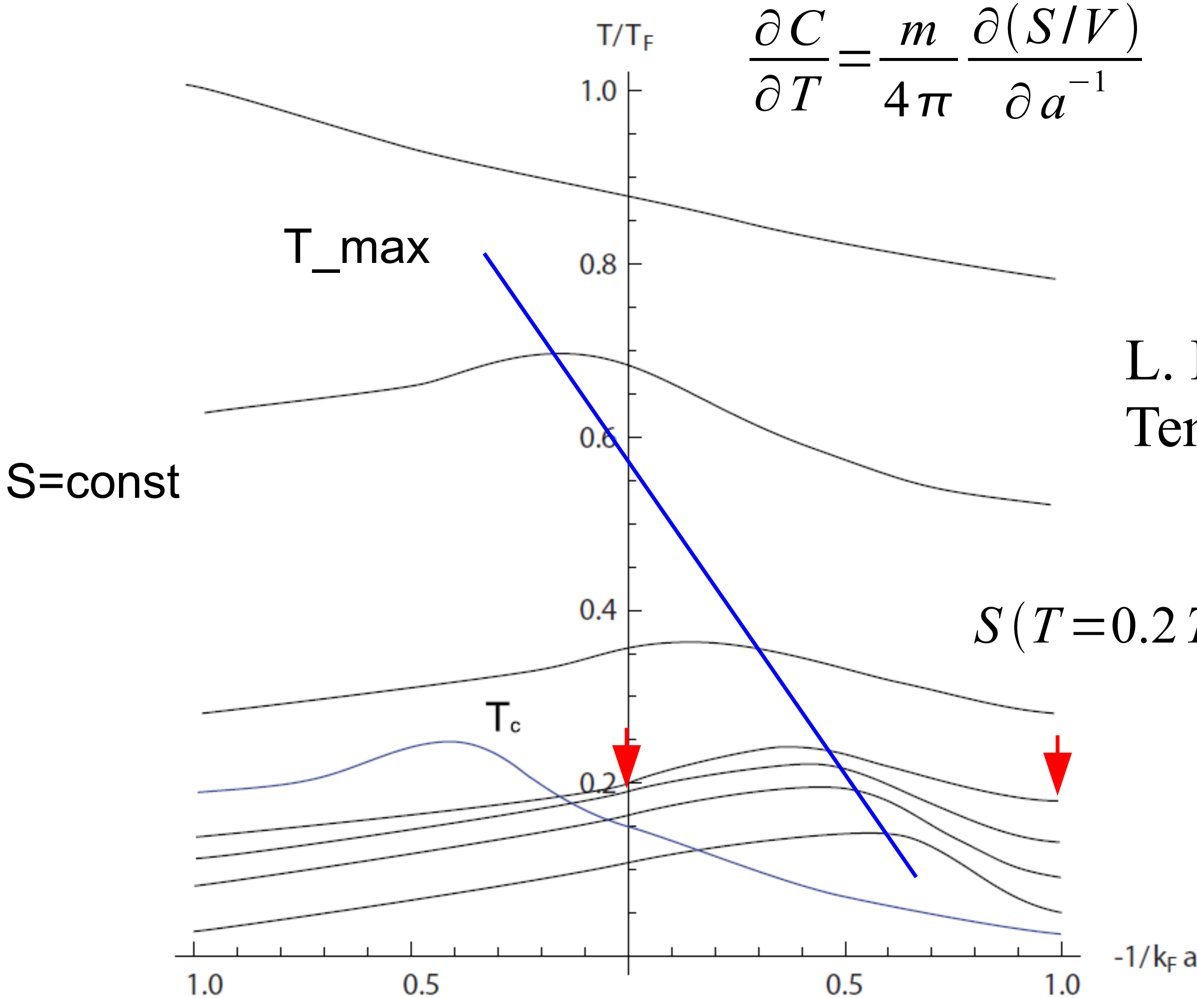


FIG. 2. (Color online) Sketches of isentropes of a balanced two-component Fermi gas, from which one can infer the temperature dependence of $C(T)$.

