The BCS - BEC Crossover In Arbitrary Dimensions

Zohar Nussinov\textsuperscript{1,2,∗} and Shmuel Nussinov\textsuperscript{3,†}

\textsuperscript{1}Department of Physics, Washington University, St. Louis, MO 63160-4899, USA
\textsuperscript{2}Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
\textsuperscript{3}School of Physics and Astronomy, Tel Aviv University, Ramat-Aviv, Tel Aviv 69978, Israel

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Cold atom traps and certain neutron star layers may contain fermions with separation much larger than the range of pair-wise potentials yet much shorter than the scattering length. Such systems can display universal characteristics independent of the details of the short range interactions. In particular, the energy per particle is a fraction $\xi$ of the Fermi energy of the free Fermion system. Our main result is that for space dimensions $D$ smaller than two and larger than four a specific extension of this problem readily yields $\xi = 1$ for all $D \leq 2$ whereas $\xi$ is rigorously non-positive (and potentially vanishing) for all $D \geq 4$. We discuss the $D = 3$ case. A particular unjustified recipe suggests $\xi = 1/2$ in $D = 3$.

I. INTRODUCTION

Bose-Einstein condensates (BEC) in dilute atomic gases were achieved in 1995 for rubidium, sodium, and lithium [1]. Recently, with the production of cold atomic gases close to the Feshbach resonance [2], these systems provided a vehicle for the study of the BCS to BEC crossover. The (BCS) superconducting and Fermi superfluid are mixed systems harboring quasi-free and pair correlated fermions. In the dilute strong coupling molecular BEC, all fermions are relatively tightly bound into pairs forming a unique macroscopic state. Several theoretical studies have been carried, e.g. [3]. Many of these works report on very interesting universal aspects of the BCS to BEC transition. In such dilute systems with an inter-particle separation much greater than the range of the pair-wise potential yet far shorter than the scattering length, the value of the energy density at this crossover is independent of specific details. This universal energy density is only dimension dependent. Direct results on the three dimensional system are hard to obtain and numerical works have been extremely valuable. As is well known from a multitude of other arenas, a dimensional generalization of original problems posed in three dimensions to arbitrary dimensions often allows us an analytical access to original three dimensional problems (e.g. the well known $\epsilon = 4 - D$ expansion, with $D$ the spatial dimension, which has been extremely fruitful in statistical and quantum field theories, e.g. [4]). Here, we follow suite and couch the BCS to BEC crossover problem in arbitrary dimensions ($D$). We report new results on the energy per particle at the onset of this crossover in such an arbitrary dimension (suitably defined by the appearance of zero-energy two particle bound states). This extension enables us to examine crossovers in low dimensions where no condensed phases occur due to the enhanced role of low energy fluctuations. We will illustrate, both by exact variational bounds and normalization considerations, that in all dimensions $D \geq 4$ the energy per particle at the onset of the transition is rigorously bounded from above by zero. By contrast, due to localization tendencies in low dimensions ($D \leq 2$), each particle carries, on average, the mean energy of a free Fermi system at the appearance of the first two particle bound states. The physically pertinent well known question [5] concerns the energy per particle in actual transitions occurring in $D = 3$ dimensions. The determination of the energy per particle here is far more difficult. In $D = 3$, we depart from the more rigorous results in higher and lower dimensions and present a heuristic argument for recently reported numerical results [6]. These independent heuristic arguments bolster the the result attained by dimensional interpolation. The average of the exact bounds on the energies in $D = 2$ and $D = 4$, which is half the free fermion energy per particle, is not far removed from the numerical results reported in three dimensions [6]. In [6] the fraction of a half, derived here by (i) dimensional interpolation and (ii) an independent heuristic argument, is replaced by $\xi \approx 0.44$.

II. OUTLINE

We begin, in section(III), by formulating the problem and briefly reviewing numerical results. Next, in section(IV), we turn to an exact variational bound concerning this transition in high dimensions and an easier result relating to bound states in low dimensions. Finally, in section(V), we present heuristic arguments for $D = 3$. These further correlate the average energy per particle with the observed differences seen in finite size system with an even or odd particle number. In a brief appendix, we provide the specifics of the exact solution of the zero energy bound state problem in a D-dimensional spherical potential well. Throughout the text, in order to make the physics and scaling very transparent, we will often use simpler forms. Nevertheless, at the end of all calculations, we will demonstrate that our results go unchanged with the insertion of the exact zero-energy bound state solution.

\textsuperscript{∗}Electronic address: zohar@viking.lanl.gov
\textsuperscript{†}Electronic address: nussinov@post.tau.ac.il
III. FORMULATING THE PROBLEM: INTRODUCTORY AND GENERAL COMMENTS

We start by writing down the general Hamiltonian, describing \( N = 2n \) spin-1/2 Fermions in a box of size \( V = L^3 \),

\[
H(g) = \sum_i p_i^2/2m - g \sum_{i>j} V(|r_i - r_j|)
= \sum_i p_i^2/2m + \sum_j (p_j')^2/2m - g \sum_{ij} V(|r_i - r_j'|).
\]

Here, \( I, J \) (or \( i, j \)) run from 1 to \( N \) (or \( n \)) respectively. The phase space coordinates \( r_i, p_i \) and \( r'_j, p'_j \) are the positions and momenta of the “spin up” and “spin down” atoms respectively and \( -gV(r_i, r'_j) \) is the attractive short range potential in mixed pairs. These conventions for the coordinates [using upper case characters to describe the total system (both spin up and spin down) quantities and the use of lower case characters (either “primed” or “un-primed”) for spin-down and spin-up coordinates] will be consistently employed throughout this work.

Atoms of identical spin polarization cannot be in a relative S wave state where the short range interactions operate and thus, in Eq.\((1)\), we set \( V(r_i, r_j) = V(r'_i, r'_j) = 0 \). The coupling \( g \) is tuned to \( g^* \) where the first (zero energy, S wave) two-body bound state appears and the scattering length \( a \) diverges. An illustration of the standard two-particle zero energy bound state in three dimensions is provided in Fig.(1).

