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**Critique of Recent Theories and Monte Carlo
Calculation of Exchange in Solid ^3He**

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CRITIQUE OF RECENT THEORIES AND MONTE CARLO
CALCULATION OF EXCHANGE IN SOLID $^3\text{He}^\dagger$

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SUBSTITUTION OF EXCHANGE IN SOLID H_2O
 CRITIQUE OF RECENT THEORIES AND WORKS ON

Abstract

Over the last ten years, a number of dissimilar and in some cases conflicting theories of exchange in solid He^3 have appeared in the literature. A comparative evaluation is needed. To this end, it is pointed out in Part I that a fundamental theory of exchange in solid He^3 exists which yields general expressions for the matrix elements of the exchange operator. The theory constitutes an extension of Herring's work on electronic exchange, which is also the approach used by Thouless. The expressions for the matrix elements of the exchange operator appear as many-body integrals. The results of the various theories follow systematically from these expressions according to various approximations. These theories are seen to be basically calculating the same quantities, and their major differences are seen to lie in their prior treatment of the lattice dynamics.

One approximation made by most of the theories is to calculate the exchange frequencies using two-body integrals which in particular neglect the short-range correlations of an exchanging pair with their surrounding

neighbors. In Part II, a test of this approximation is reported. The $T = 0$ nearest neighbor exchange frequency is calculated by Monte Carlo integration of the full many-body surface integral expression, using the Nosanow type wavefunction. This exchange integral as it stands is not amenable to practical computation by the Monte Carlo method, in that it would attempt to calculate an extremely small number in a statistical manner. variable transformations are used to analytically remove these small factors from the integration. The calculation has been performed for different densities, and compared to the results of the two-body approximation to the full integral. The results of the full integral are considerably smaller in magnitude, though of an improved density dependence, than those of the two-body approximation. It is concluded that the many-body short-range correlation effects are important to the exchange process.

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PART I

CRITIQUE OF RECENT THEORIES OF EXCHANGE IN SOLID He^3

ERRATA

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I-44

Equation at the top of the page should read

$$\approx \underline{\underline{1}} - \dots, \text{ and not } - \underline{\underline{1}} \approx \dots$$

I-65

Right parenthesis missing on far right hand side of Eq.(5.9).

I-76

Line 6: should read Eq.(5.20), not Eq.(5.2)

I-81

The subscript Σ to the integral sign in Eq.(5.30) has been omitted.

II-7

The integral obtained by using the Nosanow-Varma choice for ϕ_0^e is slightly more complicated than that given in Eq.(2.6).

II-11

The arguments of $f^2(\quad)$ in Eq.(2.12) are $f^2(x, y, z' - \Delta)$.

II-13

The argument of the delta function in Eq.(2.17) should be $\delta(\underline{\underline{E}}_{12} - \hat{\Delta} - \Delta)$. The 6th line from the bottom should read "... lie within $\Delta/2$ of $\underline{\underline{R}}_1$ and $\underline{\underline{R}}_2$ "

II-22

Part of the page is not clearly legible. In the second line from the bottom, we have "... $B = A/8$ "

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Add to ref. 27: Proc. Phys. Soc. 86, 905 (1965).

CHAPTER 1: INTRODUCTION AND SUMMARY1. Background

Solid He^3 is a very unusual crystal because of the relatively large zero-point motion of its atoms, corresponding to an r.m.s. deviation of about 30% of the nearest neighbor distance.¹ In fact, even at $T = 0$, the solid can only be formed under pressures in excess of 30 atm. The solid which forms is characterized by a lattice constant about one-third larger than that predicted by classical theory. The traditional lattice dynamical theory² fails for solid He^3 , and only in the last ten years has a new theory emerged.³⁻⁶ In this theory the elementary excitations of the solid are determined in a self-consistent manner, and the hard-core repulsion between atoms is explicitly treated by means of short-range correlation functions.

One consequence of the large zero-point motion in solid He^3 , is an unusually large probability for two atoms in the crystal to exchange places, which leads to a comparatively large exchange interaction. The exchange energy of a pair is about three orders of magnitude larger than that of the nuclear spin magnetic dipole-dipole

interaction, though about three orders of magnitude smaller than the energy per particle.⁷⁻¹⁷ This makes solid He^3 unique among solids in that it has an exchange interaction due to the direct exchange of atoms which is the dominant nuclear spin-spin interaction. It is expected that this interaction will cause the nuclear spins to order at a temperature on the order of $1 \text{ m}^\circ\text{K}$. It leads to a complicated curve for the spin-lattice relaxation.^{7-12,14} At low temperatures, the exchange interaction has dramatic effects on the thermodynamic properties of solid He^3 . It has an important effect on the shape of the melting curve, the minimum in which makes compressional cooling possible.^{19,20} Recently, it has been shown that the theoretical lower limit of such cooling may be considerably reduced with the use of an appropriate magnetic field.^{21,22} The exchange interaction is expected to lead to a vanishing thermal expansion coefficient¹⁶ at a temperature on the order of $.2^\circ\text{K}$. Below about $50 \text{ m}^\circ\text{K}$ the behavior of $dP_V(T)/dT$ is due almost entirely to the exchange interaction, and this has been used^{16,17} to measure J .

The exchange interaction in solid He^3 has been investigated experimentally by measurements of the bulk susceptibility,¹³⁻¹⁵ the slope of the melting curve,¹⁶

$P_V(T)$,^{16,17} and by NMR determination of both transverse and longitudinal nuclear relaxation times.⁷⁻¹² The results indicate that it is antiferromagnetic and of the order of $1 \text{ m}^{\circ}\text{K}$. The exchange interaction has also received considerable theoretical treatment.²³⁻³⁰ These calculations have yielded values of the $T = 0$ nearest-neighbor exchange frequency, J , which are in order of magnitude agreement with experiment. All calculations yield a density dependence such that the magnitude of J decreases with increasing density. This feature is understood in terms of the increased density making it more difficult for two atoms to maneuver around each other in the exchange process.

The exchange interaction was first chosen²³ to have the form

$$H_X = -2 \sum_{i < j} J_{ij} \underline{I}_i \cdot \underline{I}_j, \quad (1.1)$$

where $\underline{I}_i$ is the nuclear spin operator for atom i , and J_{ij} are the exchange frequencies. Thouless²⁷ pointed out that J_{ij} should be replaced by exchange operators $\mathcal{J}_{ij}$, having matrix elements between the phonon excitations of the solid; i.e.,

$$H_X = -2 \sum_{i < j} g_{ij} \mathbf{I}_i \cdot \mathbf{I}_j \quad (1.2)$$

The reason is that the collective or phonon-like modes of the solid are much more closely spaced in energy than the size of the exchange energy, so that the exchange interaction should include the possibility of coupling these modes. The exchange frequencies J_{ij} are then identified²⁸ as

$$J_{ij} = \text{tr}(\rho_{\text{ph}} g_{ij}) \quad (1.3)$$

where ρ_{ph} is the density matrix for the phonon system. At the low temperatures for which crystalline He^3 exists, one can make the identification²⁸

$$J_{ij} \approx (g_{ij})_{00} \quad (1.4)$$

The Hamiltonian given by Eq. (1.1) may then be viewed as a low-temperature approximation to Eq. (1.2) in which the off-diagonal elements of g_{ij} are ignored, and the diagonal elements are taken according to Eq. (1.4).

2. Purpose and Summary of the Paper

Each of the above mentioned theories represents the exchange interaction by one or the other of Eqs. (1.1) and (1.2). However, they calculate the matrix elements of the exchange operator in strikingly dissimilar ways. In fact, Guyer and Zane²⁹ have suggested that Thouless²⁷ and Nosanow and Varma²⁸ have omitted an important contribution to the exchange in their calculations. These dissimilarities in formal structure of the various calculations make it difficult to comparatively evaluate their results.

The basic purpose of this paper is to point out that a fundamental theory of exchange in solid He^3 exists which yields general expressions for the matrix elements of $\mathcal{J}_{ij}$ from which all of the expressions given by the various theories may be derived according to various approximations. It constitutes an extension of the work of Herring³¹ on electronic exchange to the problem of nuclear exchange in solid He^3 , an approach which is essentially that of Thouless' paper. While we are in full agreement with Thouless' work, his formulation is not entirely sufficient for our needs; hence, we present a

more complete and explicit extension of Herring's ideas to the helium problem. With the exception of our intuitive justification of a generalized version of Herring's assumptions, the theory is basically that of Herring.

In Chapters 2-4 we develop this theory, a brief overview of which is given in the next section. The essential point is that in order to separate the complex behavior of a crystalline system into lattice dynamical effects plus exchange effects, it is convenient to utilize localized wave functions. Since a localized wave function cannot be an eigenfunction of the Hamiltonian for a system which exhibits exchange effects, the question is by what criterion should one select these functions. Herring's point is that there is a natural way of choosing them. He has given the name "home-base" functions to these special localized functions. This procedure is discussed in Chapter 2. In Chapter 3 we discuss the significance of the home-base functions in the context of the general quantum mechanical formalism, and suggest ways of calculating approximations to them. In Chapter 4 we use these functions to develop an effective Hamiltonian for solid He^3 which is separable into a lattice and an exchange part.

The eigenfunctions of this lattice Hamiltonian are home-base functions. The development of this theory emphasizes a point which has been made before in the literature;²⁸⁻³⁰ The treatment of exchange in a crystalline system must be preceded by the proper treatment of the lattice dynamics of the system.

In Chapter 5 we show that the expressions given by the various theories for the $T = 0$ exchange frequencies and for the matrix elements of the exchange operator follow systematically from our general expression derived in Chapter 4. These theories are all basically calculating the same quantities, and the major differences between them lie in their prior treatment of the lattice dynamics. We show that Guyer and Zane's criticism of the work of Thouless and of Nosanow and Varma stems from an approximation made by Guyer and Zane in their calculations.

3. Overview of the Theory

In this section we give a brief overview of the generalization of Herring's theory to be developed in detail in Chapters 2, 3 and 4. We neglect the nuclear spin magnetic dipole-dipole interaction as it is three

orders of magnitude smaller than the exchange energy.

We also neglect atomic diffusion in this work. The system is thus described by the spin-independent Hamiltonian

$$H = \sum_i \left(-\hbar^2 \nabla_i^2 / 2m \right) + \sum_{i < j} v(r_{ij}) , \quad (1.5)$$

acting on the space of antisymmetrized products of coordinate (ψ) and spin (ξ) functions, $\{G(\psi\xi)\}$. It is convenient, however, and equivalent, to first study exchange in the context of just the coordinate problem

$$H \psi = E \psi , \quad (1.6)$$

where the atoms may be considered to be distinguishable, and then at some later time add spin to the coordinate functions and antisymmetrize. Note that the spectrum of Eq. (1.6) already exhibits any energy splittings which one will eventually attribute to exchange, in that the addition of spin via the requirement of antisymmetrization simply throws out some energy levels and assigns particular spin configurations to those remaining. The presence of exchange, in the literal sense of this word, is also manifest in the coordinate eigenfunctions ψ : If exchange

is non-zero in the system, the eigenfunctions ψ are of necessity non-localized in the configuration space of the N atoms, in the sense that a given atom has a non-negligible probability of being found not just near one particular lattice site, but near many different lattice sites.

The question of the localization of the coordinate eigenfunctions of H is central to the problem of exchange. There are $N!$ points in the configuration space of the N atoms which correspond to all possible ways of placing N atoms on the N lattice sites, one to a site, which we indicate by p^P , where the index P runs over all permutations of N objects. A localized function, in our usage of the word, is sizeable only near a single one of the p^P in configuration space, while a non-localized function is sizeable near many of the points p^P which are selected in a regular way from the full set $\{p^P\}$. The point we are trying to bring out is that the existence of exchange requires the coordinate eigenfunctions ψ of H to be non-localized in the above sense, whereas were exchange zero, one could have localized eigenfunctions ψ . We are simply making a somewhat mathematical statement of the following physical picture: The atoms spend most

or their time vibrating about particular lattice sites (frequency $\sim 10^{12}$ cps). Occasionally (exchange frequency $\sim 10^8$ cps.) atoms take excursions far enough from their lattice sites to allow a number of them to exchange places. Having done so, the atoms proceed to vibrate about their new lattice sites, and so on. Were the exchange frequency zero, one would always have a given atom vibrating about the same lattice site. I-10

At the core of the theory is the assumption that the manifold* or low-lying coordinate eigenfunctions of H can be spanned by a special set of mainly localized functions, the home-base functions. The qualification "mainly" localized signifies the essential feature that two such home-base functions localized about different points p^P and $p^{P'}$ may still have some overlap. We write the home-base functions as $\{\phi_m^P\}$ where the index P refers to the particular p^P that the function is localized about, and all other indices are lumped into m . We repeat that by virtue of their localization, the home-base functions are not eigenfunctions of H . However, one may think of

* By the manifold of states $\{\psi_\mu\}$ we mean that subspace of the full Hilbert space which contains all possible linear combinations of the states ψ_μ . The states ψ_μ are said to span the manifold.

a given Φ_m^P as fairly accurately representing the behavior of the system in the neighborhood of the point p^P in configuration space. Since the lattice dynamical nature of the system is characterized by its behavior in just these regions, one may consider the home-base functions as eigenfunctions of some effective lattice Hamiltonian. The exchange interaction is then related to the coupling of various home-base functions through matrix elements like $\langle \Phi_m^P | H | \Phi_m^{P'} \rangle$.

With the above assumptions made, the rest of the derivation follows easily. The manifold of low-lying physical states is spanned by the states $\{G(\Phi_m^P \xi_K)\}$, where an index has been added to the spin function ξ_K . One writes down the characteristic equation for the eigenvalues of H in this manifold. After some manipulation it is seen that these eigenvalues may be generated by an effective Hamiltonian which contains a spin-independent part plus a spin-dependent part

$$H_{\text{eff}} = H_L + H_X \quad (1.7)$$

and acts on the space of the unsymmetrized products $\{\Phi_m^e \xi_K\}$, where e is the identity permutation. H_L is

given by

$$H_L = \sum_m |\Phi_m^e\rangle \bar{E}_m \langle \Phi_m^e| \quad (1.8)$$

where $\bar{E}_m = \langle \Phi_m^e | H | \Phi_m^e \rangle$, and the Φ_m^e are assumed to be normalized. To lowest order, H_X is given by

$$H_X \approx - \sum_{i < j} J_{ij} \frac{1}{2} (1 + \underline{\sigma}_i \cdot \underline{\sigma}_j) \quad (1.9)$$

where

$$\langle \Phi_m^e | J_{ij} | \Phi_{m'}^e \rangle = \langle \Phi_m^e | (H - \frac{1}{2} \bar{E}_m - \frac{1}{2} \bar{E}_{m'}) P_{ij} | \Phi_{m'}^e \rangle \quad (1.10)$$

We have suggested that the home-base functions may be considered as eigenfunctions of an effective lattice Hamiltonian, and so identify H_L as such. Indeed, only the $\{\Phi_m^e\}$ for $P = e$ occur in H_L , so that it describes a fictitious system in which a given atom always remains mainly localized about the same lattice site. We identify H_X as the exchange Hamiltonian, and note that it contains an exchange operator having matrix elements

between the presumably phonon-like states of the lattice Hamiltonian. Note that we could retain the higher order corrections in H_X corresponding to more complex exchanges than pair exchanges, which would result in a considerably more complicated expression than Eq. (1.9).

The effective lattice Hamiltonian acts on the truncated Hilbert space spanned by the functions $\{\phi_m^e\}$ for $P = e$. This results in a natural way from the present theory, and is equivalent to the restriction of single occupancy of the lattice sites which is used in second quantized theories of the lattice dynamics.⁴

We note that this theory may be extended to a spin-dependent Hamiltonian. In this case the home-base functions would be functions of spin as well as coordinate variables. One would antisymmetrize these functions to get possible physical states, which would then be used to diagonalize the Hamiltonian. In general, the resultant effective lattice Hamiltonian would be spin dependent as well as the exchange Hamiltonian.

CHAPTER 2: EXISTENCE OF HOME-BASE FUNCTIONS FOR SOLID HELIUM

1. Herring's Definition of Home-Base Functions for the Problem of Electronic Exchange

We begin by summarizing part of the work by Herring³¹ on electronic exchange in systems with well-separated atoms, i.e., in systems where the coupling between atoms may be taken as a weak perturbation on the system of free atoms. For convenience we suppose there is only one electron per atom. We also take the Hamiltonian of the system to be spin independent, and consider only its coordinate eigenfunctions. The ground state of such a system at infinite separation (free atoms) will be $N!$ degenerate. As we bring the atoms in to finite separations, this level will split into a band which will be well separated from all other energy levels if we don't allow the atoms to get too close. One can choose the $N!$ coordinate eigenfunctions at infinite separation, $\{\psi^\alpha\}$, so that they do not mix throughout this process, basically by utilizing the symmetry group of the Hamiltonian. Accordingly one expects a given ψ^α not to change very much, excepting of course in that the

distances between atoms have changed. Writing the coordinate eigenfunctions of the lowest band of the system at finite separation as $\{\psi^\alpha\}$, Herring proposes the correspondence:

$$\psi^\alpha \leftrightarrow \bar{\psi}^\alpha \quad (2.1)$$

where i) ψ^α and $\bar{\psi}^\alpha$ are physically similar when differences in relative positions of the atoms is accounted for. ii) The correspondence is preserved under permutation and the relevant geometric symmetry operators. iii) The correspondence preserves inner products $(\psi^\alpha | \psi^\beta) = (\bar{\psi}^\alpha | \bar{\psi}^\beta)$.

The system at infinite separation has no electron exchange, and thus one can make linear combinations of the $N!$ degenerate eigenfunctions $\{\bar{\psi}^\alpha\}$ to yield eigenfunctions for which each electron is localized about a single ion core. We write $\{\bar{\phi}^P\}$, $\bar{\phi}^P = P\bar{\phi}^e$, where the index P is a permutation operator; e , the identity permutation, and we mean that in the state $\bar{\phi}^P$, electron i is to be found only near ion P_i . Moreover the following manifolds* are equal:

* See footnote on page I-10.

$$\text{manifold } \{\bar{\Psi}^{\alpha}\} = \text{manifold } \{\bar{\Phi}^P\} . \quad (2.2)$$

Taken together, Eq. (2.1) and Eq. (2.2) provide a prescription by which one may make linear combinations of the eigenfunctions $\{\bar{\Psi}^{\alpha}\}$ at finite separation to yield functions $\{\bar{\Phi}^P\}$, $\bar{\Phi}^P = P\bar{\Phi}^e$, which Herring calls "home-base" functions, where: 1) They are not eigenfunctions, though they are legitimate wave functions. 2) They span the manifold $\{\bar{\Psi}^{\alpha}\}$. 3) They are mainly localized in the configuration space of the N electrons in the sense that for a given function, each electron is to be found mainly localized about a particular ion core. The qualification "mainly" indicates the essential feature that $\bar{\Phi}^P$ and $\bar{\Phi}^{P'}$ for $P \neq P'$ may have some overlap, which was not the case for the $\{\bar{\Phi}^P\}$. However, these functions are well enough localized that if H is the Hamiltonian,

$$(\bar{\Phi}^e | H | \bar{\Phi}^e) \gg (\bar{\Phi}^e | H P_{ij} | \bar{\Phi}^e) \gg (\bar{\Phi}^e | H P_{\text{other}} | \bar{\Phi}^e) \quad (2.3)$$

where P_{ij} is a nearest neighbor pair permutation, and P_{other} is neither the identity, nor such a pair permutation.

