Three-Body Bound States on a Lattice

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The theory of three-body bound states for particles moving on a lattice and interacting with attractive two-body pointlike potentials is presented. The applications are to bosons, fermions (no three-body bound states are found), and magnons. When a three-body bound state forms in three dimensions, it does so discontinuously. Thus there is a maximum size for the three-body bound state, of approximately two lattice constants. Some of the various analyses are relevant to magnetism and superconductivity.

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In this Letter we report on our study of three identical particles with attractive pointlike two-body interactions of strength U, on a lattice in two and three dimensions (2D and 3D.) We find several interesting and surprising results.

In the case of three bosons in 3D, there is a jump in kinetic energy at the dissociation threshold, implying a finite radius for the bound state at threshold. This phenomenon does not occur in 2D or 1D, nor with one or two particles in any dimension $d \leq 4$, and is therefore nonintuitive.

For three fermions, the Pauli principle requires the wave function to be antisymmetric with respect to interchange of at least two of them, depending on their total spin. For $S=\frac{3}{2}$ the wave function is totally antisymmetric and there is of course no interaction. Even for $S=\frac{1}{2}$, when there *is* an interaction, the three particles are unbound with respect to breakup either into a bound pair with $S=0$ and a free third particle, or into three free particles. Upon finding that there is never a three-fermion bound state, whether in 3D or 2D, we conclude that the Cooper pair is truly fundamental in the theory of superconductivity.[1] Our work in progress[2] also suggests that in 2D, four-fermion states are unstable against breakup into pairs. It should be noted that 2D is the analog of Cooper's problem as the density of one-particle states is essentially constant. Two-body bound states form at arbitrarily weak values of the coupling constant, yet three-body bound states are totally missing for fermions.

Finally, our results can be used to estimate the limits of validity of spin-wave theory as applied to the anisotropic Heisenberg ferromagnet in 3D when $J_z \geq J_x = J_y$. We consider the *long-wavelength* magnons which predominate at low T. At $J_z > 1.43 J_x$, we find a three-magnon bound state to be stable against all breakups. At $J_z > 1.67 J_x$, a two-body bound state can also form. Thus, once J_z exceeds $O(1.5 J_x)$, the very concept of magnons as elementary excitations of the ferromagnet ceases to be valid at all but the lowest temperatures, and one must deal with the bound complexes. Except in 1D there has been very little research into this topic, which appears to have interesting consequences.

We proceed to outline our procedures and give the results graphically. Divers extensions to $n>3$ particles and to repulsive forces are detailed in some companion articles[2] and in the Ph.D. thesis of one of us (S.R.).

First, consider three spinless bosons on a lattice. The "kinetic energy" (KE) of an individual particle comes from hopping from site to site, the potential energy (PE) is the result of two-body interactions. For simplicity, we take the interaction to be $-U$ for any pair of particles on the same site and zero otherwise, limiting the hopping matrix elements to connect nearest-neighbor sites on a square lattice (2D) or simple cubic lattice (3D). The bound-state eigenfunction must take the form

$$\Phi = \sum M(k_1 k_2 k_3) a_{k_1}^{+} a_{k_2}^{+} a_{k_3}^{+} |0\rangle \quad (1)$$

with M a totally symmetric function of its arguments. Total momentum $P = k_1 + k_2 + k_3$ is conserved (to within a reciprocal-lattice vector), and Schrödinger's equation $H\Phi = -W\Phi$ is satisfied by defining

$$\hat{S}(k_1) \equiv \frac{1}{N} \sum_q M(k_1, k_2+q, k_3-q) \quad (2)$$

from which it follows directly that

$$M(k_1 k_2 k_3) = U \frac{\hat{S}(k_1) + \hat{S}(k_2) + \hat{S}(k_3)}{\tau(k_1 k_2 k_3)} \delta(P - k_1 - k_2 - k_3) \quad (3)$$

where $\tau \equiv W + e(k_1) + e(k_2) + e(k_3)$, W is the binding energy with respect to free particles, and $e(k)$ are the individual kinetic energies measured relative to the bottom of the band,

$$e(k) = 3 - \cos k_x - \cos k_y - \cos k_z .$$

In 2D, the 3 is replaced by 2 and $\cos k_z$ is missing.

