The few-body problem on a lattice

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The author explores some of the inherent simplifications of "quantum lattice physics." He distinguishes between fermions and bosons and analyzes the n-body problem for each, with $n=1,2,3\ldots$ typically a small number. With delta-function (zero-range) interactions, the three-body problem on a lattice is manageable, and some results can even be extrapolated to $n\geq 4$. Such calculations are not limited to one dimension (where the well-known Bethe ansatz solves a number of n-body problems). On the contrary, studies cited are mainly in three dimensions and actually simplify with increasing dimensionality. For example, it is found that bound states of $n\geq 3$ particles in $d\geq 3$ dimensions are formed *discontinuously* as the strength of two-body attractive forces is increased, and are therefore always in the easily analyzed "strong coupling limit." In the Appendix, an exactly solved example from the theory of itinerant-electron magnetism illustrates how a rigorous solution to the few-body problem is capable of yielding information concerning the N-body problem.

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INTRODUCTION

The notion of particles "hopping" on discrete space lattices dates back to Bethe's treatment of one-dimensional magnetic materials (Bethe, 1931) or, in a different context, to the invention of Wannier functions (Wannier, 1937). In the former case, the stationary states $\mid\psi\rangle$ are eigenstates of a Heisenberg Hamiltonian H given by

$$H=-\tfrac{1}{2}J_x\sum(S_n^+S_{n+1}^-+\text{H.c.})-J_z\sum S_n^ZS_{n+1}^Z\ .$$

The reference "saturated ferromagnetic state" denoted $\mid 0\rangle$ consists of all spins "down" (i.e., for each n, $S_n^Z\mid 0\rangle=-S\mid 0\rangle$). It thus belongs to $M_Z=-Ns$ for N spins; together with the state with $M_Z=+Ns$, to which it is related by a 180° rotation, this is the state of maximum total spin. The next highest spin magnitude is $M_Z=-Ns+1$. Eigenstates that have this quantum number are plane-wave linear combinations of basis states of the type $S_n^+\mid 0\rangle$, alias "spin waves." It is natural to visualize an individual basis state $S_n^+\mid 0\rangle$ as representing a particle (a "magnon") at the nth site. In this picture, the above Hamiltonian describes the motion of such magnons from site to neighboring site, as well as their interactions (J_Z) when they are on adjacent sites. There is considerable literature on the exact solutions for this problem for arbitrary M_Z (i.e., for an arbitrary number of "particles") in one dimension, and the problem of two particles in arbitrary dimensions (do two magnons scatter or bind?) has also been satisfactorily solved (for bibliography see Mattis, 1981). This stands in sharp contrast with the study of eigenstates of three or more particles, on $d=2,3$, or higher-dimensional lattices, which has been almost totally ignored [with the important exception of three magnons in $d=2$ (Himbergen, 1977)].

Why should we care? Aside from obvious implications for ongoing research in two- or three-dimensional magnetism, the study of such pseudoparticles provides microscopic insight into the quantum mechanics of the condensed Bose-Einstein fluid, of which liquid helium remains the salient and fascinating prototype. This follows from the observation that spin operators on different sites commute, for example, $S_i^+S_j^+\mid 0\rangle=S_j^+S_i^+\mid 0\rangle$, implying that such pseudoparticles satisfy Bose-Einstein statistics. Moreover, the spins' interactions are similar to those of rare-gas atoms—attractive for two particles on nearest-neighbor sites (if $J_Z>0$), they are essentially repulsive (for kinematical reasons) when two particles are on the same site. In the extreme quantum limit $s=\frac{1}{2}$, the property of the relevant Pauli matrices $(S_i^+)^2\equiv 0$ is tantamount to a "hard-core" zero-range potential. Even for large s, only a restricted number of particles, $2s-1$, is allowed on a given site. Such a constraint has the characteristic of a "soft-core," zero-range, repulsive potential.

In the case of Wannier functions, one deals with electrons, hence with Fermi-Dirac statistics. Within a given energy band, Wannier electrons are centered about a given atomic cell. They are characterized by quantum numbers α (denoting the band) and R_i (denoting the cell coordinate or "lattice site"). As in the example of the basis set of spin states introduced above, the Wannier states are *not* eigenstates of a one-electron Hamiltonian H_0. Instead, H_0 causes Wannier particles to "hop" from lattice site to

lattice site, with hopping matrix elements derivable from the Bloch energy-band structure. The Wannier functions constitute a most satisfactory basis, often simpler than Bloch functions, in the analysis of problems in which interband matrix elements are inconsequential. The hopping matrix elements can be supplemented by an interaction Hamiltonian H', like that which, in Hubbard's model of an interacting electron gas (Hubbard, 1963), characterizes the Coulomb repulsion between two electrons of opposite spin on a given site. Hubbard's Hamiltonian has a general appearance not too different from the equation above, except that, instead of bosons, a two-component field of fermions is involved. It, too, is exactly soluble in one dimension (Lieb and Wu, 1968), while resisting exact analysis on higher-dimensional lattices.

In recent years, lattice field theories have been developed that benefit from the automatic ultraviolet cutoff and easy counting properties inherent in a finite Hilbert space. Additionally, equilibrium statistical mechanics has benefited from the simplifications of a lattice in such applications as calculations of the partition function from a transfer matrix. It has certainly been easier to treat the lattice gas (Lee and Yang, 1952) than its continuum analogs. However, in all cases, those properties directly related to the topology of space (homogeneity, isotropy, homotopy) are sacrificed. Aside from the possible loss of such relevant physics, one additional difficulty characteristic of lattice theory occurs on the technical level: the significant simplifying features of differential equations or operators as opposed to their difference counterparts are indeed lost. Without any comprehensive mathematical framework for the solution of nonlinear difference equations, the equations of statistical physics, quantum mechanics, or field theory that are formulated on a lattice are then required to be solved either by purely numerical means, or (as in current studies of critical phenomena) in the continuum approximation. Thus the lattice theories have difficulties of their own, and there is generally a need for interplay between various techniques. The present review is intended only as an introduction to, and a partial and partisan overview of, one particular methodology: that of studying a few particles on a lattice.

In treating this topic, it is convenient to distinguish the number n of particles. In the Hartree or Hartree-Fock approximations, it is possible to reduce the many-body problem to a one-body problem; in this case, the difference equations of lattice physics are hardly more challenging than the differential equations of the continuum. Proceeding to $n=2$ in the case of arbitrary interactions (subject only to the symmetry of the lattice), it is possible, by use of the translational invariance, to reduce the calculation of eigenstates to a tractable one-body problem. On a lattice, the Hamiltonian does not separate into two parts, one relating to the center-of-mass motion and the other to the internal degrees of freedom. Rather, the translational and point-group symmetries allow eigenstates to be written as product functions. Although the center of mass can indeed be factored out and the two-body problem reduced to a one-body problem, the result differs from continuum problems in that the translational energy turns out to depend on the internal quantum numbers. The result is that composite particles on a lattice have a "mass *excess*" related to the internal binding, quite different from the "mass *defect*" familiar in special and general relativity. Following upon the recent theoretical prediction of this effect (Mattis and Gallinar, 1984), the mass excess has indeed been observed and quantitatively measured by Cafolla, Schatterly, and Tarrio (1985) in experiments on excitons (bound electron-hole pairs) in a number of semiconductors.

For $n=3$ no general results are available except for zero-range interaction potentials. (In that exceptional case, discussed at length below, the eigenvalue problem reduces once more to a one-body problem.) For $n \geq 4$, no simplifications exist regardless of interactions; nevertheless, some general observations may make analysis of such cases less formidable than it seems at first sight.

It is not yet clear what the most useful applications of such work will turn out to be. We have already mentioned superfluidity. There are applications to the theory of superconductivity (do Cooper pairs have bound states of "Cooper molecules"?) and to magnetism (are there multimagnon bound states, and if so, how does their existence affect low-temperature thermodynamics?). Additionally, a number of applications have already been made to electron, surface, and exciton physics in semiconductors. A similar study of the vibrational properties of anharmonic lattices is not too far behind. For historical reasons, there is a great deal of satisfaction in solving the "three-body problem," or at least in reducing it to quadrature, in *any* context. This satisfaction will be compounded when the n-body problem ($n \geq 4$) becomes qualitatively understood. Combined with whatever knowledge already exists concerning the many-body problem (Pines, 1962), such understanding is bound to have many unforeseen consequences. It is in this hopeful vein that I offer the present review, not as an encyclopedic compendium of acquired knowledge, but as an open-ended introduction to a vital new field of study.

In the sections that follow, subjects are presented in order of increasing n, i.e., of increasing difficulty. Various applications are separately noted, and obvious opportunities for new research indicated.

I. THE ONE-BODY PROBLEM

One may investigate a single phonon, magnon, electron, or hole. Let us consider first a translationally invariant lattice. One-particle stationary states are often eigenstates of a Hamiltonian of the type

$$H=\sum J(\mathbf{R}_i-\mathbf{R}_j)a_i^* a_j \tag{1.1}$$

and take the form of plane-wave states $|\mathbf{k}\rangle$ of wave vector $\mathbf{k}$:

$$|\mathbf{k}\rangle \equiv (1/N^{1/2})\sum e^{i\mathbf{k}\cdot\mathbf{R}_j} a_j^* |0\rangle , \tag{1.2}$$

where $|0)$ is the zero-particle (vacuum) state. Here, statistics plays no role; the operators a_i^* can create fermions (electrons or holes) or bosons (e.g., magnons). The normalization of Eq. (1.2) is predicated only on the presumed orthonormal character of the basis states $a_i^*|0)$, i.e., on

$$(0|a_j a_i^*|0)=\delta_{ij} . \tag{1.3}$$

The eigenvalues are obtained by calculating the action of Eq. (1.1) on (1.2). Thus $H|\mathbf{k}\rangle=E(\mathbf{k})|\mathbf{k}\rangle$ yields the eigenvalues $E(\mathbf{k})$,

$$E(\mathbf{k})=\sum_{R_j} J(\mathbf{R}_i-\mathbf{R}_j)e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} , \tag{1.4}$$

as the lattice Fourier transforms of the hopping matrix elements $J(\mathbf{R})$.

A formally alternative method will be seen to be both instructive and useful. Assuming that

$$\Psi(\mathbf{R})\propto e^{i\mathbf{k}\cdot\mathbf{R}} \tag{1.2'}$$

(we omit the normalization constant) is an eigenstate in the first-quantized representation, then the eigenvalue equation $\mathscr{H}\Psi=E(\mathbf{k})\Psi$ requires $\mathscr{H}$ to be an operator of the form

$$\mathscr{H}\equiv E(-i\nabla) , \tag{1.1'}$$

with E the function defined in Eq. (1.4). Conversely, the eigenfunctions of (1.1') are the plane-wave states (1.2'), having eigenvalues $E(\mathbf{k})$ by inspection. There exists one difficulty, however.

Clearly, $\mathscr{H}$ commutes with ∇, the generator of the infinitesimal translations, whereas the space lattice has only discrete translational symmetry. It is thus necessary to restrict $\mathscr{H}$ to the physical subspace. In three dimensions, this is easily achieved by requiring three arbitrarily chosen noncoplanar R's in Eq. (1.2') to agree with three corresponding, distinct physical lattice sites. Starting from these, $\mathscr{H}$ can translate a particle only to other physical lattice sites.[1]

Newton's equations for the normal modes of harmonic lattices can be posed as an eigenvalue problem similar to Schrödinger's equation. They take the form $\mathscr{L}\psi=\omega^2\psi$, where ψ is a normal-mode amplitude and (in a one-dimensional, nearest-neighbor example) $\mathscr{L}$ is given as

$$\mathscr{L}=2(K/M)(1-\cos i\partial/\partial x) . \tag{1.5}$$

The ψ's are thus also plane waves of the type (1.2'), whose eigenvalues

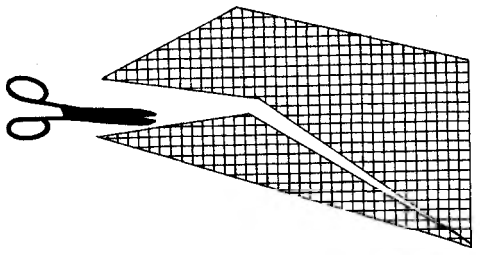

FIG. 1. Cleaving a crystal creates surface planes of various possible orientations, and cuts all bonds extending out of the surface.

$$\omega^2(k)=2(K/M)(1-\cos k) \tag{1.6}$$

yield the "dispersion relations" $\omega^2(k)$ of the normal modes.

This alternative method comes into its own when the symmetries of the problem are disturbed, as by some perturbation δH in the Hamiltonian or some change $\delta\mathscr{L}$ in $\mathscr{L}$ (reflecting a change in mass M or spring constants K about an impurity), and one finds it simple to construct the relevant Green's functions using the plane-wave states. Even more interesting is the imposition of new boundary conditions to replace the periodic boundary conditions implied by the plane-wave form. We turn to this important question next.