With this identification of \( g^* \) at hand [5], the BCS to BEC crossover problem is now formally defined in arbitrary dimension \( D \), although, due to the enhanced role of low energy fluctuations, actual condensates may form only in \( D > 2 \). Our physical interest is in \( D = 3 \). To make \( g \) dimensionless in Eq.(1), we scale \( \text{V by} \ (m\hbar^2/\pi a_0)^{-1} \) with \( a_0 \) the range of the potential and \( m \) the particle mass. We assume a dilute system with inter-particle separation \( d = 1/k_F \), much larger than \( r_0 \). In practical terms, this implies that we will always consider the limit \( r_0 \to 0 \). To avoid the well known formal “collapse problem” in which all particles may sit within the attractive potential well [as the attractive \( \text{V(r}_i, r'_j) < 0 \) for \( r_i - r'_j \leq r_0 \), we may envision a state in which all particles sit within a sphere of radius \( r_0 \)], leading to a divergent negative energy density, the problem is formulated with the provision that the limit \( r_0 \to 0 \) is taken before the thermodynamic limit is considered [5, 7]. With these definitions in tow, the problem emulates what transpires in many dilute fermionic systems (cold atom traps, neutron star layers) with separations far larger than the range of the pair potentials yet far smaller than the scattering length.

In three dimensions, scaling arguments then imply a universal form for the energy per particle

\[
\frac{E}{N} = \left(\frac{3}{5}\varepsilon_F\right)\xi,
\]

with \( \varepsilon_F \) the Fermi energy of the free fermi system. [8] The fraction \( \xi \) is independent of the specific potential \( V(r) \) chosen and is the same for all short range potentials which have a zero energy S-wave bound state. Cold dilute Fermionic atoms display many fascinating universal (and not universal) features; see, e.g., [3]. Here we will focus just on the above \( \xi \) parameter.

In actual traps, an excited zero energy state \( \psi(r) \) plays a key role. The continuum states are effected by the extended zero energy state and have negligible overlap with lower, tightly bound, states of size \( \sim r_0 \) which can be ignored unless we consider very long time scales. As any zero energy S wave bound state has the same form \( \psi(r) = \psi_0(r) = A/|r| \) outside the range of the potential for \( |r| > r_0 \), we assume just one zero energy state. For \( g = 0 \), there are two free species with \( n = N/2 \) fermions in each, and relative to Eq.(2), with the standard results

\[
E_{\text{free-fermion}} \to 3/5 \varepsilon_F, \quad n = \frac{L^3(4\pi/3)p_F^3}{(2\pi)^3},
\]

where \( p_F = \frac{\hbar^2}{2m} \) are the free particle Fermi momentum and Fermi energy respectively. Throughout, we set \( \hbar = 1 \). Thus, by definition,

\[
\xi = 1 \quad \text{for} \quad g = 0.
\]

For small \( g > 0 \) (weak attractive potentials), the BCS wave function is adequate. By contrast, for strong coupling \( g/|V(r)| < r_0 \) >> \( \varepsilon_F \), up-down spin pairs tightly bind into dimers of sizes of order, \( r_0 \), the range of the potential V. The \( n = N/2 \) dimers in the deepest bound state then behave as point-like bosons and undergo BEC (Bose-Einstein Condensation) to the traps’ ground state with \( \rho_{\text{dimer}} \sim 0 \) so that

\[
\frac{E}{N} = -\frac{|B.E.|}{2} \quad \text{if} \quad g \to \infty,
\]
with $B.E.$ the binding energy.

The focus of the current work is on the crossover between the BCS and BEC regimes wherein the initial Cooper pairs become tighter dimers [9]. The existence of a bound state renders a weak-coupling perturbation series inappropriate. Similarly, strong coupling/tight binding schemes also fail. As $g$ decreases so does the binding energy. Once $|B.E.| < \varepsilon_F$, the size of the bound state becomes larger than the average inter-particle distance: $O(m \varepsilon_F)^{-1/2} \sim d$ and antisymmetrization of spin up (and of spin down) atoms—which is negligible for small dimers—raises $E/N$ above $\frac{B.E.}{4} = 0$.

The difficulty and interest of the problem motivated several calculations. A semi-analytic approach utilizing the Padé approximation has been discussed at length in Ref. [7]. Numerical Fixed Nodal Planes-Green Function-Monte Carlo (FNPGFMC or MC) calculations were used to estimate $E(N)$ [6]. The ground state wave function of $N$ fermions in a periodic box of size $L$ was estimated by evolving (in imaginary time $\tau = -it$) an initial trial function $\Psi(r_i, r_j; \tau = 0)$ with $\exp(-H\tau)$. The short range potential $V(r_i - r_j)$ was chosen to have precisely one zero energy bound state. The lowest energy obtained to date via these methods corresponds to $\xi = 0.44$ in Eq.(2) which is consistent with present imprecise experimental values. The $L/d \sim n^{1/3} = 80^{1/3} \approx 3.5$ used there implies a box size $L$ smaller than the (infinite) scattering length. This still allows for an extraction of reliable data.

In general, the ground state energy $E/N$ decreases continuously with increasing $g$. The instability against the formation of Cooper pairs for any attractive potential adds a singular $\sim \exp(-g_c/g)$ (with $g_c$ a constant) term to $E/N$ with the continuity in $g$ maintained.

IV. EXTENSION TO ARBITRARY SPATIAL DIMENSIONALITY $D$

While the original problem is posed in $D = 3$ dimensions, it is instructive to address it in any (continuous) $D$ with the simple extension of Eqs.(2,3),

$$\frac{E}{N} = \frac{\xi}{D(2 + D)} \varepsilon_F. \quad (6)$$

To set the ground for future notation, we mention that the simple $D$ dimensional extension of the latter part of Eq.(3) has the total fermion number (per spin flavor) within a Fermi sphere of radius $p_F$ given by $n = \Omega_D L^D p_F^D/(2\pi)^D$. Here, $\Omega_D = \pi^{D/2}/\Gamma(\frac{D}{2} + 1)$ is the volume of the $D$ dimensional unit sphere.

