Zero-Temperature Equation of State of Mass-Imbalanced Resonant Fermi Gases

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Zero-temperature equation of state of mass-imbalanced resonant Fermi gases

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We calculate the zero-temperature equation of state of mass-imbalanced resonant Fermi gases in an ab initio fashion, by implementing the recent proposal of imaginary-valued mass difference to bypass the sign problem in lattice Monte Carlo calculations. The fully non-perturbative results thus obtained are analytically continued to real mass imbalance to yield the physical equation of state, providing predictions for upcoming experiments with mass-imbalanced atomic Fermi gases. In addition, we present an exact relation for the rate of change of the equation of state at small mass imbalances, showing that it is fully determined by the energy of the mass-balanced system.

Introduction.– Experiments with ultracold Fermi gases continue to move forward in their study of progressively richer quantum many-body systems, advancing our understanding of strongly interacting matter at the interface of nuclear, atomic and condensed matter physics. From the pioneering experiments realizing a condensate and determining the energy of unpolarized atomic clouds [1], research has moved on in less than a decade to experiments varying temperature and polarization [2], studies of Bose-Fermi mixtures [3], optical lattices [4], precise determinations of the equation of state [5], and the list continues (see e.g. Ref. [6] for reviews). Now many new experiments with mixtures of a variety of different fermion species (such as 6Li, 40K, 161Dy, 163Dy, 167Er) appear to be possible in the near future (see e.g. Ref. [7]), giving us an unprecedented opportunity to understand the effects of mass imbalance in strongly coupled gases. In particular, it is possible to achieve mixtures with mass imbalances smaller than the one associated with a 6Li-40K-mixture for which three-body effects are already expected to be significant [8], thus making experimental studies more challenging.

Of the wide variety of regimes explored in ultracold fermions, one has received unparalleled attention. This is the so-called “unitary” Fermi gas, which is realized by adjusting an external magnetic field on a dilute system of two fermion species, setting the system close to a broad Feshbach resonance. Since the interaction range \( r_s \) is effectively zero relative to the interparticle spacing \( n^{-1/3} \) in that limit and the \( s \)-wave scattering length \( a_s \) is very large (on the order of hundreds to thousands of Bohr radii), i.e. \( r_s \ll n^{-1/3} \ll a_s \), the system is scale-free (except for \( n \), as in a non-interacting gas). This disappearance of dynamical scales at unitarity has brought about interest from the nuclear physics area (where the unitary gas is a model for neutron matter [9] and has been proposed as a starting point for perturbative nuclear structure calculations [10]). Indeed, the strong pairing displayed at (and around) resonance results in a relatively high critical temperature (\( T_c \simeq 0.15 - 0.17 \), in units of the Fermi energy [11]) with observed pairing correlations above \( T_c \) [12], as in high-\( T_c \) superconductors. In addition, the realization that the physics of the unitary limit is directly connected to a non-relativistic conformal fixed point [13, 14], has spurred interest from the string-theory side, in connection with gauge-gravity duality [15].

In this work, we determine the zero-temperature equation of state of a mass-imbalanced unitary Fermi gas, by computing the ground-state energy as a function of the mass imbalance. As three-body effects become significant for large mass imbalances, we focus on the equation of state for mass imbalances below the one associated with a 6Li-40K-mixture. A natural question for imbalanced systems of this kind is whether they undergo a quantum phase transition at a critical imbalance. This work is a first step towards answering this question in a controlled and non-perturbative way. To our knowledge, there are no previous ab initio calculations covering the range of mass imbalances presented here.

Because the unitary regime is strongly coupled, and there is no small parameter to formulate an expansion, computational methods are needed for quantitative predictions. For a many-body problem of this kind, Monte Carlo methods are the tools of choice. However, the presence of a finite mass-imbalance introduces a “sign problem” as in systems with finite polarization, or in QCD in the presence of finite baryon density [16]. This is a serious roadblock in many fields (condensed matter, atomic physics, high- and low-energy nuclear physics). For mass-imbalanced Fermi gases, this implies that our present understanding is based on mean-field studies partly amended to account for fluctuation effects to some extent, see, e.g., Ref. [17] for early ground-breaking studies. While such studies give qualitative access to the features of these systems, it is also known that mean-field theory does not predict the energy of the mass-balanced unitary Fermi gas correctly. In fact, the mean-field result (see, e.g., Refs. [18] for reviews) for the ground-state energy is about 50% larger than the accepted values from Monte Carlo calculations [19].