In sum, Herring wants to find a set of localized

functions which span the manifold or the $\{\psi^v\}$. He uses a closely related fictitious system in which there is no exchange, the infinitely separated system, as a tool which suggests how the $\{\psi^a\}$ may be combined to yield these localized functions, the home-base functions.

2. Analogue of the Infinitely Separated System for the Solid He³ Problem

In order to extend the above ideas to our problem of nuclear exchange in solid He³, we begin by seeking an analogue to Herring's infinitely separated system. That is, we seek a fictitious system as much like the true system as possible, but which does not exhibit exchange. We suggest that to prohibit exchange of the atoms in the lattice one need only require that the relative ordering of the atoms remains unchanged. In one-dimension this simply means that, say, atom 1 always stays to the left of atom 2, etc. In three dimensions this notion is more complicated, but straight forward. One may again consider the configuration space of the N atoms. The N! points p^P in configuration space correspond to all possible ways of placing the N atoms on the N lattice

sites, one to a site. It is now possible to divide all of configuration space into $N!$ sections Ω_p such that every point in a given Ω_p is closer to a particular one of the p^P than to any of the others. The relative ordering of the atoms in the crystal is determined by which Ω_p contains the representative point of the system. Accordingly we take our fictitious system to have Hamiltonian $\bar{H} = H + \bar{V}$, where $\bar{V}$ is a potential having infinite barriers at the hyper-surfaces separating the Ω_p , and is zero elsewhere. We note that the potential $\bar{V}$ does not seriously affect the collective or phonon-like modes of the crystal, in that these modes correspond in general to small oscillations of the atoms about the lattice sites, i.e., to the behavior of the system near the points p^P which lie well within the sections Ω_p . (See Appendix A: The Hamiltonian $\bar{H}$).

The eigenfunctions of $\bar{H} = H + \bar{V}$ not only do not exhibit exchange, but by our definition of $\bar{V}$, they also apply only to a particular crystalline structure, and a particular orientation and position of the crystal. In the limit that $\bar{V}$ vanishes, we do not regain all of those highly degenerate eigenfunctions of H corresponding to other orientations and positions of the crystal, and

other crystalline structures. But we are, after all, not interested in these extra states. They may be removed by adding appropriate external constraints to H , which we assume to be done henceforth. With this in mind we may consider H and $\bar{H}$ to have the same symmetry group G , and view the more highly degenerate levels of $\bar{H}$, which we comment on shortly, to be the result of accidental degeneracy. One may take the eigenfunctions of $\bar{H}$ to be completely contained in one or another of the various sections of configuration space, and write $\{\bar{\Phi}_{m\nu j}^P\}$, where P indicates the particular section. One may also interpret the index P as indicating that atom i is localized about lattice site P_i . The index m indicates energy, while νj indicates that $\bar{\Phi}_{m\nu j}^P$ transforms irreducibly under that subgroup of G which leaves the P^{th} section of configuration space, as a whole, invariant. This subgroup is in fact just the relevant space group for the crystal. (See Appendix B: Group Theory). Since $[\bar{H}, P] = 0$ where P is any permutation of the atoms, the coordinate eigenfunctions $\{\bar{\Phi}_{m\nu j}^P\}$ of $\bar{H}$ are $N!$ degenerate in the index P . It is this degeneracy which one may view as accidental and which is largely removed in the perturbative process of turning on the exchange by going from $\bar{H} \rightarrow H$.

3. Difficulties in Application to the Helium Problem

We are now in a position to see some of the difficulties inherent in an attempt to extend Herring's theory to solid He^3 . Recall that in the electronic problem the perturbative process of bringing the system from infinite separation to finite separation was small, in that the interactions between atoms constituted a small perturbation on the system of free atoms. This fact permitted Herring to work with just the highly degenerate ground state of the infinitely separated system, and the resultant band at finite separations, and set up the correspondence given by Eq. (2.1). The analogue of the above perturbative process for our problem is to go from the system $\bar{H}$ to the system H by relaxing the constraints $\bar{V}$. This is not a small perturbation. The size of a perturbation is usually gauged by comparing the shifts in the energy levels which it incurs to the original spacing of the energy levels in the unperturbed system. In the electronic problem, the exchange energy is considerably smaller than the level spacing of the system of free atoms, and so the perturbation is small. In our problem, it is not that the exchange energy is so

large, but it is that the spectrum of $\bar{H}$ is a quasi-continuum, which makes the perturbation large. For the Hamiltonian $\bar{H}$ contains the collective or phonon excitations of the crystal, leading to a separation between energy levels on the order of $1/N$, where N is the number of atoms. Thus, as one begins to relax the constraints $\bar{V}$ in some fashion, and the degenerate levels of $\bar{H}$ begin to split, almost immediately one has states originating from various different levels beginning to cross and mix.

4. Generalization for the Helium Problem

In spite of these difficulties we feel that a generalization of the type of correspondence used by Herring can be set up between the states of H and $\bar{H}$, allowing us to define home-base functions for our problem. We shall lead up to a statement of this correspondence by discussing the nature of the perturbative process of relaxing the constraints $\bar{V}$. The arguments we make are intended to be only intuitive, as a rigorous justification is beyond our reach.

Let us imagine what a low-lying coordinate eigenfunction ψ of H looks like, knowing that the Debye frequency for

the solid ($\sim 10^{12}$ cps) is considerably larger than the exchange frequency ($\sim 10^8$ cps) at the low temperatures for which the crystal exists. One imagines the atoms spending most of their time vibrating at the Debye frequency about particular lattice sites, and only very rarely taking excursions far enough from their lattice sites to allow a number of them to exchange places. Thus, we expect the eigenfunction ψ to be large only near the points p^P in configuration space, i.e., well within the interior of the various sections Ω_p , and that it drops off and becomes very small near and at the hyper-surfaces separating the Ω_p . It was just at these hyper-surfaces that we added the rigid barriers $\bar{V}$ in defining $\bar{H} = H + \bar{V}$. Consider now a single one of the sections of configuration space, say Ω_e . As H and $\bar{H}$ are identical interior to Ω_e , any differences between the functional behavior of ψ in Ω_e and some appropriate one of the $\bar{\phi}_{m/j}^e$ must originate in only the small difference in boundary conditions at the hyper-surfaces bounding Ω_e : ψ is small at these hyper-surfaces while the $\bar{\phi}_{m/j}^e$ are required to be zero there. It is tempting to expect that

$$\psi \sim \bar{\phi}_{m/j}^e \quad \text{in } \Omega_e \quad (2.4)$$

for an appropriate choice of the indices m/j . However, this statement is only partially correct and it is because of the fact that the spectrum of $\bar{H}$ is a quasi-continuum, which in turn is due to our considering a system of a very large number of particles, that is is incomplete.

We digress momentarily to point out that the above difference in boundary conditions would constitute a small perturbation if only a small number of degrees of freedom were involved, and in this case Eq.(2.4) would be valid. Take for example, the analogue of a one-dimensional oscillator equation defined on a line segment large compared to the characteristic length appearing in the equation. Let $\bar{f}_n(x)$, and $\bar{\epsilon}_n$ be the eigenfunctions and eigenvalues corresponding to the zero boundary conditions at each end, while $f_n(x)$ and ϵ_n correspond to the boundary conditions that $f(x)$ be some small number at each end. It is not difficult to convince oneself that at least for the low-lying states one has to lowest order

$$f_n(x) \approx \bar{f}_n(x) \quad (2.5)$$

$$\epsilon_n = \bar{\epsilon}_n + \Delta\epsilon_n \approx \bar{\epsilon}_n \quad (2.6)$$

where the energy shifts $\Delta\epsilon_n$ are considerably smaller than the level spacing of the $\bar{\epsilon}_n$.

To return to the full problem, we would like to suggest the manner in which Eq. (2.4) breaks down when one goes to a system of a very large number of particles. For the sake of our intuitive argument we assume that the functions $\bar{\Phi}_{mvj}^e$ can be factored into products of $3N$ normal mode functions, and that the boundary conditions may be applied independently to each normal mode function. The first assumption is consistent with the expectation that the $\bar{\Phi}_{mvj}^e$ should be phonon-like near the point p^e . In the second we are effectively redefining the potential $\bar{V}$. It should be possible, crudely speaking, to construct a box about the point p^e using hyper-surfaces defined by constant values of one or another normal mode coordinate, such that these hyper-surfaces do not get too close to the point p^e , and such that the completed box would not overlap with its permuted counter parts about the other points p^p . That is, it should be possible to define an adequate Hamiltonian $\bar{H}$ for which the above assumption is appropriate

In the following, we will not distinguish between any such redefined $\bar{H}$ and that originally defined. Our idea is to view the perturbation or going from $\bar{H} \rightarrow H$, within the section Ω_e , as a sequence of $3N$ small perturbations whose net effect is large. We imagine systematically, one after another, altering slightly the boundary conditions for each of the normal modes. According to the previous one-dimensional example, the small change in boundary conditions for a single normal mode problem constitutes a small perturbation on that problem. This is true even for the very low frequency normal modes in that although they are more spread out than the higher frequency modes, the width of the section Ω_e in these directions is still much larger than their characteristic width. Thus, we can apply Eq. (2.5) and Eq. (2.6) individually to each normal mode in the course of this step by step perturbation, so that if we started with $\bar{\Phi}_{m\nu j}^e$ we will get some new function which we write $\hat{\Phi}_{m\nu j}^e$ such that to lowest order

$$\hat{\Phi}_{m\nu j}^e \approx \bar{\Phi}_{m\nu j}^e \quad (2.7)$$

$$\hat{E}_m = \bar{E}_m + \Delta E_m \approx \bar{E}_m \quad (2.8)$$

However, according to Eq. (2.6) each of the $3N$ normal modes can contribute an energy shift, which are then added to get ΔE_m . Since the level spacing or the $\bar{\Phi}_{m,j}^e$ is at least as small as that of its smallest frequency normal mode, it is easy to see that ΔE_m could be considerably larger than the level spacing or $\bar{H}$. The net perturbation is large. We could easily have altered the boundary conditions in a slightly different way to generate a different $\hat{\Phi}_{m,j}^e$, which would also satisfy Eq. (2.7) and Eq. (2.8) except with say ΔE_m of the opposite sign, or in fact, with $\hat{E}_m$ lying anywhere in some interval about $\bar{E}_m$ depending on the particular boundary conditions used. The size of this interval depends on the restrictions we place on these altered boundary conditions, i.e., we only allow the boundary conditions which generated the $\{\bar{\Phi}_{m,j}^e\}$ to be altered slightly. It is tempting then to identify the width of this interval with the order of magnitude of the exchange energy.

Let us reiterate the above ideas in a different manner: We would like to solve for a low-lying coordinate eigenfunction Ψ of H in the section Ω_e . To do so we must insure its continuity and the continuity

or its first derivatives across the bounding hypersurfaces of Ω_e , a process of sufficient complexity as to leave us essentially in ignorance. However, we do have an ad hoc restriction that ψ be small at these hypersurfaces. With this very incomplete knowledge we can only say that possible candidates for ψ in Ω_e are the functions $\hat{\Phi}_{m\nu j}^e$ but that depending on the particular boundary conditions the energy $\hat{E}_m$ might lie anywhere in an interval about $\bar{E}_m$ of width on the order of the exchange energy. But since this interval is much wider than the level spacing of $\bar{H}$ we might have

$$\begin{aligned}\hat{\Phi}_{m\nu j}^e &\approx \bar{\Phi}_{m\nu j}^e \\ \hat{\Phi}_{m'\nu'j'}^e &\approx \bar{\Phi}_{m'\nu'j'}^e\end{aligned}\quad (2.9)$$

where $\hat{E}_m = \bar{E}_m$, and yet where $\bar{E}_m$ and $\bar{E}_{m'}$ might differ by as much as the order of the exchange energy. Thus, we must admit the possibility that something like $c_1 \hat{\Phi}_{m\nu j}^e + c_2 \hat{\Phi}_{m'\nu'j'}^e$, where $\hat{E}_m = \hat{E}_{m'}$, is also a possible candidate for ψ in Ω_e . To allow this possibility, we correct Eq. (2.4) so that

$$\psi \approx \sum_{m\nu j} c_{m\nu j} \bar{\phi}_{m\nu j}^e \quad \text{in } \Omega_e \quad (2.10)$$

where the $\bar{\phi}_{m\nu j}^e$ occurring in the sum lie within some limited interval of the spectrum of $\bar{H}$, of order of the exchange energy. The arguments leading to Eq. (2.10) can be repeated for each of the sections Ω_p , so that we have

$$\psi_\mu \approx \sum_{Pm\nu j} c_{Pm\nu j}^\mu \bar{\phi}_{m\nu j}^P, \quad (2.11)$$

where we have added an index μ to ψ .

The arguments leading to Eq. (2.11) required that ψ_μ was small near and at the hyper-surfaces separating the various Ω_p . We suggest this is a property of all of the coordinate eigenfunctions of H which are statistically important at the temperatures for which crystalline He^3 exists. That is, in the end we are interested in evaluating thermal averages of various physical quantities for the system. Because of the Boltzmann factor we may restrict our attention to some appropriately chosen low-lying manifold of states. The question is whether indeed all of these states are small near the hyper-surfaces.

We can only say that it is consistent with the smallness of the exchange frequency measured at low temperatures that this is the case. Since the ψ_μ should be phonon-like near the various p^P , it is also illuminating to investigate this question for phonon functions. Given a phonon function $|\underline{n}\rangle$ centered about, say p^e , one can calculate the rms deviation of the system, $\langle \underline{n} | u^2 | \underline{n} \rangle^{1/2}$, about the point p^e and in the direction of one of the bounding hyper-surfaces of Ω_e :

$$\langle \underline{n} | u^2 | \underline{n} \rangle \leq \text{const. } E_{\underline{n}}/N \quad (2.12)$$

(See Appendix C: Phonon Functions). As one would expect, the higher energy phonon functions are less well localized. Yet the low-lying phonon functions, in the above sense, are well enough localized about p^e as to be quite small at the bounding hyper-surfaces of Ω_e . (See Appendix).

We now confine our attention to the low-lying states of H and $\bar{H}$. Recall that the sum in E_1 (2.11) is restricted in the sense that for a given ψ_μ of energy E_μ , the $\bar{\Phi}_{m\nu j}^P$ which occur in the sum have energies $\bar{E}_m$ lying within an interval about E_μ of width on the order

of the exchange energy. Since the low-lying states of $\bar{H}$ extend over an energy range many orders of magnitude larger than this, we expect that according to Eq. (2.11), they are sufficient to give a lowest order approximation of all but perhaps some of the highest energy low-lying ψ_μ . Furthermore, all of the arguments of this section could have been made in reverse, beginning with the states of H and then going from $H \rightarrow \bar{H}$, which would give an inverted version of Eq. (2.11) with a given low-lying $\bar{\Phi}_{m\nu j}^P$ approximated by a similarly restricted linear combination of low-lying ψ_μ .

$$\bar{\Phi}_{m\nu j}^P \approx \sum_{\mu} c_{\mu}^{Pm\nu j} \psi_{\mu} \quad (2.13)$$

Taken together, Eq. (2.11) and Eq. (2.13) define a one to one correspondence between the low-lying coordinate states of H and $\bar{H}$, such that: i) corresponding functions are functionally similar, and ii) have the same symmetry properties. The latter follows from H and $\bar{H}$ having the same symmetry group. Via this correspondence we define the home-base functions $\{\bar{\Phi}_{m\nu j}^P\}$, $\bar{\Phi}_{m\nu j}^P = P \bar{\Phi}_{m\nu j}^e$, as those particular linear combinations of the low-lying eigenfunctions of H indicated on the right hand side of

Eq. (2.13). They have the following properties: i) They are not eigenfunctions of H . ii) They span the manifold $\{\Psi_u\}$. iii) They are functionally similar to the $\{\Phi_{m\backslash j}^P\}$. In particular they have the same symmetry characteristics, and they are mainly localized in the configuration space of the N atoms. Because of this, if O_p is some non-pathological operator, we have in analogy to Eq. (2.3)

$$\langle \Phi_m^e | O_p | \Phi_m^e \rangle \gg \langle \Phi_m^e | O_p^P{}_{ij} | \Phi_m^e \rangle \gg \langle \Phi_m^e | O_p^P{}_{\text{other}} | \Phi_m^e \rangle$$

(2.14)

where we have abbreviated $m\backslash j$ by m .

CHAPTER 3: CALCULATION OF THE HOME-BASE FUNCTIONS

The purpose of the preceding chapter was to argue that home-base functions exist for solid He^3 , and to present some of their properties. In this chapter we begin with some intuitive comments as to their significance, and then suggest ways of calculating approximations to them. We point out that the functions which are commonly used to represent solids are in reality home-base functions, or approximations thereto.

It is helpful to first discuss the home-base functions in the context of the (unphysical) system of identical but distinguishable atoms represented by the coordinate eigenfunctions Ψ of H . These eigenfunctions manifest the effects of exchange, in the literal sense of this word, since they are not localized. A given atom has a significant probability in the state Ψ of being found near any lattice site. One would like to abstract from Ψ the complementary features of its lattice dynamical behavior, i.e., the highly correlated motion of the atoms vibrating about their own lattice sites, and its exchange-like behavior. This is accomplished by expressing Ψ as a linear combination of localized wavefunctions, each corresponding to a different arrangement of the atoms in

the lattice. These are the home-base functions. One may then view Ψ as representing the net effect of the system passing back and forth between these various localized states. A given one describes possible lattice dynamical behavior, while the coupling between them represents exchange.

The home-base functions are not coordinate eigenfunctions of H , because of their localization. Nor are they arbitrary localized functions. As Herring points out, there is a natural condition which they must satisfy; i.e., in the limit of vanishing exchange, the home-base functions should become eigenfunctions. In the previous chapter we suggested that such localized functions could be constructed as special linear combinations of eigenfunctions of H which are not too widely separated from each other in energy. One might conjecture that the home-base functions decay more slowly than an arbitrary localized wave function. With this in mind, it is tempting to consider the home-base functions as fairly accurately representing the system in the regions of configuration space where they are localized.

One must be careful not to take the preceding picture of exchange too literally in treating the true

system which consists of indistinguishable atoms. For example, it is not possible to physically prepare a localized state, as such a state is incompatible with both Bose and Fermi statistics. However, as will be seen in the next chapter, the home-base functions offer a mathematically convenient way whereby the energy of the true system may be expressed as a dominant part which is independent of the statistics used, plus a second term embodying the effects of the statistics. The dominant term is an expectation value of the Hamiltonian in a home-base state. To lowest order, then, it is equivalent to think of the true system as composed not only of distinguishable atoms, but atoms which stay localized about their own lattice sites. The second term involves the matrix element of H between permuted home-base states, and so it is convenient to think of this contribution to the energy as due to exchanges of the "distinguishable" atoms.