A. Surface boundary conditions

We pose a modest equation: what happens if, all other things being equal, simple periodic boundary conditions (PBC's) are replaced by those appropriate to a surface? Assume atomic planes at $x=a,2a,3a,\ldots,Na$. With periodic boundary conditions, the atoms at the right-hand edge $Na,(N-1)a,(N-2)a,\ldots$ also appear to be at $x=0,-a,-2a,\ldots$ and are joined to the atoms at the left-hand edge $x=a,2a,3a,\ldots$ by the usual bonds. When a physical surface is introduced at $x=0$, the atomic planes at $x=0,-a,-2a,\ldots$ are replaced by vacuum, and no bonds are present (see Fig. 1). Because the consequences for Wannier particles differ from those for vibrational normal modes, we shall discuss each in turn.

1. Wannier particles (electrons or holes)

As there are no hopping matrix elements to take particles into the half-space at $x\leq 0$, the appropriate boundary condition is $\psi=0$ at $x=0,-a,-2a,\ldots$. We call this "zero boundary conditions" (ZBC's).[2] The eigenvalue problem is formally the same as for PBC's:

[1]For a one-dimensional example, suppose $E(k)=2A\cos k$, hence $\mathscr{H}=Ae^{\partial/\partial x}+Ae^{-\partial/\partial x}$. It follows from the Taylor series expansion, $e^{\pm\partial/\partial x}f(x)=f(x)\pm f'(x)+1/2f''(x)\pm\cdots=f(x\pm 1)$, that if any wave function $f(x)$ is defined at $x=0$, $\mathscr{H}$ can translate it only to the other, correct, regularly spaced lattice points at $x=\pm 1,\pm 2,\ldots$. Coordinates that do not coincide with lattice points, such as $x=0.5$, do not appear in subsequent analysis. In this example, the (nearest-neighbor) hopping matrix element is A.

[2]If N is sufficiently large, we apply ZBC to the second surface at $(N+1)a$ separately. It is also important to note that, in general, the spatial axes do not necessarily coincide with the crystal axes; thus in general $a\neq a_0$, the "natural" lattice parameter (in fact, $a\leq a_0$).

$$\mathscr{H}\psi=\varepsilon\psi\ . \tag{1.7}$$

As the periodicity in the y,z plane is undisturbed, it is only necessary to take into account the motion perpendicular to the surface. Thus, if the Bloch energies (also known as the "energy-band structure") in the αth band are given by $E(k_1,k_2,k_3)$, we can set

$$\mathscr{H}=E(-i\partial/\partial x,k_2,k_3) \tag{1.8}$$

and just consider $\psi=\psi(x)$. The wave vectors k_2 and k_3 are just parameters in what turns out to be a one-dimensional problem. We now work out a trivial example.

Suppose that the band structure at a particular k_2,k_3 lends itself to the following approximation: $E(\mathbf{k})\approx A(k_2,k_3)+2B(k_2,k_3)\cos ak_1$. Then

$$\mathscr{H}\approx A(k_2,k_3)+B(k_2,k_3)(e^{a\partial/\partial x}+e^{-a\partial/\partial x})\ , \tag{1.9}$$

which indicates that particles are transferred only between nearest-neighbor planes. Thus satisfying the ZBC at $x=0$ is sufficient, and

$$\psi=(2/N)^{1/2}\sin k_1x \quad \text{for} \quad x=0,a,2a,\ldots$$

satisfies both the eigenvalue equation (1.7) and the ZBC at $x=0$. Note the important features: for every bulk E there is an eigenvalue $\varepsilon=E$ when ZBC's are imposed, but the wave functions are substantially altered. In particular, the probability of finding the Wannier particle on the nth plane is $(2/N)\sin^2k_1na\to 1/N$, independent of k at large n, exactly as with PBC's while at the surface, the probability vanishes at the band edges $[(2/N)\sin^2k_1a\to 0$ as $ka\to 0$ or $\pi]$.

But the band structure might not lend itself to this simple-minded approximation. Suppose

$$E(\mathbf{k})\approx 2A\cos ak_1+2B\cos 2ak_1\ ,$$

with A and B again functions of k_2,k_3. The procedure for solving the eigenvalue equation (1.7) for a given ε, subject to two ZBC's, $\psi(0)=0$ and $\psi(-a)=0$, as $e^{\pm 2a\partial/\partial x}$ connects next-nearest-neighbor planes, is then roughly the following:

(1) replace $\exp ik_1a$ by ζ, and solve the quartic equation

$$A(\zeta+1/\zeta)+B(\zeta^2+1/\zeta^2)=\varepsilon$$

for the four roots. They correspond to four complex values of k_1 in general.

(2) Discard any roots having $\mathrm{Im}(k_1)<0$, as they result in non-normalizable, exponentially growing states in the interior of the solid.

(3) Satisfy the two ZBC's with the remaining waves. There may remain only one solution, or as many as two linearly independent solutions. [If ε is not in an appropriate range of energies, there may be none. However, if we set $\varepsilon=E(k_1,k_2,k_3)$ then $\zeta=e^{\pm ik_1a}$ with real k_1 will always yield one solution, at least. Thus, degeneracy aside, for every eigenvalue E that exists with PBC's there will be an eigenvalue ε found for ZBC's, so the band structure is essentially unaltered in the bulk.]

One of the interesting consequences of the ZBC relates to the amplitudes of waves approaching the surface. As with the simple example worked out above, in general the ψ's must vanish near the surface, whenever ε corresponds to a bulk energy near a band extremum or to a Van Hove singularity; but even such general conclusions have to be extensively modified by the presence of surface perturbations $\delta\mathscr{H}$. Such additional complications owing to charge imbalance (surface dipole moment), bond bending, and surface reconstruction, all related to the appearance of surface states, are clearly beyond the scope of the present section on boundary conditions. The interested reader will find an extensive literature (of dedicated journals and books) on all aspects of the electronic properties of surfaces except the theory of ZBC. The systematic study of this boundary condition was undertaken some years ago by the present writer in a series of papers reviewed in Mattis, 1978.

2. Normal modes (phonons, magnons, etc.)

This case is much more difficult than the previous one. The absence of bonds connecting surface atoms to planes at $x\le 0$ affects $\mathscr{L}$ and cannot generally be expressed in terms of boundary conditions.

There are some simple exceptions. As one soluble example, suppose $\mathscr{L}$ to be of the form (1.9):

$$\mathscr{L}\approx A(k_2,k_3)+B(k_2,k_3)(2-2\cos ia\partial/\partial x)$$

everywhere except at the surface plane $x=a$, where it takes on the form

$$\mathscr{L}_s\approx A+B(1-e^{a\partial/\partial x})\ ,$$

reflecting the absence of bonds connecting to $x=0$. In this case, $\mathscr{L}_s$ can be put in the same form as the bulk if we add $B(1-e^{-a\partial/\partial x})=0$ to it, making sure that this vanishes by requiring that a boundary condition,

$$\psi(a)=\psi(0)\ ,$$

be satisfied. (This is approximately a condition of zero normal gradient, and certainly differs from ZBC's. We have no name for it.) It is satisfied by the following linear combination of $e^{\pm ik_1x}$:

$$\psi(x)\propto(2/N)^{1/2}\cos k_1(x-a/2)\ .$$

If next-nearest-neighbor bonds are involved, the effects of the surface cannot be conveniently expressed in terms of boundary conditions, and the analysis becomes thoroughly complicated. Fortunately, adequate studies of surface normal modes by other methods have been undertaken, and a lot of detailed information is now available. For a recent review, see Maradudin (1981).

B. Surface potentials

In certain semiconductors, the potentials at the surface serve to trap one or the other sign of the carrier. The

motion of Wannier particles in a region of constant electric field E ($V \propto x$) or constant charge density ρ ($V \propto x^2/2$) presents an interesting subject of study. With the imposition of a surface boundary condition, $\psi = 0$ for $x \leq 0$, both problems are well posed. In the continuum version of this problem ($\mathscr{H}_0 = -\partial^2/\partial x^2$) the eigenstates are the well-known Airy and Hermite functions, respectively. On a lattice, the eigenstates can also be obtained, and they are found to be Bessel and Mathieu functions, respectively. Let us start with the analysis of the linear potential (Gallinar and Mattis, 1985b).

1. $V(x) = |qE|x$

All states subject to this potential and to ZBC's are perforce confined; therefore the energy-level scheme (in the x direction) must be discrete. We shall assume the simplest possible band structure (1.9). The eigenstates $\psi(n)$ (we replace the plane coordinates $x = na$ by the plane indices n, for convenience) satisfy a difference equation:

$$\psi(n+1)+\psi(n-1)=(Fn-\varepsilon)\psi(n) . \tag{1.10}$$

This is precisely the difference equation satisfied by the Bessel functions of the first kind $J_\nu(z)$ (Abramowitz and Stegun, 1965), which also display the correct asymptotic properties permitting the identification

$$\psi(n) = DJ_\nu(z) , \tag{1.11}$$

where D is a normalization constant, $\nu = n - \varepsilon/F$, and $z = 2B/F$. The ZBC, which consists of finding the zeros of the Bessel functions through varying the subscripts,

$$J_{-(\varepsilon/F)}(z) = 0 , \tag{1.12}$$

provides the eigenvalue condition. Although the ε's are quantized by this procedure, each level gives rise to a separate continuum parametrized by k_2, k_3. Plots of the energy levels and comparison with the effective-mass approximation are given in Gallinar and Mattis (1985b). It is found that the effective-mass approximation is accurate only in weaks fields, when $|qEa_0|$ is less than the electronic bandwidth.

2. $V(x) = x^2/2$

This problem is best solved by means of an elementary duality transformation. Suppressing the trivial k_2, k_3 parameters, suppose we start with the "discrete Gaussian" one-particle Hamiltonian:

$$\mathscr{H} = -A(e^{\partial/\partial x}+e^{-\partial/\partial x})+x^2/2, \quad x = 1,2,3,\ldots . \tag{1.13}$$

We extend the space to $x = 0, -1, -2, \ldots$ and satisfy ZBC's by selecting only odd states. Next, we perform the canonical (duality) transformation: $x \to p - p_0$ and $p \to -x + x_0$, where p_0 and x_0 are adjustable parameters. Now $\mathscr{H}$ takes on the appearance of Mathieu's equation (Abramowitz and Stegun, 1965):

$$\mathscr{H} = (p-p_0)^2/2 - 2A\cos(x-x_0) . \tag{1.13'}$$

By Floquet's theorem, solutions are of the Bloch type:

$$\psi_{\beta,q}(x) = u_{\beta,q}(x)e^{iqx} , \tag{1.14}$$

where $u_{\beta,q}(x)$ has the periodicity of Eq. (1.13') [$u(x \pm 2\pi) = u(x)$], and β labels the new bands. Now, the original condition that $x =$ integer translates into $p =$ integer, hence $q = 0$. β becomes a quantum label for the allowed eigenstates. (While the solutions to Mathieu's equation are well documented, the details of the indicated calculation have not been carried out in the literature, to this author's knowledge, and would serve a useful purpose.)

(*Note added.* In response to this "challenge," E. Chalbaud, J.-P. Gallinar, and G. Mata [J. Phys. A (to be published)] have just performed a thorough analysis of this problem.)

A number of lattice-adapted path-integral methods have been proposed for the study of one-particle problems. We refer the interested reader to Wannier (1962) and Buot (1976) for an introduction to this methodology.

While there are a number of other instances of one-particle lattice physics that are of widespread interest (e.g., the Wannier-Aubry problem of localized or "kinky" eigenstates associated with potentials that are incommensurate with the lattice), further discussion is outside the purview of the present article. We proceed instead to a review of $n = 2$ particle states, where a surprise is in store.

II. THE TWO-BODY PROBLEM

On a lattice, no less than in the continuum, the two-body problem reduces to a standard one-body problem through the usual decoupling of center-of-mass and relative coordinates. As one example, the problem of two particles interacting via a linear potential can be reduced to Bessel's equation (1.10), with (1.12) $J = 0$, the eigenvalue equation for odd-parity states and a similar condition, $dJ/dz = 0$, yielding the even-parity states (Gallinar and Mattis, 1985b).

In one important and surprising aspect, composite particles on a lattice differ from those in the continuum. Investigation of the motion of a composite particle on a lattice finds it to depend parametrically on the internal binding. This is not the case in continuum physics, where, for example, the mass of a hydrogen molecule is precisely twice the mass of a hydrogen atom, and the mass of a water molecule is the sum of the hydrogen molecule and oxygen masses (all subject to small, relativistic, mass-defect corrections). In lattice physics, on the other hand, for $n = 2$ we are able to enunciate a fairly general rule: *the greater the internal binding energy, the greater the total mass* (or translational inertia) of the composite particle.

Qualitatively, the reason is clear: the greater the interactions, the greater the fraction of the Brillouin zone occupied by the eigenstate, hence the more complete the

localization in real space.[3] While in general $\mathscr{H}$ *cannot* be written as the sum of an internal Hamiltonian and of a Hamiltonian of the center-of-mass motion, nevertheless, because $\mathscr{H}$ commutes with the lattice symmetry operators (including the discrete translation operator), the eigenstates *do* factor to reflect these symmetries and so take the familiar form $\Psi=\Phi(\mathbf{R})F(\mathbf{r}_{12})$ with $\mathbf{R}$ the center-of-mass coordinate. However, the total energy is not an additive function of the internal and translational energy. For simple band structures, this causes a mass *excess* which can approach infinity if the entire Brillouin zone is involved in the interactions. This state of affairs is in sharp contrast with the mass *defect* of relativity theory. (In relativity, this mass defect is proportional to the binding energy of a composite particle. In the lattice theory, the mass excess is related to the amount of kinetic energy present in the bound state.) Although in both cases the nonadditivity of the energies is responsible for the variability of the total mass, the details differ. We spend the next few paragraphs elucidating the theory of the lattice-theoretic effective mass for a two-particle composite. It should also be noted that (as of the date of writing) a correspondingly general theory has not been worked out for $n \geq 3$.