To make progress in spite of the sign problem, we implement a method we proposed recently in Refs. [20, 21]. Borrowing ideas from a technique originally devised for lattice QCD [16], we introduced an imaginary mass im-
balance, such that each species has a complex mass, but
one is the complex conjugate of the other. As a result, the
sign problem is avoided. However, the data now needs to
be analytically continued to real mass imbalance. This
can be done in many ways, but the imaginary-mass calcula-
tions are performed in a fully non-perturbative fashion
without ambiguities. It should be noted that this tech-
nique has never been applied to non-relativistic systems
before. Moreover, because the system we study is simple
yet strongly coupled, our calculations may also shed light
on aspects of similar methods on the lattice QCD side.

Computational technique.– Following the notations
of Ref. [21], the Hamiltonian \(\hat{H}\) of two Fermi species,
up and down, with a zero-range interaction is

\[
\hat{H} = \int d^3x \left( \sum_{\sigma=\uparrow,\downarrow} \bar{\psi}_\sigma(x) \left( -\frac{\nabla^2}{2m_\sigma} \right) \psi_\sigma(x) + \bar{\psi}_{\uparrow}(x) \hat{\rho}_\uparrow(x) \psi_\downarrow(x) \right)
\]

and can be viewed as the sum of the kinetic operators \(\hat{T}_{\uparrow,\downarrow}\)
associated with the two fermion species and an opera-
tor \(\hat{V}\) specifying the interaction, \(\hat{H} = \hat{T}_\uparrow + \hat{T}_\downarrow + \hat{V}\). The
operators \(\hat{\rho}_{\uparrow,\downarrow}\) are the particle-density operators, and the
masses of the species are \(m_\uparrow\) and \(m_\downarrow\). To simplify the dis-
cussion of mass imbalanced systems, we define a di-

gen
mensionless imbalance parameter \(\bar{m} = (m_\downarrow - m_\uparrow) / (m_\downarrow + m_\uparrow)\),
which maps the problem to a finite interval, 0 ≤ |\bar{m}| < 1.
For convenience, we shall take units such that \(\hbar = k_B = 1\),
as well as \(m_0 = (m_\uparrow + m_\downarrow)/2 = 1\). With these conven-
tions, we have \(\bar{m} \approx 0.74\) for a \(^6\)Li-\(^4\)K mixture.

We implement a projection quantum Monte Carlo (QMC)
algorithm (see e.g. Ref. [22]) on a spacetime latt-

e ice, whereby we start with a Slater determinant \(|\psi_0\rangle\) as a
guess for the ground-state wavefunction and project pro-
towards the ground state by evolving in imaginary time.
This is accomplished by applying the transfer matrix
\(T = \exp\left(-\tau\hat{H}\right)\), which we factorize in the Trotter-Suzuki
fashion. A Hubbard-Stratonovich transformation is then
used to represent the interaction, allowing us to write the
transfer matrix as (see e.g. Ref. [22] for further details):

\[
T = \int D\sigma \ T_1[\sigma] T_\uparrow[\sigma] ,
\]

where \(D\sigma = \prod d\sigma_i / (2\pi)\), and \(\sigma_i\) is an external auxiliary
field taking values between -\(\pi\) and \(\pi\) at each point \(i\)
in the spatial lattice. The partition sum (or rather its
zero-temperature analogue) is then given by

\[
Z_0(\beta) \equiv \langle \psi_0 \ \prod_{\ell=1}^{N_\tau} T_\uparrow[\sigma] \rangle = \int D\sigma \ \det \left[ \sum_{\ell=1}^{N_\tau} T_\uparrow[\sigma] T_\uparrow[\sigma] \right].
\]

Here, \(\sigma\) is to be regarded as defined on a spacetime lat-
tice of \(N_x^2 \times N_\tau\) points, with lattice spacing \(\ell = 1\) (by
definition) in the spatial directions and \(\tau\) in the time di-
rection, \(\beta = N_\tau/\ell\). The determinant is taken over the
single-particle space of the orbitals that make up the \(N\)-
fermion state \(|\psi_0\rangle\).

