The Unitary Fermi Gas: An Overview

by

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1.1 INTRODUCTION

For a good introduction to cold-atom physics, look at the book by Pethick and Smith [1]. Then, to get a feel for the current state of research, look at the reviews [2–5].

1.2 UNIVERSALITY

First some notations. We consider here gases of two-species of nonrelativistic fermion, which we shall label a and b, that interact with an attractive and short range interaction. Let the masses be equal $m_a = m_b = m$, and the densities be denoted n_a and n_b such that the total density is $n_+ = n_a + n_b$. We shall express everything in terms of the Fermi wave-vector k_F , Fermi energy $\epsilon_F = \hbar^2 k_F^2/2m$.

At low densities, the two-body s-wave interaction dominates and can be described by the effective range expansion (see for example [6])

$$k \cot \delta_k = \frac{-1}{a_s} + \frac{r_e k^2}{2} + O(k^4).$$
 (1)

where δ_k is the phase shift at wave-vector k. This is one way of defining the s-wave scattering length a_s . (See problem P-4 to get a feel for the unitary limit.) The unitary limit corresponds to the separation of scales

$$\mathbf{r}_e \ll \mathbf{k}_F^{-1} \ll \mathfrak{a}_S. \tag{2}$$

I.e. when the density can be taken so low that the interparticle separation is much larger than the range ($k_F r_e \ll 1$), then the system is fully described by the single dimensionless combination $k_F a_S$. In this limit, all properties of the potential that are characterized by higher terms in the effective range expansion (1) (sometimes called "shape" parameters) become irrelevant and everything is characterized by the s-wave scattering length a_S .

Since the only length scales are the interparticle spacing $\propto k_F^{-1}$ and the scattering length a_S , the physics of homogeneous matter is completely described by the dimensionless parameter $(k_F a_S)^{-1}$: this set of theories describe the Bardeen-Cooper-Schrieffer (BCS)/Bose-Einstein Condensate (BEC) crossover. The unitary limit occurs when One can think of two spin states in neutrons, or two hyperfine states of an atom in cold atom, or even two different species.

It is common to drop factors of $\hbar = 1$ and mass m = 1 to obtain more "natural" units. I will endeavour to keep them in the formulae, but don't be alarmed if they go astray – just add them as needed to make up the appropriate densities.

Indeed, cold atom systems typically are unstable, with the ground state being not a gas, but a metal (lithium for example). The dilute gases realized in experiment are actually long-lived metastable states. The decay mode – via three-body scattering – is highly suppressed in the dilute limit. the scattering length is subsequently taken much larger than the interparticle spacing (1 $\ll |k_F \alpha_S|$). Then all length-scales drop out and one obtains a theory who's only dimensionful scale is set by the density $n_+ = k_F^3/3\pi^2$ (see problem P-2).

When this state was first considered, it was not at all obvious that the limit of infinite scattering length could be taken simultaneously with the zero-range limit. The potential failure of this approach would be a collapse whereby the density would increase until $k_Fr_e \sim 1$ and the shape of the potential would soften the potential, allowing the exclusion pressure to stabilize the system in a high-density state.

George Bertsch formally posed the question of the stability of dilute matter in this limit as a challenge question [7] that has since been practically (though not formally) resolved through a combination of theories and experiments. Thus, one realizes a single state of matter – the Unitary Fermi Gas (UFG) – that can arise in the dilute limit of any short-range interaction if the potential can be tuned so that $a_S \gg k_F^{-1}$. This is the sense in which the physics is "universal". This limit is not "natural": one would generically expect the the scattering length and range to have the same scale $a_S \sim r_e$. It turns out, however, that dilute neutron matter has an unnaturally large scattering length making the unitary limit physically relevant. To deal with this unnatural ordering of scales in Effective Field Theory (EFT), one must choose the appropriate subtraction scheme (see [10, 11] for details and [12] for a pedagogical overview).

As a result of this universality we can define the thermodynamics of the theory in terms of a single dimensionless parameter $\xi \approx 0.37$ – known as the Bertsch parameter – through the energy density:

$$\mathcal{E}(\mathbf{n}_{+}) = \xi \mathcal{E}_{\mathsf{FG}}(\mathbf{n}_{+}) \tag{3}$$

where $\mathcal{E}_{FG}(n_+)$ is the energy density of the free Fermi gas (see problems P-1 and P-2). Despite the simplicity of the thermodynamics, the system itself is highly correlated and lacks any perturbative expansion parameter. Thus, measuring and computing the *value* of ξ has been a major challenge over the past decade (see Fig. 13 of [13] for the historical set of values given for ξ).

1.3 AWAY FROM UNITARITY

When one departs from the unitary limit – finite T, a_S , r_e , polarization $n_a - n_b \neq 0$ etc., additional length scales enter the problem and the thermodynamic functions depend on dimensionless functions of

various dimensionless ratios (see problem P-6). For example, at finite polarization, it is useful to characterized the thermodynamic functions by dimensionless functions of the dimensionless ratio n_b/n_a . As one introduces more length scales, these functions become multidimensional and one quickly runs out of enough information to accurately parametrize them. Currently, the finite-temperature characterization has received the most rigorous characterization from the Massachusetts Institute of Technology (MIT) group [14].

Perhaps the most interesting physics lies in the polarized Fermi gas, where many exotic phases may exist including P-wave superconductors, crystalline super-solids (Larkin-Ovchinnikov Fulde-Ferrel (LOFF) states), and gapless superconductors (see figure 1).



Figure 1: (Figure 1 from [15].) Conjectured zero-temperature grand canonical phase diagram after [16]. Scaling relations allow this twodimensional projection of the three parameters $(\mu, \alpha_S, \delta\mu)$. The chemical potential asymmetry $\delta \mu = (\mu_a - \mu_b)/2$, and the s-wave scatteringlength a_S are expressed in units of the s-wave gap $\Delta_{\delta\mu=0}$ and density $n_{\delta\mu=0}$ of the symmetric state with the same parameters μ and a, but with $\delta\mu = 0$. The phase P₁ – a gapless superfluid with single Fermi surface in [16] – is a P-wave superfluid/BEC phase. The phase P_2 – a two-component Fermi-liquid in [16] – is a two-component P-wave phase. There may be additional P-wave phases (for instance in the breached pair phases) near the s-wave Feshbach resonance. Likewise, the exact nature of the phase(s) labeled "LOFF?" has yet to be determined. The dotted lines in the BEC and BCS regimes represent sample trajectories of constant a_S and $\delta\mu$. A trap provides a radially varying μ , and would comprise concentric shells of the various phases crossed by these trajectories starting from the crosses at the center of the trap.

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1.4 PHYSICAL REALIZATIONS

As mentioned before, dilute neutron matter – as expected in the shells of neutron stars – is well modelled by the UFG on account of the unnaturally large neutron-neutron scattering length $a_{nn} \approx -18.9(4)$ fm [17]. Many qualitative properties of dilute neutron matter may thus be studied with the UFG, though quantitative calculations need to take into account the effects of the rather large effective range $r_{nn} \approx 2.75(11)$ fm [19].

The UFG can be realized directly in systems of trapped neutral alkali atoms (⁶Li is the most commonly studied isotope). These systems are tuned through a Feshbach resonance [20] by adjusting an external magnetic field so that a bound-state in a closed channel is brought to zero-energy. This resonance allows different hyperfine states of the atoms to interact over large inter-particle separations even though their range is extremely small (set by the van der Waals interactions). Through various cooling techniques (see the demo http://www.colorado.edu/physics/2000/bec/evap_cool.html), cold-atom experiments can study cool quantum-degenerate gases comprising ~ 10⁶ particles. (See [21] for a review of the experimental techniques.)

In addition to tuning the interactions, one can control the particle number and population imbalance. Systems can also be produced with different interacting species, or a variety of different hyperfine states to study multi-component systems. In addition to s-wave Feshbach resonances, many resonances in higher partials such as P-wave interactions have been identified. (See [22] for a review of known resonances.)

Through precise control of magnetic and optical traps, 1D tubes, 2D planes, and a variety of 3D systems can be studied. Recent interest has concerned optical lattices – spatially varying potentials – which can be used to study lattice models, or to further control interactions. Optical traps can also be used to manipulate the systems: for example, by stirring the system, the MIT group observed regular vortex lattices [23] – an indication that superfluidity had be achieved. One typically images these systems destructively through photo-absorption imaging, but other techniques are being developed. See [21] for a review.