L. Luo and J. E. Thomas, J. Low Temp. Phys. **154**, 1 (2009)

$$S(T=0.2\,T_F, a \to 0^-) = S(T=0.2\,T_F, 1/a=0)$$

At unitarity, T_max>0.2 T_F

Joaquín E. Drut, Timo A. Lähde, Timour Ten, arXiv:1012.5474

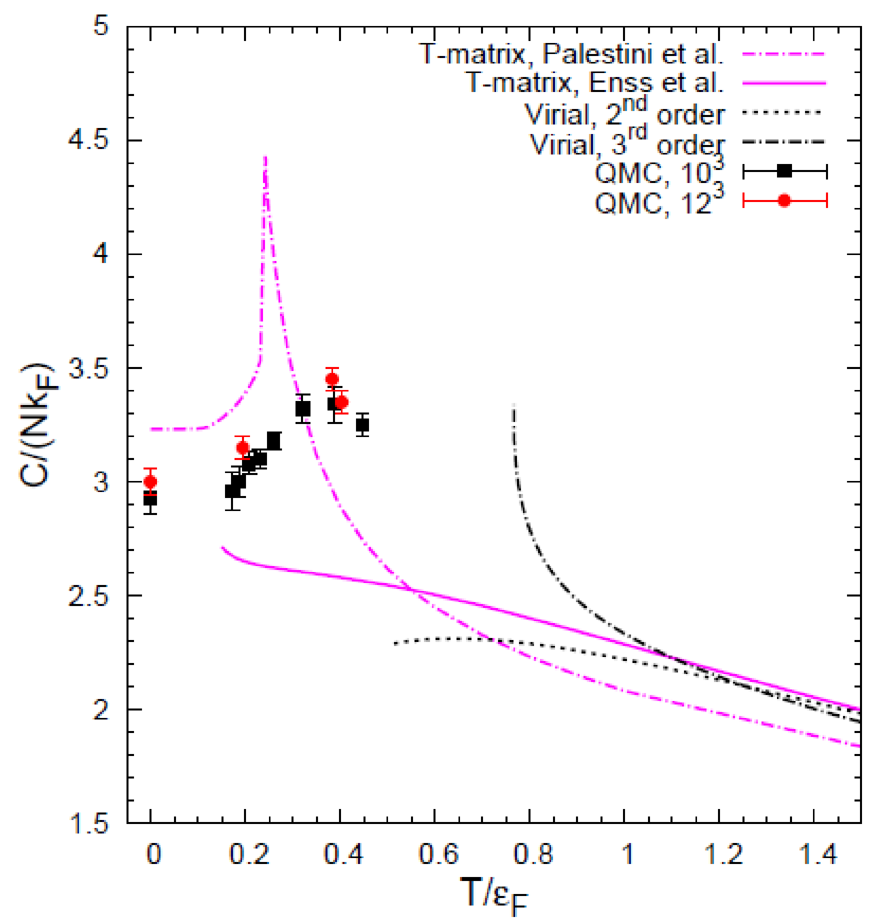
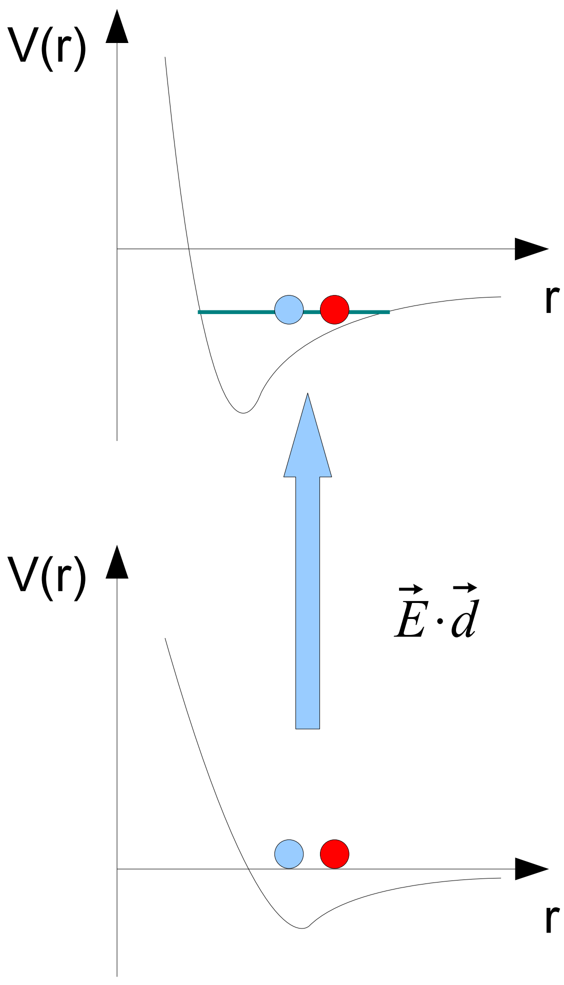