In what follows, we (i) establish by localization tendencies in dimensions $D \leq 2$ that $\xi(D \leq 2) = \xi(g = 0) = 1$. We then (ii) illustrate that $\xi(D \geq 4) \leq 0$ by relying on divergence, at short length scales, of the wave function normalization. This simple scaling consideration is then made rigorous for all continuous dimensions $D > 4$ by employing a variational bound with the use of an “orbital” Slater determinant wavefunction. (Regrettfully, we have not been able to devise a wavefunction which will lead to new stringent variational bounds on the three-dimensional problem.)

Putting all of the pieces together, we find by extending the problem to any dimension $D$ while insisting on having precisely one zero energy bound state that $\xi$ is non-trivial only within the interval $2 < D < 4$. From this perspective, the only interesting integer dimensionality is, in fact, the original $D=3$.

There may be other extensions of the problem which might be non-trivial in all dimensions. Many systems simplify at $D \to \infty$ and a mean field approach may apply there also to Fermionic problems [12]. It has been argued that a certain class of diagrams dominates in this limit the perturbative series in an appropriate effective field theory and can be analytically summed in certain fashions to yield $\xi(D = \infty) = \frac{4}{9}$ [13] or $\frac{4}{9}$ [14].

In what briefly follows, we employ the above continuation with a primary focus on energetics (i.e., the existence of a zero energy $S$ wave bound state) rather than on the infinite scattering length. We find the resulting simple values $\xi = 1$ for all (continuous) dimensions smaller than $D = 2$ and $\xi \leq 0$ for all $D \geq 4$ interesting on their own right.

A. Low Dimensions ($D \leq 2$)

Localization tendencies present in low dimensions afford us with a direct result. Purely attractive potentials $V(r)$ have zero energy bound states in one and two dimensions [10], for any strength and $g$. It follows that a bound state appears immediately as the two body attraction is introduced, i.e. $g^* = 0^+$. As the energy fraction $\xi(g)$ is continuous in any dimension $D$, we find that

$$\xi = \xi(g = 0) = 1, \quad D \leq 2. \quad (7)$$

Similar incarnations of localization tendencies in low dimensions have proven very useful in other arenas (e.g. [15] in which a scaling theory of localization suggested $D = 2$ as the marginal dimension for the appearance of metallic states).

B. High Dimensions ($D \geq 4$)

1. Energy attained by Normalization conditions

Next, let us assume that the potential $V$ vanishes outside the range $r_0$. Volume normalization factors aside, the spin-up spin-down, zero energy, pair wave function for relative separation $|r| > r_0$ is $\phi(r) = A_D/r^{D/2-1}$, with $A_D$ a dimension dependent numerical constant. The following is a very interesting observation: the integral representing the normalization of this zero energy wave function, $\int d^D r |\phi(r)|^2$, diverges at small $r$ for $D \geq 4$. We consequently find that in $D \geq 4$ dimensions most of the normalization of the zero energy bound state wave function is concentrated near $|r| = r_0^*$ and the dimers formed are actually compact—just like for large coupling in $D=3$. Hence, we can again neglect the overlap of
the different dimers and attendant kinetic energy due to antisymmetrization in the spin up coordinates \( \{ \phi_i \} \) and separately in the spin down positions \( \{ \phi'_i \} \). The strong coupling result Eq. (5) applies and we have: \( E/N = \frac{|B_c E|}{2} \leq 0 \). Thus, we find that \( \xi \) may vanish (or become negative) for all dimensions greater than four,

\[
\xi \leq 0, \quad D \geq 4.
\]  

(8)

In the marginal dimension \( D = 4 \), the size of the dimers is just barely \( r_0 \) (where the attractive potentials operate) and the upper bound may be more easily saturated with a potentially vanishing \( \xi (D = 4) \).

2. A Variational Upper Bound

To substantiate the above arguments, and directly derive Eq.(8), we next employ a 2n-body ansatz wave function \( \Psi(\{r_1, r_2, \ldots, r_n; \{r'_1, \ldots, r'_n\} \) and show that in all continuous dimensions \( D > 4 \), we have \( H[\Psi] = 0 \). The ansatz \( \Psi \) has the form of a Slater “orbital” determinant. It represents the state of \( n \) dimers, say, \( \phi(\{r_1 - r'_1\}) \ldots \phi(\{r_n - r'_n\}) \) with \( \phi(|r_i - r'_j|) \) the zero energy bound state, antisymmetrized over all the \( n! \) permutations: \( P = i \rightarrow (p(i)), \ i = 1, \ldots, n \) of the \( n \) spin-up atoms:

\[
\Psi = \sum_P (-1)^P \Phi(P) \quad \Phi(P) = \prod_{i=1}^n \phi(r_i - r'_{p(i)})
\]  

(8)

with \( (-1)^P \) the parity of the permutation \( P \). Here, \( \phi(r_i - r'_{p(i)}) \) represent normalized, zero energy, pair wavefunctions. The further required antisymmetrization over the \( n \) spin-down atoms simply scales \( \Psi \) : \( \Psi \rightarrow ([n!]\Psi) \) and is redundant. We note that \( \Psi \) can be expressed as a determinant,

\[
\det \begin{pmatrix}
\phi(r_1 - r'_1) & \phi(r_1 - r'_2) & \cdots & \phi(r_1 - r'_n) \\
\phi(r_2 - r'_1) & \phi(r_2 - r'_2) & \cdots & \phi(r_2 - r'_n) \\
\vdots & \vdots & \ddots & \vdots \\
\phi(r_n - r'_1) & \phi(r_n - r'_2) & \cdots & \phi(r_n - r'_n)
\end{pmatrix}.
\]  

(9)

We can use the variational ansatz \( \Psi \) in any dimension \( D \) to obtain a variational upper bound on the \( N \)=2n-body ground state energy and on the corresponding \( \xi \):

\[
E(2n) = \frac{2nD}{D+2} \xi_F \xi \leq \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}.
\]  

(10)

Clearly,

\[
\langle \Psi | H | \Psi \rangle = \sum_{P, P'} \langle \Phi(P) | H | \Phi(P') \rangle,
\]  

(11)

with a similar expression for \( \langle \Psi | \Psi \rangle \).

