

Theory of rf-Spectroscopy of Strongly Interacting Fermions

M. Punk and W. Zwerger

Physik-Department, Technische Universität München, James-Frank-Str., D-85748 Garching, Germany

(Received 5 July 2007; published 25 October 2007)

We show that strong pairing correlations in Fermi gases lead to the appearance of a gaplike structure in the rf spectrum, both in the balanced superfluid and in the normal phase above the Clogston-Chandrasekhar limit. The average rf shift of a unitary gas is proportional to the ratio of the Fermi velocity and the scattering length with the final state. In the strongly imbalanced case, the rf spectrum measures the binding energy of a minority atom to the Fermi sea of majority atoms. Our results provide a qualitative understanding of recent experiments by Schunck *et al.*

DOI: [10.1103/PhysRevLett.99.170404](https://doi.org/10.1103/PhysRevLett.99.170404)

PACS numbers: 03.75.Ss, 05.30.Fk, 32.30.Bv

According to the 50 yr old microscopic theory of Bardeen, Cooper, and Schrieffer, the phenomenon of superfluidity in a system of fermions is connected with the formation of bound pairs. In the weak coupling limit, where the formation of pairs and their condensation appears simultaneously, the transition to the superfluid state is associated with the appearance of a gap in the fermionic excitation spectrum. For strong coupling, however, this simple connection is no longer valid and bound pairs of fermions may exist even in the normal state. This phenomenon is well known from the pseudogap phase in high temperature superconductors, where a d -wave pairing gap appears on the Fermi surface at temperatures far above the superconducting transition temperature [1]. A much simpler example is realized by ultracold fermions near a Feshbach resonance, which provide a perfectly controllable model system to study the effects of strong pairing interactions [2]. In the case of an equal population of the two hyperfine states undergoing pairing, the ground state is superfluid at arbitrary values of the scattering length. A microscopic signature of pairing in ultracold Fermi gases has first been obtained by Chin *et al.* [3] through rf spectroscopy. The rf field drives transitions between one of the hyperfine states $|2\rangle = |\downarrow\rangle$ which is involved in the pairing and an empty hyperfine state $|3\rangle$ which lies above it by an energy $\hbar\omega_{23}$ due to the magnetic field splitting of the bare atom hyperfine levels. In the absence of any interactions, the spectrum exhibits a sharp peak at $\omega = \omega_{23}$. Pairing between the two lowest hyperfine states $|1\rangle$ and $|2\rangle$ leads to an upward shift of this resonance. The shift essentially follows the two-particle binding energy on the BEC-side of the crossover but stays finite on the BCS side, where the appearance of a bound Cooper pair is a many-body effect

[3]. A theoretical explanation of these observations can be given by extending the BCS description of pairing to the strong coupling regime and neglecting interactions involving state $|3\rangle$ [4,5]. In a homogeneous system, the resulting rf spectrum exhibits a peak at energies around Δ^2/μ , which is of the order of the energy gap $\Delta \approx 0.5\varepsilon_F$ at the unitarity point. Since pairing appears already in the normal state above T_c , the rf shift does not directly measure the superfluid order, however [5]. The importance of understanding the relation between rf spectra and the nature of the many-body states involved, is underlined by recent experiments in imbalanced gases [6]. There, a shift in the rf spectrum is observed which hardly changes between the balanced superfluid and a normal ground state beyond a critical population imbalance, where superfluidity is destroyed by a sufficiently large mismatch of the Fermi energies even at $T = 0$ (this is the analog of the Clogston-Chandrasekhar limit in superconductors). In this Letter, we present a theory of rf shifts in both balanced and imbalanced Fermi gases, which provides a qualitative understanding of these observations. In particular, we show that the average frequency shift in the balanced superfluid at unitarity (i.e., at infinite scattering length) is linear in the Fermi velocity and inversely proportional to the scattering length a_{13} . In the nonsuperfluid state beyond the Clogston-Chandrasekhar limit, pair fluctuations give rise to sharp peaks in the rf spectrum which are associated with the binding of $|\downarrow\rangle$ -pairs even in the absence of long range phase coherence.