FIG. 3: (Color online) Summary of results for $C/(Nk_F)$ as a function of T/ϵ_F. The solid datapoints are determined from the large k/k_F behavior of $n(k)$, and the errorbars are dominated by systematics related to the residual fluctuations in the plateaux, as shown in Fig. 2. Also shown are the results of the virial expansion of Ref. [29], as well as the t-matrix calculations of Refs. [27, 28].

Photoassociation



A resonant electrical field E, coupled to the electronic dipole moment, converts fermions into a molecular state which loses from the trap.

The loss rate of the atoms from the trap

$$\Gamma \propto \langle \psi_1^+(\vec{r})\psi_2^+(0)\psi_2(0)\psi_1(\vec{r})\rangle$$

Expt: G. B. Partridge, K. E. Strecker, R. I. Kamar, M. W. Jack, R. G. Hulet, Phys. Rev. Lett. 95, 020404 (2005).

coupled to the closed channel

$$\frac{dN(t)}{dt} = -\frac{\Omega^2}{\gamma}\frac{4\pi a_{bg}V}{m\mu_b \Delta B}\left(\frac{1}{a_{bg}}-\frac{1}{a}\right)^2 \boxed{C}$$

$$\Omega = \langle f|d|i\rangle$$

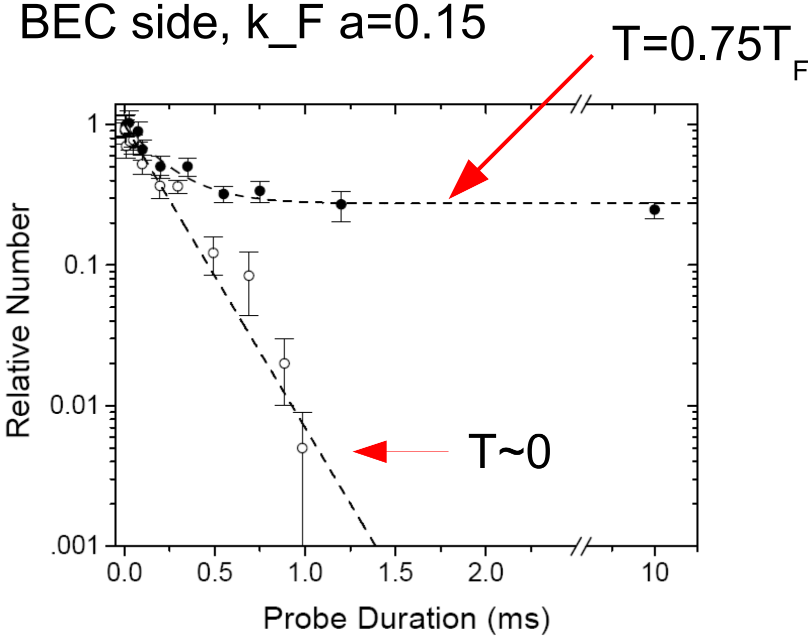
F. Werner, L. Tarruell, and Y. Castin, Eur. Phys. J. B **68**, 401(2009)