The local potential limit, say, \( r_0 \rightarrow 0 \) in the “square well” spherical potential

\[
V(\mathbf{r}) = -V_0 \Theta(\mathbf{r}_0 - |\mathbf{r}|)
\]  

(12)

implies for all dimensions \( D > 2 \) the following “selection rule” for non-vanishing \( \langle \Phi(P') | V_{i,j} | \Phi(P) \rangle \) matrix elements appearing when the 2n-body Hamiltonian (1) is substituted in Eq. (11) above.

Before going into the details of the variational calculations, let us quickly give the reader a glimpse of the final results derived below and their implication. The calculation detailed in this subsection illustrates that for the value of \( V_0 \) in Eq.(12) (the analog of \( g \) in Eq.(1)) which secures a single zero-energy bound, state we have a variational state (i.e. \( |\Psi\rangle \) of Eq.(9)) for which the corresponding energy \( E_{var} = 0 \). This result then implies (by Eqs.(6,10)) that \( \xi \leq 0 \).

For any \( V_{i,j} \) among the \( n^2 \) spin-up–spin-down potentials we have, for all \( D > 2 \) with a local \( V(\mathbf{r}) \) producing one zero energy bound state, the following relation

\[
\langle \Phi(P') | V_{i,j} | \Phi(P) \rangle = 0 \quad \text{if no } p(i) = j \text{ and no } p'(i) = j.
\]  

(13)

To prove this claim, we perform first (among the \( 2n \) \( d^D r_1 d^D r'_j \) integrations involved in evaluating the above matrix element) the integrals \( \int d^D r_i \int d^D r'_j \) over the coordinates \( r_i \) and \( r'_j \) appearing in the particular potential term \( V(r_i - r'_j) \) considered.

Both \( r_i \) and \( r'_j \) appear in the product \( \Phi(P) \) of Eq.(8) but, by assumption, in different \( \phi \) factors. The same holds for \( \Phi(P') \). Thus, the integration over \( r_i \) and \( r'_j \) is of the form,

\[
\int d^D r_i \int d^D r'_j | \phi(r_i - r'_p(i)) \overline{\phi(r_i - r'_{p'(i)})} | \phi(r_{p^{-1}(i)} - r'_j) | V(r_i - r'_j) | \phi(r_{p^{-1}(i)} - r'_j)| \overline{|\phi(r_{p^{-1}(i)} - r'_j)|} \overline{|\phi(r_{p^{-1}(i)} - r'_j)|}.
\]  

(14)

with \( p^{-1} \) the permutation inverse to \( p \). The condition for having one zero energy S wave bound state in the square well potential of (12) in the \( D=3 \) case is well known (see Fig.(1)),

\[
V_0 = \hbar^2 \left( \frac{\pi^2}{4} \right) \frac{1}{mr_0^2}.
\]  

(15)

By dimensional considerations, the same condition for one zero energy bound state holds in all dimensions \( D > 2 \) wherein the constant \( \pi^2/4 \) is replaced by some other, dimension dependent, numerical factor \( c_D \),

\[
V_0 = \hbar^2 \frac{c_D}{mr_0^2}.
\]  

(16)

In the general \( D \) dimensional problem, \( c_D \) of Eq.(16) is fixed by normalization of the zero-energy wavefunction \( \phi(r) \). In the appendix, we briefly present the solution to the a zero-energy bound state in a \( D \)-dimensional spherical potential well.

By changing variables \( (r_i, r'_j) \rightarrow (r_i, r_{i,j}) \) with \( r_{i,j} = (r_i - r'_j) \), the local \( V(\mathbf{r}_{i,j}) \) implies that \( r_i = r'_j \) in the arguments of all the four \( \phi \) factors appearing above which generally keep finite arguments and bound \( \phi \) values. Neglecting small variations of \( \phi(r) \) away from \( r \sim 0 \), the integral \( \int d^D r V(\mathbf{r}) \) over the \( D \) dimensional sphere of radius \( r_0 \) where the square well potential is non-vanishing yields the factor \( V_0 r_0^D \Omega_D \). This multiplicative factor is, by virtue of Eq.(16), proportional to \( [c_D r_0^{(D-2)}] \). In dimensions \( D > 2 \), this factor vanishes as \( r_0 \rightarrow 0 \) and, as claimed earlier, so does the
complete matrix element. This is not the case in dimensions $D < 2$ for which $\xi = 1$.

Next, we consider dimensions $D > 4$. In this case, the zero energy bound states

$$\Phi(r_1, r'_{p(i)}) = L^{-D/2} \phi(r_i - r'_{p(i)}),$$  \hspace{1cm} (17)

with (see the Appendix for details),

$$\phi(r_i - r'_{p(i)}) = A_\star |r_i - r'_{p(i)}|^{-(D-2)}$$

for $|r_i| \equiv |r_i - r'_{p(i)}| > r_0$;

and $\phi(r_i - r'_{p(i)}) \sim A_\star r_0^{-(D-2)}$ for $0 < |r_i| < r_0$,  \hspace{1cm} (18)

where $A_\star \approx (r_0^{(D-2)/2})$. Exact forms are provided by Eqs.(A3,A4, A8, A9). The comparison between Eq.(18) and the exact forms is provided in Eq.(A7). The scaling of the results with $r_0$ (which we will shortly obtain) becomes more transparent with the use of Eq.(18). With the incorporation of Eq.(A7) and its ensuing discussion, the results which we will obtain using Eq.(18) will further enable as a rigorous upper bound on the matrix value elements to be discussed. As seen from Eq.(18), the wavefunctions $\phi$ are strongly localized at $|r_i| \sim r_0$ implying stronger selection rules for non-zero matrix elements:

$$\langle \Phi(P')|\Phi(P)\rangle = 0 \text{ unless } P = P',$$  \hspace{1cm} (19)

and

$$\langle \Phi(P')|V(r_i - r'_{j})|\Phi(P)\rangle = 0 \text{ unless } j = p(i) = p'(i).$$  \hspace{1cm} (20)

Eq.(20) implies that also $\langle \Psi|H|\Psi\rangle$, the numerator of Eq.(10), has only diagonal contributions. Namely,

$$\langle \Phi(P')|H|\Phi(P)\rangle = 0 \text{ unless } P = P'.$$  \hspace{1cm} (21)