Consider the reasonably general lattice Hamiltonian $\mathscr{H}$, comprising motional energy (KE) for two particles, not necessarily of the same species:

$$\mathscr{H}\mathscr{E}=E_1(-i\nabla_1)+E_2(-i\nabla_2) \tag{2.1}$$

and an attractive interaction potential $V(\mathbf{R}_i-\mathbf{R}_j)$. *If V is sufficiently attractive* and the statistics permit it, in the ground state (Ψ_0) both particles will reside on the same site. Taking the translational invariance of the lattice into account, we see that the (variational) ground state is of the form

$$\Psi_{0,\mathbf{K}} \approx (1/N^{1/2}) \sum_j e^{i\mathbf{K}\cdot\mathbf{R}_j}\delta(\mathbf{R}_i-\mathbf{R}_j) \ . \tag{2.2}$$

Now, a representation of the discrete delta function (Kronecker delta)

$$\delta(\mathbf{R})=(1/N)\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} \tag{2.3}$$

allows us to evaluate the variational ground-state energy ε_0 as a function of translational momentum $\mathbf{K}$:

$$\begin{aligned}\varepsilon_0(\mathbf{K}) &= (\Psi_0 \,|\, \mathscr{H} \,|\, \Psi_0) \\ &= \langle E_1\rangle + \langle E_2\rangle + V(\mathbf{0}) \ , \end{aligned} \tag{2.4}$$

where $\langle E_1\rangle = \int d^3k \ E_1(\mathbf{k})/\Omega$, $\Omega \equiv \int d^3k$ = volume of the first Brillouin zone, and $\langle E_2\rangle$ is given similarly. Both are independent of $\mathbf{K}$, as is $V(\mathbf{0})$. It follows that, to the extent that Ψ_0 is an accurate variational state, the bandwidth of the composite particle vanishes in the strong coupling limit. (One also states more imaginatively, although somewhat less accurately, that in this limit the translational mass of the composite particle is infinite.)

It is obvious that slightly bound states or unbound scattering states have a translational mass of approximately the sum of the two constituents. m_1, the "effective mass" of the first constituent and m_2, that of the second, are tensors, the components of which are obtained by inverting expressions of the form

$$(1/m)_{ij} \equiv \partial^2 E(\mathbf{k})/\partial k_i \partial k_j \,|_{k_{\min}} \ , \tag{2.5}$$

where the derivatives are to be evaluated at the point where $E(\mathbf{k})$ has its minimum. The effective mass of *any* stationary state of energy $\varepsilon(\mathbf{K})$ of the composite particle (not just the ground state) is defined by an identical expression, with $\varepsilon(\mathbf{K})$ replacing $E(\mathbf{k})$.

For lattices or band structures with cubic symmetry, if the components k_i are picked along principal axes, one infers that the cross terms ($i \neq j$) vanish and that the three diagonal components ($i=j$) are equal. In that case, we can assign a scalar effective mass m_1 or m_2 to the constituent particles and to the composite one, M, as well. (In the effective-mass approximation, $M=m_1+m_2$ as in continuum theory.)

One important composite particle of solid-state physics is the *exciton*. The literature distinguishes between the highly mobile Wannier-Mott exciton [an electron from the conduction band and a hole from the valence band of a semiconductor, interacting by a Coulombic attractive potential in any of the hydrogenic bound states (Knox, 1963)] and the Frenkel exciton [a localized atomiclike excitation (Davydov, 1962)], which proceeds by diffusion. To this we must add the "mathematical" exciton (for want of a better name) associated with itinerant-electron magnetism, which we treat separately in the Appendix. [Excitons are not the only objects of study. Among other two-particle composites of solid-state physics that have been considered at one time or another, one should also mention the Cooper pair of the BCS theory of superconductivity (fermions) and the bound-magnon (boson) pair of magnetism.]

We shall now prove that the Wannier-Mott and Frenkel excitons are merely extreme cases of a "generic exciton" (highly mobile when weakly bound and localized when strongly bound) by calculating the effective mass M of the composite particle (Mattis and Gallinar, 1984). The present illustration applies specifically to "simple cubic" band structures although with minor changes it also works for "body-centered-cubic" band structures (and should be qualitatively valid for all other "simple" band structures). The final result is Eq. (2.14) below.

Let $E_1(\mathbf{k})=W_1\varepsilon(\mathbf{k})/3$ and $E_2(\mathbf{k})=W_2\varepsilon(\mathbf{k})/3$, where

$$\varepsilon(\mathbf{k}) \equiv 3-\cos k_x-\cos k_y-\cos k_z \ . \tag{2.6}$$

By conservation of momentum, the interaction scatters $\mathbf{k}_1=\eta\mathbf{P}$ and $\mathbf{k}_2=(1-\eta)\mathbf{P}$ into $\mathbf{k}_1+\mathbf{k}$ and $\mathbf{k}_2-\mathbf{k}$ (mod

[3]Quantitatively, the range and "shape" of the interactions and the "statistics" of the particles (which forbid certain eigenstates) also play nontrivial roles.

any reciprocal-lattice vector $\mathbf{K}_n$) with matrix element $gV(\mathbf{k})/N$. We introduce a coupling constant g for convenience, setting $g=1$ at the end of the calculation. $\mathbf{P}$, the total momentum, is conserved (mod any $\mathbf{K}_n$); η is an adjustable parameter.

All *scattering states* of $\mathscr{H}$ can be written in the form

$$|\mathbf{k}_1\mathbf{k}_2\rangle = |\mathbf{k}_1,\mathbf{k}_2\rangle + (1/N)\sum_k L(\mathbf{k})\,|\mathbf{k}_1+\mathbf{k},\mathbf{k}_2-\mathbf{k}\rangle\ , \tag{2.7}$$

whereas all *bound states,* labeled by a discrete quantum number β, take the form

$$|\beta\rangle = (1/N^{1/2})\sum_{\mathbf{k}} F(\mathbf{k})\,|\mathbf{k}_1+\mathbf{k},\mathbf{k}_2-\mathbf{k}\rangle\ . \tag{2.8}$$

Sums over $\mathbf{k}$ are limited to the first Brillouin zone. Writing $\mathscr{H}\,|\beta\rangle = E\,|\beta\rangle$ we obtain an integral equation

$$F(\mathbf{k}) = -(g/N)\sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}')[E(\mathbf{k}',\eta,\mathbf{P})-E]^{-1}F(\mathbf{k}')\ , \tag{2.9}$$

where

$$\begin{aligned} E(\mathbf{k}',\eta,\mathbf{P}) &\equiv E(\mathbf{k}_1+\mathbf{k}',\mathbf{k}_2-\mathbf{k}') \\ &\equiv E_1(\mathbf{k}'+\eta\mathbf{P}) \\ &\quad + E_2[-\mathbf{k}'+(1-\eta)\mathbf{P}] + E_g\ . \end{aligned} \tag{2.10}$$

E_g is the energy gap, the smallest energy required to produce an electron and a hole in the material. We shall find only bound states for energy eigenvalues $E<E_g$, while scattering states occupy the region $E\geq E_g$. The former exist only for sufficiently attractive potentials ($gV<0$). (The Coulomb attraction qualifies; it always possesses an infinity of them.[4]) The principal advantage of Eq. (2.9) is that it concerns only bound states. If there are none, it has no solutions. We turn to this equation first, and analyze scattering states [Eq. (2.7)] last.

To obtain the desired results concerning the total mass M, we are not required to be able to solve Eq. (2.9), only to note that it has the form of an integral equation (symbolically $F=\mathbf{K}\cdot F$), the kernel of which depends on $\mathbf{P}$ and has matrix elements given by

$$\begin{aligned} K_{\mathbf{k}\mathbf{k}'}(\mathbf{P}) = -(g/N)V(\mathbf{k}-\mathbf{k}')\{&E_1(\mathbf{k}'+\eta\mathbf{P}) \\ &+E_2[-\mathbf{k}'+(1-\eta)\mathbf{P}] \\ &+\Delta_{\mathbf{P}}(g)\}^{-1}\ , \end{aligned} \tag{2.11}$$

with $\Delta(g)\equiv E_g-E=$binding energy (≥ 0 when a bound-state solution exists), displaying the dependence on coupling constant g explicitly. The bound-state energy consists of two parts: kinetic energy (KE) and potential energy (PE). By Feynman's theorem, $\mathrm{PE}=-g\Delta'(g)$. Thus, in the bound state,

$$\mathrm{KE} = -[\Delta(g)-g\Delta'(g)]\ . \tag{2.12}$$

The strategy is as follows: one first sets $\mathbf{P}=0$ and assumes a binding energy $\Delta_0(g)$. Choosing an appropriate direction for infinitesimal $\mathbf{P}$, and an appropriate η, one manipulates $K_{\mathbf{k}\mathbf{k}'}(\mathbf{P})$ into the form $K_{\mathbf{k}\mathbf{k}'}(\mathbf{0})$. This requires infinitesimal changes in Δ and g. On the other hand, because the effective mass M is a scalar we have $\Delta_p(g)=\Delta_0-(1/2M)P^2+O(P^4)$ with which to define M.

The following quantities are required: $W\equiv W_1+W_2$ [this is the KE in the case of *maximum localization,* in the sense of Eq. (1.4); it is *not* the maximum KE, which is $2W$], $\mathbf{P}=(p,p,p)$, and η chosen to cancel odd terms in p in the denominator of the kernel. This last requires

$$W_1\sin\eta p = W_2\sin(1-\eta)p\ . \tag{2.13}$$

Now we need to define three new quantities in terms of the old:

$$\alpha\equiv[W_1\cos\eta p + W_2\cos(1-\eta)p]/W\ ,$$

$$g^*\equiv g/\alpha,\quad \Delta^*\equiv(1/\alpha)(\Delta_p+W)-W\ .$$

The kernel $K_{\mathbf{k}\mathbf{k}'}(p)$ can be brought back to the form $K_{\mathbf{k}\mathbf{k}'}(0)$ with the substitutions g^* for g and Δ^* for Δ_p. After some minor additional algebraic manipulations involving the comparison of Δ^* (g^*) with the expansion of Δ_p (g) in powers of P^2, one obtains a formula for the total mass M of the composite particle in each discrete bound level β:

$$M_\beta = (m_1+m_2)/(1-\mathrm{KE}_\beta/W)\ . \tag{2.14}$$

The smaller the spatial extent of a given state β, the greater KE_β. As stated above, the maximum value of KE in a bound state is W, in which limit the exciton mass is $M=\infty$ ("Frenkel exciton"). At the opposite extreme, in a spatially extended state KE can be quite small and $M\approx m_1+m_2$ in accord with the continuum approximations to the "Wannier-Mott exciton." In physically important cases of Coulomb interactions, if the modifications imposed by the lattice (see footnote 4) still permit the virial theorem to remain approximately valid, then $\mathrm{KE}_n=\mathscr{R}/n^2$, where $\mathscr{R}$ is the appropriate Rydberg and n the principal quantum number. Equation (2.14) becomes

$$M_n = (m_1+m_2)/(1-\mathrm{c}/n^2),\quad n=1,2,\ldots \tag{2.15}$$

and $\mathrm{c}\equiv\mathscr{R}/W$. This result has been confirmed experimentally in a number of semiconducting materials by

[4]On the cubic lattice (where it must satisfy the discrete analog of Poisson's equation) we take the Coulomb interaction to be of the form $gV(k)\approx -2\pi e^2/\kappa\varepsilon(\mathbf{k})$, with $\varepsilon(\mathbf{k})$ defined in Eq. (2.6) and κ the dielectric constant. At small k this reduces to the usual $-4\pi e^2/\kappa k^2$, while exhibiting the crystal symmetries $V(\mathbf{k}+K_n)=V(\mathbf{k})$ at all $\mathbf{k}$. Conversely, in real space, the lattice Fourier transform of the proposed function exhibits satisfactory limiting behaviors: $\tilde{V}(R)\to -e^2/\kappa R$ at large R, and at $R=0$, $\tilde{V}(0)=-e^2/\kappa a_1$ (where a_1 is a constant of the order of the lattice parameter a_0).

Cafolla, Schatterly, and Tarrio (1985). In the Frenkel limit, there is a two-body (dipolar-resonance) mechanism, which we have ignored so far, but which allows the entity to move as a whole. When this modification is made in Eq. (2.14), one finds a result only slightly more complicated:

$$1/M=[(1-\mathrm{KE}/W)/(m_1+m_2)]+1/M_F\ , \qquad (2.16)$$

where a combination of parameters denoted M_F is then the (relatively large) limiting mass (for a detailed derivation, see Gallinar and Mattis, 1985a). In the large-mass limit, the scattering of excitons by phonons becomes relatively important. Instead of wavelike propagation, one now expects diffusive behavior. For recent information concerning the properties of excitons, alone and in interaction with each other and with such other particles as phonons and photons, the reader is referred to the compendium by Rashba and Sturge (1982).