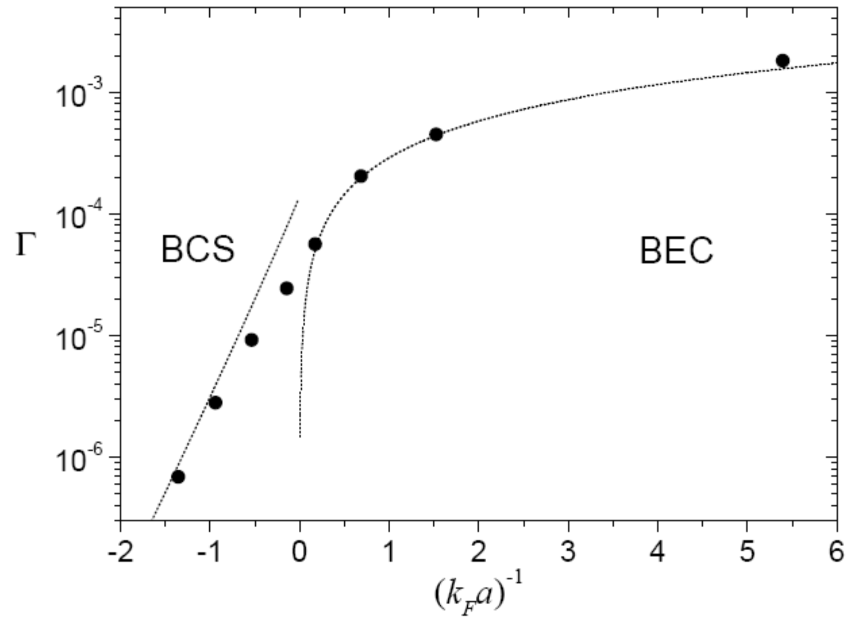
S. Zhang and A.J. Leggett, Phys. Rev. A 79, 023601 (2009)

Photoassociation of ^{6}Li

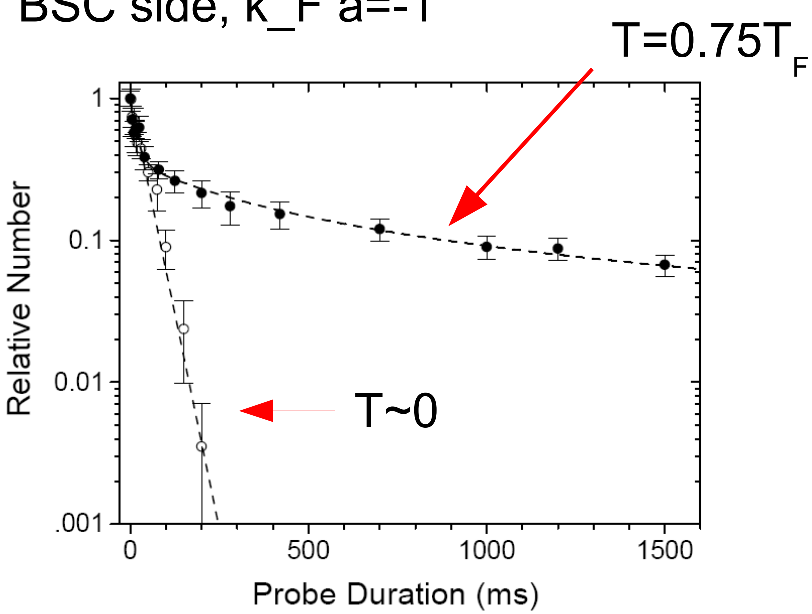
G. B. Partridge, K. E. Strecker, R. I. Kamar, M. W. Jack, R. G. Hulet, Phys. Rev. Lett. 95, 020404 (2005).