In Eq. (2), we observe that the fermion determinant
factorizes into a determinant for each fermion species. In
the absence of mass imbalance, and if the interaction is
purely attractive (\(\bar{g} > 0\) in our convention), these de-
terminants are real and identical. The product is thus
positive semidefinite and can therefore be used as a prob-
ability measure in a QMC calculation. In the presence
of a finite mass imbalance, on the other hand, this is
no longer the case, which spoils the naive application of
QMC methods. By using an imaginary mass imbalance,
however, the determinants become complex conjugates
of each other, which again makes their product positive
semi-definite and therefore amenable to standard QMC
methods [21]. In finite temperature calculations, it is in
principle also possible to calculate at finite spin imbal-
ance via imaginary chemical potential differences [20].

To connect the bare lattice theory to the physical
parameters (namely the scattering length \(a_s\)), we uti-
lize Lüscher’s formula [23] for the relation between the
phase shift and the energy eigenvalues of the two-body
problem in a box. As the lattice eigenvalues depend
directly on the bare coupling \(\bar{g}\) and the reduced mass
\(m_r = (m_0/2)(1 - \bar{m}^2)\), it is a simple matter to tune these
to match the desired physics, see, e.g., Refs. [24, 25] for
details. This results in \(\bar{g}(\bar{m}) = \bar{g}(\bar{m} = 0)/(1 - \bar{m}^2)\).

Data Analysis.– In the present work, we focus on the
(dimensionless) equation of state \(\xi(\bar{m})\), which is defined
as the ratio of the energy of the interacting \(N\)-body
problem evaluated at a given \(\bar{m}\), to the energy of the
corresponding non-interacting mass-balanced Fermi gas.
For \(\bar{m} = 0\), this definition matches the one of the so-called
Bertsch parameter. To be more specific, we calculated the
\(\beta\epsilon_F\)-dependence of systems of many particles in cubic
lattices of different sizes (see Table II), and for imaginary-
mass imbalances in the range \(\bar{m} \in 0, 0.025, 0.05, \ldots , 1\).
Here, \(\epsilon_F\) denotes the Fermi energy of the non-interacting
gas at the same density. The data was then extrapolated
to large \(\beta\epsilon_F\) in a standard fashion [25].

For each set of parameter values \((N_x, N, \beta\epsilon_F, \bar{m})\) we
used approximately 500 decorrelated samples of the aux-
iliary field, which yields a statistical uncertainty of the
order of 5%. The lattice length and energy units were set
by the spatial lattice spacing \(\ell = 1\), and the imaginary-
time spacing \(\tau = 0.05\) (in the units determined by \(\ell\)). To
perform the analytic continuation from imaginary to real
\(\bar{m}\), we employed an ansatz for the form of the equation
of state as a function of \(\bar{m}\), to which we fit the data.

Results.– Naturally, an analytic continuation of the
data is only meaningful if the partition sum \(Z_0\) is an ana-
lytic function of \(\bar{m}\) in a finite domain about \(\bar{m} = 0\).

\[\text{Footnote:} \text{For the lattices and particle numbers studied here, we have found that the analytic continuation could be performed before or after the extrapolation to } \beta \epsilon_F \rightarrow \infty \text{ without significant change in the results.}\]
In practice, however, little is known about the analytic properties of the full partition sum. Therefore any analytic insight is important to guide the continuation. A very first understanding of the \( \bar{m} \)-dependence of the equation of state \( \xi \) can be obtained from the free mass-imbalanced Fermi gas. In that case, \( \xi_{\text{free}} = E_{\text{free}}(\bar{m})/E_{\text{tree}}(0) = 1/(1 - \bar{m}^2) \) for real-valued \( \bar{m} \). Note that the partition sum is invariant under \( \bar{m} \to -\bar{m} \).