Within linear response theory, which is adequate for rf pulses short compared to the Rabi oscillation period of the bare 2–3 transition, the number of particles transferred from state $|2\rangle$ to state $|3\rangle$ per unit time is given by

$$I(\omega) \sim \int dt d^3x d^3x' e^{i(\mu_3 - \mu_1 - \omega_L)t} \langle [\psi_3^\dagger(x, t) \psi_1(x, t) \psi_1^\dagger(x', 0) \psi_3(x', 0)] \rangle, \quad (1)$$

where $\omega = \omega_L - \omega_{23}$ denotes the detuning of the rf field from the bare 2–3 transition. Since particles in state $|3\rangle$ have a nonvanishing interaction with those in states $|1\rangle$ and $|2\rangle$ [7], the response function in Eq. (1) does not factorize into one particle functions, making a full calculation of the spectrum very difficult. Nevertheless, near $T = 0$, where only a single peak is observed in the rf spectrum, its position can be determined from a sum rule approach [8]. In particular, the first moment $\bar{\omega} = \int d\omega \omega I(\omega) / \int d\omega I(\omega)$ is given by

$$\hbar \bar{\omega} = \frac{\bar{g}_{12} - \bar{g}_{13}}{N_2 - N_3} \left(\frac{\langle H'_{13} \rangle}{\bar{g}_{13}} - \frac{\langle H'_{12} \rangle}{\bar{g}_{12}} \right). \quad (2)$$

Here H'_{13} and H'_{12} denote the interaction Hamiltonians between the respective states, while N_2 and N_3 denote the total number of particles in states $|2\rangle$ and $|3\rangle$. The \bar{g}_{ij} are the bare interaction constants arising in the pseudopotential interaction Hamiltonian

$$H'_{ij} = \bar{g}_{ij} \int d^3x \psi_i^\dagger(x) \psi_j^\dagger(x) \psi_j(x) \psi_i(x). \quad (3)$$

They are related to their renormalized values $g_{ij} = 4\pi\hbar^2 a_{ij}/m$ by

$$\frac{1}{\bar{g}} = \frac{1}{g} - \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\varepsilon_{\mathbf{k}}}, \quad (4)$$

where a_{ij} are the s -wave scattering lengths between states i and j , m is the mass of the particles and $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/2m$ the single particle energy. Note that the interaction g_{23} between states 2 and 3 drops out quite generally, because H'_{23} and H_{RF} commute. Moreover, there is no shift of the rf peak if the interaction strengths g_{12} and g_{13} are equal, a case, where all interaction effects are cancelled exactly [8,9]. Since $\langle H'_{13} \rangle$ is of order N_3 , the first term in (3) is negligible compared to the second term if $N_2 \gg N_3$. The average shift of the rf spectrum then simplifies to

$$\hbar \bar{\omega} = \frac{\langle H'_{12} \rangle}{N_2} \left(\frac{\bar{g}_{13}}{\bar{g}_{12}} - 1 \right) \rightarrow \frac{\langle H'_{12} \rangle}{N_2 \Lambda} \frac{\pi}{2} \left(\frac{1}{a_{13}} - \frac{1}{a_{12}} \right). \quad (5)$$

Here, the second form is obtained by expanding $1 - \bar{g}_{13}/\bar{g}_{12}$ to leading order in the upper cutoff Λ of the momentum integral in (4). Evidently, for vanishing interactions $\bar{g}_{13} = g_{13} \equiv 0$ with state 3, the rf shift just measures the (negative) interaction energy per particle in the state 2. Within a pseudopotential description, however, the interaction energy $\langle H'_{12} \rangle \sim \Lambda$ diverges linearly with the cutoff. It is thus sensitive to the range of the interactions, which is set equal to zero in the pseudopotential. In terms of the spectrum $I(\omega)$, this divergence shows up as a slow decay $I(\omega) \sim \omega^{-3/2}$ at large frequencies, leading to a divergent first moment, as is easily seen within a BCS description with a constant gap Δ . Remarkably, for finite interactions $g_{13} \neq 0$, the second form of (5) gives a result for the frequency shift which is well defined and finite in the limit $\Lambda \rightarrow \infty$. As shown by Tan [10], the total energy of the balanced gas can be obtained from the momentum distribution $n_{\mathbf{k}}$ via $E = 2\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} (n_{\mathbf{k}} - C/k^4)$ up to a constant, which is irrelevant for the calculation of the limit $\langle H'_{12} \rangle/\Lambda$. Here C is the constant arising in the asymptotic behavior $\lim n_{\mathbf{k}} = C/k^4$ of the momentum distribution at large momenta. Evidently, the interaction contribution to the total energy is just $\langle H'_{12} \rangle = -2C\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}/k^4 \sim -C\Lambda$. Introducing a dimensionless constant s via $C = s k_F^4$, the shift of the rf spectrum