The essential feature of a crystal is that its atoms or molecules are localized about lattice sites. What does one mean by a crystal when the various particles can, by means of exchange, wander throughout the system? The ability to construct home-base functions out of the

statistically important coordinate eigenfunctions of the system is a possible answer. It is tempting to think that this procedure breaks down at the point of instability of the solid with respect to the liquid; however, the existence of a superheated solid phase suggests that this cannot be correct. One would expect exchange still to be relatively small in such a superheated solid state. Thus, the point at which it would become impossible to construct home-base functions would in all likelihood correspond to the point at which the superheated crystal would become intrinsically unstable, and would not be directly related to the solid-liquid phase transition.

How does one calculate home-base functions for solid helium? One apparent possibility is to add a localizing potential to H , e.g.,

$$H + \lambda \sum_{i < j} (\underline{r}_i - \underline{R}_i) \underline{G}_{ij} (\underline{r}_j - \underline{R}_j)$$

and solve for the eigenfunctions of this combined Hamiltonian in the limit of small λ . This procedure is analogous to the use of an infinitesimal external magnetic field in the case of a ferromagnetic system to

obtain states with the spontaneous magnetization pointing in a chosen direction. However, the Hamiltonian in the magnetic case has degenerate eigenfunctions corresponding to the various different directions of the magnetization, and the infinitesimal perturbation simply selects out one of them. This procedure fails for our problem: The home-base functions for the various arrangements of the atoms in the lattice are not eigenfunctions of H . It would, however, apply to the fictitious exchangeless system with Hamiltonian $\bar{H}$ which was introduced in the previous chapter.

³¹Herring has suggested a possible approach in his work on the electronic problem. The many-body potential of the electrons contains a set of permutationally equivalent local potential wells centered about points p^P in configuration space corresponding to the various ways of assigning the electrons to the ion cores. He constructs a truncated potential by eliminating the attractive part of all but one of these local wells, leaving that about, say, p^e undisturbed. The resultant truncated Hamiltonian has eigenfunctions mainly localized about p^e ; and since the truncated potential is identical to the original for a considerable distance about p^e , these functions, with

the exception of their localized nature, should accurately describe the system. An application of this procedure to solid helium is straightforward, though more complicated. For the many-body potential of solid helium contains local wells corresponding not only to the various permuted arrangements of the atoms in a given lattice structure, but also to different lattice structures, i.e. bcc and hcp, and perhaps structures with vacancies. Furthermore, due to the large zero-point motion of the atoms, the equilibrium configuration of a given lattice structure will be represented by a point which is not centered in the appropriate local well; in fact, it is likely to be on a "shoulder" well away from the minimum. With these matters in mind, one first chooses the lattice structure of interest, which determines the points p^P and sections Ω_p of configuration space. To truncate the potential, one sets the attractive part of the pair interactions to zero if the representative point of the system is not in, say, Ω_e . We identify the eigenfunctions of the resultant truncated Hamiltonian as approximations to the home-base functions $\{\Phi_m^e\}$. Again since the potential is identical to the original for a considerable

distance about p^e , we may reasonably expect this procedure to yield a good approximation.

Note that the harmonic approximation used in standard lattice dynamical theories² is a more severe form of just the kind of truncation we are discussing. The true many-body potential is replaced by a single generalized parabolic well, tailored to fit a single local well of the true potential, say that about p^e , according to its curvature at p^e . Phonon wave functions are thus approximations to home-base functions of the true Hamiltonian.

The truncated Hamiltonian has a variational principle, so that one could determine approximations to its eigenfunctions. In practice one would usually take a localized variational Ansatz appropriate to a particular lattice structure, in which case the true Hamiltonian could be used -- the form of the Ansatz serving the same function as the truncated Hamiltonian. This is of course precisely what has been done in previous calculations for solid He³. We emphasize that the functions calculated by Nosanow and coworkers³ must be viewed as approximations to the home-base functions and not to the true eigenfunctions of H.

CHAPTER 4: DERIVATION1. The Effective Hamiltonian

We are now in a position to derive the effective Hamiltonian using a procedure due to Herring.³¹ The effective Hamiltonian generates the low-lying eigenvalues of the system, and appears as the sum of a lattice part and an exchange part. Very briefly, the procedure is to set up the secular equation for these eigenvalues using matrix elements of the true Hamiltonian H in a very special basis, which involves the home-base functions defined in Chapter 2.

Since He^3 atoms are spin one-half fermions, we must add spin functions to the low-lying coordinate eigenfunction $\{\psi_\mu\}$ or H , and antisymmetrize. Let ξ_k be a product spin function for the N atoms with k indicating the possible 2^N spin states. The physical eigenstates of the system are then $\{G \psi_\mu \xi_k\}$ where G is the antisymmetrizer:

$$G = N!^{-1} \sum_P (-1)^P P \quad (4.1)$$

where $P = P^{(x)} P^{(\sigma)} = P^{(\text{space})} P^{(\text{spin})}$. We will occasionally omit these superscripts if the use of the

operator is unambiguous. It is understood that in running over the possible values for μ and k that the expression $G(\Psi_\mu \xi_k)$ will sometimes be zero and will sometimes duplicate functions. This is not a difficulty in that we are concerned with the manifold* or the states $\{G(\Psi_\mu \xi_k)\}$.

We now show that the manifold of physical eigenstates $\{G(\Psi_\mu \xi_k)\}$ is equal to the manifold $\{G(\Phi_m^e \xi_k)\}$ where the Φ_m^e are those home-base functions for which atom i is mainly localized about lattice site i . (We have abbreviated the indices m, j by the single index m). To see that this is the case recall that in Chapter 2 we suggested that the manifolds $\{\Psi_\mu\}$ and $\{\Phi_m^P\}$ were equal, where in the latter expression we intend P as well as m to take all possible values. Accordingly the manifolds $\{G\Psi_\mu \xi_k\}$ and $\{G\Phi_m^P \xi_k\}$ must also be equal. Now note that

$$\begin{aligned}
 G\Phi_m^P \xi_k &= G(P^{(r)} \Phi_m^e) \xi_k \\
 &= GP\Phi_m^e (P^{(o)})^{-1} \xi_k \\
 &= \pm G\Phi_m^e \xi_k.
 \end{aligned}
 \tag{4.2}$$

* See footnote page I-10.

where $\xi_k = P^{(\sigma)} \xi_k$, and $G P = \pm G$. Thus taking a different value for P in $G(\Phi_m^P \xi_k)$ one simply generates the same states all over again. Any single value will do, and we choose $P = e$, the identity. It is worth noting that for each choice of the combined index mk , the states $G(\Phi_m^e \xi_k)$ are non-zero and linearly independent.

To write the secular equation for the low-lying eigenvalues of the system, one may take the matrix elements of H in any basis spanning the manifold $\{G(\Psi_\mu \xi_k)\}$. We have just shown that the states $\{G(\Phi_m^e \xi_k)\}$ constitute such a basis, so that we have the eigenvalues E being the solution of

$$\det \left[\langle G\Phi_m^e \xi_k | H | G\Phi_n^e \xi_q \rangle - E \langle G\Phi_m^e \xi_k | G\Phi_n^e \xi_q \rangle \right] = 0,$$

where the matrix element multiplying E occurs because while they are linearly independent, the states $G(\Phi_m^e \xi_k)$ are in general not orthogonal. Using the facts that $[H, G] = 0$ and $G^2 = G$ one has

$$\det \left[\langle \Phi_m^e \xi_k | H | \Phi_n^e \xi_q \rangle - E \langle \Phi_m^e \xi_k | G | \Phi_n^e \xi_q \rangle \right] = 0 \quad (4.3)$$

At this point, the basic purpose behind the home-base

function formulation is clear: Eq. (4.3) can be greatly simplified because the home-base functions $\{\phi_m^e\}$ are mainly localized in the same region of configuration space. With reference to Eq. (2.14) one sees that the matrix elements in Eq. (4.3) are dominated by the identity and nearest neighbor pair permutations in the expansion Eq. (4.1) for G .

Before continuing, we make a slight digression. The home-base functions were determined as certain localized functions which would span the manifold $\{\psi_\mu\}$. There are certainly many sets of localized functions which would serve the same purpose. For example we could make orthogonal linear combinations of the functions $\{\phi_m^e\}$ for $P = e$ to construct another set spanning the original set. If the corresponding linear combinations were made in turn for each of the sets $\{\phi_m^P\}$, fixed P , we would have a new set of localized functions equally adequate for our purpose. With this leeway, it is a straight forward extension of Herring's definition of home-base functions to take them such that

$$\langle \phi_m^e | H | \phi_n^e \rangle \propto \delta_{mn} \quad (4.4)$$

and

$$\langle \Phi_m^e | \Phi_n^e \rangle = \delta_{mn}$$

We shall see that this is equivalent to taking the home-base functions as eigenfunctions of the lattice Hamiltonian.

To continue, we slightly rephrase Eq. (4.3). We seek a matrix $\underline{\underline{U}}$ such that*

$$\underline{\underline{U}} \left[\langle \Phi_m^e \xi_k | G | \Phi_n^e \xi_q \rangle \right] \underline{\underline{U}}^\dagger = (N!)^{-1} \underline{\underline{1}} \quad (4.5)$$

or

$$\underline{\underline{U}}^\dagger \underline{\underline{U}} = N! \left[\langle \Phi_m^e \xi_k | G | \Phi_n^e \xi_q \rangle \right]^{-1} \quad (4.6)$$

in which case we have

$$\det (N! \underline{\underline{U}} \left[\langle \Phi_m^e \xi_k | H G | \Phi_n^e \xi_q \rangle \right] \underline{\underline{U}}^\dagger - E \underline{\underline{1}}) = 0 . \quad (4.7)$$

Using the localization properties Eq. (2.14), and the conditions given by Eq. (4.4) we get

* $\underline{\underline{U}}$ is not a unitary operator.

$$N: \left[\langle \Phi_m^e \xi_k | G | \Phi_n^e \xi_q \rangle \right]$$

$$= \frac{1}{2} \sum_{i < j} \left[\langle \Phi_m^e \xi_k | P_{ij} | \Phi_n^e \xi_q \rangle \right]$$

so that from Eq. (4.6) we have to first order

$$\underline{U} = \underline{U}^\dagger = \frac{1}{2} + \frac{1}{2} \sum_{i < j} \left[\langle \Phi_m^e \xi_k | P_{ij} | \Phi_n^e \xi_q \rangle \right]. \quad (4.8)$$

Similarly

$$N: \left[\langle \Phi_m^e \xi_k | H G | \Phi_n^e \xi_q \rangle \right] = \left[\bar{E}_m \delta_{mn} \delta_{kq} \right]$$

$$= \sum_{i < j} \left[\langle \Phi_m^e \xi_k | H P_{ij} | \Phi_n^e \xi_q \rangle \right]. \quad (4.9)$$

where

$$\bar{E}_m = \langle \Phi_m^e | H | \Phi_m^e \rangle. \quad (4.10)$$

Note that we are taking the Φ_m^e to be normalized.

Substituting Eq. (4.8) and Eq. (4.9) into Eq. (4.7) one has to first order

$$\det \left[\bar{E}_m \delta_{mn} \delta_{kq} - \sum_{i < j} \langle \Phi_m^e | \mathcal{J}_{ij} | \Phi_n^e \rangle \langle \xi_k | P_{ij}^{(\sigma)} | \xi_q \rangle - E \delta_{mn} \delta_{kq} \right] = 0 \quad (4.11)$$

where

$$\langle \Phi_m^e | \mathcal{J}_{ij} | \Phi_n^e \rangle = \langle \Phi_m^e | (H - \frac{1}{2} \bar{E}_m - \frac{1}{2} \bar{E}_n) P_{ij}^{(\sigma)} | \Phi_n^e \rangle. \quad (4.12)$$

The secular equation given by Eq. (4.11) now has the form

$$\det \left[\langle \Phi_m^e \xi_k | H_{eff} | \Phi_n^e \xi_q \rangle - E \delta_{mn} \delta_{kq} \right] = 0 \quad (4.13)$$

where

$$H_{eff} = H_L + H_X \quad (4.14)$$

$$H_L = \sum_m | \Phi_m^e \rangle \bar{E}_m \langle \Phi_m^e | \quad (4.15)$$

$$H_X = - \sum_{i < j} \mathcal{J}_{ij} \frac{1}{2} (1 + \underline{\sigma}_i \cdot \underline{\sigma}_j) \quad (4.16)$$

since $P_{ij}^{(\sigma)} = \frac{1}{2}(1 + \underline{\sigma}_i \cdot \underline{\sigma}_j)$ where $(1/2)\underline{\sigma}_i = \underline{I}_i$ is the nuclear spin operator for atom i . It is customary to

neglect the constant term in H_X , giving

$$H_X = - 2 \sum_{i < j} g_{ij} \mathbf{I}_i \cdot \mathbf{I}_j . \quad (4.16')$$

The effective Hamiltonian H_{eff} acting on the space of unsymmetrized products $\{\Phi_m^e \xi_k\}$ gives a first order approximation to the low-lying eigenvalues of the true Hamiltonian H acting on the properly symmetrized space $\{G(\Psi_{ij}^e \xi_k)\}$. We note that higher order corrections can be included in H_{eff} by retaining in the derivation more complex permutations than pair permutations. These corrections will be spin dependent and will appear as a more complicated H_X . With this extension in mind, note that all effects of the statistics appear in H_X ! This is more strikingly illustrated by repeating the derivation for a Bose system, say He^4 . One diagonalizes H in the manifold $\{S \Phi_m^e\}$, where S is the symmetrizer, rather than in $\{G \Phi_m^e \xi_k\}$. Except for the difference in mass, the same H_L obtains, while H_X becomes to lowest order

$$H_X = \sum_{i < j} g_{ij} \quad (4.17)$$

with g_{ij} also defined by Eq. (4.12). Furthermore, by

virtue of the localization properties of the $\{\phi_m^e\}$ given by Eq. (2.14) one sees that H_L is the dominant part of H_{eff} . To lowest order, then, one can neglect the statistics in solid He^3 and He^4 , in which case their differences in behavior are due only to the mass difference, facts which are well known.

The Hamiltonian H_L has all of the characteristics one would expect of a lattice Hamiltonian, and we identify it as such. One thinks of lattice dynamical behavior as the highly correlated behavior of a system of atoms undergoing oscillations about their own lattice sites, i.e. the behavior of the system near a given one of the points p^e , say p^e , in configuration space. The eigenfunctions of H_L , the home-base functions $\{\phi_m^e\}$ for $p = e$, are all mainly localized about the point p^e , so that each atom does remain mainly localized about its own lattice site. Furthermore, it is just in the neighborhood of p^e that the functions $\{\phi_m^e\}$ may be considered as accurately representing the true system. One can also show (See Appendix B: Group Theory) that the symmetry group of H_L is in fact, just the space group used in standard lattice dynamical problems.

We now direct our attention to the spin dependent part of Eq. (4.14), the Hamiltonian H_X , which we identify as the exchange Hamiltonian. It has the usual Heisenberg form except that the exchange integral is replaced by an exchange operator having matrix elements between the states of the lattice Hamiltonian. These matrix elements, given by Eq. (4.12), are basically of the form

$$\langle \phi_m^e | H | \phi_n^p \rangle , \quad (4.18)$$

since the $\bar{E}$ terms occur essentially to correct for the lack of orthogonality between ϕ_m^e and ϕ_n^p . As is clear from their indices, there are two differences between the states ϕ_m^e and ϕ_n^p : a number of atoms in the latter appear interchanged with respect to the former; and they correspond to two different lattice vibrational states, if $m \neq n$. Since neither of these states are eigenfunctions of H , they will be coupled via a matrix element such as given by Eq. (4.18). One may interpret this matrix element crudely as the frequency with which the system passes from one of these states to the other and then back again. This is clearly the process of exchange, with the additional feature that there can be a simultaneous

change in the lattice dynamical state of the system. We have simply given an intuitive paraphrase of what is obvious from Eq. (4.12): The exchange operator can couple different states of the lattice Hamiltonian. Thouless²⁷ has implied that this coupling is probably only significant between lattice states differing in energy by less than or on the order of the diagonal part of J_{ij} , i.e., about 10^{-3} °K. Since the lattice states are presumably phonon-like, and their spectrum a quasi-continuum, there are certainly a very large number of such states lying within this interval about any given state. Furthermore, one can show (See Appendix B: Group Theory) that there are no selection rules for the matrix elements given by Eq. (4.12), meaning that two phonon-like states of H_L with different momentum can be coupled: Accordingly, the exchange operator can create, destroy, and scatter phonons, as has been pointed out by Thouless. The non-conservation of phonon momentum makes sense physically in that phonons can scatter off of spin waves. It also leads to the possibility of spin-lattice relaxation in solid He³ due to the exchange interaction, a matter which has been discussed in the literature.^{18,27} Finally, we point out that the measured exchange frequency has been

identified²⁸ as

$$J_{ij} = \text{Tr}(\rho_L \mathcal{J}_{ij}) \quad (4.19)$$

where ρ_L is the density matrix for the lattice Hamiltonian.

To conclude this section we point out that the formalism of this chapter reduces trivially in the case of a two-body problem. Consider the effective two-body Hamiltonian

$$h = t_1 + t_2 + v(12) + U(1) + U(2) \quad (4.20)$$

where t_1 and t_2 are the kinetic energies of two atoms, $v(12)$ the interaction between them, $U(1)$ the effective potential seen by atom 1 due to all of the other atoms of the lattice excepting atom 2, and similarly for $U(2)$. The $T = 0$ exchange frequency for the pair is

$$J_{12} = \langle \phi | (h - \bar{\epsilon}) P | \phi \rangle \quad (4.21)$$

$$\bar{\epsilon} = \langle \phi | h | \phi \rangle$$

where ϕ is the normalized home-base function given by

$$\phi = (\psi^+ + \psi^-) / \sqrt{2} \quad (4.22)$$

and where ψ^+ and ψ^- are the lowest symmetric and anti-symmetric coordinate eigenfunctions of h . Since the Hamiltonian given by Eq. (4.20) is formally identical to that for two electrons belonging to a pair of hydrogen atoms, we refer the reader to Herring³¹ for more detailed comments. We note that the disadvantage of trying to study exchange in a large many-body system by using an effective two-body model is that one loses the exchange operator, and can only hope to calculate the $T = 0$ exchange frequency given by Eq. (4.21).