We turn now to the scattering states, Eq. (2.7). To obtain algebraic equations, we evaluate

$$\langle \mathbf{k}_1,\mathbf{k}_2 \,|\, \mathscr{H}-E \,|\, \mathbf{k}_1,\mathbf{k}_2\rangle=0$$

and

$$\langle \mathbf{k}_1+\mathbf{k},\mathbf{k}_2-\mathbf{k} \,|\, \mathscr{H}-E \,|\, \mathbf{k}_1,\mathbf{k}_2\rangle=0\ ,$$

obtaining from the first

$$E=E(\mathbf{k}_1,\mathbf{k}_2)+(g/N^2)\sum_{\mathbf{k}'} L(\mathbf{k}')V(-\mathbf{k}') \qquad (2.17a)$$

and from the second

$$L(\mathbf{k})=\left[gV(\mathbf{k})+(g/N)\sum_{\mathbf{k}'} L(\mathbf{k}-\mathbf{k}')V(\mathbf{k}')\right] \times[E-E(\mathbf{k}_1+\mathbf{k},\mathbf{k}_2-\mathbf{k})]^{-1}\ . \qquad (2.17b)$$

In the thermodynamic limit ($N\to\infty$) one replaces $(1/N)\sum_k$ by $\Omega^{-1}\int d^3k$, and the singular integral in Eq. (2.17a) yields a complex energy:

$$E=E(\mathbf{k}_1,\mathbf{k}_2)+(1/N)(\delta\varepsilon+i/2\tau)\ . \qquad (2.18)$$

We indicate the real shift in energy (related to the usual phase shift) by $\delta\varepsilon/N$, the imaginary part (related to the lifetime τ) by $1/2\tau N$. The calculation of both requires the solution of the integral equation (2.17b), generally an involved, numerical task.

While the $1/N$ ensures that the energies of scattering states are substantially unaffected by the interaction and interlace the unperturbed energies, this is not the case for the wave functions, which are significantly affected in the scattering region.

For the calculation of effects that are sensitive to this (such as optical matrix elements), Eq. (2.17b) must be solved for the $L(\mathbf{k})$'s. Although in lattice physics there are few of the simplifying features of continuum scattering theory with central potentials, such as the decomposition into partial waves, in special cases one finds useful "tricks" here, too. For example, in the special case $V(k)=$const (zero-range potential), Eqs. (2.17) become trivial. Their solution in the two cases of interest ($V>0$ and $V<0$) are left as an exercise for the reader. Other information is available in Rashba and Sturge (1982). Leaving aside other topics in the lattice physics of $n=2$ particles, we now turn to $n=3$.

III. THE THREE-BODY PROBLEM

"The quantum-mechanical three-body problem compounds the difficulty of the classical problem ... approximation schemes are based more on physical insight than on mathematical credential and work far better than they ought ...."

(R. Amado, 1981)

Although this quote concerns the three-body problem in the continuum (nuclear or atomic physics), the reader may be reassured to know the following.

(1) The three-body problem in three or higher dimensions for short-range interactions is *simpler on a lattice* than in the continuum. Assuming the particles interact via two-body potentials only, the three-body bound states (when they exist) are generally in the strong coupling limit, and approximations based on this principle converge well.

(2) For short-range, attractive, two-body forces of arbitrary strength, the number of distinct three-body bound states with substantial binding energies is small, of $O(1)$. In three or higher dimensions, such states appear (and disappear) *discontinuously* as the coupling constant is varied. In two (or fewer) dimensions, bound states appear continuously, for arbitrarily weak attractive forces.

(3) There exists a three-dimensional anomaly: near the threshold for two-body bound states to form, an infinite number of extremely weakly-bound three-body states appear (Efimov, 1970). This phenomenon is known from continuum theory. Whether in the lattice theory or in the continuum, it apparently exists only in three dimensions (Bruch and Tjon, 1979).

This section starts with the zero-range (delta-function) interactions, the closest to being exactly soluble. In fact, for delta-function interactions in one dimension, Bethe's ansatz does essentially resolve the many-body problem, as shown in a great body of literature, including (but not limited to) Lieb and Mattis (1966), Yang (1967), Gaudin (1967), and Lowenstein (1981). Unfortunately, this phase-shift approach is inoperative in two dimensions or higher. Therefore the present review deals only with the far less well understood (not to say obscure) applications in two or higher dimensions. They are a recent concern; the publications we shall review appeared during the period 1982—1984. Clearly the field is in its infancy and much work remains to be done.

Following a recapitulation of these recent results for zero-range interactions, we shall examine the statement of the problem for arbitrary forces, whether attractive, repulsive, or mixed, and assess the prospects for a complete analysis.

A. Trion

Consider a Frenkel exciton in the strong coupling limit: one electron and one hole on the same lattice site. Will it bind one extra hole? The answer in three dimensions is yes, if the bandwidth of the electrons is approximately three times greater than that of the holes. (If the bandwidth of the holes is three times that of electrons—an unlikely situation—then the exciton can bind one extra electron. If the bandwidths are similar, i.e., if the ratio of bandwidths lies between $\frac{1}{3}$ and 3, then *no* trion is stable in three dimensions.)

The analysis is straightforward: when the two holes are neighbors, the electron can hop from one to the other without loss of potential energy. If the energy gained by this process is greater than that lost by localizing the second hole, the trion is stable. Only band energies (KE) are involved; the potential energy of the exciton is so great that the energy to ionize it (even virtually) is presumably unavailable. The original solution in d dimensions was obtained with the help of lattice Green's functions for spinless particles (Schilling and Mattis, 1982). Later work (Schilling and Mattis, 1983a) incorporated the spin variables and calculated the translational mass of the trion for all ranges of the parameters, while another paper treated one hole in the presence of N excitons (Schilling and Mattis, 1983b).

One of the most interesting results of these investigations concerns the motility of the composite particle. While the Frenkel exciton is immobile [see discussion following Eq. (2.4) above] and the extra hole is presumed to be at least three times more massive than the electron, the composite *does* move (in three-dimensional lattices). (For the calculations and graphical details, see the above-cited reference.) This is an instance, which might be considered somewhat unusual, when the introduction of an extra particle helps *reduce* the mass of a composite.

B. Donor atoms

It is a longstanding premise of semiconductor physics that a donor atom can bind one electron (of either spin) but, because of the Coulomb repulsion, not two. Of course, this depends on the nature and range of the forces. (Subject to some technical modifications due to band-structure degeneracies, similar considerations apply to *acceptors* and the *holes* which reside on them.) We distinguish between short- and long-range forces.

(1) Short-range forces: The attractive one-body potential $-v$ of the impurity atom has a bound state that can accommodate two mobile particles. We have studied the effects of a repulsive zero-range two-body potential of strength U on this bound state, estimating the curve $U_c(v)$ above which the two-body bound state becomes unstable against ionization of one of the particles. When this occurs, the one-particle bound state (the ground state) becomes degenerate, so that at temperature T the effective binding energy is shifted by a term $-kT\ln 2$. The difficulty of this particular three-body problem is that one of the particles (the immobile impurity atom) differs from the other two; the resultant integral equation is rather awkward (Rudin and Mattis, 1984). The continuum version of this problem studied by Klaus and Simon (1980) should apply in the effective-mass limit.

TABLE I. Total binding energies of various ions in rydbergs $\equiv m^*e^4/2\hbar^2\kappa^2$

Excess valency Z and number of bound particles N	Calculated E_0 (Kalia *et al.*, 1984)	Experimental E_0 (Moore, 1949)
$Z=1,\ N=1$	-1	-1
$Z=1,\ N=2$	-1.056	?
$Z=2,\ N=1$	-4	-4
$Z=2,\ N=2$	-5.807	-5.807
$Z=2,\ N=3$	-6.10	?
$Z=3,\ N=2$	-14.56	-14.56
$Z=3,\ N=3$[a]	-17.34	-15.0
$Z=3,\ N=4$[a]	-18.05	?

[a]Calculated E_0 is for N *bosons* (this simulates valence-band degeneracy for acceptors in germanium). Experimental E_0 is for physical atoms (H,He,Li), with spin-$\frac{1}{2}$ *fermions.*

(2) *Coulomb potentials:* In estimates of such quantities as thresholds for bound states, the effective-mass approximation (EMA) should prove adequate for the Coulomb potential, because of its emphasis on long wavelengths (see footnote 4). We may then appropriate a theorem of Lieb's (1984) which limits the number of bound electrons to $N<2Z+1$ (e.g., allowing H^- but forbidding H^{--}). If the Coulomb attraction is given by potentials $-1/r_1-1/r_2$ and the two-body repulsion is modeled by[5] A/r_{12}, then at or above some A_c, the two-body bound state is unstable against ionizing one of the mobile particles [just as in (1) above]. It has been proven (Hoffmann-Ostenhof, Hoffmann-Ostenhof, and Simon, 1983) that the two-body bound state has a square-integrable eigenfunction at threshold (A_c), while above threshold it is just a scattering state. Thus the bound state forms *discontinuously,* a feature characteristic of the three-body problem, as we shall see in later sections of this review.

Following the discovery of multiply charged acceptor states in germanium by Haller *et al.* (1983), attention has focused on what might heretofore have seemed a purely academic problem. The variational methods of Hylleraas (Hylleraas and Midtdal, 1956) have been extended by Wu and Falicov (1984) to a variety of Z and N. An in-principle exact Green's-function solution of the few-body problem (based, however, on Monte Carlo sampling techniques and thus necessarily subject to numerical error) has also been carried out by Kalia, Vashishta, and Lee (1984), with the results [in general agreement with Wu and Falicov and in excellent agreement with experimental data on atoms and ions (Moore, 1949)] shown in Table I.

[5]Although the introduction of a parameter A is a mathematical artifice, there may be additional *physical* justification if the dielectric screening (which is frequency and wavelength dependent) affects the two-body (repulsive) potential differently from the one-body forces.

C. Three bosons

The case of three identical particles in a state symmetric under permutations is the simplest of the three-body problems. It lends itself to a reasonably complete analysis (Mattis and Rudin, 1984; Rudin, 1984). While interesting in its own right (e.g., for the binding or scattering of three magnons or three phonons), the steps leading from the analysis of $n=2$ to 3 to 4, etc., particles are presumed helpful in the ultimate understanding of the N-body problem.

We treat the three-body bound states and the scattering states separately, starting with the bound states, which take on the form

$$|\Psi_\beta\rangle=(1/N)\sum F(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\,|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle\ . \tag{3.1}$$

The label (β) serves to distinguish these discrete states when there are several of them. We suppress it for typographical simplicity in what follows. The total momentum $\mathbf{P}=\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3\ (\mathrm{mod}\mathbf{K}_n)$ is also a good quantum number, labeling each eigenstate in the cases of interactions which preserve the discrete translational symmetries of the lattice. The band energies (KE) for the three identical particles at $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_3$ are

$$E(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)=\varepsilon(\mathbf{k}_1)+\varepsilon(\mathbf{k}_2)+\varepsilon(\mathbf{k}_3)\ , \tag{3.2}$$

where the one-body energies are presumed to have their minima $\varepsilon(\mathbf{k})=0$ at $\mathbf{k}=\mathbf{0}$, as in the example of Eq. (2.6). Thus the energy eigenvalues E are negative for bound states and positive for scattering solutions. An additional feature concerns the states in which two particles are bound and one is free; these also may have negative E, although they are not three-body bound states and cannot be written in the form (3.1) with a continuous amplitude F. We shall deal with those later.