$$\hbar \bar{\omega} = s \frac{4\varepsilon_F^2}{n_2} \left(\frac{1}{g_{12}} - \frac{1}{g_{13}} \right) \quad (6)$$

of the balanced gas is completely determined by the universal constant s , the Fermi energy $\varepsilon_F = \hbar^2 k_F^2/(2m)$ of the balanced, noninteracting gas and the renormalized interaction constants g_{12} and g_{13} . The expression is finite for all coupling strengths g_{12} and evolves smoothly from the BCS to the Bose-Einstein condensation (BEC) limit. Within an extended BCS description of the ground state wave function, the product $s^{(0)} 4\varepsilon_F^2 \equiv \Delta^2$ is precisely the square of the gap parameter. In weak coupling, our result then coincides with that obtained by Yu and Baym [8], except for the mean field shift, which is not contained in the reduced BCS Hamiltonian. In the BEC-limit, where the BCS ground state becomes exact, the asymptotic behavior $\Delta_{\text{BEC}} = 4\varepsilon_F/\sqrt{3\pi k_F a_{12}}$ gives $\hbar \bar{\omega} = 2\varepsilon_b(1 - a_{12}/a_{13})$, where $\varepsilon_b = \hbar^2/ma_{12}^2$ is the two-particle binding energy. It is straightforward to show that this is precisely the average shift for bound-free transitions following from a detailed calculation of the rf spectrum in the molecular limit by Chin and Julienne [11]. The most interesting regime is that around the unitarity limit $1/g_{12} = 0$. At this point, the average rf shift is given by $\bar{\omega} = -0.46v_F/a_{13}$, which varies like the *square root* of the Fermi energy $\varepsilon_F = mv_F^2/2$. The constant $s = 0.098$ is obtained from the recent calculations of the crossover thermodynamics by Haussmann *et al.* [12]. Our result for the homogeneous gas can be compared directly with locally resolved rf spectra by Shin *et al.* [13]. Accounting for the enhancement of the local Fermi velocity at the trap center by a factor ≈ 1.25 due to the attractive interactions, the predicted average shift $\bar{\omega} = 2\pi \times 28.9$ kHz [14] is considerably larger than the measured position of the peak near 15 kHz. This is probably due to the fact, that $\bar{\omega}$ has a considerable contribution from the higher frequency part of the spectrum. A crucial prediction of our theory is the linear behavior of the average rf shift with the Fermi momentum. Experimentally, the spatial resolution necessary to distinguish this from the naive ε_F scaling has not yet been achieved [13].

To discuss the situation with a finite imbalance, it is convenient to introduce two distinct chemical potentials for the states undergoing pairing, defined by $\mu_{\uparrow} = \mu + h$ and $\mu_{\downarrow} = \mu - h$. Since the ground state of the spin balanced gas is a superfluid with a gap for fermionic excitations, it will be stable over a finite range $h < h_c$ of the chemical potential difference. In the BCS limit, the associated Clogston-Chandrasekhar critical field $h_c = \Delta_{\text{BCS}}/\sqrt{2}$ is exponentially small. Near the unitarity point, the absence of a second energy scale implies that the critical field h_c beyond which a nonzero polarization appears, is on the order of the bare Fermi energy ε_F of the balanced two-component Fermi gas. From fixed node diffusion Monte Carlo calculations the resulting numerical value in the continuum case at unitarity is $h_c = 0.96\mu \approx 0.4\varepsilon_F$ [15]. The phase for $h > h_c$ is a nonsuperfluid, polarized