An exciting possibility is to use cold-atoms systems to simulate neutron matter, or even Quantum Chromo-Dynamics (QCD). This program is in its infancy, but progress in cold-atom technology has been extremely rapid, and it is likely that simple simulators can be realized in the near future. (For example, people have explored the possibility of engineering interactions with a finite range to simulate neutron matter [24], as well as attempted to model dynamical gauge fields [25].)

2.1 PERTURBATIVE TECHNIQUES

The two limiting cases of the BEC/BCS crossover admit perturbative treatment. In the BEC limit, one can describe the system in terms of tightly-bound bosonic dimers and excess fermions (if polarized). One can explicitly solve the two, three, and four-body problems to obtain the properties of these weakly interacting components, and then perform perturbation theory. For example, solving the two-body problem (problem P-4), one finds that the bosonic dimer has a binding-energy of $E_B = \hbar^2/ma_S^2$. Likewise, one can compute the dimer-fermion scattering length a_{FB} by solving the three-body problem, and the dimer-dimer scattering length a_{BB} by solving the four-body problem. Including these, we obtain the following energy for the BEC limit:

$$\mathcal{E}(n_F, n_B) = -E_B n_B + \frac{3}{5} \frac{\hbar^2}{2m} (6\pi^2)^{2/3} n_F^{5/3} + f_{FB} n_F n_B + \frac{1}{2} f_{BB} n_B^2, \quad (4)$$

where $n_B = n_b$ is the number of dimers (tightly bound "bosons") and $n_F = n_a - n_b$ is the number of unpaired fermions. The couplings are determined from the scattering length $a_S > 0$ using few-body methods [26–28]:

$$f_{BB} = \frac{\pi \hbar^2}{m} a_{BB} a_S \approx \frac{\pi \hbar^2}{m} 1.2 a_S, \qquad (5a)$$

$$f_{FB} = \frac{\pi \hbar^2}{m} a_{FB} a_S \approx \frac{\pi \hbar^2}{m} 3.54 a_S, \qquad (5b)$$

$$E_{\rm B} = \frac{\hbar^2}{m} a_{\rm S}^{-2} \tag{5c}$$

Deep in the BEC limit, the couplings become weak and the many-body system may be treated perturbatively as an expansion in $k_F \alpha_S$ (here k_F is typically defined in terms of the total density $k_F = (3\pi^2 n_+)^{1/3}$ as before).

Likewise, when the bare attraction between the fermions is weak, the scattering length becomes small and negative. In this BCS limit, one may perturbatively expand in powers of $k_F \alpha_S$, but one must first deal with the infrared (IR) singularities associated with the wellknown BCS instability. This probably is highlighted by our lack of understanding about the nature of polarized superfluid phases, even

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We consider only $n_a \ge n_b$ so that any excess (unpaired) fermions are of type a and there are $n_F = n_a - n_b$ of these (per unit volume). The remaining fermions are all paired into $n_B = n_b$ dimers. in this weak-coupling regime. There may be many possible partially polarized states – even at weak coupling – but one needs to know the IR structure of these states to be able to compare their energies. The BCS superfluid state appears as an instability in the normal state, and one might discover a hint of a new state from a perturbative calculation, but as is well known, one cannot reach the BCS perturbatively from the normal state, even though the system has weak interactions.

Many proposed phases exist, include crystalline LOFF states, gapless superfluids, and P-wave superconductors, but the best one can do is to compare the energies of these various states. In principle, the true ground state at finite polarization might be something very different, and if it is separated by a first-order transition from the other states, then there might not even be a perturbative signal in the form of an instability. To truly understand what is happening in these interesting regimes, one needs a reliable *ab initio* method or experiment. Once one has identified the IR structure of the ground state, then these perturbative techniques allow one to quantify what happens in the deep **BEC** and **BCS** limits (see Fig. 1). Unfortunately, they do not help at all for quantifying what happens in the unitary limit where $k_F a_S$ diverges.

Another perturbative approach developed by Son and Nishida [29] is known as the ϵ expansion. The idea here is to do a dimensional expansion about 4D in $\epsilon = 4 - d$. There is no strictly four-dimensional unitary limit - the dimers collapse and require an effective range to stabilize them – but in $4 - \epsilon$ dimensions, the dimers become small (they scale like ϵ) so that the theory looks like a weakly interacting gas of dimers and perturbative calculations can be applied to this gas of tightly bound dimers. This allows one to compute quantities and then extrapolate back to d = 3 dimensions. Unfortunately, to answer questions about d = 3 one needs to take $\epsilon = 1$ which is no-longer a small parameter. One can play a similar game expanding about the 2D gas in $\epsilon = d - 2$. In this case, the unitary 2D gas is non-interaction (see problem P-4) and again one can compute as desired. One can then interpolate between d = 2 and d = 3 by making assumptions about the asymptotic forms of the series and one obtains, for example, very reasonable values for the Bertsch parameter.

Finally, one can perform a perturbative virial expansion in μ/T that works at high temperatures, but this does not shed any light on the interesting physics below the superfluid phase transition.

Unfortunately, the assumptions made to perform the interpolation are known to be incorrect, but this opens the door to the possibility that somehow one can learn about the asymptotic properties of the expansion, thereby correcting these results. In summary, the unitary regime admits no perturbative expansion. This should be evident since there is only one length scale: all physical quantities of interest have the same scale! Nothing is small.

2.2 NON-PERTURBATIVE TECHNIQUES

2.2.1 Mean-field Approach

To gain an intuitive understanding as to what might be happening at unitarity, one typically turns to a mean-field analysis (see problem P-8). The mean-field approach provides a simple physical picture for what is happening, and can provide qualitative suggestions about the potentially relevant physics. The unitary gas, however, demonstrates that one cannot trust mean-field models quantitatively.

2.2.2 Density Functional Theory

A related approach, is to use the intuition developed with a meanfield model to develop a Density Functional Theory (DFT) to describe the system. In principle, DFT is an exact approach: The Hohenberg-Kohn theorem [33] establishes the existence of a functional E[n] of the density $n(\vec{x})$ such that the energy and density of the ground state in *any* external potential $V(\vec{x})$ may be found by minimizing:

$$\min_{\mathfrak{n}(\vec{\mathbf{x}})} \mathbb{E}[\mathfrak{n}] + \int d^3 \vec{\mathbf{x}} \, \mathbb{V}(\vec{\mathbf{x}}) \mathfrak{n}(\vec{\mathbf{x}}). \tag{6}$$

The problem is that the form of the functional E[n] might be extremely complicated and non-local. The way to proceed is to make some assumptions about the form. In particular, a useful variation due to Kohn and Sham [34] introduces an auxiliary "kinetic" density $\tau(\vec{x})$ so that the equations of motion after minimization describe quasiparticles. If one also introduces an anomalous (pairing) density $\nu(\vec{x})$, then it turns out that a three-parameter local energy density works very well for describing the UFG is

$$\mathcal{E}_{SLDA} = \alpha \frac{\tau_{+}}{2m} + \beta \mathcal{E}_{FG}(n_{+}) + g \nu^{\dagger} \nu.$$
(7)

The parameter α describes the inverse effective mass of the quasiparticles in the theory, the parameter β rectifies the missing Hartree terms in the mean-field theory, and the third parameter (hidden in g) sets the pairing strength. The standard variational mean-field result is obtained when one sets $\alpha = 1$ and $\beta = 0$.

There are still some subtleties with the zero-range limit: the local form of ν and τ_+ here are divergent, and the coupling *g* must be taken to zero in such a way that the $\Delta = -g\nu$ is held fixed. See [35] and the references therein

There are some reasonable caveats: check the theorem for details.

for details.

This simple three-parameter model, does an exceptional job of modelling homogeneous systems in the UFG. In particular, it seems to properly capture all of the finite-size (shell) corrections for particles in a periodic box, even all the way down to $N_+ = 2$ [36]. Corrections in the form of gradients are currently being explored.

One big advantage of **DFT** approaches is that they can be trivially extended to investigate time-dependent phenomena. See [35] for details.

2.2.3 Diagrammatic Resummation

One may also go beyond the perturbative by summing certain infinite subsets of diagram, and various methods in the literature rely on summing the ladders of the T-matrix. These include both self-consistent and non–self-consistent approximation depending on whether the bare (G_0) or renormalized (G) propagators are included. The mixed (G_0G) approximation exhibits a pseudo-gap (see section 3.3), but does not agree quantitatively with thermodynamic quantities. The self-consistent (GG) approximation, on the other hand, seems to fare much better with the quantitative thermodynamics, but does not have a pseudo-gap. Unfortunately, at unitarity, neither method is under control and the errors are unknown: It is quite possible that the apparent quantitative agreement is accidental. Various T-matrix expansions play an important role in describing the polaron (see section 3.2 and problem P-7). See the references in [38] for a recent discussion and review of some of these methods.