To better understand the effect of fermion interactions on the functional form of \( \xi(\bar{m}) \), we consider a mean-field analysis. In Refs. [21, 26], it was found that the radius of convergence \( r_{\bar{m}} \), associated with the \( \bar{m} \)-dependence of the partition sum is maximal for the unpolarized system, \( r_{\bar{m}} = 1 \). For the mean-field equation of state as a function of (real-valued) mass-imbalances, we obtain \( \xi_{\text{mf}}(\bar{m}) = \xi_{\text{mf}}(\bar{m} = 0)/(1 - \bar{m}^2) \), where \( \xi_{\text{mf}}(\bar{m} = 0) \approx 0.6 \). Thus, the conventional Bertsch parameter \( \xi_{\text{mf}}(\bar{m} = 0) \) completely determines the coefficients of an expansion in powers of \( \bar{m}^2 \). The analyticity of the mean-field equation of state in the range \( 0 \leq \bar{m} < 1 \) can be understood from the fact that the system does not undergo a (quantum) phase transition from the superfluid phase to a normal phase as function of \( \bar{m} \) for \( N_\uparrow = N_\downarrow \) (see e.g., Ref. [26]). Indeed, the existence of a phase transition at a given critical value \( \bar{m}_{ct} \) would be associated with a non-analytic behavior of \( \Sigma_0 \), and therefore with a non-analytic behavior of the observables.

Beyond the mean-field approximation, an analysis of the analytic properties of the full partition sum is difficult. From the path-integral representation Eq. (2), however, it is a simple matter to derive an exact differential equation for the equation of state:

\[
\frac{\partial \langle \hat{H} \rangle}{\partial \bar{m}^2} = \frac{1}{1 - \bar{m}^2} \left( \langle \hat{H} \rangle - \langle \hat{T}_\Sigma \rangle \right),
\]

where \( \langle \hat{T}_\Sigma \rangle = \frac{1}{2} \left( \langle \hat{T}_\uparrow + \hat{T}_\downarrow \rangle - \frac{1}{\bar{m}} \langle \hat{T}_\uparrow - \hat{T}_\downarrow \rangle \right) \), and the mass derivative is taken along the line of constant physics, i.e. such that the two-body scattering parameters remain constant. We may interpret the quantity \( \langle \hat{T}_\Sigma \rangle \) as a measure of the difference between the kinetic energies of the spin-up and down fermions in the presence of an interaction. Indeed, \( \langle \hat{T}_\Sigma \rangle = 0 \) for the free gas for all \( \bar{m} \), as well as for the interacting mass-balanced system. The initial condition for the differential equation (3) is given by the energy of the mass-balanced system, and the dimensionless equation of state \( \xi \) is given by \( \xi(\bar{m}) = \langle \hat{H}(\bar{m}) \rangle / E_{\text{tree}}(\bar{m} = 0) \). Note also that the mean-field equation of state is obtained from the differential equation (3) by setting \( \langle \hat{T}_\Sigma \rangle \to 0 \). Our analytic insight into the \( \bar{m} \)-dependence of the equation of state suggests that it may be insufficient to fit our QMC data to a low-order truncation of a polynomial in \( \bar{m}^2 \). Below, we therefore only fit our data for small \( \bar{m} \) to a polynomial in \( \bar{m}^2 \) to show that our numerical data obeys \( \partial \langle \hat{H} \rangle / \partial \bar{m}^2 \big|_{\bar{m}=0} = \langle \hat{H} \rangle |_{\bar{m}=0} \), which follows from Eq. (3) and \( \langle \hat{T}_\Sigma \rangle = 0 \) at \( \bar{m} = 0 \). To provide a global description of our QMC data for imaginary-valued mass imbalances, we employ a Padé approximant:

\[
\xi(\bar{m}) = \frac{\xi(\bar{m} = 0)}{1 + \xi_M \bar{m}^2},
\]

where \( \xi(\bar{m} = 0) \) and \( \xi_M \) are the only two fit parameters. Note that this ansatz violates the constraint \( \partial \langle \hat{H} \rangle / \partial \bar{m}^2 \big|_{\bar{m}=0} = \langle \hat{H} \rangle |_{\bar{m}=0} \) if \( \xi_M \neq 1 \). While we could consider more sophisticated approximants to include this constraint, we have found that our present ansatz already provides a reasonable parameterization for the equation of state for \( 0 \leq |\bar{m}| < 1 \) (see below).