To illustrate Eq.(19), let us assume that $P$ and $P'$ differ minimally: $p(i) = p'(i)$ for all $i > 2$, but $p(1) = 1$, $p(2) = 2$ and $p'(1) = 2$, $p'(2) = 1$. The overlap in Eq.(19) is then

$$L^{-2D} \int d^D r_1 d^D r'_1 d^D r_2 d^D r'_2 \phi(r_1 - r'_1)\phi(r_2 - r'_2)$$

$$\times \phi(r_1 - r'_2)\phi(r_2 - r'_1) L^{-nD} \prod_{i,j>2} \int d^D r_i d^D r'_j \langle \phi(i, p(i))|\phi(i, p(i))\rangle. \hspace{1cm} (22)$$

Turning to Eq.(22), we assume that $p(i) = j$ but $p'(i) \neq j$ and prove that the matrix element $\langle P'|V_{pi}|P\rangle$ vanishes for $D > 4$. Recall that when also $p(i) \neq j$ we showed that this matrix element vanishes in all $D > 2$. Unlike that previous case, we have here only three (rather than four) $\phi$ functions in which $r_i$ and/or $r'_j$ appear. Factors of $L$ aside, the relevant two integrations on $r_i$ and $r'_j$ in the analog of Eq.(14) are now:

$$\int d^D r_i \int d^D r'_j V(r_i - r'_j)\phi(r_i - r'_{p(i)})\phi(r_{p(i)} - r'_j)\phi(r_i - r'_j)$$

$$= A_\triangle \Theta_0^2 \int d^D r |\Theta(r_0 - |r|)| (|\kappa r|)^{1-D/2} I_{p(i)}^{(D-1)}(\kappa r)|\phi(r_i - r'_{p(i)})|\phi(r_{p(i)} - r'_j)\phi(r_i - r'_j).$$  \hspace{1cm} (23)

where we invoke Eq.(A4). In particular, as seen from the appendix, the wavenumber $\kappa = c_D^{1/2}/r_0$. In Eq.(23), we employ, once again, $p^{-1}$ for the inverse permutation, $r = r_i - r'_j$, is the argument of the square well potential, and $\phi(r_i - r'_j) = \phi(r)$. 

The last line of Eq.(22) denotes a normalized integral (equal to one). In the first integral over the 4 variables $\{r_1, r'_{1,2}\}$, the number of integration variables is equal to the number of wavefunctions $\{\phi(r_i - r'_j)\}$ appearing in the integrand. For each of the two particle wavefunctions $\phi(r_i - r'_j)$, we insert Eq.(18) (or the exact Eqs.(A3,A4) derived within the appendix) with $A_\triangle \approx r_0^{(D-2)/2}$. Insofar as scaling with $r_0$ is concerned, all integrals over products of wavefunction forms of Eq.(18) multiplying $A_\triangle$ amount to product of either integrals of the type $I_\triangle = \int_{r|>r_0} d^D r |r|^{2-D}$ or of the form $I_\triangle = \int_{|r|<r_0} d^D r$. Constant factors aside, both $I_\triangle$ and $I_\star$ scale as $r_0^{(D-4)/2}$. The four normalization prefactors of $A_\triangle$ (with $A_\triangle \approx r_0^{2(D-4)/2}$), originating from the four factors of $\phi$ in the top two lines of Eq.(22), lead to an additional factor of $r_0^{2(D-4)}$ in tow. Thus, in the final analysis, when the integrals are segregated into all possible terms for $|r_i - r'_j| > r_0$ and for $|r_i - r'_j| < r_0$ and Eq.(18) or Eqs.(A3, A4) are inserted, we find that all terms scale as $A_\triangle \approx r_0^{2(D-4)}$ as $r_0 \to 0$. This signals that the factor in the first two lines of Eq.(22) vanishes as $r_0 \to 0$ and thus so does the entire overlap of Eq.(19). We can readily verify that for larger mismatches between $P$ and $P'$ the overlap vanishes as a higher power of $r_0$. Now, in the diagonal case, with $p(1) = 1$ and $p'(2) = 2$ the product of the four normalization factor cancels and $\langle \Phi(P')|\Phi(P)\rangle = 1$. [16]
In what briefly follows, to flesh out more crisply the simple scaling form of this term, we may replace the exact Bessel function form of Eq.(A4) and instead invoke Eq.(18) to replace the last factor \( \phi(r) \) for \( r < r_0 \) in the upper line of Eq.(23). The result which we will obtain in this fashion will go unchanged if we employ the exact Bessel function form of Eq.(23), see [17]. With the insertion of Eq.(18), the \( d^D r \) integration of Eq.(23) yields

\[
V_0 \int_0^{r_0} d^D r \left[ \frac{\hbar^2}{2m} (2D-2) \right] = \Omega_D V_0 \frac{\hbar^2}{r_0^2} \rightarrow 0 \quad \text{for } D > 4,
\]

in the limit \( r_0 \rightarrow 0 \). Here, the definition of \( c_D \) was invoked from Eq.(16). The peculiar form given in the square braces of Eq.(24) follows from Eq.(18) with the approximate \( A_\infty \approx (r_0^{(D/2)-2}) \). The incorporation of the exact Bessel function form of Eq.(A4) in Eq.(23) whose derivation is detailed in the appendix does not alter this simple result [17]. This concludes the proof of Eq.(20).

\[
\langle \Phi(P')|H_{i,j}|\Phi(P) \rangle = \langle \phi(1,p'(1)) \ldots \phi(n,p'(n)) | V_{i,j} - \frac{\hbar^2}{2m} (\nabla_i^2 + \nabla_j^2) | \phi(1,p(1)) \ldots \phi(n,p(n)) \rangle. \tag{26}
\]

This holds for each \( \Phi(P) \) and, hence, for the full Slater orbital ansatz of Eq.(9) \( \Psi \) in \( D > 4 \) dimensions,

\[
H|\Psi\rangle = E(2n) = -n\epsilon|\Psi\rangle. \tag{29}
\]

Thus, the total energy of the system is just that of \( n \) independent Bose-Einstein condensed dimers. When the binding energy \( \epsilon \rightarrow 0 \) we have \( E(2n) \rightarrow 0 \) and for the variational orbital Slater determinant of Eq.(9), we find \( \xi_{\var}(D > 4) = 0 \) as claimed. By the standard variational theorem, this proves that for continuous \( D \),

\[
\xi(D > 4) \leq 0. \tag{30}
\]

The exact variational result fortifies the conclusion arrived at earlier (subsection IV B 1), with Eq.(8) in particular) via normalization considerations. In the final analysis, normalization was present in our slightly elaborate variational bound and ultimately dictated the scaling form of our expressions with \( r_0 \) (see, e.g., Eq.(22), [16]) as \( r_0 \rightarrow 0 \).