We mention one final form of resummation: the so-called bold diagrammatic Monte Carlo (MC) scheme. Here one uses a MC algorithm to integrate a large set of Feynman diagrams (see for example [39, 42]). Although this allows for a summation of high order diagrams (order ~ 10), as with any diagrammatic approach, this can not access nonperturbative physics (and can certainly not probe through a phase transition). To overcome this limitation, one must manually include some infinite ladder summations – the "bold" diagrams – and the proponents of this method argue that this allows the method to access regimes of interest. The process appears to work with systems above T_c , but the choice of ladders, order, etc. seem rather arbitrary and not everyone is convinced that errors are under control with this method.

Unfortunately, none of these approaches provides a rigorous quantitative method for understanding the UFG. For this, we must turn to Quantum Monte Carlo (QMC) calculations or experiments.

2.2.4 Monte-Carlo Calculations

Most MC algorithms applied to cold-atom systems use some sort of MC update to evolve a wavefunction

The bold-diagrammatic MC algorithms are a notable exception.

2.2.4.1 Fixed-Node Green's Function Monte Carlo

One way of dealing with the sign problem is to perform a QMC calculation over a restricted set of wavefunctions. The Fixed-Node Green's-Function MC (GFMC) (FNGFMC) algorithm starts with a particular wavefunction Ψ_V and evolves this forward in imaginary time by $e^{-\hat{H}\tau}$ while holding the nodes (zeros) of the wavefunction fixed. Formally, this is equivalent to performing a full MC calculation on the projected space of wavefunction that all have the same nodal structure as the initial state Ψ_V . Thus, if Ψ_V can be chosen to have the same nodal structure as the ground state, then one will obtain the ground-state properties of the system. The advantage of working with a set of states with fixed nodes is that one can ensure the measure for the MC integral remains positive – thereby solving the sign problem.

The nodal structure of the ground state, however, is not known, and so one must choose a physically motivated guess for Ψ_V . (Knowing the IR structure of the state you are interested in comes in handy at this point.) The result of the MC calculation is thus only an upper bound on the true ground state energy. To improve this bound, the wavefunction is then parametrized with a handful of parameters that affect the nodal structure, and the MC calculation is repeated while varying these parameters to lower the bound as much as possible.

The FNGFMC algorithm operates in the continuum – one instead uses some basis of functions (typically plane waves). Thus, the continuum limit is not an issue, but one must ensure that the basis set is large enough. The challenge is thus to extrapolate to the thermodynamic limit of infinite volume. It turns out that a DFT make be formulated that works both in finite volumes, and in the thermodynamic limit. Furthermore, this DFT is consistent with the QMC calculations, thereby providing a tool for extrapolating to the continuum limit. Some of the best bounds for ξ have been obtained using DFT extrapolated FNGFMC calculations [36].

This process has provided some of the most accurate quantitative calculations to date of cold-atom systems – even for symmetric systems where other methods have no sign problem. Unfortunately, the results are only strictly reliable as upper bounds. Another advantage of this

method, however, is that it can be directly applied to polarized systems where there is a sign problem. Armed with a good understanding of the IR structure of the polarized phase, one hopes to provide some quantitative understanding with this approach.

One other potential limitation of the **FNGFMC** method is that it requires potentials to be formulated in position space. This is not a problem for cold-atom systems, but makes implementing some of the representations of nuclear forces somewhat tricky. For further details about this method, see [44], and for some recent results, see [36].

2.2.4.2 Auxiliary Field Path Integral Monte Carlo

Another *ab initio* approach is to compute quantities directly from the partition function (for more details, see [35]). The partition function and average of an observable \hat{O} are calculated according to

$$Z(\beta, \mu, V) = \operatorname{Tr} \left\{ \exp[-\beta(\widehat{H} - \mu \widehat{N})] \right\},$$
$$O(\beta, \mu, V) = \frac{\operatorname{Tr} \left\{ \widehat{O} \exp[-\beta(\widehat{H} - \mu \widehat{N})] \right\}}{Z(\beta, \mu, V)},$$

where $\beta = 1/T$ (in this example we will take Boltzmann's constant to be $k_B = 1$ so that temperature is expressed in units of energy). In order to be able to calculate these quantities one first factorizes the statistical weight using the Trotter formula:

$$\exp[-\beta(\widehat{H} - \mu \hat{N})] = \prod_{j=1}^{N_{\tau}} \exp[-\tau(\widehat{H} - \mu \hat{N})]$$
(8)

where $\beta = N_{\tau}\tau$. The next step is to decompose the exponentials on the right hand side into exponentials that depend separately on the kinetic and potential energy operators. The second order expansion is (higher orders require more effort, see [45–48]):

$$\exp\left[-\tau(\hat{\mathbf{H}} - \mu\hat{\mathbf{N}})\right] = \exp\left[-\frac{\tau(\hat{\mathbf{K}} - \mu\hat{\mathbf{N}})}{2}\right]\exp(-\tau\hat{\mathbf{V}})\exp\left[-\frac{\tau(\hat{\mathbf{K}} - \mu\hat{\mathbf{N}})}{2}\right] + O(\tau^{3}), \quad (9)$$

where $\hat{\mathbf{K}}$ is the kinetic energy operator, whose dispersion relation, for momenta smaller than the cut-off, is given by $\varepsilon_{\vec{k}} = \hbar^2 k^2 / 2m$.

In order to efficiently evaluate the term containing the interaction, one has to replace it by the sum (or integral) of one body terms. This can be done with the Hubbard-Stratonovich (HS) transformation [49].

The transformation is not unique, and one takes advantage of this freedom to ensure an efficient summation (or integration) scheme. In our case, due to the simplicity of the interaction term, a discrete HS transformation can be applied, similar to that in [50]:

$$\exp[-g\tau\hat{n}_{a}(\vec{r})\hat{n}_{b}(\vec{r})] = \frac{1}{2} \sum_{\sigma(\vec{r},\tau_{j})=\pm 1} [1 + A\sigma(\vec{r},\tau_{j})\hat{n}_{a}(\vec{r})] [1 + A\sigma(\vec{r},\tau_{j})\hat{n}_{b}(\vec{r})],$$
(10)

where $A = \sqrt{\exp(-g\tau) - 1}$, τ_j labels the location on the imaginary time axis, $j = 1, ..., N_{\tau}$, and $\sigma(\vec{r}, \tau_j)$ is a field that can take values ±1 at each point on the space-time lattice.

One thereby renders all fermionic operations one-body in nature, allowing them to be directly applied to the state. The cost is that one must now use MC to perform the sum over the $\sigma(\vec{r}, \tau_j)$ field configurations. The advantages of this transform is discussed, for example, in [50, 51]. One can show that the measure is positive definite for symmetric systems $\mu_{\alpha} = \mu_{b}$. The sign problem in other cases can sometimes be cured by properly choosing the HS transformation [52].

The many-fermion problem is thus reduced to an Auxiliary Field Quantum Monte Carlo problem (Auxiliary-Field QMC (AFQMC)), to which the standard Metropolis algorithm can be applied. In contrast to the FNGFMC algorithm, the AFQMC algorithm is an *ab initio* method, providing unbiased estimates (providing convergence is achieved), however, it is afflicted by the sign problem, and so has been of limited used when discussing polarized phases. For more details, see [51, 53–61], and the review [35].

2.2.4.3 *Lattice Methods*

Finally, one can apply more standard lattice techniques to calculate properties of the UFG. Several groups have explored lattice techniques, including [62], [13, 64, 65], and [66]. These approaches use an Euclidean time lattice formalism, developing a lattice action, and tuning the interactions to reproduce the phase shifts in a periodic box as given by the so-called Lüscher formula [67]

$$k \cot \delta_{k} = \frac{1}{\pi L} S(\eta), \quad \eta = \left(\frac{Lk}{2\pi}\right)^{2}, \quad S(\eta) = \lim_{\Lambda \to \infty} \left[\sum_{\vec{n}} \frac{\theta(\Lambda^{2} - n^{2})}{n^{2} - \eta} - 4\pi\Lambda\right].$$

In principle, these methods seem very attractive – by carefully tuning the lattice operators, for example, they should be able to probe the unitary limit, even with small lattice volumes. In practise, however,

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There are more general HS transformations that allow σ to take continuous values in both compact and infinite domains.

these methods seem to disagree with the preponderance of evidence, including the most recent high-precision experiment at MIT which found $\xi = 0.376(4)$ [14]; consistent with AFQMC results and FNGFMC bounds [36]. For example, the earliest lattice calculations of ξ [62] found very small values $\xi \leq 0.33(1)$ while the more recent calculations find somewhat larger values $\xi \gtrsim 0.39(1)$. The latter results have not been fully extrapolated to the continuum limit, but comparison with FNGFMC bounds is troubling: the lattice results seem to exhibit much stronger finite-size (shell) effects, many of which contradict the variational upper bound provided for by the FNGFMC method.