BEC side, k_F a=0.15

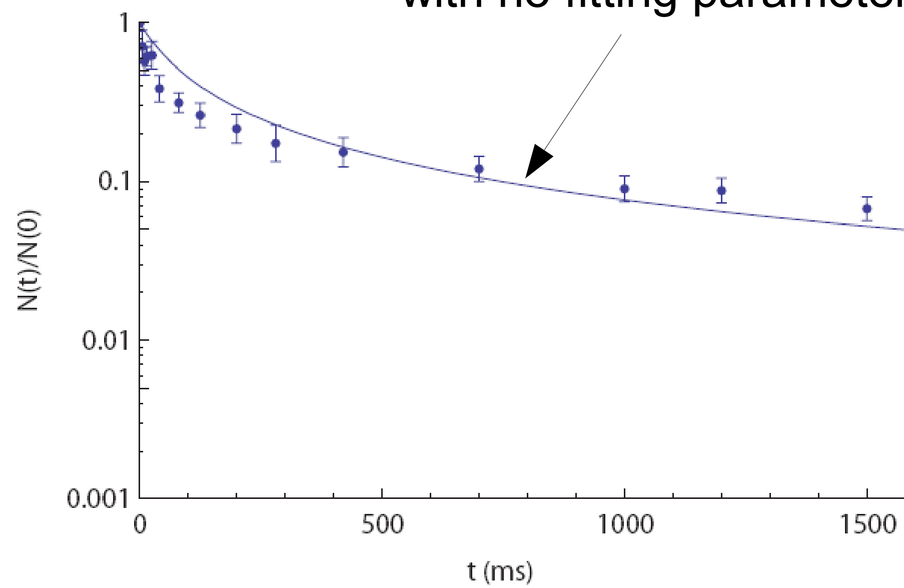




BSC side, k_F a=-1



Virial expansion theoretical result with no fitting parameters



Future questions

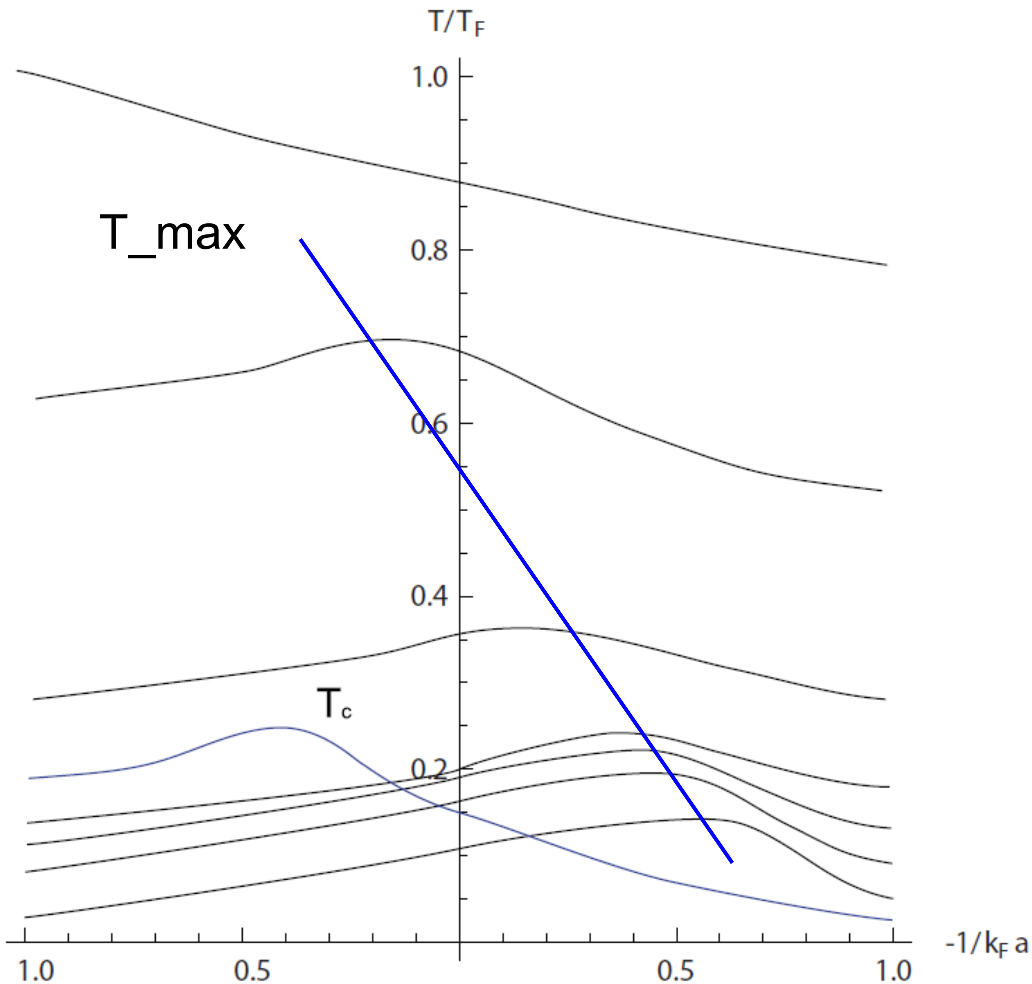