V. HEURISTIC CONSIDERATIONS FOR \( \xi(D = 3) \)

The extension of the problem to arbitrary continuous dimension \( D \) allowed us to firmly establish that \( \xi = 1 \) in \( D \leq 2 \) and \( \xi = 0 \) in \( D \geq 4 \) (with the particular point \( D = 4 \) accessed by general normalization conditions; our rigorous variational bound \( \xi(D > 4) \leq 0 \) held for all continuous \( D > 4 \). These
results suggest that in a lowest order $\epsilon$ expansion interpolating between these two limits, $\xi(D = 3) \approx 1/2$. [Or, if the upper bound in the variational inequality for all continuous large $D$, $\xi(D > 4) \leq 0$ is not saturated for the marginal $D = 4$, that, more generally, $\xi(D = 3) \leq 1/2$.] This is, remarkably, not far from the results obtained by very intensive numerical work [6] (which led to an upper bound of $\xi(D = 3) \approx 0.44$). Unfortunately, we have not been able to attain direct potent bounds on the three dimensional problem which are close to the numerically attained values. In the current section, we attack the harder $D = 3$ problem by a heuristic approach. This approach, although imprecise, may shed light on some of the observed physics in three dimensions. Similar to the simple minded dimensional interpolation result it, too, suggests that $\xi(D = 3) \approx 1/2$. As an additional bonus, this allows for a heuristic argument for even-odd oscillations numerically observed.

Unlike the normalization of the zero energy bound state, which for $|r| > r_0$ is uniform in $|r| = |r_i - r_j|$, the kinetic energy,

$$\int d^d r (\nabla \phi(r))^2 = \int d^d r A^2 / |r|^2,$$  \hspace{1cm} (31)

is mostly concentrated at small $|r| \sim r_0 << d$ values. In the last equality of Eq.(31), we inserted the well known $(D = 3)$ zero-energy S-wave wavefunction form outside a potential well, $\phi = \frac{1}{|r|^2}$. As a consequence of this concentration of kinetic energy, a zero energy bound state of a mixed $(i, j')$ pair, can manifest over any smooth background function $B$ of all other variables by a $\frac{1}{|r_i - r_j'|}$ enhancement at distances $|r_i - r_j'|$ smaller than typical particle spacing. (Due to antisymmetry, the $i^{th}$ spin up atom is equally likely to bind with any one of the $n$ down spin atoms at $r_j'$, with $j = 1, ..., n$.)

This is indeed the case for the wave functions serving as the staring point of the above MC where correlations in mixed pairs are introduced via a Jastrow product $\Psi$,

$$\Psi = B \times J \equiv B \prod_{j=1 \ldots n} \phi(|r_i - r_j'|),$$ \hspace{1cm} (32)

where the background $B$ of free Fermion Slater determinants or BCS form accounts for the antisymmetrization.

The other $(n-1)$ factors of the form $\frac{1}{|r_i - r_j'|}$ with $k$ different from $j$ still allow for $\Psi \sim \frac{C}{|r_i - r_j'|}$ for $|r_i - r_j'| << d$. Thus, let the remaining $(n-1)$ down spin atoms form a cubic lattice of spacing $d$, the triply periodic product, $\prod_{j=1 \ldots n-1} \phi(|r_j' - r_i|)$, is then invariant under the point symmetry group of the simple cubic lattice. Its finite extrema are at the centers of the n cubes (each of volume $d^3$) and C varies slowly for $|r| << d$.

This suggests (yet does not justify) the following ad-hoc approach which yields $\xi = 1/2$. The potentials $V(|r_i - r_j'|)$ involve atom pairs yet the kinetic energy is a sum over single atoms:

$$\sum_{I=1 \ldots N=N} \frac{p_I^2}{2m} = \sum_{i=1 \ldots n} \frac{p_i^2}{2m} + \sum_{j=1 \ldots n} \frac{(p_j')^2}{2m}.$$  \hspace{1cm} (33)

We formally associate kinetic energies with pairs by using the identity:

$$\sum_{I=1 \ldots N=2n} \frac{p_I^2}{2m} = \sum_{I,J=1 \ldots N} \frac{1}{2m(N+1)} \sum_{I < J=1 \ldots N} (p_I - p_J)^2,$$  \hspace{1cm} (34)

where $P^2_{\text{tot}} = \sum p_j^2 = 0$ was subtracted cancelling all $I < J$ terms $(p_I \cdot p_J)$. Next, we separate the contribution to the Hamiltonian of same (up-up, down-down) and mixed spin pairs with the potentials included in the second term:

$$H = H_{\text{same}} + H_{\text{mixed}}$$

$$= \frac{1}{2m(N+1)} \sum_{i \leq l = 1 \ldots n} (p_i - p_l)^2$$

$$+ \frac{1}{2m(N+1)} \sum_{j < k = 1 \ldots n} (p_j' - p_k')^2$$

$$+ \sum_{i,j=1 \ldots n} \frac{(p_i - p_j')^2}{2m(N+1)} - gV(r_i, r_j').$$  \hspace{1cm} (35)

For $g = 0$ the kinetic terms in $H_{\text{same}}$ and $H_{\text{mixed}}$ are equal up to $1/N$ corrections.