Unfortunately, all these methods seem to give the same results at some of the simpler points where there are reliable few-body methods. This includes the $N_+ = 2$ systems (which have analytical solutions from the two-body problem), and the $N_+ = 4$ and $N_+ = 6$ harmonically trapped gases which enjoy a high-precision few-body method [68]. The lattice methods are promising in principle, but these disagreements need to be understood before further progress is made.

3.1 POLARIZED PHASES

Not much is known about the phases of polarized matter in the **BEC/BCS** crossover. As has been mentioned, many possibilities exist, including P-wave superfluid states, crystalline LOFF states, states with deformed Fermi surfaces [69], and others, but no reliable calculations exist to address this question rigorously. Part of the problem is that one encounters a sign-problem as one moves away from $n_{\alpha} = n_{b}$ symmetric matter. Another part is that the IR structure of possible phases is not particularly well understood – if it were, then perhaps a good ansatz could be make for the nodal structure of the wavefunction, allowing **FNGFMC** to attack the problem. One approach is to "ignore" the sign problem and hope that it is not too bad. This yields some information about polarized properties, such as the size of the gap, but precision results are lacking.

Experiments should in principle have no problem studying these phase, and indeed, they have been probed. However, they typically occupy a small shell on the outside of trap. The crystalline LOFF phases, for example, require a substantial physical volume to allow the crystal structure to develop. This might be possible with flat-bottom traps, but as of yet, experimentalists have yet to explore these phases seriously.

3.2 POLARON

The question about whether or not induced P-wave superfluidity can exist and be seen at unitarity as suggested in [15] has not been fully resolved. Perturbative analysis [15] suggested yes; Born-Oppenheimer analyses suggested no [70]; Most recently, uncontrolled diagrammatic summations suggest yes [71]. Reliably resolving this question would be helpful to guide experimental searches for these exotic phases.

3.3 PSEUDO-GAP

Some QMC calculations of the spectral function at finite temperature suggest that, even above the critical temperature $T > T_c$, the single-

The group at **MIT** is apparently undertaking a systematic study of the polarized equation of state as they did with the symmetric state in [14], so the situation may be somewhat remedied in the near future. particle dispersion relationship still has a "gap" [58]. This "pseudogap" phenomenon can be easily understood in the BEC limit where the critical temperature T_c is related to the phase coherence of the bosonic dimers, whereas the "gap" – the energy required to split pairs – is at a much higher scale set by the pair binding energy. The "pseudo-gap" in this context appears in the single-particle dispersion as a negative chemical potential:

$$E_{k} = \sqrt{\left(\frac{\hbar^{2}k^{2}}{2m} - \mu\right)^{2} + |\Delta|^{2}}.$$
 (11)

When $\mu < 0$, the spectral gap is $\sqrt{|\mu|^2 + |\Delta|^2}$, which remains even above $T > T_c$ where $\Delta = 0$.

The unitary point lies in a regime with positive chemical potential, however, so the naïve picture would suggest no pseudogap. Some calculations see a signature for a pseudogap (for example the non-selfconsistent T-matrix summation) while others do not (including the self-consistent T-matrix approach). Even the experimental evidence for a pseudogap is suspect since current analyses are based on the Thomas-Fermi (TF) approximation, and properties of the homogeneous phases can get mixed up by the trapping geometry. This point was discussed extensively in a recent workshop at the Institute for Nuclear Theory (INT):

 http://www.int.washington.edu/talks/WorkShops/int_11_1/ See the talks from the afternoon of 17 May 2011 starting with Randeria's overview "Pairing Pseudogap in Strongly Interacting Fermi Gases".

3.4 DISAGREEMENT BETWEEN LATTICE METHODS

As discussed in section 2.2.4.3, the lattice-based approaches, although nice formally, disagree with other QMC based methods. Compare, for example, the extremely small values of ξ found in [62, 72, 73], and the shell structure seen in [13, 65] with the values and lack of shell structure seen in the FNGFMC and DFT approaches used in in [36]. This disagreement needs to be understood and resolve before further progress with lattice methods is made for cold-atom systems.

3.5 NOVEL PROPERTIES

Cold atom experiments are increadibly diverse with their abiliity to trap various species, to tune interactions, and to apply various potentials, from confining particles to lower dimensions, to embedding the particles in optical lattices. This opens the door to simulation: If one finds an interesting system, then there is a chance that experiments may be able to simulate it. In this way, one can use cold atom systems to check and benchmark calculations. The interplay between computing to analyze properties of cold atom systems, and designing cold atom systems to simulate theories that are difficult to compute will likely be a hot topic of research in the near future.

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P-1 FREE FERMION PROPERTIES

Consider a gas of two-species of non-interacting (free) non-relativistic Fermions described by the Hamiltonian

$$\widehat{\mathbf{H}}_{0} = \int \frac{d\vec{k}^{3}}{(2\pi)^{3}} \frac{\hbar^{2}k^{2}}{2m} \left(\widehat{\mathbf{a}}_{k}^{\dagger} \widehat{\mathbf{a}}_{k} + \widehat{\mathbf{b}}_{k}^{\dagger} \widehat{\mathbf{b}}_{k} \right) = \int d^{3}\vec{k} \frac{\hbar^{2}k^{2}}{2m} \left(\widehat{\mathbf{a}}_{k}^{\dagger} \widehat{\mathbf{a}}_{k} + \widehat{\mathbf{b}}_{k}^{\dagger} \widehat{\mathbf{b}}_{k} \right).$$

This serves as the reference point for expressing quantities of the UFG. Derive the following quantities for the energy E_{FG} , number density n_+ , and chemical potential $\mu = \epsilon_F$ for the ground state of a homogeneous T = 0 gas:

$$\mathcal{E}_{FG}(\mathfrak{n}_{+}) = \frac{3}{5}\mathfrak{n}_{+}\varepsilon_{F}(\mathfrak{n}_{+}) \propto \mathfrak{n}_{+}^{5/3}, \qquad (\text{energy})$$

$$n_{+} = n_{a} + n_{b} = \frac{k_{F}^{3}}{3\pi^{2}}, \qquad k_{F} \equiv (3\pi^{2}n_{+})^{1/3}, \qquad (\text{number density})$$

$$\mu_{+} = \frac{\partial \mathcal{E}_{FG}}{\partial n_{+}} = \epsilon_{F}(n_{+}) = \frac{k_{F}^{2}}{2m} \propto n_{+}^{2/3}, \qquad \text{(chemical potential)}$$
$$P_{FG} = \frac{2}{3} \mathcal{E}_{FG}. \qquad \text{(pressure)}$$

These implicitly define the Fermi wave-vector k_F , Fermi energy ε_F , and energy density \mathcal{E}_{FG} of the free Fermi gas at fixed number density n_+ .

P-2 symmetric unitary fermi gas at t = 0

Using dimensional analysis, show that the symmetric T = 0 Unitary Fermi Gas (UFG) must have an equation of state:

$$\mathcal{E}(n_{+}) = \xi \mathcal{E}_{FG}(n_{+}) \propto n_{+}^{5/3}$$
 (P-2.1)

$$\mu_{+} = \xi \varepsilon_{\mathrm{F}}(\mathfrak{n}_{+}) \tag{P-2.2}$$

where ξ is a dimensionless parameter (called the Bertsch Parameter). Argue that the pressure P is related to the energy density \mathcal{E} by

$$\mathcal{P} = \frac{2}{3}\mathcal{E}.$$
 (P-2.3)

This is simply a consequence of the lack of scales and holds also for the non-interacting gas.

Here we introduce a useful notation: $\mathbf{d}^3 \vec{\mathbf{k}} \equiv \mathbf{d}^3 \vec{\mathbf{k}}/(2\pi)^3$. This is analogous to $\hbar = \hbar/2\pi$ and our normalizations shall be such that all factors of 2π in the Fourier transform appear with measure of momentum integrals.