The two-body forces scatter each pair individually. Thus

$$(\mathscr{H}-E)\,|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle=[E(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)-E]\,|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle+(g/N)\sum_{\mathbf{k}}V(\mathbf{k})[\,|\mathbf{k}_1+\mathbf{k},\mathbf{k}_2-\mathbf{k},\mathbf{k}_3\rangle$$
$$+\,|\mathbf{k}_1+\mathbf{k},\mathbf{k}_2,\mathbf{k}_3-\mathbf{k}\rangle+|\mathbf{k}_1,\mathbf{k}_2+\mathbf{k},\mathbf{k}_3-\mathbf{k}\rangle]\ . \tag{3.3}$$

One obtains equations for the amplitudes (F's) by making use of the Schrödinger equation $(\mathscr{H}-E)\,|\Psi\rangle=0$:

$$\langle\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\,|\,\mathscr{H}-E\,|\,\Psi\rangle=0\ , \tag{3.4}$$

which yields

$$F(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)[E(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)-E]+(g/N)\sum_{\mathbf{k}}V(\mathbf{k})[F(\mathbf{k}_1+\mathbf{k},\mathbf{k}_2-\mathbf{k},\mathbf{k}_3)+F(\mathbf{k}_1+\mathbf{k},\mathbf{k}_2,\mathbf{k}_3-\mathbf{k})+F(\mathbf{k}_1,\mathbf{k}_2+\mathbf{k},\mathbf{k}_3-\mathbf{k})]=0\ . \tag{3.5}$$

If the lattice is in three dimensions, this is an integral equation in six dimensions, down from nine by conservation of momentum.[6] We make use of the permutation symmetry $F(\mathbf{a},\mathbf{b},\mathbf{c})=F(\mathbf{b},\mathbf{a},\mathbf{c})=\cdots=F(\mathbf{c},\mathbf{b},\mathbf{a})$ to rewrite the above in the form

$$F(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)[E(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)-E]$$
$$+[J(\mathbf{k}_1;\mathbf{k}_3)+J(\mathbf{k}_3;\mathbf{k}_2)+J(\mathbf{k}_2;\mathbf{k}_1)]=0\ , \tag{3.6}$$

where[7]

$$J(\mathbf{k}_1;\mathbf{k}_2)\equiv(g/N)\sum_{\mathbf{k}}V(\mathbf{k}-\mathbf{k}_1)F(\mathbf{k},\mathbf{k}_2,\mathbf{P}-\mathbf{k}-\mathbf{k}_2)\ . \tag{3.7}$$

Subject to mild restrictions (see footnote 7) on the functional forms of V and F, one finds

$$J(\mathbf{k}_1;\mathbf{k}_3)=J(\mathbf{k}_2;\mathbf{k}_3),\quad J(\mathbf{k}_2;\mathbf{k}_1)=J(\mathbf{k}_3;\mathbf{k}_1)\ ,$$
$$J(\mathbf{k}_1;\mathbf{k}_2)=J(\mathbf{k}_3;\mathbf{k}_2)\ .$$

Thus there are three distinct J's and three coupled integral equations [each of type (3.7), with F given in (3.6)] with which to solve for the allowed three-body bound state energies E and corresponding amplitudes F. As $E<0$ in these states, we define $W\equiv-E=$binding energy ≥ 0. We start the analysis with the zero-range attractive interaction, $gV(\mathbf{k})=-U$, constant in $\mathbf{k}$. $J(\mathbf{k}_1;\mathbf{k}_2)$ then ceases to depend on the first variable, and we write it as a function of the second variable alone, $J(\mathbf{k}_2)$. The integral equations [(3.6) and (3.7)] become

$$J(\mathbf{k}_2)=(U/N)\sum_{\mathbf{k}}[J(\mathbf{k}_2)+J(\mathbf{k})+J(\mathbf{P}-\mathbf{k}-\mathbf{k}_2)]$$
$$\times[E(\mathbf{k},\mathbf{k}_2,\mathbf{P}-\mathbf{k}-\mathbf{k}_2)+W]^{-1}\ . \tag{3.8}$$

The symmetry of the denominator allows one to substi-

[6] In the continuum theories, conservation of angular momentum and special transformations of coordinates serve to simplify the equations further, although the generality is subsequently spoiled by the need to choose separable (and unphysical) two-body interactions (Amado, 1972; Phillips, 1977). Unfortunately, aside from the delta-function interaction, we have found no such simplifications in the lattice theory.

[7] We eliminate $\mathbf{k}_3$ by conservation of momentum and assume that $V(\mathbf{k})$ in the first Brillouin zone, as well as the F's, are periodically repeated in the second, third, etc., zones (as is automatically the case for all properly defined lattice functions). This property, unlike the usual cutoffs, affords the convenience of arbitrary changes in the origin of the integrations. We also assume $V(-\mathbf{k})=V(\mathbf{k})$ whenever convenient.

tute $J(\mathbf{k})$ for $J(\mathbf{P}-\mathbf{k}-\mathbf{k}_2)$ in the numerator. Combining the terms in $J(\mathbf{k}_2)$ we obtain

$$J(\mathbf{k}_2)[1-UI_W(\mathbf{k}_2)] = (2U/N)\sum_{\mathbf{k}} J(\mathbf{k})/[E(\mathbf{k},\mathbf{k}_2,\mathbf{P}-\mathbf{k}-\mathbf{k}_2)+W] . \tag{3.8'}$$

Finally, defining $S(\mathbf{k}_2)=J(\mathbf{K}_2)[1-UI_W(\mathbf{k}_2)]^{1/2}$, we obtain

$$S(\mathbf{k}_2)=(2U/N)\sum_{\mathbf{k}} S(\mathbf{k})\{R_W(\mathbf{k})R_W(\mathbf{k}_2) \times[E(\mathbf{k},\mathbf{k}_2,\mathbf{P}-\mathbf{k}-\mathbf{k}_2)+W]\}^{-1} , \tag{3.9}$$

where

$$R_W(\mathbf{k}_2)\equiv[1-UI_W(\mathbf{k})]^{1/2} ,$$
$$I_W(\mathbf{k}_2)\equiv(1/N)\sum_{\mathbf{k}} 1/[E(\mathbf{k},\mathbf{k}_2,\mathbf{P}-\mathbf{k}-\mathbf{k}_2)+W] . \tag{3.10}$$

I_W is a generalized "Watson's integral" (Joyce, 1972; Glasser, 1972). It is related to the lattice Green's functions (Katsura *et al.*, 1971). The derivation of Eq. (3.9) could have been performed starting with $J(\mathbf{k}_1)$ or $J(\mathbf{k}_3)$; it is thus valid for any $\mathbf{k}$, and we rewrite it in a more "natural" form,

$$S(\mathbf{k})=(2U/N)\sum_{\mathbf{q}} S(\mathbf{q})/R_W(\mathbf{k})R_W(\mathbf{q})[E(\mathbf{q},\mathbf{k},\mathbf{P}-\mathbf{q}-\mathbf{k})+W]$$
$$=(2U/\Omega)\int d^3q\, S(\mathbf{q})/R_W(\mathbf{k})R_W(\mathbf{q})[E(\mathbf{q},\mathbf{k},\mathbf{P}-\mathbf{q}-\mathbf{k})+W] \tag{3.11}$$

or, more symbolically, in the form of an integral equation, $\lambda\mathbf{S}=\mathbf{K}\cdot\mathbf{S}$, where

$$K_{\mathbf{kq}}=(2U/\Omega)\{R_W(\mathbf{k})R_W(\mathbf{q})[E(\mathbf{q},\mathbf{k},\mathbf{P}-\mathbf{q}-\mathbf{k})+W]\}^{-1} \tag{3.11'}$$

subject to $\lambda=1$. This kernel is positive, invariant under the cubic group O_h, and compact (integrable) except in the neighborhood of $R_W(\mathbf{k})\to 0$, i.e., where the two-body bound states just start to appear.[8] [The discovery of an infinite number of Efimov states (Efimov, 1970) near this threshold starts with the observation of such a divergence related to a "resonance" in the two-body spectrum.] We also note that if the binding energy W for three bodies is less than for two-body bound states, $R_W(\mathbf{k})$ can become imaginary—causing the integral equation to fail to have any acceptable solutions. We therefore seek bound states in the region $W>$ binding energy of two-particle states.

The integral equation (3.11') is unusual, in that the eigenvalue λ is always set equal to 1, while the usual eigenvalue in quantum theory, the energy parameter W, appears nonlinearly (in R as well as in the explicit denominator.) Nor does any simplification result from fixing W and varying U, as the latter also appears nonlinearly in a number of places. Thus numerical solution for $W(U)$ is required. There are at least two systematic approaches to this: (1) expansion of $S(k)$ in cubic harmonics (Bethe and von der Lage, 1947), (2) "strong coupling" expansion of kernel in powers of $(W+b)^{-1}$, where b is a fixed constant. The first converges faster and is numerically more accurate—the binding energies are obtained to $O(1\%)$. The second, when the expansion is carried out to leading terms, is only tolerably accurate (a few percent accuracy), but qualitatively and intuitively more useful than the first.

To proceed, we must fix the unit of energy, related to the one-particle bandwidths in Eq. (3.2). In one dimension, we shall take $\varepsilon(k)=1-\cos k$, in two dimensions $\varepsilon(\mathbf{k})=2-\cos k_x-\cos k_y$, and in three dimensions

$$\varepsilon(\mathbf{k})=3-\cos k_x-\cos k_y-\cos k_z . \tag{3.12}$$

Consider the case of three dimensions and the (strong coupling) expansion

$$1/(\varepsilon+W)=1/(W+3) +(\cos k_x+\cos k_y+\cos k_z)/(W+3)^2 +\cdots . \tag{3.13}$$

Note that such expansions converge absolutely, are efficient under an integral sign (many of the trigonometric terms are projected out, or are small), and are tantamount to considering the motion of the particle on the lattice as a sort of perturbation. *They are unique to lattice physics*: in continuum theory, $\varepsilon\approx\mathbf{k}^2$ and no similar expansion exists.

The expansion in harmonics also demonstrates the essentially localized nature of the bound-state problem. Upon lattice Fourier transformation, Eq. (3.11') takes on the aspect (Rudin, 1984)

$$\lambda\Psi(\mathbf{R}_i)=\sum_J K(\mathbf{R}_i\,|\,\mathbf{R}_j)\Psi(\mathbf{R}_j) . \tag{3.14}$$

The real (lattice) space kernel $K(\mathbf{R}\,|\,\mathbf{R}')$ is

$$K(\mathbf{R}\,|\,\mathbf{R}')=(1/\Omega^2)\int\int d^3k\, d^3q\, K_{\mathbf{kq}}e^{i(\mathbf{q}\cdot\mathbf{R}'-\mathbf{k}\cdot\mathbf{R})} . \tag{3.14a}$$

It also is a nonlinear function of W and U; $W(U)$ has to be adjusted to yield the desired eigenvalue $\lambda=1$ and corresponding eigenfunction Ψ. The method of expansion follows upon the realization that (with some exceptions) K decreases rapidly as each R_i and R_j increases from 0, also varying with the distance R_{ij} between them. Thus a first approximation yields $K(\mathbf{0}\,|\,\mathbf{0})=1$, from which we obtain

[8] Compare $R_W=0$ with the equation for two-body bound states (2.9), when $-gV=U$ and, as a consequence, $F(k)=$const.

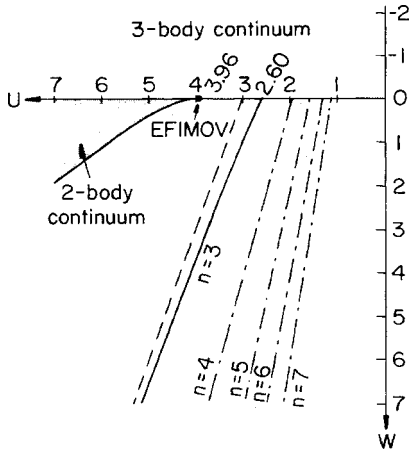

FIG. 2. Binding energy W of n-body bound state vs strength U of an attractive two-body potential in three dimensions. The shaded three-body continuum represents free particles, the shaded two-body continuum represents two-particle bound states with one (or more) free particle. The fundamental three-boson bound state labeled $n=3$ is asymptotic to the straight dashed line of slope 3. The excited bound state and/or "Efimov states" all lie within a point of radius 0.1 at the "tricritical point" $U_c(2)=3.96$. There are no three-fermion bound states for this zero-range interaction. Dot-dashed lines labeled $n=4,5,6,7$ are binding energies estimated from scaling arguments, with $U_c(n)\approx 7.92/n$. From Mattis and Rudin, 1984.

a first estimate of $W(U)$. If we now also retain some smaller terms[9] $K(0\,|\,\delta_j)$, the secular determinant obtained from Eq. (3.14) yields a more accurate equation:

$$K(0\,|\,0)+6\,|\,K(0\,|\,\delta_j)\,|^2=1\ . \tag{3.15}$$

In iteratively adjusting W to satisfy such equations, we are obliged to evaluate six-dimensional integrals (3.14a) at *each step* of the iteration. This causes conflicting requirements of accuracy: if integrations take too many steps, there is not sufficient time for small-step iterations. If the integrals are inaccurate, it does not help to be able to take small increments in W. Finally, one must determine the number of shells to be retained in successive improvements of (3.15)—each successive shell brings in a larger number of ever smaller integrals. Fortunately, the Korobov-Hlawaka "quasi-Monte Carlo" procedure (Korobov, 1963) offers an efficient method for evaluating precisely the type of integrals we need. This method (reviewed in English by Stroud, 1971) takes advantage of periodicity in the integrands[10] to evaluate integrals with high precision, and, ultimately, this is what renders our procedures practical.

In the case of the strong coupling expansion, the expansion parameter is $(W+9)^{-1}$ for three particles, rather than $(W+3)^{-1}$ as indicated in Eq. (3.13). Thus convergence is more rapid than it might have seemed at first sight. [It may be even more rapid for $n>3$ particles or in $d>3$ dimensions, where the expansion parameter is $(W+nd)^{-1}$ for n particles in d dimensions, allowing relatively primitive strong coupling methods to "... work far better than they ought," as we shall argue below.]

In the accompanying figures we show graphically a summary of the original results (Mattis and Rudin, 1984). The numerical and error analysis, with additional commentary, are to be found in Rudin (1984). In Fig. 2, the three-body binding energy in three dimensions is plotted (solid curve). The infinite number of Efimov states have energies all lying within the indicated dot.

Although the estimates for $n=4,5,\ldots$ (dot-dashed curves) come from scaling-type arguments, they agree very well with zeroth-order strong coupling analysis of the respective bound-state equations (*vide infra*).

Figure 3 shows the binding curve or three bosons in $d=2$ dimensions. (As in one dimension, there is always a bound state for potentials in two dimensions, provided merely they are attractive on balance.)

The surprise comes in Fig. 4, which indicates that at threshold, the three-body bound state in three dimensions is formed discontinuously. (While the total binding energy W increases smoothly from zero as U is increased beyond threshold, its constituent KE and PE jump to opposite, finite values at threshold.) This is the consequence of the finite slope (recall Feynman's theorem) of $W(U)$ at U_c, and is found to be a property of all $n\geq 3$ particle bound states for all dimensions $d\geq 3$ (and, conceivably, for $n\geq 4$ in two dimensions,[11] although this has not yet been established).