We next discuss our QMC results for \( \xi(\bar{m}) \), beginning with small values of \( \bar{m} \). Our analytic calculation predicts that \( \partial \langle \hat{H} \rangle / \partial \bar{m}^2 \big|_{\bar{m}=0} = \langle \hat{H} \rangle |_{\bar{m}=0} \), i.e. the curvature of the equation of state at \( \bar{m} = 0 \) is fully determined by the Bertsch parameter \( \xi(0) \). Our QMC data for imaginary mass imbalances agrees with this statement as seen from a fit to the ansatz \( \xi(\bar{m}) = \xi(\bar{m} = 0) - \xi(1) \bar{m}^2 \), see Table I. For the fit, we have only used data for \( \bar{m} \leq 0.4 \) as obtained from a \( 1/N_x \)-extrapolation of the original QMC data for \( N_x = 8, 10, 12 \) to the infinite-volume limit while keeping the density \( N/N_x^3 \approx 0.05 \) fixed. We chose this (relatively low) density to (at least partially) avoid finite-range effects. The continuum limit can be reached by studying the low-density limit. Already the data for the smallest lattice size, \( N_x = 8 \), agrees within error bars

<table>
<thead>
<tr>
<th>( N/N_x^3 )</th>
<th>( \xi(\bar{m}=0) )</th>
<th>( \xi^{(1)} )</th>
<th>( \chi^2/\text{dof} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.414 ± 0.012</td>
<td>0.461 ± 0.181</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table I. Estimates for the Bertsch parameter \( \xi(\bar{m}=0) \) and the curvature \( \xi^{(1)} := d\xi(\bar{m})/d\bar{m}^2 \big|_{\bar{m}=0} \) for real mass imbalance in the large-volume limit, fitting with \( \bar{m} \leq 0.4 \).

<table>
<thead>
<tr>
<th>( N_x )</th>
<th>( N )</th>
<th>( \xi(\bar{m}=0) )</th>
<th>( \xi_M )</th>
<th>( \chi^2/\text{dof} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>24</td>
<td>0.449 ± 0.002</td>
<td>0.496 ± 0.010</td>
<td>0.9</td>
</tr>
<tr>
<td>10</td>
<td>46</td>
<td>0.431 ± 0.002</td>
<td>0.631 ± 0.011</td>
<td>2.0</td>
</tr>
<tr>
<td>12</td>
<td>80</td>
<td>0.444 ± 0.002</td>
<td>0.532 ± 0.010</td>
<td>0.4</td>
</tr>
<tr>
<td>∞</td>
<td>-</td>
<td>0.420 ± 0.007</td>
<td>0.693 ± 0.111</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table II. Parameters for the global fit function given in Eq. (4) for a fixed density \( N/N_x^3 \approx 0.05 \) as obtained from three different particle numbers \( N = N_\uparrow + N_\downarrow \) (\( N_\uparrow = N_\downarrow \)) and volumes \( N_x^3 \). The error bars of these fits result from statistical and large-\( \beta_{xy} \)-extrapolation errors. Estimates in the large-volume limit (\( N_x \to \infty \) with fixed \( N/N_x^3 \approx 0.05 \)) are also shown, where a \( 1/N_x \)-extrapolation of the data was performed before the fit.