2. The Surface Integral Expression

The expression given by Eq. (4.12) for the matrix elements of the exchange operator $\mathcal{J}_{ij}$ can be put in another form following a procedure due to Herring. Consider first a diagonal element for a nearest neighbor pair exchange. The overlap between ϕ_m^e and $P_{ij}\phi_m^e$ will be important only near the hyper-surface separating Ω_e and

$\Omega_{p_{ij}}$, and so to lowest order one can neglect the contribution to the integral outside of the combined region of these two adjacent sections. One views Φ_m^e and $\bar{E}_m$ as an eigenfunction and corresponding eigenvalue of the truncated Hamiltonian discussed in Chapter 3. Since the truncated Hamiltonian is identical to H within Ω_e , one has for use in Eq. (4.12):

$$\begin{aligned} (H - \bar{E}_m) | \Phi_m^e \rangle &= 0 \quad \text{except in } \Omega_{p_{ij}} \\ (H - \bar{E}_m) P_{ij} | \Phi_m^e \rangle &= 0 \quad \text{except in } \Omega_e \end{aligned} \quad (4.23)$$

Let Σ be an extension of the hyper-surface separating Ω_e and $\Omega_{p_{ij}}$ such as to divide all of configuration space into a "near" half containing Ω_e , and a "far" half containing $\Omega_{p_{ij}}$. Using Eq. (4.23), Eq. (4.12) becomes

$$\langle \Phi_m^e | \mathcal{P}_{ij} | \Phi_m^e \rangle \approx \int_{\text{near}} \Phi_m^{e*} (H - \bar{E}_m) P_{ij} \Phi_m^e d\tau \quad (4.24)$$

One then integrates by parts the kinetic energy terms in H .

$$\langle \Phi_m^e | \mathcal{J}_{ij} | \Phi_m^e \rangle \approx$$

$$\begin{aligned} & (-\hbar^2/2m) \int \sum d\vec{S} \cdot \left[\Phi_m^e \vec{\nabla}_{3N}^* P_{ij} \Phi_m^e - (P_{ij} \Phi_m^e) \vec{\nabla}_{3N} \Phi_m^e \right] \\ & + \int_{\text{near}} (P_{ij} \Phi_m^e) \left[(H - \bar{E}_m) \Phi_m^e \right]^* d\tau \end{aligned} \quad (4.25)$$

Using Eq. (4.23) again, and noting that $\sum$ is midway between the points p^e and p^{ij} one has

$$\langle \Phi_m^e | \mathcal{J}_{ij} | \Phi_m^e \rangle \approx \frac{\hbar^2}{m} \Re \int \sum d\vec{S} \cdot (P_{ij} \Phi_m^e) \vec{\nabla}_{3N} \Phi_m^e \quad (4.26)$$

where the direction of the surface element $d\vec{S}$ is from the near to the far side of $\sum$, $\Re$ means real part of, and $\vec{\nabla}_{3N}$ is the 3N dimensional gradient. (This is just Herring's Eq. (4.19)³¹ for the case of one electron per atom).

The derivation can be repeated for the off-diagonal elements of Eq. (4.12):

$$\langle \phi_m^e | \mathcal{J}_{ij} | \phi_n^e \rangle \approx$$

$$\begin{aligned} & (\hbar^2/2m) \int_{\Sigma} d\vec{S} \cdot \left[(P_{ij} \phi_n^e) \vec{\nabla} \phi_m^{e*} - \phi_m^{e*} \vec{\nabla} (P_{ij} \phi_n^e) \right] \\ & + \frac{1}{2} (\bar{E}_m - \bar{E}_n) \int_{\text{near}} \left[\phi_m^{e*} P_{ij} \phi_n^e - (P_{ij} \phi_m^e)^* \phi_n^e \right] d\tau \end{aligned} \quad (4.27)$$

where we have used the fact that

$$\int_{\text{far}} \phi_m^{e*} P_{ij} \phi_n^e d\tau = \int_{\text{near}} (P_{ij} \phi_m^e)^* \phi_n^e d\tau.$$

Crudely speaking, the surface and volume integrals in Eq. (4.27) are of the same order of smallness in the overlap of ϕ_m^{e*} and $P_{ij} \phi_n^e$. Since the matrix elements of $\mathcal{J}_{ij}$ which are expected to be significant are those for $\bar{E}_m - \bar{E}_n$ of the order of the diagonal part of $\mathcal{J}_{ij}$, which is small, one has to lowest order for these matrix elements:

$$\langle \phi_m^e | \mathcal{J}_{ij} | \phi_n^e \rangle \approx$$

$$(\hbar^2/2m) \int d\vec{S} \cdot \left[(P_{ij} \phi_n^e) \vec{\nabla}_{3N} \phi_m^{e*} - \phi_m^{e*} \vec{\nabla}_{3N} P_{ij} \phi_n^e \right] \quad (4.28)$$

$\sum$

which is just the result of Thouless²⁷.

CHAPTER 5: CRITIQUE OF VARIOUS THEORIES OF EXCHANGE IN SOLID HE³

1. Introduction

A number of papers treating exchange in solid He³ have appeared in the literature over the last ten years. In this chapter we show that these theories may be deduced from the development of the last three chapters according to various approximations, which we discuss critically.

There are two general classes of theories: 1) The theories in the first class may be viewed as first choosing approximations to the home-base functions. The resultant expressions for $(\mathcal{G}_{ij})_{mn}$ may be cluster expanded by means of the same expansions used in the various theories. Their results are reproduced by approximating $(\mathcal{G}_{ij})_{mn}$ by the two-body terms in these expansions. In two cases, this description should be qualified: Because of their choice for the ground state home-base function, Bermendes and Primakoff²³ do not need to cluster expand. Also, Thouless²⁷ leaves his expression for $(\mathcal{G}_{ij})_{mn}$ in the form of a many-body integral. 2) The theories in the second class begin by reducing the full many-body problem, without exchange,

to an effective two-body Schroedinger equation, which describes a nearest neighbor pair of atoms with the rest of the lattice represented by an effective potential seen by these two atoms. The two-body equation is then modified to allow the atoms to exchange. We have pointed out previously that exchange is easily understood in such two-body systems without resorting to the concept of home-base functions. Nevertheless, the formalism of the preceding chapters when applied to a two-body system does result in expressions completely equivalent to those ordinarily used. Thus, the $T = 0$ exchange frequency for the pair of atoms is given by Eq. (4.21), and one may view the theories in this class according to their approximations of the home-base functions appropriate to the two-body Hamiltonian. It should be noted that the drawback of working with an effective two-body problem is that one can only hope to calculate the $T = 0$ exchange frequency J_{ij} which we identify with $(J_{ij})_{00}$. The fact that one really has an exchange operator is lost when one reduces the N -body problem to an effective two-body problem.

At this point we should like to emphasize one particular approximation which is made by all of the theories except that of Thouless: The exchange frequencies are

calculated by two-body integrals involving a Gaussian function for the two atoms multiplied by a correlation function for the pair. These expressions neglect the short range correlations of the exchanging pair of atoms with their surrounding neighbors. We shall show in a subsequent paper that these many-body effects are important to the exchange process; i.e. that exchange is a many-body effect. Such correlations make it more difficult for two atoms to maneuver around each other in the process of exchange, an effect that will be more pronounced at higher densities. By neglecting these correlations one will get a magnitude for J which is too large, and its density dependence will be too "flat". Not only do the above theories neglect these correlations, but in general, they already obtain magnitudes of J which are too small. This suggests that there is still more to be learned about the details of an accurate calculation of J . We do not mean to suggest that the neglect of the many-body effects accounts for the poor density dependence obtained by a number of the theories, although it certainly is a factor. For, as has been pointed out in the literature,²⁸⁻³⁰ the density dependence as well as the magnitude for J depends crucially on the size and density dependence assumed for

the Gaussian parameters. This is precisely a point we have tried to emphasize in this paper: An investigation of exchange must be preceded by a proper treatment of the lattice dynamical behavior of the system.

2. Early Theories

The treatment of exchange in the pioneering work on solid He³ by Bernades and Primakoff²³ (BP) is characterized by taking the ground state home-base function ϕ_0^e to be a product of single atom functions:

$$\phi_0^e \approx \prod_i \phi_i(i)$$

$$\phi_i(j) = C \exp[-n^2(\underline{r}_j - \underline{R}_i)^2/2] \quad (5.1)$$

In this case Eq. (2.12) for the $T = 0$ exchange frequencies $J_{ij} = (J_{ij})_{00}$ becomes:

$$J_{ij} = \langle ij | (t_1 + t_2 + v_{\text{eff}}(12)) | ji \rangle - \langle ij | (t_1 + t_2 + v_{\text{eff}}(12)) | ij \rangle$$

$$+ 2\Delta \sum_{\mathbf{k}} \left[\langle i\mathbf{k} | v_{\text{eff}}(12) | j\mathbf{k} \rangle - \langle i\mathbf{k} | v_{\text{eff}}(12) | i\mathbf{k} \rangle \Delta \right] \quad (5.2)$$

$$|ij\rangle = \phi_i(1)\phi_j(2)$$

$$|ji\rangle = \phi_j(1)\phi_i(2)$$

$$\Delta^2 = \langle ij | ji \rangle$$

$$t_i = \hbar^2 v_i^2 / 2m$$

and following BP we have replaced the Lennard-Jones potential $v(r)$ by the truncated potential

$$v_{\text{eff}}(r) = v(r) \exp(-\lambda r^{-10}). \quad (5.3)$$

BP neglect the last two terms in Eq. (5.2), terms which must appear in the expression for J_{ij} since $\phi_i(1)$ and $\phi_j(1)$ are not orthogonal.³² The last term is likely to be small, but one can show that the second (including the minus sign) is of the same order and sign as the first term. With this correction, BP would have obtained an even larger value, in magnitude, for the nearest neighbor exchange frequency than the value $J = -.02^\circ\text{K}$, which they calculated for an hcp lattice of nearest neighbor distance

$R = 3.80 \text{ \AA}$. This value is about a factor 20 larger than experiment.

The excessive size of BP's value of J is due in large part to their use of a rather small Gaussian parameter, $\alpha = .9 \text{ \AA}^{-1}$, which allows too much overlap between the wavefunctions in Eq. (5.2). This choice of α is in turn due to their incomplete treatment of the short-range correlations, which they include phenomenologically for the potential energy according to Eq. (5.3), but do not include for the kinetic energy. Minimization of their expression for the ground state energy with respect to α tends to select an overly small value of this parameter, since the kinetic energy goes as α^2 while the potential energy at small α is prohibited from becoming too large due to the cut off incorporated into V_{eff} . BP neglect the fact that the kinetic energy cannot continue to decrease as α decreases in that a given atom is always constrained to vibrate within the box presented by the hard-core repulsive forces of its neighbors.

Two other early theories should be mentioned, that due to Saunders²⁴ and a revision of the same theory presented by Garwin and Landesman²⁵. In these works the pair correlations are introduced in a more fundamental

way than in BP. However, the single particle functions are taken to be free particle functions, a feature which necessitated a heuristic derivation of the exchange integral. For this reason, we will not further discuss these theories here, but refer the reader to the critical review by Mullin.³³

3. Nosanow and Mullin and Nosanow and Varma

Nosanow and Mullin²⁶ (NM) calculated the $T = 0$ exchange frequencies $J_{ij} = (\mathcal{J}_{ij})_{\infty}$ using an Einstein approximation to the phonons and directly incorporating the short range correlations into the wave function. This calculation was generalized to finite temperatures, using a proper phonon spectrum, by Nosanow and Varma²⁸ (NV). NV's work yields expressions for the matrix elements $(\mathcal{J}_{ij})_{mn}$ and also calculates $\text{Tr}(\rho_L \mathcal{J}_{ij})$ which they identify with the finite temperature exchange frequencies. Their approximations for the home-base functions are:

$$(NM) \quad \Phi_0^e \approx \prod_i \phi_i(1) \prod_{i < j} f_{ij} \quad (5.4)$$

$$(NV) \quad \Phi_m^e \approx \phi_m \prod_{i < j} f_{ij} \quad (5.5)$$

where

$$\phi_i(j) = c \exp[-A(\underline{r}_j - \underline{R}_i)^2/2]$$

and where ϕ_m are eigenfunctions of a system of coupled simple harmonic oscillators, m standing for the set of occupation numbers. The functions f_{ij} are the short-range correlations given by

$$f_{ij} = \exp\left\{-K \left[(\sigma/r_{ij})^{12} - (\sigma/r_{ij})^6 \right]\right\} \quad (5.6)$$

The form of Eqs. (5.4) and (5.5) is suggested by the usual expectation that the low-lying excitations of a crystal are phonon like. In addition, the large zero-point motion in solid He^3 necessitates an explicit treatment of the short-range correlations between atoms.

To simplify the complicated integrals for $(f_{ij})_{mn}$ given by Eq. (2.12), one employs a cluster expansion. Because of the special dependence of $(f_{ij})_{mn}$ on atoms i and j , it is natural to begin with the two-body terms for the pair (i,j) , then sum over k for the three body terms (i,j,k) , etc. With the exception of this rather logical alteration, we employ precisely the cluster expansions used by NM and NV. Retaining only the two-body

terms, one gets from cluster expanding Eq. (2.12):*

$$(NM) \quad (J_{ij})_{\infty} \approx 4 \frac{\langle \phi_i(i) \phi_j(j) f_{ij} | (H_{ij} - \epsilon_{ij}) | \phi_j(i) \phi_i(j) f_{ij} \rangle}{\langle \phi_i(i) \phi_j(j) f_{ij} | \phi_i(i) \phi_j(j) f_{ij} \rangle} \quad (5.7)$$

$$(NV) \quad (J_{ij})_{mn} \approx 4 \frac{\langle \phi_m f_{ij} | (H_{ij} - \frac{1}{2} \epsilon_{ij}^m - \frac{1}{2} \epsilon_{ij}^n) P_{ij} | \phi_n f_{ij} \rangle}{\langle \phi_m f_{ij} | \phi_m f_{ij} \rangle^{1/2} \langle \phi_n f_{ij} | \phi_n f_{ij} \rangle^{1/2}} \quad (5.8)$$

where

$$H_{ij} = t_i + t_j + v_{ij}$$

* NM and NV's convention for J_{ij} or J_{ij} is a factor of four larger than the more standard convention we have used in arriving at Eq. (2.12), thus this factor in Eq. (5.7) and Eq. (5.8). See Appendix D: Conventions. One should also be aware that NV's equations (3.10), (4.1), and (4.2) contain an erroneous extra factor of 2. This factor has been omitted in (4.3) and subsequent equations, so their numerical results are not affected. In any case, in comparing with experiment, attention must be paid to the convention used. For example, Panczyk and Adams¹⁷ use the standard convention for J , so that both NM and NV's values of J should be divided by four to enable comparison with that experiment.

$$\epsilon_{ij} = \frac{\langle \phi_i(i) \phi_j(j) f_{ij} | H_{ij} | \phi_i(i) \phi_j(j) f_{ij} \rangle}{\langle \phi_i(i) \phi_j(j) f_{ij} | \phi_i(i) \phi_j(j) f_{ij} \rangle}$$

$$\epsilon_{ij}^m = \frac{\langle \phi_m f_{ij} | H_{ij} | \phi_m f_{ij} \rangle}{\langle \phi_m f_{ij} | \phi_m f_{ij} \rangle}.$$

After some algebra one can show that Eq. (5.7) is just NM's expression for J_{ij} . Similarly Eq. (5.8) gives NV's results for the diagonal matrix elements $(J_{ij})_{mm}$, however, is slightly different from their expression for the off-diagonal elements. This is because NV neglected the fact that the states $\mathcal{U}(\phi_m \xi)$ and $\mathcal{U}(\phi_n \xi)$ for $m \neq n$, where ξ is a spin function, are not orthogonal.

Note that the equivalent surface integral for exchange given by Eq. (2.26) can also be cluster expanded according to NM and NV. One gets in the NM case

$$(J_{ij})_{00} = (4\hbar^2/m) \int_{\Sigma} d\vec{S} \cdot \phi_i(j) \phi_j(i) f_{ij} \vec{\nabla}_6 (\phi_i(i) \phi_j(j) f_{ij}) \quad (5.9)$$

taking $\phi_i(i) \phi_j(j) f_{ij}$ normalized; Σ is the hyper-surface in the six dimensional space (r_i, r_j) midway between the

points (R_i, R_j) and (R_j, R_i) . According to Herring's derivation, Eq. (5.9) and Eq. (5.8) would be equivalent if the functions

$$[\phi_i(i)\phi_j(j) \pm \phi_i(j)\phi_j(i)]f_{ij} \quad (5.10)$$

were eigenfunctions of H_{ij} . Guyer³ has pointed out that they are not. Instead, they are likely to be eigenfunctions of a Hamiltonian such as

$$H_{ij}^G = H_{ij} + U_{ij}(i) + U_{ij}(j) \quad (5.11)$$

where $U_{ij}(i)$ represents the effective field seen by atom i due to all other atoms except atom j . Eq. (5.9) is thus equivalent to Eq. (5.7) with H_{ij} replaced by H_{ij}^G . We shall argue later that this latter calculation is essentially that of Guyer and Zane.²⁹ It is consistent with their results that we find Eq. (5.9) gives an improved density dependence and about the same magnitude for J as NM's calculations using Eq. (5.7). (See Fig. 1) However, the density dependence is still too flat. Thus, while the inclusion of the potentials $U_{ij}(i)$ in the two-body Hamiltonian does improve the result for J , this only

accounts for part of the difference between the results of NM and Guyer and Zane. We shall see later that the major cause of the difference lies in the different density dependence assumed for the Gaussian constants in the two theories.

Guyer and Zane have criticized the work of NM and NV suggesting that the use of a correlation function in Eqs. (5.7) and (5.8) which is independent of symmetry effects, i.e. $P_{ij} f_{ij} = f_{ij}$, leads to the omission of what they call the interaction contribution to exchange. We show in a later section that this criticism rests on an approximation made in their calculations, and not made by NM and NV. Thus, Eqs. (5.7) and (5.8) as they stand do indeed contain both tunneling and interaction contributions to exchange.

The calculations of NM and NV involve two basic approximations: approximating the home-base functions, and the subsequent cluster expansion. We discuss the latter first. NM and NV cluster expanded simultaneously with respect to the statistics and the short range correlations. One may view the approach of our work as cluster expanding with respect to statistics alone, for

Mullin³² has shown that cluster expansion with respect to the statistics can yield the same result as the procedure of expanding the antisymmetrizer. Such an expansion is likely to be good, as there is a small parameter involved--the overlap between localized functions appropriate to different assignments of the atoms to the lattice sites. The question, then, is how successful is NM and NV's cluster expansion of the short-range correlations as far as a calculation of exchange is concerned. To test this, we performed a Monte Carlo calculation of the full expression for $(g_{ij})_{00}$ and compared it to its cluster expanded approximation. We find that the cluster expanded approximation is poor, basically because of the many-body effects discussed in the introduction to this chapter. This calculation will be described in a subsequent paper. Note that NM and NV defined the exchange frequencies only after having used their cluster expansion, and so to improve their calculation one would have to go through the kind of formalism given in the preceding chapters of this paper.

It is apparent that without the use of the cluster expansion, NM and NV's calculations would lead to values

of J with an improved density dependence, but a magnitude even smaller than the results they obtained. NV suggest that their choice of f_{ij} according to Eq. (5.6) presents an overly severe hard core, which would clearly give a too small value for $|J|$. One might also ask if the Gaussian function, which is chosen according to its behavior when the atoms are near the lattice sites, is inaccurate, in fact too small, when the atoms are far from their lattice sites. This is a subtle question as it is the combined effect of the "tail" of the Gaussian and the short-range part of the pair-correlation functions which should accurately represent the "tail" or the home-base function. One feature which is clearly crucial to the calculations of NM and NV, as well to the other theories, is the determination of the Gaussian constants, or phonon frequencies as the case may be, and their density dependence. A slight variation in these parameters can cause a large change in the results for J . It seems likely that NM and NV's use of a correlation function which over emphasizes the hard core would lead, in minimization of the ground-state energy, to Gaussians which are too broad at high densities. This may be an important factor in their obtaining a too "flat" density dependence for J .