P-3 NATURAL UNITS

The lack of length scales for the UFG allows us to express everything in terms of the total number density n_+ or the Fermi wave-vector $k_F \equiv (3\pi^2 n_+)^{1/3}$. It is also common to set $\hbar = 1$ and the mass m = 1, thereby defining a set of "natural" units. Show that energies, momenta, etc have the following length dimensions in these units:

$$[T] = L^2$$
, $[E] = L^{-2}$, $[P] = [\mathcal{E}] = L^{-5}$, $[n_+] = L^{-3}$, $[p] = [k] = L^{-1}$

I will try to keep the factors of ħ and m in the critical formulae, but don't be alarmed if they go astray – just add them as needed to make up the appropriate densities.

P-4 TWO-BODY PROBLEM

Solve the Schrödinger equation for the two-particles interacting with an attractive short-range radially symmetric potential V(r) of your choice. (A square well will work fine, or perhaps use the Pöschl-Teller form sech²(r) which admits a supersymmetric solution. If you have not seen the supersymmetric method for solving quantum mechanics problems, do yourself a favour and look it up [74]: it is very amusing and useful for finding analytic solutions.)

Parametrize your potential with two parameters: a strength g and a range r_e . I.e. $gV(r/r_0)$. Adjust the strength of your potential so that the potential has a bound state with zero energy E = 0. This potential has an infinite s-wave scattering length $a_s = 0$. Take the range of the potential $r_0 \rightarrow 0$ to zero and adjust the strength g so that the bound-state remains at E = 0. This is the unitary limit. Is the potential stronger or weaker than a delta-function? What does this "unitary" limit look like in d = 2 dimensions? (Hint: How weak do you need to make the attractive potential in order for the bound state to disappear?) What about d = 4 dimensions?

Now consider the BEC limit where the interaction becomes stronger. The scattering length will become positive and $k_F a_S$ will be a small positive number. Solve for the binding energy of the two-body system and show that it behaves like

$$E_{\text{bind}} = \frac{\hbar^2}{\mathrm{ma}_{\mathrm{S}}^2}.$$
 (P-4.1)

For details, see Erich Mueller's tutorial http://people.ccmr.cornell. edu/~emueller/tutorials.html and play with the Java Applets to get a feel for this limit.

Since m = 1, it is common to call n₊ simply the "density" rather than "number density", even

when keeping m explicit.

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P-5 UNITARY HAMILTONIAN

The Unitary Fermi Gas (UFG) can be defined through the Hamiltonian

$$\widehat{H}_{\rm UFG} = \int \frac{d\vec{k}^3}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} \left(\widehat{a}_k^{\dagger} \widehat{a}_k + \widehat{b}_k^{\dagger} \widehat{b}_k \right) + \int d^3 \vec{x} \, \widehat{n}_a(\vec{x}) \widehat{n}_b(\vec{y}) V(\|\vec{x} - \vec{y}\|)$$

where $\hat{\mathbf{n}}_{a}(\vec{x}) = \hat{\mathbf{a}}^{\dagger}(\vec{x})\hat{\mathbf{a}}(\vec{x})$ is the density operator, where the twobody interaction potential V(r) is taken to zero range as described in problem P-4. Since the physics is universal, one need not restrict oneself to local interactions. An alternative formulation that is useful in calculations is to use a separable potential

$$\begin{split} \widehat{\mathbf{H}}_{\mathrm{UFG}} &= \int \frac{d\vec{k}^{3}}{(2\pi)^{3}} \frac{\hbar^{2}k^{2}}{2m} \left(\widehat{\mathbf{a}}_{k}^{\dagger} \widehat{\mathbf{a}}_{k} + \widehat{\mathbf{b}}_{k}^{\dagger} \widehat{\mathbf{b}}_{k} \right) + \\ &+ \int d^{3}\vec{k} \, d^{3}\vec{p} \, d^{3}\vec{q} \, V_{\parallel \vec{p} - \vec{q} \parallel} V_{\parallel \vec{p} - \vec{q} + 2\vec{k} \parallel} \widehat{\mathbf{a}}_{\vec{p} + \vec{k}}^{\dagger} \widehat{\mathbf{a}}_{\vec{p}} \widehat{\mathbf{b}}_{\vec{q} - \vec{k}}^{\dagger} \widehat{\mathbf{b}}_{\vec{q}}. \end{split}$$
(P-5.1)

One can also use a contact interaction with an appropriate cutoff:

$$\widehat{\mathbf{H}}_{\text{UFG}} = \int \frac{d\vec{k}^{3}}{(2\pi)^{3}} \frac{\hbar^{2}k^{2}}{2m} \left(\widehat{\mathbf{a}}_{k}^{\dagger}\widehat{\mathbf{a}}_{k} + \widehat{\mathbf{b}}_{k}^{\dagger}\widehat{\mathbf{b}}_{k}\right) + g \int d^{3}\vec{x} \,\delta^{(3)}(\vec{x})\widehat{\mathbf{n}}_{a}(\vec{x})\widehat{\mathbf{n}}_{b}(\vec{x})$$
(P-5.2)

but recall from problem P-4 that the limiting interaction is substantially weaker than a δ -function potential. This theory needs to be computed with a regulator, either a momentum space cutoff Λ , or perhaps with dimensional regularization (see [76]). One must then match the regulated theory to a physical observable like the phase shifts (1) to determine the relationship between the cutoff and the coupling. This is carefully discussed in the review [77].

To get around the need for regularization, people sometimes use a "pseudo-potential" – a weaker potential of the form $\delta(r)\partial/\partial r$. These work by enforcing the appropriate short-range boundary conditions on the many-body wavefunction whenever two particles approach each others (valid in the limit $\vec{x} \rightarrow \vec{y}$ for any particle a at \vec{x} and any particle b at \vec{y}):

$$\psi(\dots, \vec{x}, \vec{y}, \dots) \propto \frac{1}{\|\vec{x} - \vec{y}\|} - \frac{1}{a_{\rm S}} + O(\|\vec{x} - \vec{y}\|).$$
(P-5.3)

A full parametrization of pseudo-potentials can be described with the use of appropriately defined generalized functions (analogues of the Dirac δ -function) as described by Shina Tan [78].

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One of the challenges of studying the **UFG** on the lattice is to appropriately define the lattice interaction so that it approaches the appropriate unitary limit as you take the continuum limit. This is somewhat non-trivial, and the reader is referred to the discussions in [13, 65].

P-6 AWAY FROM UNITARITY

The energy density \mathcal{E} and pressure \mathcal{P} of a polarized $(n_a \neq n_b)$ in the unitary limit can be expressed as [79]

$$\mathcal{E}(n_a, n_b) = \frac{3}{5} a \left(n_a g(x) \right)^{5/3}, \quad a = \frac{(6\pi^2)^{2/3} \hbar^2}{2m}, \qquad x = \frac{n_b}{n_a}, \quad (P-6.1)$$

$$\mathcal{P}(\mu_{a},\mu_{b}) = \frac{2}{5}b(\mu_{a}h(y))^{5/2}, \quad b = \frac{1}{6\pi^{2}}\left(\frac{2m}{\hbar^{2}}\right)^{3/2}, \quad y = \frac{\mu_{b}}{\mu_{a}} \quad (P-6.2)$$

where the non-perturbative physics is described by the dimensionless functions g(x) and h(y) of the dimensionless ratios $x = n_b/n_a$ and $y = \mu_b/\mu_a$.

Show that convexity of the thermodynamic functions $\mathcal{E}(n_a, n_b)$ and $\mathcal{P}(\mu_a, \mu_b)$ is guaranteed (necessary and sufficient) by the convexity of the dimensionless functions g(x) and h(x). This the reason for this somewhat complicated parametrization. Recall that first-order phase transitions are denoted by kinks in \mathcal{P} but flat lines in \mathcal{E} (corresponding to the Maxwell construction). Finally, show how g(x) and h(y) are constrained by the form of the symmetric energy density and the value of ξ , and by the form of the free energy density of a completely polarized gas $n_b = 0$. (See [79] for details.)

The completely polarized gas occurs when $y = \mu_b/\mu_a$ is less than some critical negative value denoting the energy of a single impurity (polaron) of type b immersed in a sea of particles of type a. See problem P-7.

