Self-Consistent Selection of a Ferromagnetic Representation for the Heisenberg-Exchange Model

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The Heisenberg magnetic-exchange Hamiltonian is written in second-quantized form and a 1/V factor is extracted, where V is the volume of the system. Using Umezawa's self-consistent method, a unitarily inequivalent representation is selected in which the Hamiltonian obviously describes a ferromagnetic system; a result not at all obvious since the original Hamiltonian is completely symmetric and there is no reason *a priori* for expecting it to describe an asymmetric ferromagnetic configuration. All higher-order terms are accounted for, and the representation is picked out without using the adiabatic theorem, which is typically used in the self-consistent method. Inequivalence of various representations is discussed and validity is added for using an exchange integral depending only on relative distance between lattice sites and, in particular, on nearest neighbors.

I. INTRODUCTION

As is well known, Von Neumann¹ proved that for systems with a finite number of degrees of freedom any Hilbert-space specification is equivalent up to a unitary transformation to any other provided the canonical commutation (anticommutation) relations are preserved.

However, for systems with infinitely many degrees of freedom (i.e., for fields) not all irreducible representations of the commutation (anticommutation) relations are unitarily equivalent as has been shown by various authors. Van Hove² and Friedrichs³ were the first to study various representations of the canonical commutation and anticommutation relations, but the phenomenon of inequivalent representations was not given much attention by physicists until the appearance of papers by Wightman and Schweber, ⁴ and Haag⁵ around 1955. Wightman and Schweber showed the existence of uncountably many unitarily inequivalent representations of the canonical commutation and anticommutation relations. More mathematical details were given in two papers by Gärding and Wightman.⁶ Other important works on inequivalent representations for the canonical commutation and anticommutation relations have been written by Segal, ⁷ Araki and Woods, ⁸ Ezawa, ⁹ Araki and Wyss, ¹⁰ Klauder and McKenna, ¹¹ and Klauder, McKenna, and Woods.¹² Recently, Hatch and Benson have proposed a theorem to help clarify the typical statements for inequivalent representations with respect to the usual "change of representation" in quantum mechanics.¹³

With the idea of unitarily inequivalent representations becoming established, Umezawa, aided by a few others, began developing a self-consistent method for picking out physically relevant representations. The method essentially involves transforming the original set of variables in which the Hamiltonian is written to the physical set of variables in which the Hamiltonian becomes diagonalized and bilinear in annihilation and creation operators of the physical Fock space. The limit as $V \rightarrow \infty$ is used to eliminate higher-order terms, and this is usually done through use of the adiabatic theorem.¹⁴ However, in our model we use a different technique than the adiabatic theorem, which will impose certain conditions upon the interaction. A synopsis of Umezawa's self-consistent method as applied to many-body systems will be given in Sec. II.

For our system we will take a three-dimensional lattice of N Fermions at temperature T = 0 °K contained in a box of volume V with periodic boundary conditions, and we will eventually proceed to the limit as $V \rightarrow \infty$, $N \rightarrow \infty$, such that $N/V = \rho$, the density. The Heisenberg magnetic-exchange Hamiltonian H will be used to describe the spin effects of our system. Using second-quantized spin operators, we are able to extract a 1/V factor in front of H, arriving at the form of the model to which we can apply Umezawa's methods. We will then proceed to show that there exists a representation where H explicitly describes a ferromagnetic system, a result not at all obvious since His symmetric under spin rotations, whereas a ferromagnetic configuration is asymmetric under spin rotations. This representation will be found without using the adiabatic theorem, and it will be shown inequivalent to all other representations. These results will be discussed in Sec. III.

II. SELF-CONSISTENT METHOD OF UMEZAWA

We begin the study of our physical system by writing down an appropriate Hamiltonian $H = H_0$ $+ H_{int}$ for the system and second-quantizing it. It gives in general nonlinear equations which we then try to solve in order to deduce the results which can be compared with experiments. Umezawa,