4. Thouless

Thouless²⁷ first pointed out the necessity of using an exchange operator for solid He^3 , and discussed the essential physical ideas behind that operator. His work is based on that of Herring, as is the work of the present paper. While our treatment of exchange in solid He^3 is in full accord with that of Thouless, it also constitutes both a more general and explicit theory than his. For example, the derivation used by Thouless yields the surface integral expression for the matrix elements of the exchange operator given by Eq. (4.28), but not the equivalent volume integral given by Eq. (4.12). Furthermore, he rather intuitively specifies the wavefunctions appearing in the surface integral as the wavefunction appropriate to a single one of his cavities plus its extensions into the various ducts connected to the cavity. It is clear that this is just a home-base function. We have described these functions more explicitly, and suggested ways of calculating approximations to them. Finally, it has been an essential feature of our presentation that a proper treatment of exchange in solid He^3 requires the simultaneous

treatment of the lattice Hamiltonian, which Thouless does not explicitly introduce.

5. Guyer and Zane

The theory of exchange presented by Guyer and Zane²⁹ (GZ) is of the second type mentioned in Sec. 1--they start with an effective two-body Schroedinger equation. Accordingly, they are limited to a calculation of the $T = 0$ exchange frequency for the pair of atoms under consideration, which they take to be nearest neighbors. GZ have obtained the best density dependence for J of the various theories. As they point out, this is largely due to the density dependence which they have determined for their Gaussian constant. While we are in agreement with this feature of their theory, we are in some doubt as to their calculated magnitude for J , because of certain approximations in their paper.

We first outline the GZ approach. They wish to calculate the eigenvalues ϵ_{12}^+ and ϵ_{12}^- of the two-body Schroedinger equation

$$h(12) \psi_{12}^{\pm}(12) = \epsilon_{12}^{\pm} \psi_{12}^{\pm}(12) \quad (5.12)$$

corresponding to the lowest spatially symmetric and antisymmetric eigenfunctions. The exchange frequency, with GZ's convention (See Appendix D: conventions), is given by

$$J = \epsilon_{12}^{+} - \epsilon_{12}^{-} \quad (5.13)$$

To calculate an approximation to J , one can approximate $\psi_{12}^{\pm}(12) \approx |1 \pm X\rangle$, $P|1\rangle = |X\rangle$, giving

$$\epsilon_{12}^{\pm} \approx \frac{\langle 1 \pm X | h(12) | 1 \pm X \rangle}{\langle 1 \pm X | 1 \pm X \rangle} \quad (5.14)$$

To first order in the overlap this gives

$$J = 2 \frac{\langle 1 | (h(12) - \bar{\epsilon}) | X \rangle}{\langle 1 | 1 \rangle} \quad (5.15)$$

$$\bar{\epsilon} = \frac{\langle 1 | h(12) | 1 \rangle}{\langle 1 | 1 \rangle}$$

which is precisely* Eq. (4.21) suggested by the present paper, as well as the form of Eq. (5.7) used by Nosanow and Mullin.

GZ present two calculations of exchange, the first giving their tunneling approximation; the second a more involved calculation yielding both tunneling and interaction contributions to exchange. We briefly review these calculations to point out particular approximations that have been made. The first is precisely a calculation of Eq. (5.14) for $\epsilon_{12}^{\pm}$, and thus Eq. (5.15) for J , taking $|1 \pm X\rangle$ according to GZ(54). Note that Eq. (5.14) may be written

$$\epsilon_{12}^{\pm} \approx \frac{\langle 1 \pm X | h(12) | 1 \rangle}{\langle 1 \pm X | 1 \rangle} \quad (5.16)$$

and taking $h(12) = h_{12}^B(12) + \Delta U_2(1) + \Delta U_1(2)$ this becomes

$$\epsilon_{12}^{\pm} \approx \frac{\langle 1 \pm X | h_{12}^B(12) | 1 \rangle}{\langle 1 \pm X | 1 \rangle} + 2 \frac{\langle 1 \pm X | \Delta U_2(1) | 1 \rangle}{\langle 1 \pm X | 1 \rangle} \quad (5.17)$$

*There is a factor of two difference due to conventions.

GZ make the approximation

$$h_{12}^B(12) | 1 \rangle \approx \epsilon_{12} | 1 \rangle \quad (5.18)$$

where $| 1 \rangle = \phi_1(1)\phi_2(2)g(r_{12})$, in arriving at their equation GZ(55) for ϵ_{12}^* . It is this approximation which eliminated the interaction terms from their first calculation, and not the form of either Eq. (5.14) or Eq. (5.15). For the eigenfunction of $h_{12}^B(12)$ involves the correlation function $g(\underline{r}, \Delta)$, or $g_{12}(12)$, defined by GZ(48); the correlation function $g(r_{12})$ is presumably identical to $g(r; \Delta)$ defined by GZ(49). If we write the eigenvalue of GZ(49) as $\epsilon_{12}' - 2\epsilon_0$ so as to distinguish it from the eigenvalue of GZ(48), a comparison of these two equations* shows that

$$h_{12}^B(12) | 1 \rangle = \epsilon_{12}' | 1 \rangle + \theta(\underline{r}) | 1 \rangle \quad (5.19)$$

$$\theta(\underline{r}) = \left[-\frac{\hbar^2}{m} \frac{\partial^2}{\partial r^2} + \frac{\hbar^2 \alpha^2}{m} (\Delta - \underline{\Delta} \cdot \hat{r}) \right] g'(r)/g(r)$$

*Both GZ(48) and GZ(49) contain an erroneous factor of $1/2$, also pointed out by Brandow.⁶

where $\underline{r} = \underline{r}_{12}$ is the relative coordinate of the two atoms, $r = |\underline{r}|$, $\hat{r} = \underline{r}/r$, and $g'(r) = dg(r)/dr$. Accordingly, GZ's "tunneling" calculation should have yielded

$$J \approx 4 \frac{\langle X | \Delta U_2(1) | 1 \rangle}{\langle 1 | 1 \rangle} + 2 \frac{\langle X | \theta(\underline{r}) | 1 \rangle}{\langle 1 | 1 \rangle} \quad (5.20)$$

$$- 2 \frac{\langle 1 | \theta(\underline{r}) | 1 \rangle}{\langle 1 | 1 \rangle} \frac{\langle X | 1 \rangle}{\langle 1 | 1 \rangle}$$

rather than just the first term of this expression given by GZ(55). We show that $\langle X | \theta(\underline{r}) | 1 \rangle$ is essentially GZ's interaction term. Since $\phi_1(1)\phi_2(2)\phi_1(2)\phi_2(1)g^2(r)$ depends only on $r = |\underline{r}|$, the angular integration over $\Delta \cdot \hat{r}$ in $\theta(\underline{r})$ gives zero.

$$\langle X | \theta(\underline{r}) | 1 \rangle = - (\hbar^2/m) \langle \phi_1(2)\phi_2(1)g(r) | (2/r) | \phi_1(1)\phi_2(2)g'(r) \rangle$$

$$+ (\hbar^2 \sigma^2 \Delta/m) \langle \phi_1(2)\phi_2(1)g(r) | \phi_1(1)\phi_2(2)g'(r) \rangle \quad (5.21)$$

One recognizes the second term in Eq. (5.21) as GZ's interaction term, except for a numerical factor. If one views $g'(r)$ crudely as acting like $\delta(r-\sigma)$ where σ is

the size of the hard core in $v(12)$, one sees that the ratio of the first and second terms in E_4 . (5.21) is like -1 to $\alpha^2 \Delta \sigma / 2$ respectively, where $\alpha^2 \Delta \sigma / 2 = 0(10)$ for the densities that GZ considered. Thus, the second term in Eq. (5.21) dominates. The same kind of rough analysis suggests that the third term in E_4 . (5.2) is two or three orders of magnitude smaller than the second. One thus has

$$J \approx 4 \frac{\langle X | \Delta U_2(1) | 1 \rangle}{\langle 1 | 1 \rangle} \quad (5.22)$$

$$+ (2\hbar^2 \alpha^2 \Delta / m) \frac{\langle \phi_1(2) \phi_2(1) g(r) | \phi_1(1) \phi_2(2) g'(r) \rangle}{\langle 1 | 1 \rangle}$$

which is precisely the form of GZ's full expression for J except that the interaction term here is twice that of GZ.* We discuss this difference shortly. The point we wish to emphasize is that a calculation of J using Eq. (5.15)

* The interaction term here is actually four times as large as that appearing in the GZ paper, but the result in the paper should be a factor of two larger. (Private Communication, R. A. Guyer.)

where $|1\rangle$ and $|X\rangle$ involve a correlation function depending on $r = |\underline{r}_{12}|$ will include both tunneling and interaction aspects of exchange. Thus, while the calculations of Nosanow-Mullin, and Nosanow-Varma are clearly approximations to J , the nature of the approximation is not simply that the interaction contributions to exchange have been ignored.

In GZ's second calculation, it would seem that the approximation given by Eq. (5.18) is used inconsistently, so that some of the terms which are neglected in the first calculation are retained in the second. Consider GZ(58). Since $g_{12}^{\pm}(12)$ is eventually to be replaced by $g(r_{12})$, and the equation integrated over the half space Γ_D , one may write

$$\epsilon_{12}^{\pm} \approx \frac{\langle \bar{1} | h_{12}^B(12) | 1 \rangle \pm \langle \bar{1} | h_{12}^B(21) | X \rangle}{\langle \bar{1} | 1 \rangle \pm \langle \bar{1} | X \rangle} + 2 \frac{\langle 1 | \Delta U_2(1) | 1 \pm X \rangle}{\langle 1 | 1 \pm X \rangle} \quad (5.23)$$

where the integration over Γ_D is indicated by the $|\bar{1}\rangle$ in the first term, which we define to be $|1\rangle$ in Γ_D , and zero elsewhere. The ΔU terms in GZ(58) are already in

the form of expectation values, so they are not affected by the integration procedure. In going from GZ(58) to GZ(59), use is made of the fact that $h_{12}^B(21) | X \rangle = t_D h_{12}^B(12) | 1 \rangle + (2\hbar^2 \alpha^2 / m) \Delta \cdot \hat{r} \frac{g'(r)}{g(r)} | X \rangle$ where $t_D = \phi_1(2)\phi_2(1)/\phi_1(1)\phi_2(2)$. By making the approximation Eq. (5.18) in GZ(59) it would seem that one is approximating

$$h_{12}^B(21) | X \rangle \approx \epsilon_{12} | X \rangle + (2\hbar^2 \alpha^2 / m) \Delta \cdot \hat{r} \frac{g'(r)}{g(r)} | X \rangle \quad (5.24)$$

which is not consistent with the permuted equivalent of Eq. (5.18), namely $h_{12}^B(21) | X \rangle \approx \epsilon_{12} | X \rangle$. The results of GZ's second calculation are obtained by substituting Eqs. (5.18) and (5.24) into Eq. (5.23). Note that

$$\langle \bar{1} | \Delta \cdot \hat{r} \frac{g'(r)}{g(r)} | X \rangle = \frac{\Delta}{4} \langle \phi_1(1)\phi_2(2)g(r) | \phi_1(2)\phi_2(1)g'(r) \rangle \quad (5.25)$$

where factors of 1/2 come from the angular integration of

$\Delta \cdot \hat{r}$, and from converting the integral over Γ_D to that overall space. Combining Eqs. (5.23)-(5.25), one has for J

$$J = 4 \frac{\langle X | \Delta U_2(1) | 1 \rangle}{\langle 1 | 1 \rangle} \quad (5.26)$$

$$+ (\hbar^2 \omega^2 / \Delta / m) \frac{\langle \phi_1(2) \phi_2(1) g(r) | \phi_1(1) \phi_2(2) g'(r) \rangle}{\langle 1 | 1 \rangle}$$

which is GZ's expression.*

We would like to point out that the essential reason behind the partial separation or tunneling and interaction effects in the GZ calculations, is their use in Eq. (5.17) of $| 1 \rangle = \phi_1(1) \phi_2(2) g(r_{12})$ involving a correlation function invariant under permutation of the atoms. For in this case

$$\langle X | \Delta U_2(1) | 1 \rangle \quad (5.27)$$

is negative independent of the interaction $v(12)$, since the effect of the interaction appears only through

* See footnote page I-76.

$g(r_{12})Pg(r_{12}) = g^2(r_{12}) \geq 0$, and $\Delta U_2(1)$ is always negative. However, for this same reason, this choice of $|1\rangle$ can only be an approximation to the eigenfunction of $h_{12}^B(12)$. Thus, one also obtains a contribution to the exchange from the first term in Eq. (5.17) involving $g(r_{12})g'(r_{12})$ whose sign can be affected by the correlation function. GZ refer to this former contribution to exchange as tunneling; the latter, the interaction contribution. Note that a perfectly valid alternate calculation would be to take $|1\rangle = \phi_1(1)\phi_2(2)g_{12}(12)$, which is the eigenfunction of $h_{12}^B(12)$. In this case there would be only the ΔU terms in the expression for J . However, Eq. (5.27) would involve $g_{12}(12)Pg_{12}(12) = g_{12}(12)g_{12}(21) \neq g_{12}(12)^2$. One could no longer claim the sign of Eq. (5.27) to be independent of $v(12)$, i.e., both tunneling and interaction effects would be in the same term. Ebner and Sung³⁰ have pointed this out in saying that GZ got their interaction terms, meaning really the $g'(r_{12})$ terms, because of the approximation $g(r_{12}) \approx g_{12}(12)$. However, either calculation is a valid first order calculation of $\epsilon_{12}^{\pm}$ and thus J , and the resultant values of J , whether expressed as a sum of tunneling and interaction terms, or as some combined term,

should agree to lowest order.

There is another, and somewhat more convenient way of calculating J for GZ's two body model. The surface integral expression for J follows rigorously from the Schroedinger equation given by Eq. (5.12). We refer the reader to Thouless (his Eqs. (11)-(15)) for the details. One has

$$J = \epsilon_{12}^+ - \epsilon_{12}^- = (2\hbar^2/m) \int_{\Sigma} d\vec{S} \cdot (\mathbf{P}\phi) \vec{\nabla}_6 \phi \quad (5.28)$$

where Σ is the surface separating the direct space Γ_D from the exchanged space Γ_X , and ϕ is the home-base function given by

$$\phi = (\psi_{12}^+(12) + \psi_{12}^-(12)) / \sqrt{2} . \quad (5.29)$$

GZ have consistently approximated $\psi_{12}^{\pm}(12) \approx |1 \pm X\rangle$, so that one should get their results from

$$J \approx (2\hbar^2/m) \int d\vec{S} \cdot \phi_1(2)\phi_2(1)g(r_{12}) \vec{\nabla}_6(\phi_1(1)\phi_2(2)g(r_{12})) \quad (5.30)$$

where we assume $|1\rangle = \phi_1(1)\phi_2(2)g(r_{12})$ to be normalized.

We have calculated Eq.(5.30) using GZ's Gaussian values and correlation function; see Fig. 1. Their correlation function appropriate for a nearest neighbor distance of $R = 3.48 \text{ \AA}$ was used at all densities. We find the same density dependence as GZ, but a magnitude (near $R = 3.48 \text{ \AA}$) about a factor of eight smaller. Note that the interaction term in GZ's calculation is of the opposite sign and more than a factor of two smaller in magnitude than their tunneling term. Since we have suggested according to Eq.(5.22) that the interaction term should have an additional factor of two, this might explain the above discrepancy in the magnitude of J . In Fig. 2 it is seen that the density dependence of J is largely due to that of the Gaussian constant used. It is likely that GZ's use of a more realistic correlation function than NM and NV in determining this constant and its density dependence, has lead to GZ's improved density dependence for J .

6. Ebner and Sung

Ebner and Sung³⁰ (ES) have calculated J in best agreement with experiment. The choice of the Gaussian constant, and its density dependence, is again crucial. Their treatment of exchange is also of the second class mentioned in the

introduction of this chapter. They begin with an effective two-body Schroedinger equation which they have derived using Green's function techniques.

$$\bar{H}_{ij}(1,2) \psi^{\pm} = \epsilon^{\pm} \psi^{\pm} \quad (5.31)$$

(The use of $\psi^{\pm}$ is our notation). The energies are calculated by approximating $\psi^{\pm}$ in Eq. (5.31) by

$$\psi^{\pm} \approx (\phi_i(1)\phi_j(2)\chi_{ij}(1,2) \pm \phi_i(2)\phi_j(1)\chi_{ij}(2,1))/\sqrt{2}, \quad (5.32)$$

multiplying the equation by $\phi_i(1)\phi_j(2) \pm \phi_i(2)\phi_j(1)$, and integrating. Taking $J = (\epsilon^{+} - \epsilon^{-})/2$, this leads to first order to (we present the complex conjugate for convenience).

$$J \approx \frac{\langle \phi_i(1)\phi_j(2)\chi_{ij}(1,2) | (\bar{H}_{ij}(1,2) - \bar{\epsilon}) P | \phi_i(1)\phi_j(2) \rangle}{\langle \phi_i(1)\phi_j(2)\chi_{ij}(1,2) | \phi_i(1)\phi_j(2) \rangle} \quad (5.33)$$

where

$$\bar{\epsilon} = \frac{\langle \phi_i(1)\phi_j(2)\chi_{ij}(1,2) | \bar{H}_{ij}(1,2) | \phi_i(1)\phi_j(2) \rangle}{\langle \phi_i(1)\phi_j(2)\chi_{ij}(1,2) | \phi_i(1)\phi_j(2) \rangle} \quad (5.34)$$

In a manner similar to Guyer and Zane, ES split $\bar{H}_{ij}(1,2)$ into a biased part $H_{ij}(1,2)$ plus corrections, according to their equation ES(22). Furthermore

$$H_{ij}(1,2)\phi_i(1)\phi_j(2)\chi_{ij}(1,2) = \lambda_0\phi_i(1)\phi_j(2)\chi_{ij}(1,2) \quad (5.35)$$

Accordingly, $H_{ij}(1,2)$ acting to the left in Eq. (5.33) and Eq. (5.34) results in its cancellation in Eq. (5.33).