Finally, show that one obtains an analogous parametrization for finite temperature using the dimensionless function $h_T(z)$ where $z = \mu/T$ [55] with the same convexity properties as before:

$$\mathcal{P}(T,\mu) = \frac{2}{5} b \left(Th_T(z) \right)^{5/2}, \qquad z = \frac{\mu}{T}.$$
 (P-6.3)

P-7 POLARON

Consider a single fermion of species b (polaron) immersed in a sea of non-interacting fermions of species a. For attractive interaction, the particle b is drawn into the sea with a "binding" energy E < 0. At unitarity, there are no length scales in the problem other than the interparticle spacing k_F^{-1} for species a, so we must have

$$E_b = c \epsilon_F(n_a) \tag{P-7.1}$$

for some universal dimensionless number c. One can get an upper bound on this number variationally by considering the following variational state proposed by Chevy [80]

$$|\Psi\rangle = \phi_{0} |FG\rangle |\vec{p}\rangle + \sum_{\substack{q \le k_{F} \\ k > k_{F}}} \phi_{k,q} \widehat{a}_{k}^{\dagger} \widehat{a}_{q} |FG\rangle |\vec{p} + \vec{q} - \vec{k}\rangle.$$
(P-7.2)

The first term $|FG\rangle |\vec{p}\rangle$ is the filled Fermi sea of species a (all states $k \le k_F$ are filled) and the polaron b in momentum state \vec{p} . The second term is a linear combination of all states where a single a particle of momentum \vec{q} with $q \le k_F$ is excited out of the Fermi sphere to a state \vec{k} with $k > k_F$ and the polaron b has momentum $\vec{p} + \vec{q} - \vec{k}$ so that the total momentum of the system \vec{p} remains conserved. Compute the variational energy of this state using a Hamiltonian of your choice to obtain an upper bound for the polaron binding energy E_b by setting $\vec{p} = 0$ (one can estimate the effective polaron mass by looking at the dispersion relationship for non-zero momenta \vec{p}).

In what follows, we shall use the simplified notation $|FG\rangle \equiv |FG\rangle |\vec{p}\rangle$ and $|kq\rangle \equiv \hat{a}_{k}^{\dagger} \hat{a}_{q} |FG\rangle |\vec{p} + \vec{q} - \vec{k}\rangle$.

Note that there are four overlaps. The $|\phi_0|^2$ contribution from $\langle FG|FG \rangle$, a contribution $\phi_0^{\dagger}\phi_{k,q}$ and its conjugate from the overlap $\langle FG|kq \rangle$, and two contributions from the overlap of $\langle kq|kq \rangle$ after the contractions are performed. To simplify the calculation in the shortrange limit, you may neglect the "particle-hole" contribution where one sums over only the finite set of hole states $q < k_F$. In the shortrange limit, this will remain finite while the coupling constant $g \rightarrow 0$ (see problem P-4) and so it will vanish.

By varying the resulting equations with respect to ϕ_0 and $\phi_{k,q}$ subject to the normalization constraint $\langle \Psi | \Psi \rangle = 1$, one obtains the

These are also valid for $\vec{\mathbf{p}} \neq \vec{\mathbf{0}}$.

following set of equations, where the binding energy E_b enters as the Lagrange multiplier for the normalization constraint condition:

$$mE_{b} = \sum_{q < k_{F}} \frac{1}{\frac{1}{4\pi a_{S}} + \frac{I(E)}{m}}$$
(P-7.3a)

. 2

$$\frac{I(E)}{m} = \sum_{k>k_F} \frac{1}{m\epsilon_{k,q} - mE_b} - \sum_k \frac{1}{2m\epsilon_k}, \qquad (P-7.3b)$$

$$\epsilon_{k,q} = \epsilon_k - \epsilon_q + \epsilon_{\vec{p}+\vec{q}-\vec{k}} - \epsilon_p, \quad \epsilon_k = \frac{k^2}{2m}.$$
 (P-7.3c)

This implicit equation for E_b can be solved numerically to obtain $E_b < -0.6066 \cdots \epsilon_F(n_a)$. This should be compared with QMC calculations $E_b = -0.58(1)\epsilon_F(n_a)$ [81] and $E_b = -0.594(6)\epsilon_F(n_a)$ [82], as well as with higher-order resummation $E_b = -0.6158\epsilon_F(n_a)$ [83] which agrees with the diagrammatic QMC results [42] (but which are quoted without errors). One can show that the variational approximation discussed here corresponds diagrammatically to the non–self-consistent T-matrix analysis mentioned earlier.

An outstanding question is whether the induced P-wave interaction between two polarons is attractive. The perturbative calculations in [15] from both BEC and BCS limits suggest that they are attractive with increasing magnitude towards the unitary limit (leading to the suggestion that a P-wave superfluid state might be observable). However, this is contradicted by an estimate from the Born-Oppenheimer approximation of heavy polarons ($m_b \gg m_a$) which finds that the P-wave interactions become repulsive at unitarity [70]. Recent diagrammatic resummations [83] suggest again that the interaction may be attractive. None of these is completely reliable and the question remains unresolved.

P-8 MEAN-FIELD ANALYSIS

The Eagle-Leggett [84] approach to understanding the BEC/BCS crossover is to apply a mean-field model. I like to think of this in the following way: define a purely quadratic Hamiltonian \hat{H}_0 that contains variable parameters. For the problem at hand, one uses (the integration over all momenta \vec{k} has been suppressed)

$$\widehat{H}_{0} = \left(\frac{\hbar^{2}k^{2}}{2m} + U\right)\widehat{a}_{k}^{\dagger}\widehat{a}_{k} + \left(\frac{\hbar^{2}k^{2}}{2m} + U\right)\widehat{b}_{k}^{\dagger}\widehat{b}_{k} + \Delta\widehat{a}_{k}^{\dagger}\widehat{b}_{-k}^{\dagger} + \Delta^{\dagger}\widehat{b}_{-k}\widehat{a}_{k}.$$

where the parameters U_{α} and U_{b} characterize the self-energy, and Δ characterizes the "gap". Feynman [87] shows that one can obtain

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Since the polarons are identical fermions, the s-wave interaction must vanish by symmetry.

a variational bound for the thermodynamic potential of any other Hamiltonian \widehat{H} as

$$\Omega \le \Omega_0 + \left\langle \widehat{\mathbf{H}} - \widehat{\mathbf{H}}_0 \right\rangle_0 \tag{P-8.1}$$

where Ω_0 is the thermodynamic potential of \hat{H}_0 and the expectation value is taken with respect to the thermodynamic ensemble for the quadratic model \hat{H}_0 . Since \hat{H}_0 is quadratic, it may be diagonalized and so that Ω_0 may be computed. The ensemble described by opH₀ also only contains two-body correlations: hence, any expectation values can be decomposed into pairs which may also be evaluated:

$$\langle \widehat{\mathbf{a}}^{\dagger} \widehat{\mathbf{b}}^{\dagger} \widehat{\mathbf{b}} \widehat{\mathbf{a}} \rangle_{0} = \underbrace{\langle \widehat{\mathbf{a}}^{\dagger} \widehat{\mathbf{a}} \rangle_{0} \langle \widehat{\mathbf{b}}^{\dagger} \widehat{\mathbf{b}} \rangle_{0}}_{\text{Hartree}} - \underbrace{\langle \widehat{\mathbf{a}}^{\dagger} \widehat{\mathbf{b}} \rangle_{0} \langle \widehat{\mathbf{b}}^{\dagger} \widehat{\mathbf{a}} \rangle_{0}}_{\text{Fock}} + \underbrace{\langle \widehat{\mathbf{a}}^{\dagger} \widehat{\mathbf{b}}^{\dagger} \rangle_{0} \langle \widehat{\mathbf{b}} \widehat{\mathbf{a}} \rangle_{0}}_{\text{pairing}}. \quad (P-8.2)$$

The right-hand-side of (P-8.1) may be thus be computed for any Hamiltonian \widehat{H} and one can then vary the parameters U_{α} , U_{b} , and Δ in \widehat{H}_{0} to obtain a variational bound – the mean-field model.