Finite KE at threshold indicates that when the bound state forms, it has finite size [and presumably, a total mass M greatly in excess of the effective-mass value, $M\gg nm$; the first study of the dependence of M on U for three-body complexes has been undertaken only recently (Rudin, 1985b), and much remains to be done].

Because the maximum size at threshold is finite, es-

[9] δ_j may be any of the six nearest neighbors of 0; by symmetry, at $\mathbf{P}=0$ all six $K(0\,|\,\delta_j)$ are equal to each other and to their conjugates $K(\delta_j\,|\,0)$.

[10] In our case, the periodicity exists in $\mathbf{k}$ space (from Brillouin zone to Brillouin zone,) so that, in practice, we carry out our procedures in reciprocal space and not in "direct" (lattice) space.

[11] The failure of Eq. (3.17) to predict the correct U_c for $n=2$ (it yields $U_c=6$, far from the correct value 3.96) is just further evidence that, unlike $n\geq 3$, the bound-state threshold for the two-body problem is not yet in the strong coupling limit in three dimensions. One estimates the number of dimensions at which the two-body problem becomes strongly coupled at threshold by calculating when the threshold KE_c becomes finite. If U_c is finite (as it must be for short-range forces in $d>2$ dimensions), then $\mathrm{KE}_c\propto dW/dU\,|_{W=0}$, i.e., both are finite or both vanish. It is simple to see that the latter is proportional to $(\int dk\,k^{d-5})^{-1}$, with $0<k<k_{\mathrm{cutoff}}$, so that $\mathrm{KE}_c=0$ for $d\lesssim 4$ and is finite for $d>4$. It follows that the strong coupling expansions will converge even for the two-body problem, on lattices in $d>4$ dimensions. A rigorous analysis of such questions has been given by Klaus and Simon (1980) in the continuum theory (i.e., in the EMA for lattice theories).

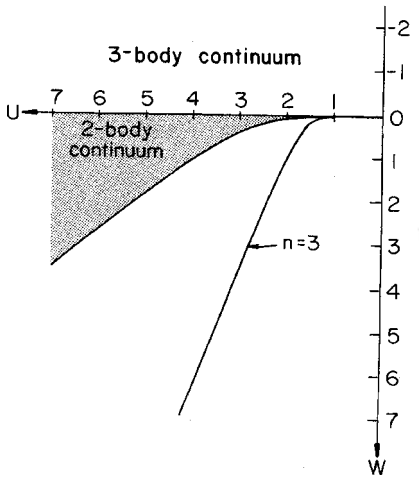

FIG. 3. Binding energy W vs strength of an attractive two-body potential U in two dimensions. Here, all thresholds for $n \geq 2$ are $U_c(n)=0$. There is no Efimov point in two dimensions, nor have three-fermion bound states been found for any value of the zero-range interactions (Rudin, 1985a).

timated at no more than two lattice constants, the bound state of $n \geq 3$ particles is borne into the strong coupling regime. (By way of comparison, at threshold, the two-body bound state is infinitely large; crossover to strong coupling occurs at $W \gg 1$.) Now, let us recall the variational ansatz for the Frenkel exciton, Eq. (2.4), which was

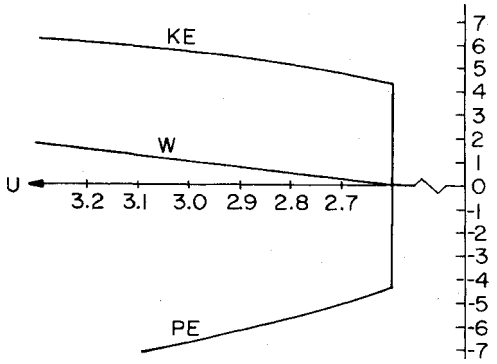

FIG. 4. Kinetic and potential energies in the three-body bound state vs strength U of an attractive two-body potential in three dimensions (Mattis and Rudin, 1984). As U is increased (note break in horizontal scale) the three-boson threshold is approached at $U_c(3)=2.60$. There, the kinetic and potential energies jump discontinuously, although their algebraic sum (W) grows continuously from 0. Finite kinetic energy at threshold implies that the bound state has a small size (estimated at $\lesssim 2$ lattice constants at threshold and decreasing to 0 with increasing U). While appearing anomalous, such discontinuity is in fact a normal consequence of finite-range forces and of lack of available phase space near $k=0$, occurring for bound states of $n \geq 2$ particles in $d \geq 2$ dimensions, provided (by extension of the arguments in footnote 11) that $nd > 8$.

found to be reasonably accurate in the strong coupling limit, and let us use it to estimate the binding energy for $n \geq 3$ in $d \geq 3$ dimensions. The quantity $\langle E_1 \rangle = d$ for hypercubic lattices in d dimensions. Thus, on such lattices, the variational procedure yields estimates of the binding energy W,

$$W \approx -(\mathrm{PE}_{\min}) - nd \quad (n,d \text{ both} \geq 3) \tag{3.16}$$

for arbitrary interactions. Comparison with the zero-range calculations is encouraging; there, Eq. (3.16) in three dimensions reduces to

$$W \approx \tfrac{1}{2} n(n-1)U - 3n \ , \tag{3.17}$$

which, for $W=0$ threshold, yields $U_c = 6/(n-1)$. These estimated values ($U_c=3$ for $n=3$,2 for $n=4,\ldots,6/n$ for $n \to \infty$) agree quite satisfactorily with the exact value 2.60 for $n=3$ and remarkably well with the values shown in Fig. 2 (see footnote 11), obtained from quite independent arguments (Rudin, 1984) for $n \geq 4$. The slopes at $W > 0$ are given by $dW/dU = (1/2)n(n-1)$.

For nearest-neighbor interactions $-U_1$ (and hard-core zero-range repulsion), the minimum potential energy for use in Eq. (3.16) is that of a compact "solid droplet." Neglecting surface terms, for $n \gg 2d$ the potential energy of an n-particle solid rapidly approaches $-nU_1 d$; thus

$$W \approx nU_1 d - nd \quad \text{(nearest-neighbor attraction)} \ , \tag{3.18}$$

and $U_{1c} \approx 1$ independent of n,d (when $n \gg 2d \gg 1$). Because of the hard cores forcing particles to be a finite distance apart, in this case the energy is extensive, the energy per particle, $W/n = d(U-1)$, is finite and, unlike the zero-range attraction, this model has a proper thermodynamic limit. For n not so large, where many of the particles are at the surface of a solid droplet of small radius, one should estimate W more closely by studying the "surface particles" more carefully.

D. Fermions

Obviously, zero-range interactions have no effects on spinless fermions, nor among fermions of parallel spin, as Ψ always vanishes where the interaction is nonzero. But, surprisingly, even *with* spin there are no bound states relative to two bound fermions and one free particle, for three fermions. In strong coupling, this result can be seen to be a direct consequence of the lack of binding of trions made of particles of equal mass (substitute fermion of spin "up" for hole, fermion of spin "down" for electron, in Sec. III.A above, or in Schilling and Mattis, 1982). It is less obvious in weak coupling.

An integral equation for the bound state of three fermions can be obtained by analogy with the bosons. The wave functions are totally antisymmetric in space and spin, but as spin does not occur in H, we can deal with functions in direct-lattice (or reciprocal) space alone. For each irreducible representation of the permutation group S_3 there is a corresponding Young tableau. We have al-

ready argued that the eigenstates that can be written as one-column Young tableaux, partners of the states of spin $\frac{3}{2}$ (all spins up), cannot "feel" the zero-range interactions. Turning to the space functions transforming as two-column Young tableaux, we observe that the totally symmetric function $F(k_1,k_2,k_3)$ in Eq. (3.1) is here replaced by a function $F(k_1,k_2\,|\,k_3)$, symmetric (or antisymmetric) in the first two variables, but not in all three. After algebraic manipulations mirroring Eqs. (3.2)–(3.9), for the soluble case of the delta-function attractive potential $-U$ we finally obtain an integral equation quite similar to Eq. (3.11'), albeit with significant changes:

$$\lambda\mathbf{S}=\mathbf{K}\cdot\mathbf{S}\ ,$$

where

$$K_{\mathbf{kq}}=-(U/\Omega)\{R_W(\mathbf{k})R_W(\mathbf{q})[E(\mathbf{q},\mathbf{k},\mathbf{P}-\mathbf{k}-\mathbf{q})+W]\}^{-1} \tag{3.19}$$

subject to $\lambda=1$. All our investigations have led to the conclusion that, whatever the choice of U and $W>0$, outside of the region of two-body bound states one has $\lambda<1$, and therefore this equation can never be satisfied.

This can be seen qualitatively through the expansion of the denominator:

$$[E(\mathbf{q},\mathbf{k},\mathbf{P}-\mathbf{k}-\mathbf{q})+W]^{-1} =(9+W)^{-1}+[C(\mathbf{q})+C(\mathbf{k}) +C(\mathbf{P}-\mathbf{K}-\mathbf{q})](9+W)^{-2}+\cdots\ , \tag{3.20}$$

where $C(\mathbf{k})\equiv\cos k_x+\cos k_y+\cos k_z$. If we just retain these leading terms in the expansion, we see that $K_{\mathbf{kq}}$ is the sum of seven separable kernels—the term in $(9+W)^{-1}$ and the six summarized by $C(\mathbf{k})+C(\mathbf{q})$—plus the following separable kernels which we shall discuss individually:

$$-(U/\Omega)[R_W(\mathbf{k})R_W(\mathbf{q})(9+W)^2]^{-1}[\cos(P_x/2-k_x)\cos(P_x/2-q_x)+\cdots+\cos(P_z/2-k_z)\cos(P_z/2-q_2) -\sin(P_x/2-k_x)\sin(P_x/2-q_x)+\cdots+\sin(P_z/2-k_z)\sin(P_z/2-q_z)]\ . \tag{3.21}$$

The aforementioned first seven terms plus the first three in Eq. (3.21) all yield intrinsically negative contributions to λ. The only possible positive contributions to λ are those arising from the last three terms involving the sine functions in (3.21). Taking $S(\mathbf{k})$ to be "p wave," i.e.,

$$S(\mathbf{k})=\sin k_\alpha/R_W(\mathbf{k})\ , \tag{3.22}$$

where $\alpha=x$, y, or z, we find that 12 of the 13 separable kernels vanish, with the remaining one yielding

$$\lambda=U(9+W)^{-2}T(U,W)\ , \tag{3.23}$$

where T is an integral:

$$T(U,W)=(1/\Omega)\int d^3q\,\sin^2q_x[1-UI_W(\mathbf{q})]^{-1} \tag{3.24}$$

and I given in Eq. (3.10). Near the curve $W_2(U)$ that designates the threshold for two-body bound-state formation (given by the vanishing of the denominator, $1-UI=0$), numerical evaluation indicates the right-hand side of Eq. (3.23) to be always <1. [The likeliest candidate for a solution is the neighborhood of the Efimov point, $W=0$, $U=3.96$. But, because of the numerator $\sin^2q$, T remains finite at this point while $U(9+W)^{-2}$ is quite small there, $3.96/81=0.049$. Thus it is theoretically possible, but seemingly unlikely, that a three-fermion bound state exists in the immediate neighborhood of the Efimov point.] Far from this region, $T<\frac{1}{2}$ and we estimate the right-hand side to be always <0.04. Thus, within the expansion (3.20), we are unable to obtain $\lambda=1$, as required in a bound state. In two dimensions, similar calculations exclude such bound states at small U, while in one dimension Bethe's ansatz allows exact analysis which here precludes three-fermion bound states for all U (Takahashi, 1970; also discussed by Rudin, 1984). Finally, to the extent that all U in $d\geq 4$ can be considered strong coupling, by analogy with the trion we conclude: *no binding.* In conclusion, we remark that while this shows the BCS concept of "Cooper pairs" (as a stable composite particle of fermions with attractive forces) to be a sound idea in all dimensions, it does not necessarily exclude formation of composite Cooper-pair molecules. This problem remains open at the time of writing.

IV. SCATTERING THEORY

For repulsive potentials, all low-lying states lie in the continuum. Even for attractive forces, most states lie there too. We can immediately see the complications arising in the latter case by comparing two possible scattering events.

(1) A bound two-particle state $|\Psi_\beta\rangle$ *[e.g., Eq. (2.8)], momentum* $\mathbf{P}$*, scatters from a third particle.* Ignoring permutation symmetry for the moment, the (exact) scattering states $|\beta,\mathbf{k}_3)$ are of the general form

$$|\beta(\mathbf{P}),\mathbf{k}_3)=|\beta(\mathbf{P}),\mathbf{k}_3\rangle+(1/N)\sum F_{0\beta}(\mathbf{q})\,|\beta(\mathbf{P}+\mathbf{q}),\mathbf{k}_3-\mathbf{q}\rangle +(1/N)\sum[F_{1\gamma}(\mathbf{q})\,|\gamma(\mathbf{k}_2+\mathbf{k}_3+\mathbf{q}),\mathbf{k}_1-\mathbf{q}\rangle+F_{2\gamma}(\mathbf{q})\,|\gamma(\mathbf{k}_1+\mathbf{k}_3+\mathbf{q}),\mathbf{k}_2-\mathbf{q}\rangle+F_{3\gamma}(\mathbf{q})\,|\gamma(\mathbf{k}_1+\mathbf{k}_2+\mathbf{q}),\mathbf{k}_3-\mathbf{q}\rangle] +1/N^2\sum\sum\sum F(\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3')\delta(\mathbf{k}_1'+\mathbf{k}_2'+\mathbf{k}_3'-\mathbf{P}-\mathbf{k}_3)\,|\,\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3'\rangle\ , \tag{4.1}$$

with sums over all two-particle states (γ) and various wave vectors.