The remaining terms give

$$\begin{aligned} J = \int \phi_i(1)\phi_j(2)\chi_{ij}(1,2) [v_{ij}(1)+v_{ij}(2)-u_i(1)-u_j(2)] \\ [\phi_i(2)\phi_j(1) - \gamma\phi_i(1)\phi_j(2)] d^3r_1 d^3r_2 \end{aligned} \quad (5.36)$$

where

$$\gamma = \int \phi_i(1)\phi_j(2)\phi_i(2)\phi_j(1)\chi_{ij}(1,2) d^3r_1 d^3r_2$$

and

$$1 = \int \phi_i^2(1)\phi_j^2(2)\chi_{ij}(1,2) d^3r_1 d^3r_2 \quad .$$

An unusual feature of ES's calculation is the linearity of the various matrix elements in the correlation function $\chi_{ij}(1,2)$. Since $\chi_{ij}(1,2)$ is determined by an equation similar to that of Guyer and Zane for $g(r_{12})$, this has the effect of using a "softer-core" correlation function, which partially explains why ES's results for J are somewhat larger in magnitude than those of other calculations.* Furthermore, by requiring this linearity, the two-body surface integral expression for J is not derivable from the two-body Schroedinger equation. That is, one gets non-vanishing volume integrals in addition to the surface integral, as ES have shown. These features are the result of ES's multiplying Eq.(5.31) by $\phi_i(1)\phi_j(2) \pm \phi_i(2)\phi_j(1)$ rather than by the approximation to $\psi^\pm$ given by Eq.(5.32). Their reason is clearly that $\chi_{ij}(1,2)$ first appeared in their formalism as the correlation function part of a Green's function. In spite of this, however, it would seem that as long as Eq.(5.32) is a good approximation, one would calculate $\epsilon^\pm$ more accurately by taking the expectation value of $\bar{H}_{ij}(1,2)$ in the states given by Eq.(5.32). With

* Evaluation of Eq.(5.30) with $g(r_{12})$ replaced by $\chi_{ij}(1,2)^{1/2}$ gives $|J|$ about twice that for $g(r_{12})$ replaced by $\chi_{ij}(1,2)$.

this change, Eq.(5.33) would be precisely of the form of Eq.(4.21), and the two-body surface integral given by Eq.(5.9) or Eq.(5.30) would obtain. We have evaluated this integral using ES's Gaussian constants and their correlation function; see Fig. 1. Their correlation function for $R = 3.58 \text{ \AA}$ was used at all densities.

To compare Eq.(5.36) to the calculations of Guyer and Zane, first note that Guyer and Zane neglect their analogue of the term containing γ , assuming that the potentials are very small where $\phi_i^2(1)\phi_j^2(2)\chi_{ij}(1,2)$ is significant. Accordingly, with the exception of the linearity in $\chi_{ij}(1,2)$, Eq.(5.36) is precisely the alternate calculation we mentioned in the previous section. That is, in the language of the Guyer-Zane paper, ES are choosing $|1\rangle$ actually to be the eigenfunction of $h_{12}^B(12)$. Thus, they do not get separate tunneling and interaction terms for J , but both effects combined in a single term.

The results of evaluating the two-body surface integral for various choices of Gaussian constants (see Fig. 4) and correlation functions (see Fig. 5) appear in Fig. 2. Two conclusions are evident. First, the density dependence and magnitude of J are due largely to the density dependence and

size of the Gaussian constant. Secondly, both features of J are affected to a much lesser extent by the choice of one or another of the correlation functions used by NM, GZ, or ES. We should note that the results presented in Fig. 2 have not taken the density dependence of the various correlation functions into account. For example, Guyer and Zane have pointed out that their correlation function behaves like $\theta(r - 2.30)$ at $R = 3.39 \text{ \AA}$ and $\theta(r - 2.45)$ at $R = 3.76 \text{ \AA}$. Evaluation of the two-body surface integral for these two step functions yielded the same density dependence for each, while the magnitude of J using the former was about a factor of two larger than the latter. Thus, this effect is considerably smaller than the change in density dependence due to the different choices of Gaussian values.

PART II

MONTE CARLO CALCULATION OF EXCHANGE IN SOLID He^3

CHAPTER 1: INTRODUCTION, RESULTS, AND CONCLUSIONS

In the previous paper, Part I, fundamental arguments were used to show that the exchange frequencies in solid He^3 should be given by certain many-body integrals involving all of the variables of the system. It was pointed out that the calculations²³⁻³⁰ which have appeared in the literature effectively constitute two-body approximations to these integrals, which in particular neglect the short-range correlations between an exchanging pair of atoms and their surrounding neighbors.* It is the purpose of this paper, Part II, to report a test of this approximation. Using the Nosanow-Mullin²⁶ wave function, the full many-body expression for the $T = 0$ nearest neighbor exchange frequency J has been evaluated using the Monte Carlo integration technique, and the result compared to that of the corresponding two-body

*Thouless²⁷ has presented a two-body Monte Carlo calculation of exchange in solid He^3 which is to some extent the converse of this procedure. He has taken the short-range hard-core interaction as the only interaction between the particles. Thus, he considers two hard spheres in a box with rigid walls, the box representing the surrounding neighbors of the pair. The lattice dynamical aspects of the crystal are inadequately treated in this model.

approximation. We believe this to be the first many-body calculation of exchange in solid He^3 .

Of the equivalent many-body volume and surface integral expressions for J presented in Part I, it was felt that the many-body surface integral, given by Eq.(4.26), would be easier to calculate. For the volume integral generates a small number as the difference of two large numbers. As it stands, however, the surface integral is not directly amenable to Monte Carlo integration. J is a very small number in order of magnitude. One must rearrange the integral so that the order of magnitude of J is generated in an analytical rather than in a statistical manner in the course of the Monte Carlo integration. This is accomplished by certain variable transformations, and is the subject of Chapter 2. In Chapter 3, we discuss the procedure of the computer calculation, and point out that one can take advantage of the much stronger dependence of the integral on the pair of exchanging atoms to considerably shorten the running time needed for convergence.

The Monte Carlo integration of the full many-body expression for J was performed at four densities; the

results are presented in Table 1. and in Fig.6, along with those of the two-body approximation, given by Eq.(5.9) in Part I. The Monte Carlo value for the magnitude of J was found to range from a factor of 3 to 6 smaller than that of the two-body approximation for $R = 3.75\text{\AA} \rightarrow 3.45\text{\AA}$ respectively. The reason is clear. The hard cores of the atoms surrounding a given pair tend to make it more difficult for that pair of atoms to maneuver around each other in the process of exchange. The full calculation takes these many-body correlations into account, in contrast to the approximate calculation, and thus, should yield a smaller magnitude for J . These effects should become more pronounced at higher densities, which leads to the above difference in density dependence. The density dependence of the Monte Carlo calculation is much improved over that of the two-body approximation. For comparison, we also calculated the six-dimensional Monte Carlo integral obtained from the full integral by fixing all but the exchanging pair of atoms at their lattice sites. This describes the exchange of two atoms in an otherwise rigid lattice. The results for the magnitude of J were found to range from about the same as the full integral at $R = 3.75\text{\AA}$ to about a factor of four

smaller at $R = 3.45\text{\AA}$. They are also quite sensible. One would expect that the exchanging pair of atoms effectively sees "softer" hard cores around it if the surrounding atoms are moving. The full integral incorporates this dynamical aspect of the many-body correlations, and thus is somewhat larger in magnitude than the rigid lattice integral, which does not. Again the effect is more pronounced at the higher densities. Conversely, we note that at low density ($R = 3.75\text{\AA}$) the effect of the many-body short-range correlations is mostly static, i.e., simply due to the presence of atoms surrounding the exchanging pair.

In conclusion, we point out that in this calculation, the many-body short-range correlations are seen to have a very important effect on both the magnitude and density dependence of J . In general, the detailed nature of such effects will depend on the particular correlation function used. We have used the Nosanow correlation function, which, it should be pointed out, has a somewhat too "hard" hard core. The essential point of this paper is that a calculation of exchange in solid He^3 should include an investigation of these many-body short-range correlation effects on the exchange process.

CHAPTER 2: THE INTEGRAL

In this chapter we present the full many-body surface integral expression for the $T = 0$ nearest neighbor exchange frequency using Nosanow-Mullin's choice for the ground state home-base function. The integral, as it stands, is not yet amenable to practical computation by the Monte Carlo technique. We examine these difficulties and show how they may be circumvented.

Nosanow and Mullin approximate the ground state home-base function ϕ_0^G by

$$\phi = C \prod_i \exp \left[-A(\underline{r}_i - \underline{R}_i)^2 / 2 \right] F \quad (2.1)$$

where $F = \prod_{i < j} f(r_{ij})$, $r_{ij} = |\underline{r}_i - \underline{r}_j|$, $f(r) = \exp(-K\gamma(r))$,

$$\gamma(r) = (\sigma/r)^{12} - (\sigma/r)^6,$$

and where $\underline{r}_i$ and $\underline{R}_i$ are the position vectors of the atoms and lattice sites respectively. We assume ϕ to be normalized. The surface integral expression is given by E_1 . (4.26) in the previous paper,

$$J_{12} = (\hbar^2/m) \int_{\Sigma} d\vec{S} \cdot (\vec{v}_{3N} \phi) \nabla_{12} \phi \quad (2.2)$$

where (1,2) is a nearest neighbor pair, and the hypersurface Σ is defined by $\underline{r} \cdot \underline{\Delta} = 0$ where $\underline{r} = \underline{r}_1 - \underline{r}_2$ and $\underline{\Delta} = \underline{R}_1 - \underline{R}_2$. The direction of $d\vec{S}$ is normal to Σ and directed from the "near" side ($\underline{r} \sim \underline{\Delta}$) to the "far" side ($\underline{r} \sim -\underline{\Delta}$). Thus

$$d\vec{S} \cdot \vec{\nabla}_{3N} = dS \hat{\Delta} \cdot (\vec{\nabla}_2 - \vec{\nabla}_1) / \sqrt{2} \quad (2.3)$$

where $\hat{\Delta} = \underline{\Delta} / \Delta$ and $\Delta = |\underline{\Delta}|$. Note that on Σ

$$\hat{\Delta} \cdot (\vec{\nabla}_2 - \vec{\nabla}_1) \sum_i (\underline{r}_i - \underline{R}_1)^2 = 2\Delta, \quad (2.4)$$

so that

$$\begin{aligned} J_{12} &= -(\hbar^2 A \Delta / \sqrt{2}) m \int_{\Sigma} dS \phi P_{12} \phi \\ &\quad - (\hbar^2 K \sqrt{2}) m \int_{\Sigma} dS \phi (P_{12} \phi) \hat{\Delta} \cdot (\vec{\nabla}_2 - \vec{\nabla}_1) \sum_{i < j} \eta(r_{ij}) . \end{aligned} \quad (2.5)$$

The second integral vanishes since dS , $\phi(P_{12}\phi)$ and

$\sum_{i < j} \eta(r_{ij})$ are invariant under the permutation P_{12} , while

$\hat{\Delta} \cdot (\vec{\nabla}_2 - \vec{\nabla}_1)$ changes sign. Furthermore, since $P_{12}\phi = \phi$ on the hyper-surface Σ , we have

$$J_{12} = - (\hbar^2 A \Delta / \sqrt{2} m) \int_{\Sigma} dS \phi^2. \quad (2.6)$$

Note that this same form obtains for the $T = 0$ nearest neighbor exchange frequency had we used the Nosanow-Varma choice for ϕ_0^e , given by Eq. (5.5) of the previous paper, although the factor in front of the integral would be more complicated.

The Monte Carlo integration technique has been fully described in the literature.³⁴ Briefly, one would like to evaluate the integral

$$I = \int G(\underline{x}_1, \dots, \underline{x}_N) V(\underline{x}_1, \dots, \underline{x}_N) d\underline{x}_1 \dots d\underline{x}_N \quad (2.7)$$

where the function G is non-negative and normalized. One samples configurations of the system,

$R^{(i)} = (\underline{x}_1^{(i)}, \underline{x}_2^{(i)}, \dots, \underline{x}_N^{(i)})$, according to the probability distribution $G(R^{(i)})$, and approximates the integral by

$$I \approx \frac{1}{n} \sum_{i=1}^n V(R^{(i)}) \quad (2.8)$$

where n is the number of such samples. In the limit of large n , the right hand side of Eq. (8) approaches 1. For more practical detail we refer the reader to McMillan.³⁴ However, we point out that the manner of determining the $R^{(i)}$ involves only the ratio of G for the various configurations. Thus, one need only know G to within a multiplicative constant, and the Monte Carlo integration will effectively use $G/\langle G \rangle$, as can be seen by setting $V = 1$ in Eq. (2.8).

To evaluate Eq. (2.6) by the Monte Carlo technique, we take $G = \phi^2$, since ϕ^2 must be normalized. It would seem that we should then take* $V = \delta(z)$, where for convenience we have assumed that Δ points in the positive z direction, in which case $\sum$ is specified by $z = 0$. There are difficulties, however. With this choice of V , the integral given by Eq. (2.8) is proportional to the fraction of the configurations $\{R^{(i)}\}$ lying in the "surface". The $R^{(i)}$ are chosen according to the distribution ϕ^2 , which contains the factor

* In the computer calculation one must take the "surface" to have a finite, though small, width. One would use

$$\delta(z) \simeq \begin{cases} 1/d & \text{if } |z| < d/2 \\ 0 & \text{otherwise} \end{cases}.$$

$$\exp[-A(z-\Delta)^2/2 - A(x^2+y^2)/2] f^2(r) \quad (2.9)$$

where again $\underline{r} = (x, y, z) = \underline{r}_1 - \underline{r}_2$. The fraction of the total number of configurations $\{R^{(i)}\}$ generated which lie within the "surface" will be of order

$$d\sqrt{A} \exp[-A(\Delta^2 + \sigma^2)/2] \quad (2.10)$$

where d is the width of the "surface". The correlation function $f^2(r)$ behaves roughly like $\theta(r-\sigma)$. For typical numbers: $A = 1.30 \text{ \AA}^{-2}$, $\Delta = 3.75 \text{ \AA}$, $\sigma = 2.56 \text{ \AA}$, and say $d = .05 \text{ \AA}$, this fraction is $O(10^{-7})$. The problem is that we are asking the Monte Carlo technique to generate an extremely small number in a statistical manner. One would have to run the program for a prohibitive length of time to determine J in this manner. That is, for a meaningful result one would want at least $O(10^2)$ configurations lying in the "surface", which would necessitate generating $O(10^9)$ configurations $R^{(i)}$. For a 54 particle system, a realistic time for the generation of a single $R^{(i)}$ by computer is $O(10^{-3} \text{ sec})$. Accordingly, this calculation would take $O(10^6)$ sec.

Two features account for the smallness of J . The

surface $\int$ occurs at the "tail" of the Gaussian part of ϕ^2 , leading to a factor of $\exp(-A\Delta^2/2)$. Secondly, the hard-core interaction between atoms 1 and 2, represented by $f^2(r_{12})$, cuts out the most sizeable part of this Gaussian "tail", leading to an additional factor of $\exp(-A\sigma^2/2)$. Guyer and Zane²⁹ have discussed these matters. The remedy to the above difficulties is to remove these factors analytically from the integration. We do so by two coordinate transformations: The first transforms the surface to the center of the Gaussian. The second is a point transformation³⁸ which removes most of the hard-core interaction between atoms 1 and 2.

We discuss these transformations. Since only the relative coordinates of atoms 1 and 2 are affected, we shall suppress all other variables in the following for visual convenience. In this abbreviated notation, Eq.(2.6) appears

$$J_{12} \propto \int \exp[-A(x^2+y^2)/2 - A(z-\Delta)^2/2] f^2(x,y,z) \delta(z) dx dy dz \quad (2.11)$$

There are two steps: i) The factor $\exp(-A\Delta^2/2)$ is easily handled by setting $z = z' - \Delta$.

$$J_{12} \propto \exp(-A\Delta^2/2) \int \exp[-A(x^2+y^2)/2 - A(z'-\Delta)^2/2] f^2(x,y,z'-\Delta) \delta(z'-\Delta) dx dy dz' \quad (2.12)$$

ii) To treat the factor $\exp(-A\sigma^2/2)$, let $x = \xi \cos \theta$,
 $y = \xi \sin \theta$.

$$J_{12} \propto \exp(-A\Delta^2/2) \int dz' \delta(z'-\Delta) \exp[-A(z'-\Delta)^2/2] \cdot \int_0^{2\pi} d\theta \int_0^\infty d\xi \xi \exp(-A\xi^2/2) f^2(\xi \cos \theta, \xi \sin \theta, z'-\Delta) \quad (2.13)$$

But since $z' = \Delta$ in the integral, we have a factor $f^2(\xi)$. Thus, there is essentially no contribution to the integral for $\xi \ll \sigma$ where $\rho \lesssim \sigma$ and is determined in principle as follows: For a finite system, ϕ^2 is bounded above, and so we require $f^2(\rho)(\phi^2)_{\max}$ to be negligible. Note that $f^2(\xi)$ drops off extremely rapidly for $\xi < \sigma$. Since we do the calculation for a 54 particle system, this condition is easily satisfied for a relatively large ρ . Thus, one can replace the lower limit of the ξ integration by ρ . In practice one tests the choice of ρ by seeing that the

result of integration does not change on decreasing ρ .

To continue, we define $\zeta = \xi - \rho$, $x' = \zeta \cos \theta$, and $y' = \zeta \sin \theta$ so that Eq. (2.13) becomes:

$$\begin{aligned}
 J_{12} \propto & \exp[-A(\Delta^2 + \rho^2)/2] \\
 & \cdot \int \exp[-A(x'^2 + y'^2)/2 - A(z' - \Delta)^2/2] \\
 & \cdot t^2(x' + \rho \cos \theta, y' + \rho \sin \theta, z' - \Delta) \\
 & \cdot \exp(-A\zeta\rho) (1 + \rho/\zeta) \delta(z' - \Delta) dx' dy' dz'
 \end{aligned}
 \tag{2.14}$$

We now explicitly exhibit the other variables, and give the combined coordinate transformation in its general form. Let $\{\tilde{\underline{x}}_i\}$ be the original coordinates of the atoms and $\{\underline{x}_i\}$ the transformed coordinates. Note that only the relative coordinates of atoms 1 and 2 are affected by the transformation. Then

$$\begin{aligned}
 \tilde{\underline{x}}_1 &= \underline{x}_1 - \Delta/2 + (\underline{x}_{12} - \Delta) \frac{\rho}{2|\underline{x}_{12} - \Delta|} \\
 \tilde{\underline{x}}_2 &= \underline{x}_2 + \Delta/2 - (\underline{x}_{12} - \Delta) \frac{\rho}{2|\underline{x}_{12} - \Delta|} \\
 \tilde{\underline{x}}_i &= \underline{x}_i \quad i = 3, \dots, N
 \end{aligned}
 \tag{2.15}$$

while the expression for J_{12} is

$$J_{12} = (-\hbar^2 A \Delta / \sqrt{2} m) e^{-A(\Delta^2 + \rho^2)/2} \int \phi^2(\{\underline{x}_i\}) v(\{\underline{x}_i\}) d\underline{x}_1 \dots d\underline{x}_N \quad (2.16)$$

$$v = \frac{F^2(\{\tilde{\underline{x}}_i\})}{F^2(\{\underline{x}_i\})} e^{-A\rho |\underline{x}_{12} - \underline{\Delta}|} \left(1 + \frac{\rho}{|\underline{x}_{12} - \underline{\Delta}|}\right) \delta(\underline{x}_{12} \cdot \underline{\Delta} - \Delta^2) \quad (2.17)$$

$$\frac{F^2(\{\tilde{\underline{x}}_i\})}{F^2(\{\underline{x}_i\})} = \frac{f^2(\tilde{r}_{12})}{r^2(r_{12})} \prod_{i=1,2} \frac{f^2(\tilde{r}_{1i})}{f^2(r_{1i})} \frac{f^2(\tilde{r}_{2i})}{f^2(r_{2i})}.$$

Note that the surface now occurs where ϕ^2 is of $O(1)$. Furthermore, the correlation function $f^2(\tilde{r}_{12})$ does not constitute a severe cut off since $\tilde{r}_{12} = |\underline{x}_{12} - \underline{\Delta}| + \rho$, and thus $\tilde{r}_{12} \geq \rho$. One need not worry about v diverging due to the factors $f^2(r_{12})$, $f^2(r_{1i})$ and $f^2(r_{2i})$ in the denominator, for such configurations of the system are not selected by $\phi^2(\{\underline{x}_i\})$. In practice we find that $\tilde{\underline{x}}_1$ and $\tilde{\underline{x}}_2$ almost always lie within $\Delta/2$ of $\underline{x}_1$ and $\underline{x}_2$ respectively. Thus, only the contributions to v due to atoms 1 and 2 and their first few neighbors are important.