mixture of the different spin states. For large enough fields, the system will eventually be completely spin polarized. At unitarity, the associated saturation field h_s was determined by Chevy [16] using a variational calculation of the energy change μ_\downarrow associated with adding a single \downarrow -particle to a Fermi sea of \uparrow -particles. This leads to an upper bound $\mu_\downarrow \leq -0.60\mu_\uparrow$ at the unitarity point, where $\mu_\uparrow = 2^{2/3}\varepsilon_F$ is the Fermi energy of the completely spin polarized gas. The saturation field thus obeys the inequality $h_s \geq 0.8\mu_\uparrow = 1.27\varepsilon_F$. At unitarity, therefore, there is a wide regime $h_c < h < h_s$ of an intermediate phase between the balanced superfluid and a fully polarized gas. While superfluidity is quenched in this phase, the strong interactions between particles in states $|1\rangle$ and $|2\rangle$ still give rise to large frequency shifts in the rf spectrum, as will be shown below. To study the effect of pairing fluctuations on the imbalanced Fermi gas above the Clogston-Chandrasekhar limit, we calculate the pair-fluctuation spectrum from the two-fermion Green function, using a non-self-consistent T -matrix approach, similar to the approach by Combescot *et al.* [17]. Such a perturbative analysis is reasonable, since the states which are coupled through the interaction Hamiltonian are separated by an energy gap of width $2h$. A usual ladder approximation is used to incorporate the effects of the attractive $\uparrow\downarrow$ -interaction on the vertex part, whereas the self-energy is calculated at the one-loop level, including vertex corrections. The basic equations for the polarization loop L , vertex part Γ and self-energy part of the minority species Σ_\downarrow are given by (see Fig. 1, we take units such that $\hbar = 1$)

$$L(\mathbf{q}, i\Omega_n) = -\frac{1}{\beta} \sum_{\omega_m} \int \frac{d^3k}{(2\pi)^3} \mathcal{G}_\uparrow^{(0)}(\mathbf{q} - \mathbf{k}, i\Omega_n - i\omega_m) \times \mathcal{G}_\downarrow^{(0)}(\mathbf{k}, i\omega_m), \quad (7)$$

$$\Gamma(\mathbf{q}, i\Omega_n) = \frac{1}{1/\bar{g} - L(\mathbf{q}, i\Omega_n)}, \quad (8)$$

$$\Sigma_\downarrow(\mathbf{k}, i\omega_n) = \frac{1}{\beta} \sum_{\Omega_m} \int \frac{d^3q}{(2\pi)^3} \Gamma(\mathbf{q}, i\Omega_m) \times \mathcal{G}_\uparrow^{(0)}(\mathbf{q} - \mathbf{k}, i\Omega_m - i\omega_n), \quad (9)$$

where $\mathcal{G}_\uparrow^{(0)}$ and $\mathcal{G}_\downarrow^{(0)}$ are the bare Matsubara-Green's func-

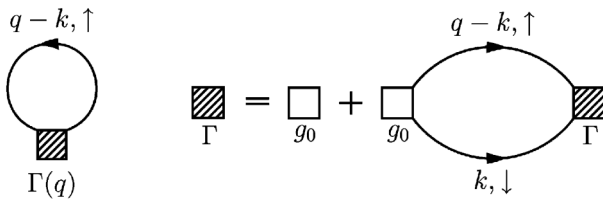


FIG. 1. Lowest order self-energy diagram for the minority component (\downarrow) Green's function and Bethe-Salpeter equation for the vertex part in ladder approximation.

tions of the majority and minority component, and $\beta = 1/k_B T$ is the inverse temperature. $\omega_n = (2n + 1)\pi/\beta$ and $\Omega_n = 2\pi n/\beta$ with $n \in \mathbb{Z}$ denote fermionic and bosonic Matsubara frequencies, respectively. After evaluating the Matsubara summation and analytic continuation, the vertex part can be calculated analytically at $T = 0$. In the regime $h > \mu$ (i.e., essentially beyond the Clogston-Chandrasekhar field $h > h_c \approx 0.96\mu$), one obtains for $\mathbf{q} = 0$, $\omega > -2\mu$

$$\Gamma^R(\mathbf{0}, \omega) = \frac{2\pi^2}{mk_{F\uparrow}} \left\{ -\frac{\pi}{2k_{F\uparrow}|a|} - 1 + \frac{1}{2} \sqrt{\frac{\omega + 2\mu}{2\mu_\uparrow}} \right. \\ \left. \times \left[\ln \left| \frac{1 + \sqrt{\frac{\omega + 2\mu}{2\mu_\uparrow}}}{1 - \sqrt{\frac{\omega + 2\mu}{2\mu_\uparrow}}} \right| + i\pi\Theta(\omega - 2h) \right] \right\}^{-1}, \quad (10)$$