To simplify the algebra, introduce the following "Nambu-Gorkov" operator

$$\widehat{\Psi}_{k} = \begin{pmatrix} \widehat{\mathfrak{a}}_{k} \\ \widehat{\mathfrak{b}}_{-k}^{\dagger} \end{pmatrix}$$
 (P-8.3)

so that the trial Hamiltonian can be written (including the integral now and including a chemical potential so that we can compute the thermodynamic potential $\Omega = E - TS - \mu N$)

$$\widehat{\mathbf{H}}_{0} = \int d^{3}\vec{k}\,\widehat{\Psi}_{k}^{\dagger} \begin{pmatrix} \frac{\hbar^{2}k^{2}}{2m} - \mu + \mathbf{U} & \Delta^{\dagger} \\ \Delta & -\frac{\hbar^{2}k^{2}}{2m} + \mu - \mathbf{U} \end{pmatrix} \widehat{\Psi}_{k}$$
(P-8.4)

up to a unimportant constant. Show that this may be diagonalized by a unitary transformation

$$\mathbf{Q} = \begin{pmatrix} u_k & v_k^{\dagger} \\ v_k & -u_k \end{pmatrix}$$
(P-8.5)

and has the spectrum

$$E_{k} = \sqrt{\left(\frac{\hbar^{2}k^{2}}{2m} - \mu + U\right)^{2} + |\Delta|^{2}}.$$
 (P-8.6)

Hence, Δ is indeed the spectral gap. Apply this to your favourite Hamiltonian, and take the zero-range limit. You should find that the

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minimum has U = 0 (there is no self-energy correction in the unitary limit) and that Δ must be chosen to satisfy the "gap" equation

$$\frac{-\mathrm{m}\Delta}{4\pi a_{\mathrm{S}}} = \int \mathrm{d}^{3}\vec{k} \left(\frac{\Delta}{2\sqrt{\left(\frac{\hbar^{2}k^{2}}{2\mathrm{m}} - \mu\right)^{2} + |\Delta|^{2}}} - \frac{\mathrm{m}\Delta}{\hbar^{2}k^{2}} \right). \tag{P-8.7}$$

This always has a "normal" solution at $\Delta = 0$, but also has a non-trivial superconducting solution $\Delta \neq 0$. The second piece may be obtained by exchanging the coupling constant g for the scattering length using the solution to the two-body scattering problem, which, for a delta-function interaction with momentum cutoff, has the form

$$1 - \frac{gm}{4\pi a_{\rm S}} = -\frac{g}{2} \int d^3 \vec{k} \, \frac{2m}{\hbar^2 k^2} = -\frac{mgk_c}{2\pi^2 \hbar^2}.$$
 (P-8.8)

The resulting expression is finite – the divergences in both terms exactly cancel – and one obtains a cutoff-independent result. (See also [76] for an approach that uses dimensional regularization).

Here are some points about the mean-field model:

- 1 This theory applies throughout the BCS/BEC crossover (just choose the appropriate a_S), thereby providing a qualitative understanding for the crossover.
- 2 There is no phase transition as a_S goes to $\pm \infty$ at unitarity. The relevant parameter a_S^{-1} behaves smoothly, as does the solution. This is the meaning of "crossover". The Cooper pairs on the BCS side evolve smoothly into the tightly bound, but coherent, dimers on the BEC side.
- 3 Solving the gap equation shows that the binding becomes tight enough somewhere on the **BEC** side of the crossover that no chemical potential $\mu = 0$ is needed to maintain a finite density. Deeper in, the attraction is so strong that a negative chemical potential is required to maintain a given density. The point at which $\mu = 0$ plays an interesting role in the discussion of polarized phases. See [16] for details.
- 4 Note, however, that a negative chemical potential does not mean that clouds will be self-bound. In particular, after scaling out the appropriate dimensions, one will find that $1/k_F a_S$ is the appropriate parameter. A density of a cloud will fall towards the outside, so for fixed a_S , this means that the outer part of the cloud approaches the unitary limit $1/k_F a_S \rightarrow \infty$. In particular, at some point, one will cross this transition point where μ becomes positive, and without a trapping potential to supply an effective *positive* μ , the cloud would evaporate, thereby reducing the density in the core, bring more of the cloud toward the unitary regime.

- 5 In the deep BEC regime, the mean-field model gets the correct dimer binding energy $E_B = \hbar^2/ma_S^2$, but fails to capture the behaviour of the fermion-dimer and dimer-dimer scattering lengths.
- 6 Formally, the mean-field theory has no Hartree-Fock terms in the zero range limit. These appear in (P-8.2) as gn_an_b where the densities n_a and n_b are finite. The pairing term, on the other hand appears as $g \langle ba \rangle^* \langle ab \rangle$ where the expectation values $\langle ab \rangle$ diverge. The zero-range limit is obtained when $g \rightarrow 0$ in such a way that $-g \langle ab \rangle \rightarrow \Delta$ is finite. Hence, the pairing contribution remains, but the Hartree (and Fock) terms vanish. At weak coupling, one can sum ladder diagrams to restore the appropriate power-counting, obtaining a Hartree term of the form $4\pi a_s n_a n_b$ that remains, even in the zero-range limit. However, the resummation destroys the variational property of the method (energies are no-longer guaranteed to be an upper bound for example).
- 7 The missing Hartree terms lead the mean-field model to completely miss some important physics. For example, the polaron would have zero-binding energy in the mean-field model (see problem P-7).

BIBLIOGRAPHY

- [1] C. J. Pethick and H. Smith, *Bose-Einsten Condensation in Dilute Gases* (Cambridge University Press, Cambridge, 2002).
- [2] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 80, 1215 (2008), 0706.3360.
- [3] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008), 0704.3011.
- [4] M. Inguscio, W. Ketterle, and C. Salomon, eds., Ultra-cold Fermi Gases, vol. 164 of International School of Physics "Enrico Fermi" (IOS Press, Amsterdam, 2007), ISBN 978-1-58603-846-5.
- [5] W. Zwerger, ed., The BCS–BEC Crossover and the Unitary Fermi Gas, vol. 836 of Lecture Notes in Physics (Springer, 2012), ISBN 978-3-642-21977-1.
- [6] H. A. Bethe, Phys. Rev. 76, 38 (1949), URL http://link.aps.org/ doi/10.1103/PhysRev.76.38.
- [7] The Many-Body Challenge Problem (мвх) formulated by G. F. Bertsch in 1999.
- [8] G. A. Baker, Jr., Phys. Rev. C 60, 054311 (1999).
- [9] G. A. Baker, Jr., Int. J. Mod. Phys. B 15, 1314 (2001).
- [10] D. B. Kaplan, M. J. Savage, and M. B. Wise, Phys. Lett. B 424, 390 (1998), ISSN 0370-2693, URL http://www.sciencedirect. com/science/article/pii/S037026939800210X.
- [11] D. B. Kaplan, M. J. Savage, and M. B. Wise, Nucl. Phys. B 534, 329 (1998), ISSN 0550-3213, URL http://www.sciencedirect. com/science/article/pii/S0550321398004404.
- [12] D. B. Kaplan (2005), nucl-th/0510023.
- [13] M. G. Endres, D. B. Kaplan, J.-W. Lee, and A. N. Nicholson, *Lattice Monte Carlo calculations for unitary fermions in a finite box* (2012), 1203.3169.

- [14] M. J. H. Ku, A. T. Sommer, L. W. Cheuk, and M. W. Zwierlein, Science 335, 563 (2012), 1110.3309.
- [15] A. Bulgac, M. M. Forbes, and A. Schwenk, Phys. Rev. Lett. 97, 020402 (2006), cond-mat/0602274.
- [16] D. T. Son and M. A. Stephanov, Phys. Rev. A 74, 013614 (2005), cond-mat/0507586.
- [17] D. E. Gonzalez Trotter, F. S. Meneses, W. Tornow, C. R. Howell, Q. Chen, A. S. Crowell, C. D. Roper, R. L. Walter, D. Schmidt, H. Witała, et al., Phys. Rev. C 73, 034001 (2006), URL http:// link.aps.org/doi/10.1103/PhysRevC.73.034001.
- [18] Q. Chen, C. R. Howell, T. S. Carman, W. R. Gibbs, B. F. Gibson, A. Hussein, M. R. Kiser, G. Mertens, C. F. Moore, C. Morris, et al., Phys. Rev. C 77, 054002 (2008), URL http://link.aps.org/doi/ 10.1103/PhysRevC.77.054002.
- [19] G. A. Miller, B. M. K. Nefkens, and I. Ålaus, Phys. Rep. 194, 1 (1990), ISSN 0370-1573, URL http://www.sciencedirect.com/ science/article/pii/0370157390901028.
- [20] H. Feshbach, Ann. Phys. (NY) 5, 357 (1958).
- [21] W. Ketterle and M. W. Zwierlein, in [4], pp. 95–287, 0801.2500.
- [22] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Rev. Mod. Phys. 82, 1225 (2010), 0812.1496, URL http://link.aps.org/doi/10. 1103/RevModPhys.82.1225.
- [23] M. W. Zwierlein, J. R. Abo-Shaeer, A. Schirotzek, C. H. Schunck, and W. Ketterle, Nature 435, 1047 (2005), ISSN 7045.
- [24] Z.-Y. Shi, R. Qi, and H. Zhai, Phys. Rev. A 85, 020702 (2012), 1108.3510.
- [25] D. Banerjee, M. Dalmonte, M. Müller, E. Rico, P. Stebler, U.-J. Wiese, and P. Zoller, Atomic Quantum Simulation of Dynamical Gauge Fields coupled to Fermionic Matter: From String Breaking to Evolution after a Quench (2012), 1205.6366.
- [26] G. V. Skorniakov and K. A. Ter-Martirosian, Sov. Phys.–JETP (1957).