The basic integral equation is obtained by substituting (3) into (2) and replacing sums by an integral over the Brillouin zone in the usual way. The similarity transformation

$$S(k) = \hat{S}(k)[1 - UI(k)]^{-1/2}, \quad (4)$$

with $I(k)$ a variant of Watson's integral,

$$I(k) \equiv \frac{1}{N}\sum_q \tau^{-1}(k, q, P - k - q), \quad (5)$$

transforms the kernel in the basic integral equation into a symmetric form $K(k|q)$, i.e., we are led to solve

$$S(k) = (2\pi)^{-d}\int_{-\pi}^{+\pi} d^d q K(k|q) S(q) \quad (6)$$

in d dimensions, where the compact, symmetric kernel

$$K(k|q) = 2U\{[1 - UI(k)][1 - UI(q)]\}^{-1/2}\tau^{-1}(k, q, P - k - q) \quad (7)$$

is a positive function, invariant under the cubic group O_h. At $P = 0$, the locus of $1 - UI(0) = 0$ [note: $I(k)$ is a function of W] and the horizontal axis $W = 0$ form the boundaries of the two-body and three-body continua, respectively, intersecting at a "tricritical point" $U_c(2)$. The three-body solutions must lie below this.

To obtain a solution, one expands $S(k)$ in (6) in Fourier "kubic harmonics"[3] and solves a secular determinant, the elements of which are six-dimensional integrals. All standard techniques for evaluating such integrals, including the Monte Carlo method, turn out inadequate—if the number of points is small enough to be usable in our iterative solution of the secular equation, the accuracy is unacceptable. And if the accuracy is within the acceptable 1% range, the length of the computation on our available computer must be measured in months. Fortunately, the unconventional Korobov-Hlawka number-theoretic "quasi Monte Carlo" method[4] devised for periodic functions, such as our S, I, and K functions, delivers the desired accuracy, with a few thousand points only, for integrations of up to nine dimensions.

The results for three identical bosons are shown in Fig. 1. There exists only one strongly bound, 1s type, bound state, with threshold at $U_c(3) = 2.60$. The curve $W(U)$ for this bound state is asymptotic to a line of slope 3 indicated by dashes in the figure. The three-body bound state appears before the two-body bound-state threshold at $U_c(2) = 3.96$ and lies well below the two-body continuum, as shown in the figure. Using $S(k)$ we calculate E_K, shown in Fig. 2, and by Feynman's theorem,