where $\Theta(x)$ is the unit step function and $k_{F\uparrow}$ is defined via $k_{F\uparrow} = \sqrt{2m\mu_\uparrow}/\hbar$. For $h > \mu$ the retarded vertex $\Gamma^R(\mathbf{q} = 0, \omega)$ has a single pole on the real axis at $\omega_0^+ = 2h - \Omega_+$ with $\Omega_+ > 0$ (note that for $h < \mu$ the vertex has two real poles). Physically, this pole describes an excitation in which two fermions with opposite spin and vanishing total momentum form a pair at the Fermi energy of the majority component with binding energy Ω_+ . A similar structure was first discussed for weak coupling by Aleiner and Altshuler [18] in the context of small superconducting grains. Remarkably, as shown in Fig. 2, the pair binding energy in units of μ_\uparrow is constant for $h > \mu$ and agrees well with the value $0.6\mu_\uparrow$ for the binding energy of a single down spin in the presence of a Fermi sea of majority atoms as calculated by Chevy [16]. The retarded self-energy for the minority component in the normal state is given by

$$\Sigma_\downarrow^R(\mathbf{k}, \omega) = \int \frac{d^3q}{(2\pi)^3} \frac{dz}{\pi} \{ n_B(z) G_{A\uparrow}^{(0)}(\mathbf{q} - \mathbf{k}, z - \omega) \\ \times \text{Im}\Gamma^R(\mathbf{q}, z) - n_F(z) \text{Im}G_{R\uparrow}^{(0)}(\mathbf{q} - \mathbf{k}, z) \\ \times \Gamma^R(\mathbf{q}, z + \omega) \}, \quad (11)$$

with n_B and n_F denoting the Bose and Fermi distributions.

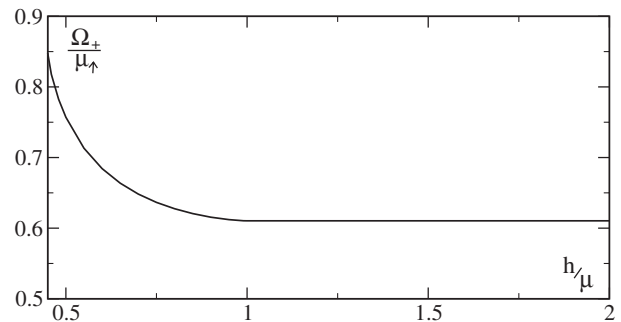


FIG. 2. Pair binding energy Ω_+ in units of μ_\uparrow at unitarity as a function of h at $T = 0$. For $h > \mu$ the binding energy is constant and given by $\Omega_+ = 0.61\mu_\uparrow$.

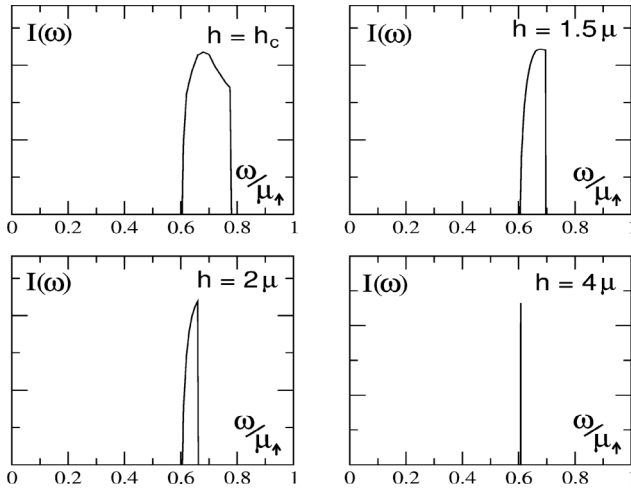


FIG. 3. rf spectra at unitarity for different imbalances at $T = 0$ (Intensity in arbitrary units; $h_c = 0.96\mu$).

This result enables us to calculate rf spectra explicitly in the limit of vanishing g_{23} and g_{13} , where the expectation value in Eq. (2) can be factorized. In this case, one obtains [4,5]

$$I(\omega) \sim \int \frac{d^3k}{(2\pi)^3} \text{Im} G_1^R(\mathbf{k}, \varepsilon_{\mathbf{k}} - \omega - \mu_1) n_F(\varepsilon_{\mathbf{k}} - \omega - \mu_1),$$