Next, we note that if the following assumptions are made:

(i) Just as for isolated up down pairs also in the N-body ground state $\Psi$, the attractions between different atoms cancel the kinetic energy of the relative motion, i.e., $\langle \Psi | H_{\text{mixed}} | \Psi \rangle = 0$, and that

(ii) turning on the coupling $g$ does not change the expectation value of $H_{\text{same}}$, then:

$$\langle E/N \rangle |_{N=even} = \frac{(n-1)}{(2n-1)} \frac{3}{5} \varepsilon_F$$

$$\approx \frac{1}{2} \left[ 1 + \frac{1}{N} \right] \frac{3}{5} \varepsilon_F.$$  \hspace{1cm} (36)

For odd $N$, say $n+1$ spin up and $n$ spin down atoms, only $n = N/2 - 1/2$ bound pairs can form. The decrease of potential attraction energy by $(N-1)/N$ produces a “gap”

$$\frac{E}{N} |_{N=2n+1} - \frac{E}{N} |_{N=2n} \approx \varepsilon_F,$$  \hspace{1cm} (37)

consistent with the finding of the MC calculations. Furthermore,

$$\xi \rightarrow 1/2 \quad \text{(as $N \rightarrow \infty$)},$$ \hspace{1cm} (38)

which is barely consistent with the variational bound $\xi < 0.43 - 0.45$ from the above calculations.[18]

VI. CONCLUSIONS

In conclusion, we examined an extension of the BCS to BEC crossover problem to arbitrary dimension $D$. We report new results on the ground state energy per particle at the crossover point by employing direct variational bounds in
high dimensions and by considering the consequences of localization in low dimensions. In particular, we find that the ground state energy per particle at the onset of the BCS to BEC crossover is zero (or negative) in all dimensions $D \geq 4$ while it is the energy of a free Fermi system in all dimensions $D \leq 2$. The interpolation of these bounds to the physical three dimensional problem leads to an energy per particle which is half that of the free fermion energy and is close to current numerical results. We outlined a simple heuristic argument for the same result which further mandates even-odd variations which are indeed seen numerically.

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APPENDIX A: THE ZERO ENERGY BOUND STATE PROBLEM IN A D-DIMENSIONAL SPHERICAL POTENTIAL WELL

Here, we provide the solution of the zero energy bound state problem in $D$ dimensions for the spherical potential well of Eq.(12) wherein the depth of the well ($V_0$) is tuned to get a zero-energy bound state. The solution is a straightforward extension of the standard $D = 1, 2, 3$ dimensional spherical potential well problems. In these, without any angular dependence, in the the “S-wave” representation (i.e. the scalar (“$l = 0$”) representation of the $SO(D)$ rotation group), the $D$-dimensional Laplacian is $\nabla^2 = [\frac{d^2}{dr^2} + \frac{D-1}{r}\frac{d}{dr}]$. This appendix explicitly illustrates how the numerical constant $c_D$ of Eq.(16) may be determined (from the implicit Eq.(A8)). Its results further allow us to compare the approximate form of Eq.(18) introduced within the text to allow a clear understanding of the scaling form of the overlap integrals with the exact form of $\phi(r)$ (Eqs.(A3,A4)). In the aftermath, it will be shown that the incorporation of the exact functional from does not change the scaling results derived in the main text (following Eq.(18)).

We proceed with the solution of the translationally invariant problem specified by the spherical potential well of Eq.(12). By translational invariance of the center of mass, the two body wavefunction

$$\tilde{\phi}(x,x') = L^{-D/2}\phi(r)$$

(A1)

with $r \equiv x' - x$. In the potential-free region ($r > r_0$), the wavefunction $\phi$ satisfies a single particle Schrödinger equation with a reduced mass $\mu = m/2$,

$$\frac{d^2}{dr^2}\phi(r) + \frac{D-1}{r}\frac{d}{dr}\phi(r) + \kappa^2\phi(r) = 0,$$

(A2)

with $\kappa = 0$. Within the spherical potential well ($r < r_0$), we have Eq.(2) with $\kappa^2 = (mV_0)/\hbar^2$. We immediately find that

$$\phi(r > r_0) = A_+ r^{2-D},$$

(A3)

while within the potential well

$$\phi(r < r_0) = A_- [\frac{1}{2}J_{\frac{D}{2}-1}(\kappa r)],$$

(A4)

with $\kappa$ and the constant prefactors $A_+$ and $A_-$ determined by continuity at $r = r_0$ and global normalization. Here, $J_{\frac{D}{2}-1}$ is a Bessel function of order ($\frac{D}{2}-1$). (Inserting $J_{\frac{D}{2}}(\kappa r) = [(\kappa r)^{-1/2}\sin \kappa r]$, the pertinent three dimensional result, illustrated in Fig.(1), is recovered.) Continuity at $r = r_0$ restraints

$$\phi(r < r_0) \approx A_+ r_0^{2-D}.$$  

(A5)

For small $r$ (i.e. $r \rightarrow 0$), employing the asymptotic form of the Bessel functions, we find that

$$\phi(r \rightarrow 0) = \frac{A_-}{\Gamma(\frac{D}{2})2^{\frac{D}{2}-1}}.$$  

(A6)

Anywhere within the potential well ($r < r_0$), the wave function

$$\phi(r < r_0) = f(\frac{r}{r_0}) A_+ r_0^{2-D},$$

(A7)

with $f(0 \leq z \leq 1)$ a bounded function satisfying $f(1) = 1$ and $f(0) = \frac{A_-}{\Gamma(\frac{D}{2})2^{\frac{D}{2}-1}}$. Within the text following Eq.(18), we set $f$ to be one and we attained vanishing overlaps in Eq.(24) in the limit $r_0 \rightarrow 0$. The incorporation of the more explicit, yet bounded, $f(z)$ given by Eq.(A4) does not alter this result. Formally, our results derived in the text can be made rigorous by deriving an upper bound which differs from the results given in Eq.(24) by a factor of $|f|_{\text{max}}$, the maximal value of $|f|$. As Eq.(24) vanishes by simple scaling, the incorporation of a finite factor leads to a vanishing upper bound, proving that Eq.(23) vanishes in the limit of small $r_0$. Although inconsequential for this bound (all that matters is its bounded norm), the prefactor $f(r/r_0)$ is everywhere positive as the zero energy ground state is nodeless and of uniform sign.