To conclude this chapter, we would like to mention an alternate and apparently feasible method for doing the

Monte Carlo integration, but which we find to be unsuccessful for the same type or practical reason discussed earlier. Indicate the Gaussian part of ϕ by ϕ_G , i.e., $\phi = \phi_G F$. We attempted to evaluate the integral given by Eq. (2.6) in terms of two Monte Carlo calculations and a one-dimensional numerical integration, i.e., as $I_1 I_3 / I_2$ where

$$\begin{aligned} I_1 &= \int \phi_G^2 F^2 / \int \phi_G^2 f^2(r_{12}) \\ I_2 &= \int \phi_G^2 F^2 / \int \phi_G^2 f^2(r_{12}) \\ I_3 &= \int \phi_G^2 f^2(r_{12}) / \int \phi_G^2 f(r_{12}) \end{aligned} \quad (2.18)$$

The numerical integration I_3 will bring out the small factors $\exp[-A(\Delta^2 + \sigma^2)/2]$, leaving the Monte Carlo integrations of I_1 and I_2 to calculate larger numbers. I_1 and I_2 were treated respectively as $3N-1$ and $3N$ dimensional Monte Carlo integrals; in each case we took the probability distribution function G to be $\phi_G^2 f^2(r_{12})$, and we took V to be $F^2/f^2(r_{12})$. The function F^2 serves basically as a cut-off, in that it is effectively zero for any configuration which has at least one pair of

atoms more closely spaced than σ . For, say, 54 particles, most of the configurations $\{R^{(i)}\}$ selected according to $\phi_G^2 f^2(r_{12})$ do have at least one such pair, and thus don't contribute to the integral. Our attempted calculation of I_2 was thus characterized by a very poor convergence, i.e. again an extremely large number of configurations would be needed to evaluate E_1 . (2.6) in this manner.

CHAPTER 3: THE NUMERICAL CALCULATION

The Monte Carlo integration of Eq.(2.16) was performed^{*} for a 54 particle bcc lattice in the shape of a cube, with atoms 1 and 2 chosen as the nearest neighbor pair lying in the center. The calculation was done at four densities, with the values for A and K taken to be the same as used by Nosanow and coworkers; see Table 1. We point out several ways in which our procedure differs from the usual one³⁴, and then discuss all of the tests we used to verify the calculation.

In the usual procedure³⁴, the sequence of configurations $\{R^{(i)}\}$ is generated by moving each atom an equal number of times. This is appropriate for an integral in which each atom is equally important. A glance at V given by Eq.(2.17), however, shows that our integral exhibits a much stronger dependence on the exchanging atoms 1 and 2 than on the others. It thus seemed intuitively clear, that, for more rapid convergence, one should vary these two atoms more frequently than the others in generating new configurations. We performed each calculation for three variation schemes:

* The Monte Carlo program used was a modification of a program very kindly furnished by Dr. R. D. Murphy.

atoms 1 and 2, each of their nearest neighbors, and each of the remaining atoms were selected in the ratios 1-0-0 respectively, 28-1-1 respectively, and 30-9-1 respectively.* The scheme 1-0-0 yields the integral obtained from Eq.(2.6) by adding delta functions to fix all atoms but 1 and 2 at their lattice sites. It corresponds to the exchanging of a nearest neighbor pair of atoms in an otherwise rigid lattice, and we refer to it as the rigid lattice calculation. We found the results of the integration using the 28-1-1 and 30-9-1 schemes to agree well within the accuracy of our results, while the results using the 1-0-0 variation were significantly lower in magnitude; see Table 2. Accordingly, it was felt that variation schemes more closely approaching the usual procedure, indicated by 1-1-1 in our notation, would yield the same results as our 28-1-1 and 30-9-1 results. We concluded that either of these schemes was adequate for determining the correct value of the integral Eq.(2.16). This conclusion was directly tested by performing the Monte Carlo integration

* The number of atoms in these categories are 2, 14, and 38 respectively. Thus 30 variations of atoms 1 and 2, 9 variations of their first neighbors, and 1 variation of the remaining atoms yields 224 configurations.

with the various variation schemes for a test function similar to the true function, and yet which could be reduced analytically to a one-dimensional integral for independent evaluation. We discuss this test later.

The calculation was performed in two ways. The first utilized a $3N$ dimensional Monte Carlo integration in which the surface had to be treated as having a finite width. The second was a $3N-1$ dimensional Monte Carlo integration in which the system was always kept on the surface. The test calculation, to be described later, showed the second approach to be more powerful.

In the $3N$ dimensional calculation, the $\{R^{(i)}\}$ were generated according to ϕ^2 . The finite surface width came from treating the delta function in V as a unit area spike of width d and height $1/d$. We found the results for d between $.04\Delta$ and $.01\Delta$ (here Δ is the nearest neighbor distance) agreed within 10%. For d much smaller than $.01\Delta$, the convergence of the calculation was not reliable. For each $R^{(i)}$ generated we also calculated $u = \underline{r}_{12} \cdot \hat{\Delta}$. This allowed us to compute

$$g(u) = \int \phi^2 \delta(u - E_{12} \cdot \hat{\Delta}) d\tau / \int \phi^2 d\tau. \quad (3.1)$$

This function was found to be Gaussian like, centered about $u = \Delta$, and of half width about $\Delta/4$. We were able to determine $g(\Delta)$ to within about 5% independent of the various interval sizes used in determining $g(u)$. It ranged from $1.8/\Delta$ to $2.0/\Delta$ for densities $\Delta = 3.75 \text{ \AA}^3$ to $3.45 \text{ \AA}^3$.

The 3N-1 dimensional calculation followed the same procedure as the above except that only $R^{(i)}$ lying on the surface were generated. Thus it calculates $J_{12}/g(\Delta)$. The virtue of this approach is that one need not worry about the effects of a finite "surface" width. The drawback is that it must be done in conjunction with the first calculation for $g(\Delta)$, and thus the overall calculation takes more than twice as long as that of the first alone.

All calculations were started from an initial configuration in which all atoms were on their lattice sites. The first 5,000 configurations were thrown away in order to remove some of the arbitrariness of the starting point. For each new $R^{(i)}$ generated, V was averaged over the current set $\{R^{(1)}, R^{(2)}, \dots, R^{(i)}\}$. It was found

that regardless of the method of particle variation used in generating the $R^{(i)}$, the determining factor in reaching convergence was the number of times that atoms 1 and 2 had been varied. Convergence was generally reached between about 10,000 and 15,000 variations of each of these atoms, and the calculations were carried out to 30,000 or more of such variations (about 225,000 configurations for the scheme 30-9-1). The statistical scatter in the values for J_{12} after convergence had been reached was about 5%. Since $g(\Delta)$ was known to about the same accuracy, our results are good to about 10%. They are presented in Table 1 and in Fig.6. A single calculation of the 3N dimensional integral using the variation scheme 30-9-1 took about 20 minutes on the CDC 6600 computer; of the 3N-1 dimensional integral, about 30 - 40 minutes.

While periodic boundary conditions were used to evaluate ϕ^2 in determining the $\{R^{(i)}\}$, they were not used in evaluating $V(R^{(i)})$. For this function basically involves the distances between atoms 1 and 2 and their first few neighbors. For this same reason it was felt that there was no need to perform the calculation for a larger number of atoms. Our 54 particle lattice already contains all

second and third neighbors of atoms 1 and 2. The parameter ρ in Eq.(2.16) was taken to be $.75 \sigma$. This was judged adequate when the choice $\rho = .70 \sigma$ was seen to give the same results as $\rho = .75 \sigma$.

Several tests were made of the program. We first replaced the full correlation function F by just $f(r_{12})$. In this case Eq.(2.6) for J_{12} reduces to a one-dimensional integral which can be computed independently by numerical integration. With the same substitution in the full program, we easily obtained agreement to two significant figures with the independent calculation. This tests our use of the variable transformations which led to Eq.(2.16). In order to present a stringent test of the full many-body nature of the integral we also replaced F by

$$F_{\text{test}} = f(r_{12}) \prod_{i < j} \exp \left[-B_{ij} (\underline{r}_{ij} - \underline{R}_{ij})^2 \right]$$

$$B_{ij} = \begin{cases} B & \text{if } i, j \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases} \quad (3.2)$$

where $\underline{r}_{ij} = \underline{R}_i - \underline{R}_j$ and $\underline{R}_i$ are the lattice vectors. The usefulness of this test function is that while the Monte

Carlo calculation of J_{12} using ϕF_{test} is of the same order of difficulty as the true calculation, the expression may be analytically reduced to a one-dimensional integral for independent computation. Furthermore, the essential feature of the true correlation function F as far as the product ϕF is concerned, is that if two nearest neighbors get too close, F will become very small. This feature is mimicked to some extent by F_{test} . The factor $f(r_{12})$ has been added since on the surface $\underline{r}_{12} \cdot \underline{R}_{12} = 0$ specified in Eq.(2-6), the Gaussian part of F_{test} does not tend to keep atoms 1 and 2 apart. The analytic evaluation of J_{12} using ϕF_{test} showed that the full integral gave the same result as the rigid lattice integral for $B/A < .01$, but was increasingly larger in magnitude for larger values of this ratio. (We took $A = 1.30 \text{ \AA}^{-2}$, $\Delta = 3.75 \text{ \AA}$, and $\log_{10} K = -.75$). This behavior is to be expected. For small B , the Gaussian part of F_{test} does not correlate the atoms. Atoms 1 and 2 are also not correlated with their neighbors if these neighbors are fixed at their lattice sites. In order to make a good test of the various variation schemes, we chose $B = 5/2$ for which the full integral was five times larger in magnitude than the rigid lattice integral. It was

immediately apparent that the Monte Carlo evaluation of Eq.(2.16) using ϕF_{test} was more difficult than the true calculation. For the function F_{test} varies more rapidly than F in going from one side to the other of the hypersurface specified in Eq.(2.16). Our Monte Carlo calculation of the $3N$ dimensional integral using ϕF_{test} thus showed such a strong dependence on the "surface" width, that we were not able to determine the value of the integral by this approach. We were able, however, to determine $g(\Delta)$ without difficulty. We thus used the $3N-1$ dimensional Monte Carlo calculation to evaluate the test integral. The results are shown in Table 3. The $30-9-1$ variation was seen to give the value for the full integral, while the $28-1-1$ variation yielded a value somewhat lower in magnitude, though much closer to that of the full integral than to that of the rigid lattice integral. Since these two variation schemes gave results in good agreement with each other for the true calculation, we concluded that they gave the value of the full integral in that case.

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APPENDIX A: THE HAMILTONIAN $\bar{H}$

The purpose of this appendix is two-fold. We point out some of the reasoning which led to the choice of $\bar{H}$ given in the text. Secondly, we illustrate the geometry involved for the case of a simple three-body system, i.e., the points p^P , the regions Ω_P , and the hyper-surfaces on which the potential $\bar{V}$ is infinite.

Working with a system of well-separated atoms, Herring could eliminate the exchanges of electrons located on different atoms by going to an infinitely separated system, without affecting the dominant field seen by the electrons --namely the electron-ion core attraction. This procedure does not work for our problem, as the field seen by a given He^3 atom is due to the proximity of its various neighboring atoms, the very particles with which it may exchange. And so we are led to take $\bar{H} = H + \bar{V}$, where H establishes the crystal, with the proper lattice constant, and $\bar{V}$ is a potential which prohibits in some manner the exchanging of atoms. A possible choice is to have $\bar{V}$ present each atom with rigid walls at the surfaces of the Wigner-Seitz cells in coordinate space. However, this choice of $\bar{V}$ constitutes a larger perturbation on H than

is necessary. For the low-frequency phonon modes are characterized by the atoms undergoing relatively large excursions from their lattice sites. A state with a large number of low-frequency phonons may have an energy not much above the ground state, and yet display a significant probability for an atom to be outside of its Wigner-Seitz cell. In making these large excursions, however, the motion of a given atom is correlated with the other atoms such that the relative particle ordering is largely maintained. Since it is a change in this ordering which is equivalent to exchange, the above possible choice of $\bar{V}$ is more restrictive than need be. We thus chose $\bar{V}$, as defined in the text, according to the criterion of particle ordering.

To visualize the geometry involved, we consider a three particle chain in one dimension. Suppose the particle-particle interaction is like a Lennard-Jones potential except that we cut off the hard-core repulsion at some large but finite value. This allows the particles to exchange. We also suppose there is a bound state of the system, with neighboring particles separated by a distance a . The configuration space for this system is three dimensional, but since we fix the center of mass of

this "crystal", we are only interested in the plane spanned by the two internal coordinates. These may be taken as

$$q_1 = -(x_2 + x_3 - 2x_1)/\sqrt{6}$$

$$q_2 = (x_2 - x_3)/\sqrt{2}$$

where x_1, x_2, x_3 are the position coordinates of the particles. Corresponding to the $N! = 3! = 6$ equilibrium configurations of the "lattice", i.e. $(x_1, x_2, x_3) = (\pm a, 0, \mp a), (\pm a, \mp a, 0), (0, \pm a, \mp a)$, there are six points in configuration space as shown in Fig. A. They are labelled p^P where P is a permutation operator in S_3 . We use cycle notation for the operators P , and e is the identity permutation. The Wigner-Seitz cells in coordinate space will be line segments of length a centered on the various "lattice" sites. The dashed lines in Fig. A indicate the potential barriers for the possible choice of $\bar{V}$ which prohibits the atoms from moving out of the Wigner-Seitz cells in which they are initially placed. The solid lines indicate the potential barriers of $\bar{V}$ as defined in the text. These lines divide the configuration

space of the relative coordinates of the particles into the six sections, the Ω_p .

Fig. A: Configuration space of the internal coordinates for a three particle chain. The points p^p are indicated. The solid lines indicate the "hyper-surfaces" dividing the configuration space into $N! = 6$ sections, Ω_p .

APPENDIX B: GROUP THEORY

In this appendix we indicate the symmetry groups of the Hamiltonian H , its harmonic approximation H_{har} , and the Hamiltonian $\bar{H}$. We point out that the lattice Hamiltonian H_L derived in Chapter 4 of Part I has the same symmetry group as H_{har} , which is the Hamiltonian usually taken in treating lattice dynamical problems.³⁵ We show that the exchange operator δ_{ij} does not conserve the momentum of the phonon-like modes of H_L .

The full many-body Hamiltonian is

$$H = (-\hbar^2/2m) \sum_i \nabla_{\underline{r}_i}^2 + \sum_{i < j} v(|\underline{r}_i - \underline{r}_j|), \quad (\text{B.1})$$

to which we can add external constraints to select states appropriate to a particular crystalline structure, and for a particular position and orientation of the crystal. We assume henceforth that this is done. The symmetry group of H is then

$$G = \mathcal{G} \otimes S \quad (\text{B.2})$$

where S is the group of permutations of the atoms, and $\mathcal{G}$ is the space group for the crystal, consisting of

combinations of the appropriate rotation, rotation-inversion, and translation operators. The symbol $\otimes$ means direct product. The action of a permutation operator is*, e.g., taking $P = (123\cdots)$ in cycle notation

$$P \underline{x}_i = (123\cdots) \underline{x}_i = \underline{x}_{i-1} \quad (\text{B.3})$$

while a translation operator

$$T_{\underline{R}} \underline{x}_i = \underline{x}_i + \underline{R} . \quad (\text{B.4})$$

If one wishes to treat a finite crystal, then the cyclic or Born-von Karman boundary conditions must be used in dealing with the translation operators. That is, after a translation one imagines slicing off the piece of crystal extending beyond the original volume and tacking it onto the opposite end of the crystal.³⁶

In the usual treatment of lattice dynamics one uses a harmonic (perhaps self-consistent) approximation to the Hamiltonian H in the neighborhood of one of the points p^P in configuration space,³⁵ say p^e . Then

* If the atoms are permuted according to P , their coordinate are permuted according to P^{-1} .

$$H_{\text{har}} = (-\hbar^2/2m) \sum_i \nabla_{\underline{x}_i}^2 + \frac{1}{2} \sum_{i,j} (\underline{x}_i - \underline{R}_i) \underline{M}_{ij} (\underline{x}_j - \underline{R}_j) \quad (\text{B.5})$$

where $\underline{x}_i$ and $\underline{R}_i$ are the positions of the atoms and lattice sites respectively. It is well known,³⁵ that the symmetry group of H_{har} is composed of translations, rotations, etc., of the displacements of the atoms from their lattice sites, and not of the atoms themselves. Thus, the "translation" by a lattice vector $\underline{r}$ moves all of the atoms by small amounts in the neighborhoods of their own lattice sites, such that the new displacement of atom i from $\underline{R}_i$ is equal to the old displacement of atom j from $\underline{R}_j$, where $\underline{R}_j + \underline{r} = \underline{R}_i$. These operators may be written in terms of the more usual geometric operators in $\mathcal{G}$ multiplied by appropriate permutation operators in S . For example, given a one-dimensional lattice with the atoms numbered from left to right, the "translation" by $\underline{R}$ where $\underline{R}$ is the nearest neighbor distance is given by

$$\underline{x}'_i = T_{\underline{R}}(123\cdots) \underline{x}_i = \underline{x}_{i-1} + \underline{R}$$

so that

$$\underline{R}_i - \underline{R}_i = \underline{R}_{i-1} + \underline{R} - \underline{R}_i = \underline{R}_{i-1} - \underline{R}_{i-1} \quad (\text{B.6})$$

where

$$\underline{R}_{i-1} + \underline{R} = \underline{R}_i .$$

We write the symmetry group of H_{har}

$$G_{\text{har}} = \mathcal{G}^{(e)} \quad (\text{B.7})$$

where we have chosen the notation intentionally in that $\mathcal{G}^{(e)}$ is isomorphic to $\mathcal{G}$, e.g.,

$$T_{\underline{R}} \text{ in } \mathcal{G} \rightarrow T_{\underline{R}}(123\cdots) \text{ in } \mathcal{G}^{(e)} . \quad (\text{B.8})$$

Because $\mathcal{G}^{(e)}$ and $\mathcal{G}$ correspond to different operator representations of the same abstract group, the differences between them are not always explicitly stated. We wish to emphasize several points: i) $\mathcal{G}^{(e)}$ is isomorphic to $\mathcal{G}$. ii) $\mathcal{G}^{(e)}$ is the subgroup of $G = \mathcal{G} \otimes S$ which leaves the neighborhood of p^e invariant. That is, an operator in $\mathcal{G}^{(e)}$ takes a point in configuration space near p^e to another point also near p^e . iii) Had the harmonic

approximation to H been made in the neighborhood of a different one of the p^P , say $p^{P'}$, then the relevant symmetry group would have been $\mathcal{G}^{(P')}$. In this case, different permutation operators would be used in the isomorphism equivalent to that given by Eq. (B.8). In general, the groups $\mathcal{G}^{(P)}$ and $\mathcal{G}^{(P')}$, for $P \neq P'$, are not the same, although they are isomorphic to each other.