(2) Three particles scatter. The incoming state is what, in the preceding expression, was one of the scattered components. Again, without regard to permutation symmetry, the general eigenstate of this type is

$$|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle = |\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle + (1/N)\sum[F_{1\beta}(\mathbf{q})\,|\,\beta(\mathbf{k}_2+\mathbf{k}_3+\mathbf{q}),\mathbf{k}_1-\mathbf{q}\rangle + F_{2\beta}(\mathbf{q})\,|\,\beta(\mathbf{k}_1+\mathbf{k}_3+\mathbf{q}),\mathbf{k}_2-\mathbf{q}\rangle + F_{3\beta}(\mathbf{q})\,|\,\beta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{q}),\mathbf{k}_3-\mathbf{q}\rangle] + 1/N^2\sum\sum\sum F(\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3')\delta(\mathbf{k}_1'+\mathbf{k}_2'+\mathbf{k}_3'-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)\,|\,\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3'\rangle\ . \tag{4.2}$$

As Faddeev has shown in the continuum theories (Faddeev, 1960; Lovelace, 1964), care must be taken to sort out the various scattering channels. Permutation symmetry must also be included in the above, if the "particle-exchange" scatterings are to be correctly incorporated. (Details can be found in recent books on scattering theory, e.g., Joachain, 1975.) It is unlikely that lattice physics simplifies the problem in general, as our lack of conservation of angular momentum is not helpful. As usual, however, the one remarkably simplifying exception is the delta-function interaction. We concentrate on it in the following analysis.

We assume two-body point interactions of strength U (here $U>0$ for repulsive forces and $U<0$ for attractive),

$$\mathscr{H}' = (U/2)\sum_i \sum_{j\neq i} \delta(\mathbf{R}_i-\mathbf{R}_j) \tag{4.3}$$

and the absence of two-body bound states β. The scattering-state equations are least formidable in appearance when applied to the case of bosons labeled by $\mathbf{k}_1=\mathbf{k}_2=\mathbf{k}_3=\mathbf{P}=0$. (The related eigenvalue is automatically symmetric under permutations.) The calculations of scattering amplitudes and energy E_0 are as follows:

$$(\mathscr{H}-E_0)\,|\,000\rangle = (3U/N-E_0)\,|\,000\rangle + (U/N)\sum_{\mathbf{k}}[\,|\,\mathbf{k},-\mathbf{k},0\rangle + |\,0,\mathbf{k},-\mathbf{k}\rangle + |\,-\mathbf{k},0,\mathbf{k}\rangle]\ , \tag{4.4a}$$

$$(\mathscr{H}-E_0)\,|\,\mathbf{k},-\mathbf{k},0\rangle = (U/N)\,|\,000\rangle + [2\varepsilon(\mathbf{k})+3U/N-E_0]\,|\,\mathbf{k},-\mathbf{k},0\rangle + (U/N)[\,|\,-\mathbf{k},\mathbf{k},0\rangle + |\,0,-\mathbf{k},\mathbf{k}\rangle + |\,\mathbf{k},0,-\mathbf{k}\rangle] + (U/N)\sum_{\mathbf{k}'\neq 0,\mathbf{k}}[\,|\,\mathbf{k}',-\mathbf{k}',0\rangle + |\,\mathbf{k}-\mathbf{k}',-\mathbf{k},\mathbf{k}'\rangle + |\,\mathbf{k},-\mathbf{k}+\mathbf{k}',-\mathbf{k}'\rangle]\ , \tag{4.4b}$$

and

$$(\mathscr{H}-E_0)\,|\,\mathbf{k}-\mathbf{k}';-\mathbf{k},\mathbf{k}'\rangle = (U/N)[\,|\,0,-\mathbf{k},\mathbf{k}\rangle + |\,0,-\mathbf{k}',\mathbf{k}'\rangle + |\,-\mathbf{k}',0,\mathbf{k}'\rangle + |\,\mathbf{k}-\mathbf{k}',0,\mathbf{k}'-\mathbf{k}\rangle + |\,\mathbf{k},-\mathbf{k},0\rangle + |\,\mathbf{k}-\mathbf{k}',\mathbf{k}'-\mathbf{k},0\rangle] + [\varepsilon(\mathbf{k})+\varepsilon(\mathbf{k}')+\varepsilon(\mathbf{k}-\mathbf{k}')+3U/N-E_0]\,|\,\mathbf{k}-\mathbf{k}',-\mathbf{k},\mathbf{k}'\rangle + (U/N)[\,|\,-\mathbf{k},\mathbf{k}-\mathbf{k}',\mathbf{k}'\rangle + |\,\mathbf{k}',-\mathbf{k},\mathbf{k}-\mathbf{k}'\rangle + |\,\mathbf{k}-\mathbf{k}',\mathbf{k}',-\mathbf{k}\rangle] + (U/N)\sum_{\mathbf{k}''}{}'[\,|\,\mathbf{k}-\mathbf{k}'',-\mathbf{k},\mathbf{k}''\rangle + |\,-\mathbf{k}'-\mathbf{k}'',\mathbf{k}'',\mathbf{k}'\rangle + |\,\mathbf{k}-\mathbf{k}',\mathbf{k}'',\mathbf{k}'-\mathbf{k}-\mathbf{k}''\rangle]\ , \tag{4.4c}$$

where a prime over the last sum indicates that $\mathbf{k}''$ must avoid those points that have already been explicitly included in preceding terms (e.g., $\neq\mathbf{k},\mathbf{k}'$, etc.). We now write the scattering eigenstate $|\,\Psi_0\rangle$ as follows:

$$|\,\Psi_0\rangle = |\,000\rangle + (1/N)\sum\mathscr{L}(\mathbf{k})[\,|\,-\mathbf{k},\mathbf{k},0\rangle + |\,0,-\mathbf{k},\mathbf{k}\rangle + |\,\mathbf{k},0,-\mathbf{k}\rangle] + (1/N^2)\sum\sum\sum\mathscr{M}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\delta(\mathbf{k}_1+\mathbf{k}_3+\mathbf{k}_3)\,|\,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle\ . \tag{4.5}$$

We note that $\varepsilon(k)$ is given in Eq. (3.12) and that the (unsymmetrized) states $|\,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle$ are shorthand for normalized plane-wave product states: $N^{-3/2}\exp i(\mathbf{k}_1\cdot\mathbf{R}_1 + \mathbf{k}_2\cdot\mathbf{R}_2+\mathbf{k}_3\cdot\mathbf{R}_3)$. The eigenstate Ψ_0 will belong to whichever symmetry class is chosen for the incoming wave (in this case, totally symmetric, corresponding to spinless boson statistics).

The coefficients $(\mathscr{L},\mathscr{M})$ are obtained through the Schrödinger equation, which is reformulated into the statement: *the right-hand sides of Eqs. (4.4a)—(4.4c) are orthogonal to* $|\,\Psi_0\rangle$. Applied to Eq. (4.4a), this statement implies

$$E_0 = 3/N\left[U\left[1+(1/N)\sum\mathscr{L}(\mathbf{k})\right]\right]\ . \tag{4.6a}$$

If we proceeded straight to the thermodynamic limit, there would be no effects of the scattering, and $E_0=0$. The interesting effects are $O(1/N)$ and even $O(1/N^2)$. [For n particles, the above expression is simply modified by replacing the prefactor $3/N$ by $n(n-1)/2N$; the value of the function $\mathscr{L}$ is also affected, but only to $O(n/N)$. To see precisely how, one compares the solutions of Eqs. (2.6)—(2.9) ($n=2$) with those for $n=3$.] We now proceed with Eq. (4.4b):

$$0=U+[2\varepsilon(\mathbf{k})+6(U/N)-E_0]\mathscr{L}(\mathbf{k}) +(U/N)[\sum_{k'}\mathscr{L}(\mathbf{k}')]+(U/N)[\mathscr{S}(-\mathbf{k})+\mathscr{S}(\mathbf{k})] , \tag{4.6b}$$

where

$$\mathscr{S}(\mathbf{k})\equiv(1/N)\sum_{k'}\mathscr{M}(\mathbf{k}'-\mathbf{k},\mathbf{k},-\mathbf{k}') .$$

The equivalent for $n=2$ is $0=U+[2\varepsilon(\mathbf{k})+(U/N)-E_0]L(\mathbf{k})+[(U/N)\sum_{\mathbf{k}'}L(\mathbf{k}')]$. We have used the invariance of $\mathscr{M}$ under permutations to arrive at Eq. (4.6b), as we now do to obtain the last equation, from (4.4c):

$$\begin{aligned}0=&2U[\mathscr{L}(\mathbf{k})+\mathscr{L}(\mathbf{k}')+\mathscr{L}(\mathbf{k}-\mathbf{k}')]\\&+[\varepsilon(\mathbf{k})+\varepsilon(\mathbf{k}')+\varepsilon(\mathbf{k}-\mathbf{k}')\\&\quad+6U/N-E_0]\mathscr{M}(\mathbf{k}-\mathbf{k}',-\mathbf{k},\mathbf{k}')\\&+U[\mathscr{S}(\mathbf{k}')+\mathscr{S}(-\mathbf{k})+\mathscr{S}(\mathbf{k}-\mathbf{k}')] .\end{aligned} \tag{4.6c}$$

If we neglect terms $O(1/N)$ in (4.6b) (i.e., let $\mathscr{L}=L$), we trivially obtain

$$\mathscr{L}(\mathbf{k})=-U[1+UI_0]^{-1}/2\varepsilon(\mathbf{k}) ,$$

where (4.7)

$$I_0=(1/\Omega)\int d^3k\,[2\varepsilon(\mathbf{k})]^{-1} .$$

Insertion of this into Eq. (4.6c) yields an inhomogeneous integral equation for $\mathscr{M}$, hence $\mathscr{S}$, and, together with Eq. (4.7), determines Ψ_0.

As long as there is no three-body bound state, Eq. (4.6a) yields the ground-state energy of three particles. By assumption following Eq. (4.3), $U>-3.96$, and the denominator $(1+UI_0)$ cannot vanish. It follows *a fortiori* that it cannot vanish for $U>-2.60$, the three-body threshold.

In principle, one can study the scattering states of $n\geq 3$ *fermions* by similar means. [The relevant Hamiltonian of hopping electrons interacting by zero-range, two-body repulsive forces, originally investigated by Hubbard (1963), now bears his name.] Starting from $|F\rangle$, the "Fermi sea" for $n\uparrow$ fermions of spin up and $n\downarrow$ fermions of spin down, one writes the expansion for an exact eigenstate $|\Psi_F\rangle$:

$$|\Psi_F\rangle=|F\rangle+(1/N)\sum_{q\neq 0}\mathbf{L}(\mathbf{q})\rho\uparrow(\mathbf{q})\rho\downarrow(-\mathbf{q})\,|F\rangle+\cdots , \tag{4.8}$$

in which $\cdots$ stands for the remaining configurations, all presumed orthogonal to those written explicitly above and to one another. The operators $\rho^m(\mathbf{q})=\sum_k c^\dagger_{m,k+q}c_{m,k}$ ($m=\uparrow$ or $\downarrow$) are density-fluctuation operators. By analogy with the boson case, the exact eigenvalue is expressed as

$$E_F=E_F^0+Un\uparrow n\downarrow/N+(U/N^2)\sum\mathbf{L}(\mathbf{q})\mathbf{P}(\mathbf{q}) , \tag{4.9}$$

in which

$$\mathbf{P}(\mathbf{q})\equiv\langle F\,|\rho\uparrow(-\mathbf{q})\rho\downarrow(\mathbf{q})\rho\uparrow(\mathbf{q})\rho\downarrow(-\mathbf{q})\,|F\rangle \tag{4.10}$$

is a quantity $O(n^2)$ and E_F^0 is the unperturbed Fermi energy ($U=0$). While superficially this procedure has the appearance of the "random-phase approximation" (Pines, 1962), Eq. (4.9) is an exact result provided the appropriate choices of $n\uparrow$ and $n\downarrow$ (not necessarily equal) are made. The real difficulty consists in obtaining $\mathbf{L}(\mathbf{q})$, a task that requires explicit knowledge of all the terms $(\cdots)$ in $|\Psi_F\rangle$. Nevertheless, estimates (as well as upper and/or lower bounds) of this function may ultimately prove of some use.

If the total number of particles is large [$O(N)$], a different approach may be more appropriate. Starting from the ferromagnetic state, one examines the effects of a small number n of "spin flips." The analysis is carried out in the Appendix for arbitrary short- or long-ranged forces. It demonstrates an interesting analogy between magnons and excitons.