$$dW/dU = (W + E_K)/U, \quad (8)$$

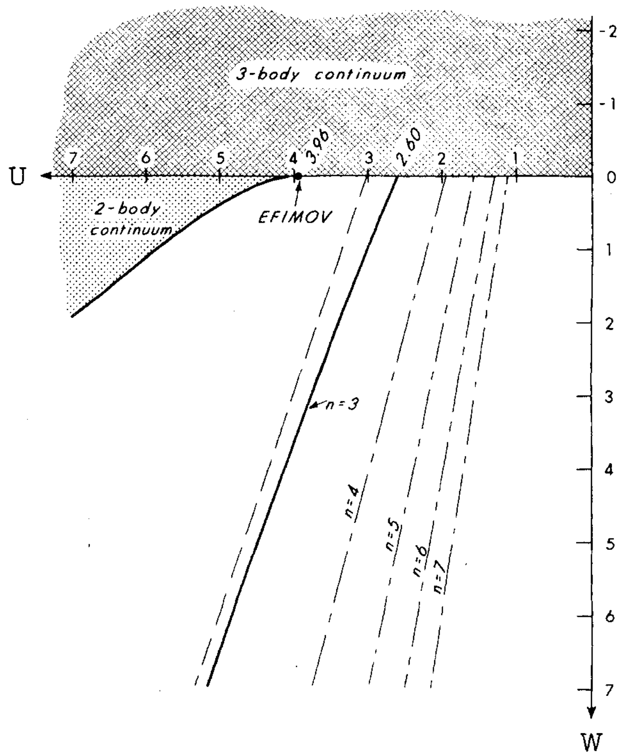

FIG. 1. Binding energy W vs strength U of attractive two-body potential in 3D. The shaded three-body continuum represents free particles, the dotted two-body continuum represents two-particle bound states with one (or more) free particle. The fundamental three-boson bound state, labeled $n = 3$, is asymptotic to the straight dashed line of slope 3. The excited bound state and "Efimov states" all lie within a point of radius of order 10^{-1} at the tricritical point $U_c(2) = 3.96$. There are no three-fermion bound states. The curves labeled $n = 4$–7 are estimated binding energies for $n = 4$–7 bosons, with $U_c(n)$ estimated as $7.92/n$ by a generalized Stenchke inequality (Ref. 5), with $U_c(n) \to 0$ as $n \to \infty$.

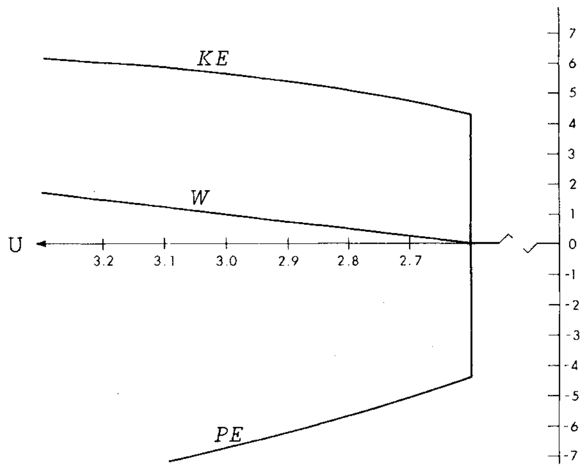

FIG. 2. As U is increased (note break in horizontal scale) the three-boson threshold is approached at $U_c(3) = 2.60$. The KE and PE both jump discontinuously at this point, while their algebraic sum (W) grows continuously from zero. The finite KE implies a finite radius $\lesssim 2$ lattice constants for the bound state at threshold, decreasing to 0 with increasing U.

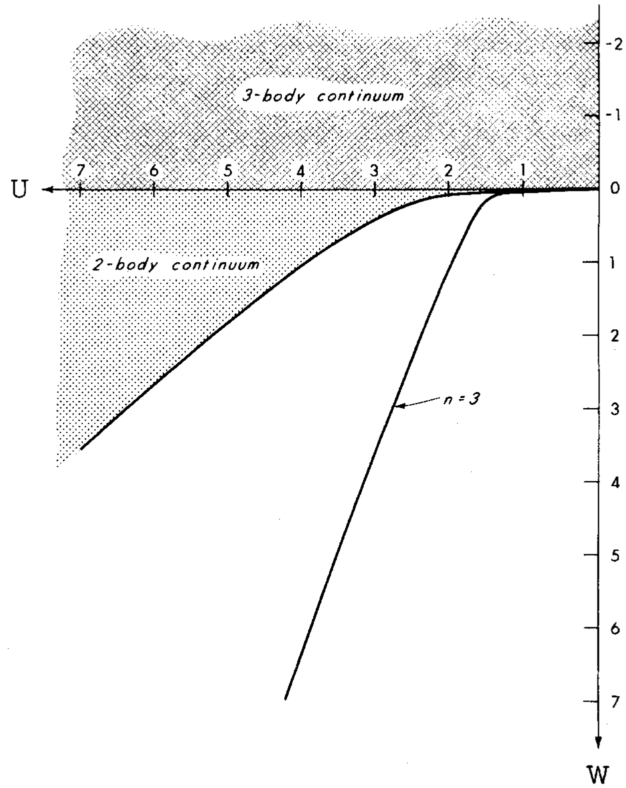

FIG. 3. Same as Fig. 1 in two dimensions. However, the curves for $n \geq 4$ have all been omitted as *all* thresholds $U_c(n) = 0$. There are *no* Efimov states in 2D, nor any three-fermion bound states.

we confirm that $dW/dU \neq 0$ at $U_c(3)$. Thus, for $U \lesssim U_c(3)$, E_K and V are both zero in the ground state, whereas for $U \gtrsim U_c(3)$, E_K and V are both finite. We estimate the *maximum* radius of the three-body bound state to be $\lesssim 2$ lattice constants. The discontinuity in E_K at threshold is shown in Fig. 2.