For completeness, we now outline the general solution. Matching the two functional forms of $\phi(r)$ and their derivatives at $r = r_0$ (and simplifying with the aid of the standard Bessel function recursion relations) leads to the implicit equation

$$1 = \frac{D}{2}J_{\frac{D}{2}-1}(\kappa r_0)$$

$$= \frac{1}{2}(\kappa r_0)J_{\frac{D}{2}}(\kappa r_0) + J_{\frac{D}{2}-2}(\kappa r_0)).$$

(A8)

The solution of Eq.(A8) enables a determination of $\kappa$ and thus of the spherical potential well $V_0$ and the constant $c_D$ in Eq.(16) which ensures a zero-energy “S-wave” state in $D$ dimensions. The amplitudes $A_+$ and $A_-$ are then determined by

$$\frac{A_-}{A_+} = \frac{r_0^{2-D}}{(\kappa r_0)^{1-\frac{D}{2}} J_{\frac{D}{2}-1}(\kappa r_0)},$$

(A9)

in conjunction with the global normalization of $\phi(r)$. Normalization demands that, up to dimension dependent numerical constants, $A_+ \approx r_0^{D/2-2}$ and consequently $A_- \approx r_0^{-D/2}$. 


[1] M. H. Andersen, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science 269, 198 (1995); K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. 75, 3969 (1995); C. C. Bradley, C. A. Sackett, J. J. Tollett and R. G. Hulet, Phys. Rev. Lett. 75, 1687 (1995); C. C. Bradley, C. A. Sackett, and R. G. Hulet, Phys. Rev. Lett. 78, 985 (1997).

[2] C. A. Regal, M. Greiner and D. S. Jin, Phys. Rev. Lett. 92, 040403 (2004); M. Zwierlein, et al., Phys. Rev. Lett. 92, 120403 (2004).

[3] R. B. Diener and T-L. Ho, Phys. Rev. Lett. 94, 090402 (2005).

[4] K. G. Wilson, Phys. Rev. Lett. 28, 548 (1972); K. G. Wilson and M. E. Fisher, Phys. Rev. Lett. 28, 240 (1972); K. G. Wilson and J. Kogut, Phys. Rep. 12, 75 (1974); J. Zinn-Justin, Quantum Field Theory and Critical Phenomena, Oxford University Press (1989).

[5] G. F. Bertsch, “Challenge Problems in Many-Body Physics”, http://www.phys.washington.edu/~mbx/george.html (1998).

[6] J. Carlson, S.-Y. Chang, V. R. Pandharipande, and K. E. Schmidt, Phys. Rev. Lett. 91, 050401 (2003).

[7] G. A. Baker, Jr., Phys. Rev. C 60, 054311 (1999).

[8] The hierarchy of scales, $a >> d >> r_0$, which is implicit here may not suffice to guarantee the same universal expression as $E/N$ could also depend on $d^2/\langle a r_0 \rangle$.

[9] A. J. Legget, in Modern Trends in the Theory of Condensed Matter, edited by A. Pekalski and R. Przystawa (Springer-Verlag, Berlin, 1980); J. R. Engelbrecht, M. Randeria, and C. sa de Melo, Phys. Rev. B 55, 15 153 (1997).

[10] Landau, Lifshitz, Quantum Mechanics (Pergamon Press), third edition (1977).

[11] E. H. Lieb and M. de Liano, J. Math. Phys. 19, 860 (1978); M. Randeria, J.-M. Duan, and L.-Y. Shieh, Phys. Rev. Lett. 62, 981 (1989).

[12] W. Metzner and D. Voldhardt, Phys. Rev. Lett. 62, 324 (1989).

[13] J. W. Steel, arXiv:nucl-th/0010066 (2000).

[14] T. Schaefer, C-W Kao, and S. R. Cotanch, arXiv:nucl-th/0504088 (2005)

[15] E. Abrahams, P. W. Anderson, D. C. Licciardo, and T. V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).

[16] In this case, we recover (by definition) the normalization integral. For a single up/down spin pair ($x, x'$) this (with the aid of Eqs. (A3, A4)) is of the forms

$$I_\geq = A_\geq^2 L^{-D} \int d^D R \int_{r > r_0} d^D r \frac{d^2 r}{r^{(D - 2)}}$$

or

$$I_\leq = A_\leq^2 L^{-D} \int d^D R \int_{r < r_0} d^D r \frac{d^2 r}{(kr)^{D - 2}}.$$  \hspace{1cm} \text{(A10)}$$

with $R = (x + x')/2$ the center of mass, whose integration cancels identically against the volume factors of $L^D$. Due to the higher power of $r$ in the denominators (viz a vis the integrals in Eq.(22)), a lower power of $r_0$ is attained in $I_\geq, I_\leq$ with respect to their permuted counterparts (see below). In $I_\geq$, the scaling is that of $A_\geq^2 r_0^{-D}$ which mandates the relation $A_\geq \approx r_0^{D/2 - 2}$ appearing in the text (Eq.(18)). The lower power of $r_0$ appearing here in the normalization integrals when no permutations are performed relative to the power of $r_0$ resulting from any integral appearing with a permutation (i.e. the scaling of of the integrals $I_\geq$ of Eq.(A10) relative to that of $I_\geq$ and $I_\leq$ defined following Eq.(22)) ensures that all integrals of the type of Eq.(22)) vanish in the $r_0 \to 0$ limit.

[17] Indeed, this may be rigorously proven by replacing the positive function $f(z)$ defined via Eq.(A7), (with the scaled radial coordinate $z \equiv r/r_0 \sim kr$), by its maximal value (denoted henceforth by $f_{\text{max}}$) in the interval $[0, 1]$ to attain an upper bound on the integral of Eq.(23). This upper bound differs from the result shown in Eq.(24) by a factor $f_{\text{max}}$. As $f_{\text{max}}$ is finite, the vanishing of Eq.(23) cannot be avoided in a spherical well of small radial extent ($r_0 \to 0$).

[18] This feature motivated the extension to unequal numbers of spin-up and spin-down atoms leading to a new exact and interesting result for the asymmetry energy, T. D. Cohen, Phys. Rev. Lett. 95, 120403 (2005) (arXiv:cond-mat/0505080)