2 The proof of Eq. (3) makes use of the Hellmann–Feynman theorem, from which it follows that \( \partial \langle \hat{H} \rangle / \partial \bar{m}^2 = \langle \partial \hat{H} / \partial \bar{m}^2 \rangle \).
well-known for the mass-balanced case \cite{19}. Increasing
significantly overestimates the ground-state energy, which is
range effects (see Table I). Our estimate in the large-volume
parameter in the large-volume
limits agrees with previous QMC studies \cite{19}, up to finite-
result from mean-field theory are also shown.

the mass imbalance, the mean-field equation of state
shows a much stronger dependence on \( \bar{m} \) than our QMC
results. For small mass imbalance, this already follows
from Eq. (3). For large real-valued mass imbalances, this
is deduced from Fig. 2. For example, for \( \bar{m} \approx 0.74 \)
(\(^{6}\)Li-\(^{40}\)K-mixture), we find \( \xi_{\text{mf}}(\bar{m})/QMC(\bar{m}) \approx 2.0 \)
when compared to our estimate for the equation of state in
the large-volume limit. Note that \( \xi_{\text{mf}} \rightarrow \infty \) for \( \bar{m} \rightarrow 1 \),
whereas the analytic continuation of the lattice data sug-
ests that \( \xi(\bar{m}) \) remains finite in this limit. This should
be taken with some care, as our results for large real-
valued mass imbalances depend strongly on the details
of the ansatz for the fit function underlying the analy-
ic continuation. However, we have checked that even
with more sophisticated fit functions (Padé approximants
with up to four parameters), the uncertainty for \( \xi(\bar{m}) \)
at \( \bar{m} \approx 0.74 \) is about 30\% at most and decreases rapidly
for decreasing mass imbalances. A detailed analysis
of \( \xi(\bar{m}) \) for various densities and lattices is beyond the
present work and will be presented elsewhere \cite{27}. For the
time being, we only would like to note that our (present)
results satisfy a rigorous variational upper bound \cite{28} and
are qualitatively in agreement with previous direct QMC
calculation for \( \bar{m} \approx 0.74 \) (\(^{6}\)Li-\(^{40}\)K mixture) \cite{29}.

Summary and Conclusions.—We have presented a first
lattice MC determination of the equation of state of res-
onantly interacting fermions with finite mass imbalance.
This \textit{ab initio}, fully non-perturbative calculation was
accomplished by implementing our recent proposal of tak-
ing the mass imbalance to the imaginary axis, where we
can calculate without a sign problem. The data thus ob-
tained was analytically continued via a simple ansatz to
real mass imbalances. To simplify this first attempt, and
provide a useful benchmark, we focused on the case of
equal particle numbers \( N_{x} = N_{j} \), such that the Fermi mo-
menta coincide, and therefore a (quantum) phase transition
at finite \( \bar{m} \) is not expected.

Although we do not aim for high accuracy in this first
study, our analysis indicates that mean-field studies not
only significantly overestimate the ground-state energy,
but also its change when the mass imbalance is increased.
This observation is already of great importance, as many
of the predictions for mass-imbalanced ultracold gases
rely on the mean-field approximation. Future experi-
ments will open up the possibility to measure at least
parts of the equation of state for \( \bar{m} \lesssim 0.7 \). Our present
calculation of the latter and, in particular, of the curva-
ture can then be tested directly.

Our work verifies that the method of imaginary mass
imbalances is feasible. It should now be possible to fur-
nish a number of predictions for an upcoming set of
ultracold-atom experiments, paving the way for future
calculations with mass imbalance in a variety of systems
and situations, e.g. away from unitarity, in various di-
dimensions, at finite temperatures, in an external potential,
and including both imaginary mass and polarization.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{(color online) Equation of state, with statistical error bars, and corresponding fit function (see Eq. (4)) for \( N_{x} = 12 \) and \( N = 80 \) \((N/N_{s}^{3} \approx 0.05)\) as a function of imaginary mass imbalance \( \bar{m} \); see Table II for the fit parameters. Our estimate in the large-volume limit (extrapolation) and the result from mean-field theory are also shown.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{(color online) Equation of state as obtained from analytic continuation of the fit function (4) (see Table II for the fit parameters) as a function of real mass imbalance \( \bar{m} \). The gray band represents an estimate of the error obtained from analytic continuation of the envelopes of our data in Fig. 1 using the ansatz (4). Our estimate in the large-volume limit (extrapolation) and the mean-field result are also shown.
\end{figure}
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