V. CONCLUSION

Lattice physics has great current appeal, although most contemporary investigations center on the many-body problems (and the use of numerical techniques in their resolution). Undoubtedly such studies will become increasingly popular as the cost of computation continues to drop further. The approach described in the present brief review is, philosophically, quite different. Here one seeks closed-form solutions (sometimes equated with "understanding") of models of one-, two- , . . . , n-body behavior. We have learned, for example, that when a bound state of three or more bosons is formed at a critical interaction U_c in three dimensions, this occurs in a discontinuous way. The Appendix illustrates a specific "many-body" problem, which can be manipulated into a "few-body" problem and consequently better understood. This is presented in the belief that there must be a number of other such cases where rigorous understanding of the few-body problem leads to the unveiling of useful physical principles.

Our review has concentrated on aspects of the n-body problem that are presently known or easily knowable. We have omitted discussions of lengthy technical questions and managed to avoid the explicit study of $n\geq 4$ particles. Although it is possible to estimate some properties for $n\geq 4$ by extrapolation from $n=3$, a rigorous formulation would facilitate several studies of great potential interest.

For example, it has been known for a while that two excitons, made of electrons and holes interacting via the Coulomb interaction, bind into a four-particle "biexcitonic molecule" (Akimoto and Hanamiura, 1972; Brinkman, Rice, and Bell, 1973).[12] As these results are all anchored in the effective-mass approximation (i.e., in continuum theory), the question of whether, *in the lattice theory,* the

[12]Recent improvements (Lee, Vashishta, and Kalia, 1983) over these early variational methods have allowed good agreement with experiment in silicon (Thewalt and McMullan, 1984).

biexcitonic molecule is bound remains unanswered and is, of course, relevant in many insulators and semiconductors other than silicon (see footnote 12).

Other problems that would benefit from a lattice analysis include the possible bound state of two Cooper pairs on a two-dimensional lattice, the ground state of four bosons, multiphonon bound states, etc. While in the continuum theories, the four-body problem can be reduced to an "effective," rather complex three-body problem (Grassberger and Sandhas, 1967; Alt, Grassberger, and Sandhas, 1970; Kroger and Sandhas, 1977), in the lattice theory there is at present no simple integral equation with which to formulate explicitly such problems in the manner of the $n=3$ body problem treated above. Just having such an equation would be of great benefit, because in many instances the strong coupling expansion [see the development surrounding Eq. (3.13)], unavailable in the continuum theories but central to the lattice theory, will, we hope, generate accurate solutions.

APPENDIX

In this appendix, we determine the stability of the ferromagnetic state of interacting fermions, by studying the spectrum of elementary and not-so-elementary excitations associated with it. Although this method cannot determine the ground state in the N-body problem, it is a simple procedure which, at least, suggests the likely instabilities.

In our example, we deal with elementary excitations (fermions) and their excitonlike bound states (bosons) and scattering states. We start with N electrons in a conduction band of an itinerant ferromagnetic metal, assuming the conduction band accommodates precisely N electrons of each spin direction. In the totally ferromagnetic state, the spin-up band is filled, while the corresponding spin-down band is empty. The energy is

$$E_{\text{Ferro}}=N\langle\varepsilon\rangle+(g/2)\sum_i{\sum_j}' V(\mathbf{R}_i-\mathbf{R}_j)\ , \tag{A1}$$

with a prime on the sum indicating $j\neq i$ (i and j span all N sites), while the factor $\frac{1}{2}$ takes care of double counting. The one-particle energies $\varepsilon(\mathbf{k})$ are as in Eq. (2.6) with $W=3$, with the averages $\langle\varepsilon\rangle$ over the Brillouin zone defined as in Eq. (2.4).

To this translationally invariant system (under the group of discrete lattice operations) we add one electron in a plane-wave ("Bloch") state characterized by $\mathbf{k}$. It has spin down, necessarily, and energy $E_1(\mathbf{k})$ relative to E_{Ferro} in Eq. (A1):

$$E_1(\mathbf{k})=\varepsilon(\mathbf{k})+g\sum_i V(\mathbf{R}_i-\mathbf{R}_j)+\mu B/2\ . \tag{A2}$$

We can as well take away one electron (add one "hole"), at an energy $E_2(\mathbf{k})$ relative to E_{Ferro} in (A1):

$$E_2(\mathbf{k})=-\varepsilon(-\mathbf{k})-g{\sum_j}' V(\mathbf{R}_i-\mathbf{R}_j)+\mu B/2\ . \tag{A3}$$

(Note the prime.) These are the two relevant types of elementary excitations or "quasiparticles" of the N-body system in an external field B.

The action of flipping the spin of a single electron among the N originally present explicitly lowers the total spin angular momentum M_z by $\hbar$, while simultaneously creating two quasiparticles, one of each type. Their joint energy is the eigenvalue of a two-particle Hamiltonian:

$$\mathscr{H}=\varepsilon(-i\nabla_1)-\varepsilon(i\nabla_2)+g[V(\mathbf{0})-V(\mathbf{R}_1-\mathbf{R}_2)]+\mu B\ , \tag{A4}$$

where μB is the extra energetic cost of lowering M_z in a magnetic field B. Out of N^2 possible eigenstates of this two-particle system, as few as N are bound states. The majority are scattering states, of the form given in Eqs. (2.7), (2.17), and (2.18). Their energies interlace the continuum $E=E_1+E_2$: *if some E are negative, the ferromagnetic state is unstable.* We leave the study of these scattering states to the reader. Here, we concentrate on the *bound states.* They take the form

$$|\Psi)=(1/N^{1/2})\sum F(\mathbf{k})\,|\,\mathbf{k}+\mathbf{Q}/2,-\mathbf{k}+\mathbf{Q}/2\rangle\ , \tag{A5}$$

where $\mathbf{Q}=(Q_1,Q_2,Q_3)$ labels the total momentum of the pair. As Ψ satisfies the Schrödinger equation, we use $(\mathscr{H}-E)\Psi=0$ to obtain equations for the amplitudes:

$$\begin{aligned}0=F(\mathbf{k})[&\varepsilon(\mathbf{k}+\mathbf{Q}/2)-\varepsilon(\mathbf{k}-\mathbf{Q}/2)+gV(\mathbf{0})+\mu B-E]\\&-(g/N)\sum V_{\mathbf{q}'}F(\mathbf{k}+\mathbf{q}')\ ,\end{aligned} \tag{A6}$$

where $V_{\mathbf{q}'}$ is the lattice Fourier transform of the two-body interaction,

$$\begin{aligned}V(\mathbf{R})&=1/N\sum V_{\mathbf{q}'}e^{i\mathbf{q}'\cdot\mathbf{R}}\\&=(1/\Omega)\int d^3q'V_{\mathbf{q}'}e^{i\mathbf{q}'\cdot\mathbf{R}}\ .\end{aligned} \tag{A7}$$

At $\mathbf{Q}=0$, Eq. (A6) [with $V(\mathbf{0})$ computed with the aid of (A7)] has the solution $F=$const, corresponding to energy eigenvalue $E=\mu B$.

For $\mathbf{Q}\neq 0$ we have to investigate specific interactions. It would be helpful to be able to study Eq. (A6) for arbitrary interaction, such as the screened Coulomb interaction for various screening lengths, but this is too difficult. So we investigate several model interactions, in order of increasing complexity. The simplest is Hubbard's zero-range interaction, $V_q=\text{const}=V(\mathbf{0})=1$ [and $V(\mathbf{R})=0$ for $\mathbf{R}\neq\mathbf{0}$], absorbing the strength of the interaction into the parameter g. For this case, we see by inspection that

$$F(\mathbf{k})\propto[\varepsilon(\mathbf{k}+\mathbf{Q}/2)-\varepsilon(\mathbf{k}-\mathbf{Q}/2)+g+\mu B-E]^{-1} \tag{A8}$$

solves Eq. (A6), reducing it into a transcendental equation for E:

$$\begin{aligned}1/g=(1/N)\sum[&\varepsilon(\mathbf{k}+\mathbf{Q}/2)-\varepsilon(\mathbf{k}-\mathbf{Q}/2)\\&+g+\mu B-E]^{-1}\ .\end{aligned} \tag{A9}$$

This equation is explicitly soluble[13] in the case $Q_2=Q_3=0$, $Q_1\neq 0$ (or any permutation). After trivial integration, the solution is found to be

$$E(Q_1)=g-[g^2+4\sin^2(Q_1/2)]^{1/2}+\mu B\ . \qquad \text{(A10)}$$

The lowest $E(Q_1)$ belongs to $Q_1=\pi$, which characterizes a state with antiferromagnetic correlations. In the absence of an external magnetic field [or in general for $|\mu B|<(g^2+4)-g$] the energy of the bound state is lower than that of the ferromagnetic configuration from which it was derived. It follows that large numbers of such antiferromagnetically correlated "excitons" (possibly $\frac{1}{3}$ of them having $Q_i\neq 0$ in each of the three principal directions) must be present in the ground state, so that the latter turns out to be rather complex layered antiferromagnet, rather than the simple ferromagnet[14] assumed initially.

Having established that a zero-range interaction of arbitrary strength g is not conducive to ferromagnetism for N electrons, it makes sense to see what happens when nearest-neighbor forces g_1 (typically associated with a Heisenberg model of magnetism) are introduced. We let

$$gV_{\mathbf{q}}=g+g_1(\cos q_x+\cos q_y+\cos q_z)\ , \qquad \text{(A11)}$$

which allows the kernel in the integral equation to be written as the sum of $2d+1$ separable kernels on the hypercubic lattice in d dimensions. In three dimensions,

$$(1/N)\sum_{\mathbf{k}'} V_{\mathbf{k}'-\mathbf{k}}F(\mathbf{k}')=g\Delta_0+g_1(\mathbf{C}\cdot\boldsymbol{\Delta}+\mathbf{S}\cdot\boldsymbol{\Gamma})\ , \qquad \text{(A12)}$$

where $C_x\equiv\cos k_x$, $\Delta_x\equiv(1/N)\sum\cos k_x' F(\mathbf{k}')$, $S_x\equiv\sin k_x$, $\Gamma_x\equiv(1/N)\sum\sin k_x' F(\mathbf{k}')$, etc., and $\Delta_0\equiv(1/N)\sum F(\mathbf{k}')$. With $Q_2=Q_3=0$ and $Q_1\neq 0$, many of the quantities vanish or simplify, and one can obtain the energy eigenvalues E explicitly as solutions of a cubic equation. Leaving algebraic details aside, we find that when the external field is set at zero ($B=0$), *any* choice of $g_1>0$, together with *any* choice of $g>0$, leads to an energy lower than that of the ferromagnetic state, with $Q_1=\pi$ being inevitably favored. *Introduction of more distant repulsive interactions cannot change this state of affairs,* as we may use the bound-state energies of the Hamiltonian with zero-range or nearest-neighbor repulsive interactions as variational upper bounds on the solutions to an arbitrary-range repulsive potential. Omitting details of a formal proof, one states the resulting *theorem.*

The saturated ferromagnetic state of N electrons in the N available Wannier states of a single conduction-band model of an itinerant ferromagnet [in *arbitrary* dimension d, for *arbitrary* repulsive interactions $gV(\mathbf{R})\geq 0$] is *always* unstable against some state with less than maximum magnetization. (While we can only conjecture that the true ground state has $M_Z\approx 0$, we can be certain that some nontrivial antiferromagnetic correlations do exist in the ground state.)

The ground state of $N-1$ electrons in the N available Wannier states of a single conduction-band model of an itinerant ferromagnet in the Hubbard model (zero-range repulsion U) is known, in the particular limit $U\to\infty$ (Nagaoka, 1966). This problem is equivalent to that of a single hole moving in a medium in which each site is occupied by ↑ or ↓; the motion of the hole creates a "wake" in the sea of localized spins, from which it follows that the ferromagnetic state (all spins ↑ or all spins ↓) has the lowest energy (Nagaoka, 1966). Combining the tendency for antiferromagnetism at a half-filled band with the tendency for ferromagnetism associated with a few holes at large U, one can construct a reasonable phase diagram in the U,n plane of the Hubbard model (see, for example, Mattis, 1981, p. 256) and a reasonable picture of the origins of itinerant-electron magnetism.

The point of this appendix? Simply that, however incomplete it may be, the examination of $n=1$ and 2 problems yields information on the many-body ground state which might be difficult to obtain by other than numerical-experimental means. Pursuit into the $n=3$ and 4 problems may be even more helpful, although, as we have seen, the difficulties increase rapidly with n.

[13]Moreover, the choices $Q_1=Q_2\neq 0$, $Q_3=0$ allow the evaluation of Eq. (A9) in terms of elliptic integrals, while $Q_1=Q_2=Q_3\neq 0$ leads to a Watson's integral, also calculable in terms of elliptic functions (Joyce, 1972; Glasser, 1972).

[14]It is already well known from the point of view of many-body theory (see the exact solution in one dimension in Lieb and Wu, 1968, or various approximate studies in three dimensions, bibliography in Mattis, 1981) that the ground state for N electrons in the Hubbard model is not ferromagnetic. But the complex layered antiferromagnetic state discussed in the present text is not the only candidate ground state. One should also examine bound states (see footnote 13) (or if there are none, the scattering states) with $Q_1=Q_2=Q_3=\pi$, to see if they possibly have energies lower than the eigenvalues (A10). At values of the coupling constant where they do, the familiar Néel-type correlations in the ground state become more likely.

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