if state $|3\rangle$ is initially empty. In Fig. 3 we have numerically evaluated the resulting rf spectra at unitarity for different fields above the Clogston-Chandrasekhar limit. The calculation explains two features which are seen in the experimental data [6], namely, the shift of the rf peak due to pairing fluctuations in the normal state and the decreasing linewidth with increasing population imbalance. The onset of the rf spectrum coincides with the pair binding energy $\Omega_+ \approx 0.6\mu_1$ for $h > h_c$, which is independent of the imbalance. In the presence of a finite $|1\rangle - |3\rangle$ interaction, the detailed spectrum $I(\omega)$ cannot be calculated analytically. Its first moment, however, is again determined by the sum rule Eq. (5). Evaluating the interaction energy $\langle H'_{12} \rangle$ using the variational wave function of Chevy [16], it turns out that the resulting average rf shift for an almost completely polarized gas is equal to $\bar{\omega} = -0.34\hbar k_{F1}/ma_{13}$. Because of the sharpness of the peak in this limit, the average shift in the strongly imbalanced gas coincides with the experimentally observed peak position. For the parameters in [13], we obtain an average rf shift $\bar{\omega} = 2\pi \times 17$ kHz at the trap center for strong imbalance, close to the observed value in the balanced case. Our theory thus accounts for the observation by Schunck *et al.* [6], where an average over the trap is involved, that there is hardly any difference in the rf shift between the balanced and strongly imbalanced gas.

In conclusion, we have given a theory of rf spectra in ultracold Fermi gases which includes interactions between all three states involved. In the balanced unitary gas, the average rf shift is proportional to $-sv_F/a_{13}$, where s is a universal constant characterizing the fermion momentum distribution at large wave vectors. In the imbalanced case, the rf spectrum exhibits a sharp peak arising from the binding energy of a $\uparrow\downarrow$ -pair which is finite even in the nonsuperfluid state. Including a finite value of a_{13} , the resulting average shift is close to the peak shift in the balanced case.

We gratefully acknowledge very helpful discussions with W. Rantner, Yong-il Shin, and M. Zwierlein. This work was supported by the DFG Forschergruppe ‘‘Strong Correlations in multiflavor ultracold Quantum Gases’’.

Note added in proof.—Equivalent results for the rf shift of balanced gases have been obtained independently by Baym *et al.* [19]. In fact, our value for the prefactor in $\bar{\omega} = -0.46sv_F/a_{13}$ agrees well with the value obtained in this reference, using a different method.

-
- [1] P. Lee, N. Nagaosa, and X.G. Wen, *Rev. Mod. Phys.* **78**, 17 (2006).
 - [2] See, e.g., I. Bloch, J. Dalibard, and W. Zwerger, arXiv:0704.3011.
 - [3] C. Chin *et al.*, *Science* **305**, 1128 (2004).
 - [4] J. Kinnunen, M. Rodriguez, and P. Torma, *Science* **305**, 1131 (2004).
 - [5] Y. He, Q. Chen, and K. Levin, *Phys. Rev. A* **72**, 011602 (2005).
 - [6] C.H. Schunck *et al.*, *Science* **316**, 867 (2007).
 - [7] S. Gupta *et al.*, *Science* **300**, 1723 (2003).
 - [8] Z. Yu and G. Baym, *Phys. Rev. A* **73**, 063601 (2006).
 - [9] M.W. Zwierlein *et al.*, *Phys. Rev. Lett.* **91**, 250404 (2003).
 - [10] S. Tan, arXiv:condmat/0505200.
 - [11] C. Chin and P.S. Julienne, *Phys. Rev. A* **71**, 012713 (2005).
 - [12] R. Haussmann *et al.*, *Phys. Rev. A* **75**, 023610 (2007). Note that the dependence $n_{\mathbf{k}} \rightarrow C/k^4$ and the corresponding value of $s \approx 0.1$ at T_c has been determined earlier in R. Haussmann, *Phys. Rev. B* **49**, 12975 (1994).
 - [13] Y. Shin *et al.*, *Phys. Rev. Lett.* **99**, 090403 (2007).
 - [14] The values for a_{13} have been taken from M. Bartenstein *et al.*, *Phys. Rev. Lett.* **94**, 103201 (2005).
 - [15] C. Lobo *et al.*, *Phys. Rev. Lett.* **97**, 200403 (2006).
 - [16] F. Chevy, *Phys. Rev. A* **74**, 063628 (2006).
 - [17] R. Combescot *et al.*, *Phys. Rev. Lett.* **98**, 180402 (2007).
 - [18] I.L. Aleiner and B.L. Altshuler, *Phys. Rev. Lett.* **79**, 4242 (1997).
 - [19] G. Baym *et al.*, arxiv:0707.0859.