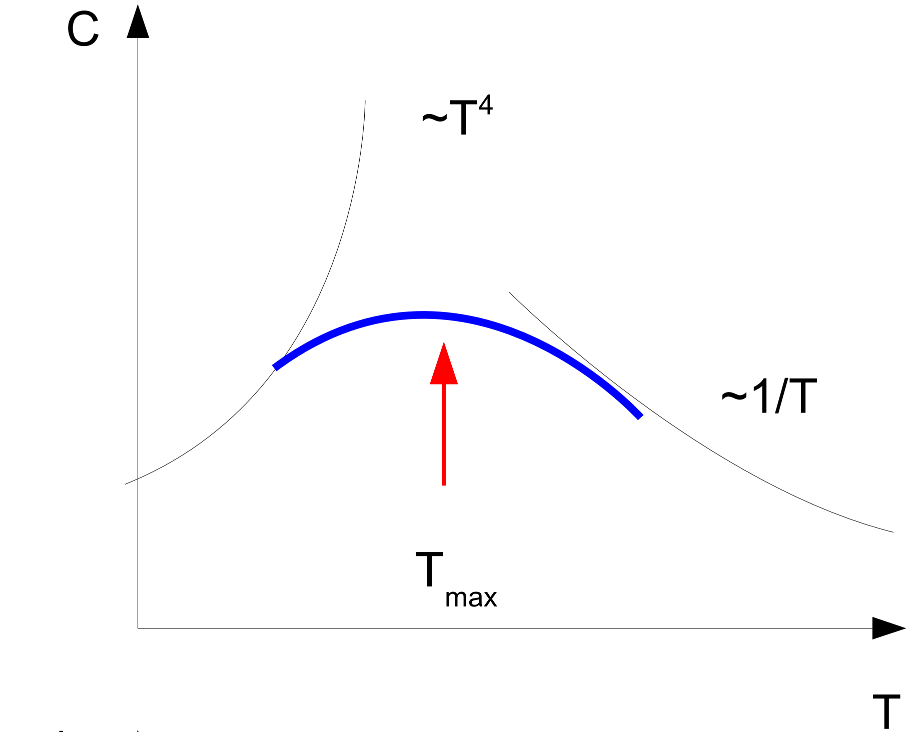
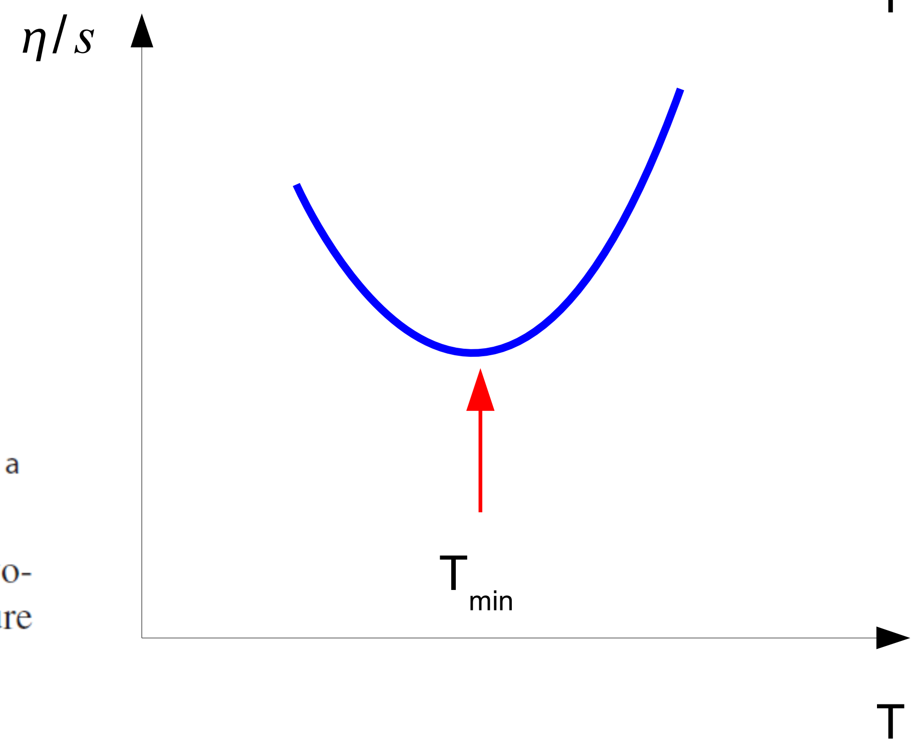


FIG. 2. (Color online) Sketches of isentropes of a balanced two-component Fermi gas, from which one can infer the temperature dependence of $C(T)$.





Thank You

谢谢