The Hamiltonian $\bar{H}$ is defined as

$$\bar{H} = H + \bar{V} \quad (\text{B.9})$$

where $\bar{V}$ consists of infinite barriers at the hyper-surfaces in configuration space separating the regions $\{\Omega_p\}$. The equation of the hyper-surface separating two adjacent regions, say Ω_p and $\Omega_{p'}$, may be given by

$$\sum_i \left[(P\mathbf{r}_i - \mathbf{R}_i)^2 - (P'\mathbf{r}_i - \mathbf{R}_i)^2 \right] = 0 \quad (\text{B.10})$$

Since all lattice sites $\mathbf{R}_i$ are contained in the sum over i , the geometric operators in $\mathcal{G}$ leave Eq. (B.10) invariant. The permutation operators in S take the various hyper-surfaces such as specified by Eq. (B.10) one into another, and thus, also leave $\bar{V}$ invariant. The symmetry group G

is accordingly at least a subgroup of that of $\bar{H}$. It is convenient to consider $\bar{H}$ as having this same symmetry group, and to view the degeneracy in its spectrum unaccounted for by G as accidental. That such additional degeneracy is present is clear from the fact that one can choose the eigenfunctions of $\bar{H}$ to lie completely in one or another of the various sections Ω_p . That is, one has eigenfunctions which do not transform according to irreducible representations of the symmetry group G . Let such eigenfunctions be $\{\bar{\Phi}^P\}$. To complete the labelling we add an energy index m , and then refer to the appropriate subgroup $\mathcal{G}^{(P)}$ of G which leaves Ω_p invariant to get indices v_j corresponding respectively to particular irreducible representations and basis elements of $\mathcal{G}^{(P)}$. One may take the eigenfunctions of $\bar{H}$ to be $\{\bar{\Phi}_{m,v_j}^P\}$.

It was pointed out in Chapter 2 that the correspondence between the states in the low-lying manifolds of H and $\bar{H}$ is preserved under the symmetry operations of G . Thus, the home-base functions $\{\Phi_{m,v_j}^P\}$ have the same symmetry characteristics as the eigenfunctions $\{\bar{\Phi}_{m,v_j}^P\}$ of $\bar{H}$. The lattice Hamiltonian defined in Chapter 4 of Part I has the form

$$H_L = \sum_{m\nu j} |\Phi_{m\nu j}^e\rangle \bar{E}_m \langle \Phi_{m\nu j}^e| \quad (B.11)$$

so that it is clear that its symmetry group is $\mathcal{G}^{(e)}$, i.e., just the space group usually used in treating lattice dynamical problems.

The matrix elements of the exchange operator between states of the lattice Hamiltonian are

$$\langle \Phi_{m\nu j}^e | \mathcal{J}_{ii'} | \Phi_{m'\nu'j'}^e \rangle = \langle \Phi_{m\nu j}^e | (H - \frac{1}{2} \bar{E}_m - \frac{1}{2} \bar{E}_{m'}) P_{ii'} | \Phi_{m'\nu'j'}^e \rangle \quad (B.12)$$

We note that $\Phi_{m\nu j}^e$ and $P_{ii'} \Phi_{m'\nu'j'}^e = \Phi_{m'\nu'j'}^{P_{ii'}}$ transform irreducibly according to two distinct subgroups of G , $\mathcal{G}^{(e)}$ and $\mathcal{G}^{(P_{ii'})}$, neither of which is a normal subgroup of G . Accordingly, group theory does not provide any selection rules for the matrix element Eq. (B.12). In particular, it should be possible for $\mathcal{J}_{ij}$ to couple two phonon-like modes of the lattice Hamiltonian of different momentum, i.e., different ν values. This is clear physically in that it should be the combined phonon and spin wave momentum which should be a conserved quantity, and neither separately.

APPENDIX C: PHONON FUNCTIONS

In this appendix, we present an order of magnitude estimate of the extent to which phonon functions are localized. That is, a ground-state phonon wave function is given by

$$\exp\left[-\frac{1}{2} \sum_{i,j} (\underline{x}_i - \underline{R}_i) \underline{G}_{ij} (\underline{x}_j - \underline{R}_j)\right], \quad (\text{C.1})$$

where the matrix G is positive definite (we eliminate the center of mass motion) and where $\underline{x}_i$ and $\underline{R}_i$ are the atom and lattice position vectors respectively. The function Eq. (C.1) clearly peaks at the point p^e in the configuration space of the N atoms and then drops off as one moves away from p^e . The question is how fast do these functions drop off. We can partially answer this question by calculating $(\underline{n} | v^2 | \underline{n})^{1/2}$ where $|\underline{n}\rangle$ is a phonon function and v is the deviation of the system from the point p^e in a particular direction d . We are most concerned with the r.m.s. deviation of the system in the direction of some neighboring point p^p to p^e , as this is the direction of closest approach of the hyper-surfaces bounding Ω_e to the point p^e . Using appropriate parameters for solid He^3 ,

we estimate $\langle \underline{n} | v^2 | \underline{n} \rangle$ in this direction, for the low-lying states $|\underline{n}\rangle$, to be roughly one-third the distance to the hyper-surface. We suggest, then, that these states are small near the bounding hyper-surfaces of Ω_e .

The phonon functions $|\underline{n}\rangle$ will be eigenfunctions of a harmonic Hamiltonian describing a fictitious harmonic lattice, which we take to be bcc, with lattice sites $\underline{R}_i$. We take the point p^e to be

$$p^e = (\underline{R}_1, \underline{R}_2, \underline{R}_3, \dots, \underline{R}_N)$$

and the neighboring point p^p to be

$$p^{p12} = (\underline{R}_2, \underline{R}_1, \underline{R}_3, \dots, \underline{R}_N)$$

so that the direction $\underline{d}$ is

$$\underline{d} = (-\underline{R}_{12}, \underline{R}_{12}, 0, 0, \dots, 0) \quad (C.2)$$

where $\underline{R}_{12} = \underline{R}_1 - \underline{R}_2$. Let the displacement of the system from p^e be

$$\underline{u} = (\underline{u}_1, \underline{u}_2, \dots, \underline{u}_N) \quad (C.3)$$

where $\underline{u}_i$ are the displacements of the individual atoms from their lattice sites. The displacement of the system in the direction d is then

$$v = \underline{u} \cdot \underline{d} / |\underline{d}| = \frac{1}{\sqrt{6}} \sum_{\alpha=1}^3 (u_{2\alpha} - u_{1\alpha}) \quad (C.4)$$

where $\alpha = x, y, z$ and where we have taken

$$\underline{R}_{12} = \frac{R}{\sqrt{3}} (1, 1, 1)$$

with R being the nearest neighbor distance.

Using the standard expressions for the real normal modes, and taking the polarization matrices to be diagonal, one has

$$v = \frac{2}{\sqrt{3N}} \sum_{\underline{k}\alpha} \overline{\sin(\underline{k} \cdot \underline{R}_{12}/2)} \alpha_{\underline{k}\alpha\sigma} \quad (C.5)$$

The bar over the sum restricts $\underline{k}$ to lie in one particular half of the first Brillouin zone. We have assumed the origin to be at $(\underline{R}_1 + \underline{R}_2)/2 = 0$, and the standing waves corresponding to $\alpha_{\underline{k}\alpha\sigma}$ for $\sigma = 2$ to be zero at this origin. The index α is again x, y , or z . Using the fact that

$$m\omega_{\underline{k}}^2 \langle \underline{n} | q_{\underline{k}\alpha\sigma}^2 | \underline{n} \rangle = \hbar\omega_{\underline{k}} (n_{\underline{k}\alpha\sigma} + 1/2) \quad (C.6)$$

one has

$$\langle \underline{n} | v^2 | \underline{n} \rangle = \frac{4\hbar}{3Nm} \overline{\sum_{\underline{k}\alpha} \frac{\sin^2(\underline{k} \cdot \underline{R}_{12}/2)}{\omega_{\underline{k}}}} (n_{\underline{k}\alpha 2} + 1/2) \quad (C.7)$$

where $\omega_{\underline{k}}$ are the frequencies and $n_{\underline{k}\alpha\sigma}$ the occupation numbers of the normal modes $q_{\underline{k}\alpha\sigma}$.

We treat the phonon frequencies in the Debye approximation. For a bcc lattice one has

$$\omega_{\underline{k}} \approx \frac{\omega_D R}{4.3} |\underline{k}|$$

where ω_D is the Debye frequency. We use the small k approximation to $\sin^2(\underline{k} \cdot \underline{R}_{12}/2)$, and also average over the angles

$$\sin^2(\underline{k} \cdot \underline{R}_{12}/2) \approx k^2 R^2 / 8.$$

With these approximations Eq. (C.7) becomes

$$\langle \underline{n} | v^2 | \underline{n} \rangle \approx \frac{3}{Nm\omega_D} \overline{\sum_{\underline{k}\alpha} \hbar\omega_{\underline{k}} (n_{\underline{k}\alpha 2} + 1/2)}. \quad (C.8)$$

For the ground state,

$$\langle 0 | v^2 | 0 \rangle \simeq \frac{3}{4m_D} E_0/N \quad (C.9)$$

where an extra factor of 1/2 comes from the fact that Eq. (C.8) contains only modes with $\sigma = 2$. The ground state energy in the Debye approximation is

$$E_0 = \frac{9}{8} \hbar \omega_D N$$

so that

$$\langle 0 | v^2 | 0 \rangle \simeq .8 \frac{\hbar}{m_D} \simeq .6 \text{ \AA}^2 \quad (C.10)$$

where we have taken m the mass of a He^3 atom, and

$\hbar \omega_D / k_B = 20^\circ \text{K}$. Thus,

$$\langle 0 | v^2 | 0 \rangle^{1/2} \simeq .8 \text{ \AA} \quad (C.11)$$

which should be compared to

$$|d|/2 = \sqrt{2} R/2 \simeq 2.5 \text{ \AA} \quad (C.12)$$

which is the distance in configuration space from p^0 to the hyper-surface bounding Ω_e and lying halfway between p^0 and p^{12} ; R is the nearest neighbor distance $R \approx 3.6 \text{ \AA}$. The ratio is thus one to three.

The low-lying excited states of interest will have energies on the order of $k_B T$ above the ground state, where $k_B T \ll \hbar \omega_D$. According to Eqs. (C.8) and (C.9), the estimate given for $\langle 0 | v^2 | 0 \rangle^{1/2}$ will apply to these states also.

APPENDIX D: CONVENTIONS

It has been pointed out^{17,30} that a number of conventions are currently in use for the definition of the exchange frequency (or operator) in solid He³. That is, if ϵ_{ij}^+ and ϵ_{ij}^- are appropriately defined singlet and triplet energies for the pair (i,j) then

$$J_{ij} = \alpha(\epsilon_{ij}^+ - \epsilon_{ij}^-) \quad (D.1)$$

where α has been taken as 1/2, 1, and 2. These conventions cannot affect the exchange Hamiltonian as a whole since it must generate the singlet-triplet energy splittings for each pair of atoms; nor can they affect the predicted nuclear spin ordering temperature, T_N , for the same reason. The particular convention used for J_{ij} must then be balanced by an appropriate numerical factor in front of the Heisenberg Hamiltonian.

To illustrate these matters we give a brief intuitive derivation of the Heisenberg Hamiltonian. Note that

$$\epsilon_{ij}^{\pm} = \frac{1}{2}(\epsilon_{ij}^+ + \epsilon_{ij}^-) \pm \frac{1}{2}(\epsilon_{ij}^+ - \epsilon_{ij}^-). \quad (D.2)$$

Now if $\underline{I}_i$ is the nuclear spin of atom i , then

$$\left(\frac{1}{2} + 2\underline{I}_i \cdot \underline{I}_j \right) = \begin{cases} -1 & \text{in the singlet state} \\ +1 & \text{in the triplet state} \end{cases} \quad (\text{D.3})$$

Thus

$$\epsilon_{ij}^{\pm} = \text{Direct terms} - (\epsilon_{ij}^{+} - \epsilon_{ij}^{-}) \underline{I}_i \cdot \underline{I}_j \quad (\text{D.4})$$

Now one sums over all of the pairs (i,j) making sure not to count them twice. The Heisenberg Hamiltonian comes from the spin dependent terms:

$$H_X = - \sum_{i < j} (\epsilon_{ij}^{+} - \epsilon_{ij}^{-}) \underline{I}_i \cdot \underline{I}_j \quad (\text{D.5})$$

In terms of Eq. (D.5), the Néel temperature for bcc solid He^3 is given by³⁷

$$T_N = 1.38 | \epsilon^{+} - \epsilon^{-} | / k_B \quad (\text{D.6})$$

where $\epsilon^{\pm}$ correspond to a nearest neighbor pair.

According to the above, the following expressions must be consistent:

$$J_{ij} = \alpha(\epsilon_{ij}^+ - \epsilon_{ij}^-) \quad (D.1)$$

$$H_X = \frac{1}{\alpha} \sum_{i < j} J_{ij} \mathbf{I}_i \cdot \mathbf{I}_j \quad (D.7)$$

$$T_C = (1.38/\alpha) \cdot |J| / \kappa_B \quad (D.8)$$

In those cases where an exchange operator is defined, one replaces $\epsilon_{ij}^{\pm}$ by $(\epsilon_{ij}^{\pm})_{mn}$ and J_{ij} by $(J_{ij})_{mn}$. Various different factors may be seen in front of the Heisenberg Hamiltonian according to whether one writes $\sum_{i < j} = \frac{1}{2} \sum_{i, j}$ or uses the Pauli spin operators $\sigma_i = 2\mathbf{I}_i$. The more standard convention is $\alpha = 1/2$, while some of the NMR work uses $\alpha = 1$.¹⁷ We list some of the papers and the conventions they use:

$$\alpha = 1/2$$

Herring³¹

Thouless²⁷

Bernardes and Primakoff²³

Ebner and Sung³⁰

This work

Panczyk and Adams¹⁷

$\alpha = 1$

Guyer and Zane²⁹
Reich⁸
Garwin and Landesman⁹
Richards, Hatton and Giffard¹⁰
Richardson, Hunt, Meyer¹¹

 $\alpha = 2$

Nosanow and Mullin²⁶
Nosanow and Varma²⁸

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Figure Captions

J is the $T = 0$ nearest neighbor exchange frequency.
All values of J are presented using the convention
 $J = (\epsilon^+ - \epsilon^-)/2$; see Appendix D. Thus the results of
NM(ref.26) and NV(ref.28) have been divided by four; and
the results of GZ(ref.29), divided by two.

R is the nearest neighbor distance.

Figure 1. J vs. R The dashed lines are the reported results
of NM(ref.26), GZ(ref.29), and ES(ref.30). The
solid lines have been calculated using the two-body
surface integral with the Gaussian values and
correlation functions of the above workers.

Figure 2. J vs. R The two-body surface integral using the
Gaussian values of NM(ref.26), GZ(ref.29), and
ES(ref.30). The solid lines were obtained using
the Nosanow correlation function. The dashed lines
were obtained using the workers own correlation
function.

Figure 3. J vs. R Some of the results in the current
literature: RHM(ref.11), PA(ref.17), NM(ref.26),
NVII(ref.28), GZ(ref.29), and ES(ref.30). The solid
lines are theoretical; the dashed lines, experimenta

Figure 4. Gaussian constant A vs. R , for NM(ref.26), GZ(ref.29 and ES(ref.30).

Figure 5. Correlation function $g(r)$ for nearest neighbors vs. r as used by NM(ref.26) [for $R = 3.75 \text{ \AA}$, $\log_{10} K = -.75$] , GZ(ref.29) [for $R = 3.48 \text{ \AA}$] , and ES(ref.30) [for $R = 3.58 \text{ \AA}$] .

Figure 6. J vs. R The Monte Carlo calculation of the full many-body surface integral for J using the NM(ref.26 wave function is indicated by "Full Monte Carlo." The "rigid lattice calculation" is obtained by including delta functions in the above integral to fix all atoms but the exchanging pair at their lattice sites. The "two-body approximation", which is the two-body surface integral mentioned in the preceding figures, is the cluster expanded approximation to the full integral, and is given by Eq.(5.9) of Part I.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6

Table 1: Results of the Monte Carlo (MC) calculation of J_{12} using the many-body surface integral expression with the Nosanow-Mullin wavefunction. The results of the two-body (TB) approximation to the full integral are presented for comparison. The results are given at four densities; Δ is the nearest neighbor distance. The values of A and $\log_{10} K$ are presented.

$\Delta(\text{\AA})$	3.45	3.55	3.65	3.75
$A(\text{\AA}^{-2})$	1.73	1.59	1.44	1.30
$\log_{10} K$	-.786	-.780	-.768	-.754
$J_{MC}(10^{-5} \text{ } ^\circ K)$	-.26 $\pm .02$	-.58 $\pm .04$	-1.3 $\pm .1$	-3.4 $\pm .2$
$J_{TB}(10^{-5} \text{ } ^\circ K)$	-1.58	-2.67	-5.17	-10.1

Table 2: Tests of the Monte Carlo calculation of J_{12} using the Nosanow-Mullin wavefunction for two density extremes. $J(I)$, $J(II)$, and $J(III)$ were calculated with the variation schemes 30-9-1, 28-1-1, and 1-0-0 respectively. All values of J_{12} are in $10^{-5} \text{ }^{\circ}\text{K}$.

Δ	3.45	3.75
$J(I)$	$-.26 \pm .02$	$-3.4 \pm .2$
$J(II)$	$-.24 \pm .02$	$-3.7 \pm .3$
$J(III)$	$-.065 \pm .004$	$-2.6 \pm .1$

Table 3: Test of the Monte Carlo calculation using the wavefunction Φ_{test} . Results compared to those of analytic computation. $\Delta = 3.75 \text{ \AA}$.

variation	Monte Carlo			Analytic	
	1-0-0	28-1-1	30-9-1	Rigid Lattice	Full Integral
$\Delta \cdot g(\Delta)$	$3.1 \pm .3$	$3.0 \pm .35$	$2.9 \pm .37$	3.05	2.98
$J(10^{-16} \text{ }^{\circ}\text{K})$	$-1.8 \pm .2$	-6.5 ± 1.2	-9.0 ± 1.6	-1.7	-8.9