Using Stenchke's inequality[5] $W_3(U) \geq 2W_2(\frac{3}{2}U)$, where W_n is the binding energy for n particles, as an *estimate*, we have $U_c(3) \approx \frac{2}{3}U_c(2)$. Strictly speaking, this estimate applies to a continuum theory only, but with $U_c(2) = 3.96$ the calculated lattice value, it predicts $U_c(3) = 2.64$, correct to 1.5%. A generalized inequality enables us similarly to estimate,

$$U_c(n) \approx (2/n)U_c(2). \tag{9}$$

Coupling this with the obvious strong-coupling asymptotic properties of the bound states as $U \to \infty$, we obtain the estimated binding energies for $n = 4, 5, \ldots$ particles shown as dot-dashed curves in Fig. 1.

A remarkable feature of the three-body problem is the infrared divergence in $K(k|q)$ near $U_c(2)$. First noted by Efimov,[6] this singularity is responsible for an *infinite* number of bound states, all s states with increasing radial quantum numbers. On the scale of Fig. 1, *all* the Efimov states lie within a dot of radius 10^{-1} at $W = 0$, $U_c(2)$! The 2s bound state found in continuum studies of the three-body problem by Amado and others[7] has also collapsed in our lattice theory, merging with Efimov's states within the aforementioned barely visible dot. While we suspect that Efimov-like states also exist for $n = 4, 5, \ldots$ particles on the lattice, we have not pursued what appears to be a purely academic point.

The estimates for two and three magnons in the anisotropic Heisenberg model quoted in the introductory remarks follow directly once we make the identification

$$U \to 2d(J_z - 1) \tag{10}$$

where d is the number of dimensions and $J_x = 1$.

The above calculations repeated on a 2D lattice show $U_c(2) = U_c(3) = \ldots = U_c(n) = 0$ and yield a unique 1s-like three-boson bound state shown in Fig. 3. As is well known,[7] there are no Efimov states in 2D. We find no excited bound states whatever for $n = 3$ particles, and do not suspect the existence of any for $n > 3$.

Turning finally to *fermions*, we can dispose of the totally antisymmetric space functions, which are noninteracting for point interactions. The two-column Young tableau representation of spin $S=\frac{1}{2}$ states results in an equation similar to Eq. (6), with K now given by

$$K(k|q)=-U\{[1-UI(k)][1-UI(q)]\}^{-1/2}\tau^{-1}. \quad (11)$$

Because of the change in sign of the kernel, the only possible solution is $2p$ like. Our numerical studies show conclusively that no such solution exists in 2D or in 3D. Thus, the three-fermion state is unstable. The basic feature which relates a lattice in 2D with the theory of superconductivity in 3D is the relatively constant, finite, one-particle density of states in the relevant ranges of energy. Thus, any number of interacting quasiparticles in the neighborhood of the Fermi energy of a metal in 3D may be, for some purposes, modeled by an equal number of interacting particles on a 2D lattice. We believe that the lack of three-body (and, we believe, four-body) bound states in 2D shows that Cooper[1] most properly selected the electron singlet pair as the basic unit of charge in a superconductor: Complexes with $3e$, $4e$, etc., are unstable against breakup into a suitable number of pairs. This fact was intuitively grasped by BCS in their variational solution of the N-body problem.

In relating the continuum literature[7] to the present discrete model, one must take various limits.[8] The details will be discussed at length elsewhere,[2] as well as the exciting applications to the study of repulsive forces in order to obtain the ground state of the $S=\frac{1}{2}$ XY model in 2D and 3D.

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[8] A correspondence between our discrete model and the potential $V_{kk'}=gf(k)f(k')$ in the continuum models is achieved by taking $f(k)=(k^2+\beta^2)^{-1}$ in the appropriate limits: $\beta\to\infty$, $g\to 0$ such that $g\beta^{-4}=U$, with $\mu/\beta=U$, $U_c(2)=\beta^{-1}$ and the scattering length

$$a_{sc}=\{[1/U_c(2)]-1/U\}^{-1}=\beta^{-1}\mu/(1-\mu).$$