- [27] D. S. Petrov, C. Salomon, and G. V. Shlyapnikov, J. Phys. B 38, S645 (2005), cond-mat/0502010.
- [28] A. Bulgac, P. F. Bedaque, and A. C. Fonseca, A dilute atomic fermi system with a large positive scattering length (2003), cond-mat/ 0306302.
- [29] Y. Nishida and D. T. Son, Phys. Rev. Lett. 97, 050403 (2006).
- [30] Y. Nishida and D. T. Son, Phys. Rev. A 75, 063617 (pages 22) (2007), cond-mat/0607835.
- [31] Y. Nishida, Phys. Rev. A 75, 063618 (pages 11) (2007).
- [32] P. Arnold, J. E. Drut, and D. T. Son, Phys. Rev. A 75, 043605 (pages 15) (2007), cond-mat/0608477.
- [33] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
- [34] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
- [35] A. Bulgac, M. M. Forbes, and P. Magierski, *The Unitary Fermi Gas: From Monte Carlo to Density Functionals*, chap. 9, pp. 305 – 373, vol. 836 of [5] (2012), 1008.3933.
- [36] M. M. Forbes, S. Gandolfi, and A. Gezerlis, Phys. Rev. Lett. **106**, 235303 (2011), **1011.2197**.
- [37] M. M. Forbes, S. Gandolfi, and A. Gezerlis (2012).
- [38] B. Šopík, P. Lipavský, M. Männel, K. Morawetz, and P. Matlock, Phys. Rev. B 84, 094529 (2011), URL http://link.aps.org/doi/ 10.1103/PhysRevB.84.094529.
- [39] E. Burovski, N. Prokof'ev, B. Svistunov, and M. Troyer, Phys. Rev. Lett. 96, 160402 (2006).
- [40] E. Burovski, N. Prokof'ev, B. Svistunov, and M. Troyer, Phys. Rev. Lett. 97, 239902 (2006).
- [41] E. Burovski, E. Kozik, N. Prokof'ev, B. Svistunov, and M. Troyer, Phys. Rev. Lett. 101, 090402 (2008), 0805.3047.
- [42] N. Prokof'ev and B. Svistunov, Phys. Rev. B 77, 020408 (pages 4) (2008), 0707.4259.

- [43] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. B 77, 125101 (2008), 0801.0911.
- [44] J. Carlson, S.-Y. Chang, V. R. Pandharipande, and K. E. Schmidt, Phys. Rev. Lett. **91**, 050401 (2003), physics/0303094.
- [45] H. A. Forbert and S. A. Chin, Int. J. Mod. Phys. B 15, 1752 (2001), nucl-th/0009068.
- [46] M. Suzuki, Phys. Lett. A 146, 319 (1990), ISSN 0375-9601.
- [47] H. Yoshida, Phys. Lett. A 150, 262 (1990), ISSN 0375-9601.
- [48] M. Creutz and A. Gocksch, Phys. Rev. Lett. 63, 9 (1989).
- [49] J. W. Negele and H. Orland, *Quantum Many-particle Systems* (Westview Press, Reading, MA, 1998), ISBN 0738200522 : 9780738200521.
- [50] J. E. Hirsch, Phys. Rev. B 28, 4059 (1983).
- [51] A. Bulgac, J. E. Drut, and P. Magierski, Phys. Rev. A 78, 023625 (2008), 0803.3238.
- [52] G. Wlazłowski and P. Magierski, Int. J. Mod. Phys. E 18, 919 (2009), 0812.0883.
- [53] A. Bulgac, J. E. Drut, and P. Magierski, Phys. Rev. Lett. 96, 090404 (2006), cond-mat/0505374.
- [54] A. Bulgac, J. E. Drut, and P. Magierski, Int. J. Mod. Phys. B 20, 5165 (2006), cond-mat/0602091.
- [55] A. Bulgac, J. E. Drut, and P. Magierski, Phys. Rev. Lett. 99, 120401 (2007), cond-mat/0701786.
- [56] P. Magierski, G. Wlazłowski, A. Bulgac, and J. E. Drut, Phys. Rev. Lett. 103, 210403 (2009).
- [57] P. Magierski, G. Wlazłowski, A. Bulgac, and J. E. Drut, Phys. Rev. Lett. 103, 210403 (2009).
- [58] P. Magierski, G. Wlazłowski, and A. Bulgac, Phys. Rev. Lett. 107, 145304 (2011).
- [59] J. E. Drut, T. A. Lähde, and T. Ten, Phys. Rev. Lett. 106, 205302 (2011), URL http://link.aps.org/doi/10.1103/PhysRevLett. 106.205302.

- [60] J. E. Drut, T. A. Lähde, G. Wlazłowski, and P. Magierski, *The equation of state of the unitary fermi gas: an update on lattice calculations* (2011), 1111.5079.
- [61] J. Carlson, S. Gandolfi, K. E. Schmidt, and S. Zhang, Phys. Rev. A 84, 061602 (2011), 1107.5848.
- [62] D. Lee, Phys. Rev. C 78, 024001 (2008), 0803.1280.
- [63] D. Lee, Lattice simulations for few- and many-body systems (2008), 0804.3501.
- [64] J.-W. Chen and D. B. Kaplan, Phys. Rev. Lett. 92, 257002 (2004), hep-lat/0308016.
- [65] M. G. Endres, D. B. Kaplan, J.-W. Lee, and A. N. Nicholson, *Lattice Monte Carlo calculations for unitary fermions in a harmonic trap*, Phys. Rev. A 84, 043644 (2011) (2011), 1106.5725.
- [66] J. E. Drut, Phys. Rev. A 86, 013604 (2012), 1203.2565.
- [67] S. R. Beane, P. F. Bedaque, A. Parreño, and M. J. Savage, Phys. Lett. B 585, 106 (2004), hep-lat/0312004.
- [68] D. Blume and K. M. Daily, C. R. Phys. 12, 86 (2011), 1008.3191.
- [69] H. Muther and A. Sedrakian, Phys. Rev. Lett. 88, 252503 (2002), cond-mat/0202409.
- [70] Y. Nishida, Phys. Rev. A 79, 013629 (2009), 0811.1615.
- [71] K. R. Patton and D. E. Sheehy, *Induced superfluidity of imbalanced Fermi gases near unitarity* (2012), 1203.6348.
- [72] D. Lee and T. Schäfer, Phys. Rev. C 73, 015202 (2006), nucl-th/ 0509018.
- [73] D. Lee, Eur. Phys. J. A 35, 171 (2008), ISSN 1434-6001, 0704.3439.
- [74] A. Valance, T. J. Morgan, and H. Bergeron, American Journal of Physics 58, 487 (1990), URL http://link.aip.org/link/?AJP/ 58/487/1.
- [75] F. Cooper, A. Khare, and U. Sukhatme, Phys. Rep. 251, 267 (1995), hep-th/9405029v2.

Revision 2:287973e981ca tip.

- [76] T. Papenbrock and G. F. Bertsch, Phys. Rev. C 59, 2052 (1999), nucl-th/9811077.
- [77] E. Braaten and H.-W. Hammer, Phys. Rep. 528, 259 (2006), cond-mat/0410417.
- [78] S. Tan (2005), cond-mat/0505615.
- [79] A. Bulgac and M. M. Forbes, Phys. Rev. A 75, 031605(R) (2007), cond-mat/0606043.
- [80] F. Chevy, Phys. Rev. A 74, 063628 (pages 4) (2006), cond-mat/ 0605751.
- [81] C. Lobo, A. Recati, S. Giorgini, and S. Stringari, Phys. Rev. Lett. 97, 200403 (pages 4) (2006), cond-mat/0607730.
- [82] S. Pilati and S. Giorgini, Phys. Rev. Lett. 100, 030401 (pages 4) (2008), 0710.1549.
- [83] R. Combescot and S. Giraud, Phys. Rev. Lett. 101, 050404 (2008), 0804.2638.
- [84] D. M. Eagles, Phys. Rev. 186, 456 (1969).
- [85] A. J. Leggett, Rev. Mod. Phys. 47, 331 (1975).
- [86] A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter*, edited by A. Pekalski and J. Przystawa (Springer, Berlin, 1980), Lecture Notes in Physics, pp. 13 – 27, proc. XVI Karpacz Winter School of Theoretical Physics.
- [87] R. P. Feynman, *Statistical Mechanics*, Advanced Book Classics (Perseus Books, Reading, Massachusetts, 1998), 2nd ed.

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