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Leplae, and Sen¹⁵ have formulated this step as a dynamical mapping between the original set of annihilation and creation operators (a_k, a_k^{\dagger}) , in terms of which the model is written down, and the physical annihilation and creation operators (b_k, b_k^{\dagger}) , in terms of which the observed stationary states are written (also referred to as quasiparticle operators):

$$a_{k} = f(b_{k}) = C + g_{k}b_{k} + h_{k}b_{k}^{\dagger} + N_{b}(b_{k}) \quad , \qquad (2.1)$$

where C stands for a constant and $N_p(b_k)$ for higher-order normal products. The expansion coefficients, such as g and h, are to be determined so that when Eq. (2.1) is inserted into the original Hamiltonian, H takes the form

$$H = \sum_{k} E_{k} b_{k}^{\dagger} b_{k} + C + Q_{V}(b_{k}) = H_{0}(b_{k}) + Q_{V}(b_{k}) , \qquad (2.2)$$

where $Q_V(b_k) \rightarrow 0$ when the volume V becomes infinite, and E_k is a c number. The b_k 's satisfy the same commutation (anticommutation) rules as the a_k 's.

In most cases the determination of the coefficients in Eq. (2.1) is carried out in two stages. First we make a canonical Bogoliubov-type transformation T from the a_k 's to the intermediate \overline{b}_k fields, and then we look for a matrix S which takes us from the \overline{b}_k 's to the b_k 's (physical fields) in such a way that

$$\overline{b}_{k} = (Z)^{1/2} b_{k} + N_{p}(b_{k}) , \qquad (2.3)$$

where Z is a c number.

Under the Bogoliubov-type transformation T and upon normal ordering our operators (denoted by : X:) and eliminating off-diagonal bilinear terms, our original Hamiltonian becomes

$$H(\overline{b}_{k}) = H_{0}(\overline{b}_{k}) + H_{int}(\overline{b}_{k}); \quad , \qquad (2.4)$$

as will be seen clearly for the model we consider in this paper. Then Umezawa proceeds to eliminate the higher-order (H_{int}) terms by employing the adiabatic theorem. This is done by taking

$$\overline{b}_{k} = S^{-1}b_{k}S, \qquad (2.5)$$

where to first order in : $H_{int}(\overline{b}_{b})$:,

$$S = 1 + (-i) \int_{-\infty}^{0} : H_{int}(t): dt$$

and

 $H_{\rm int}(t) = e^{\epsilon \, t} H_{\rm int}(b_k e^{-i E_k t}) \ , \label{eq:hint}$ with

$$\boldsymbol{\epsilon} \sim \boldsymbol{V}^{\boldsymbol{p}}, \quad -\frac{1}{3} < \boldsymbol{p} < \boldsymbol{0} \tag{2.6}$$

for large V. From Eq. (2.6), Eq. (2.4) becomes

$$H(b_k) \rightarrow S^{-1}H(b_k)S = H_0(b_k) + Q_V(b_k)$$
, (2.7)

where $Q_V(b_k)$ is an operator such that the limit of its matrix elements taken between any two states of the physical Fock representation of the b_k 's as V→∞ is zero.

The important result of using the adiabatic theorem above [essentially Eq. (2.6)] is that $Q_V(b_k)$ in Eq. (2.7) then has energy-conserving matrix elements with respect to the physical Fock-space states. It is this energy-conserving constraint that causes

$$\lim_{V \to \infty} Q_V(b_k) \to 0 \quad , \tag{2.8}$$

as will be shown in our model.

However, for the Heisenberg model we will not use the adiabatic theorem to obtain the energyconserving constraint on the matrix elements of $Q_V(b_k)$. This condition will instead be obtained by finding the condition for $[H_{bl}(b_k), H_{quad}(b_k)] = 0$, a possibility alluded to by Umezawa¹⁶ in a footnote of one of his papers, where [,] stands for the commutator, bi for bilinear, and quad for quadrilinear. For the Heisenberg magnetic-exchange model this places conditions upon the exchange integral of the interaction term as will be discussed.

III. BILINEARIZATION OF THE HEISENBERG MAGNETIC-EXCHANGE MODEL

We begin by studying a three-dimensional lattice system of N fermions, one fermion of spin- $\frac{1}{2}$ at each lattice site, at temperature T = 0°K contained in a box of volume V with periodic boundary conditions, and we will eventually proceed to the limit as $V \rightarrow \infty$, $N \rightarrow \infty$ in such a way that $N/V = \rho$, the density of the system. (The motion of ions and lattice vibrations will not be considered.) The variables that we will be concerned with for describing a fermion at lattice site 1 are the spin components S_1^* , S_1^* , S_1^* , S_1^* , and we will use the Heisenberg magnetic-exchange model Hamiltonian¹⁷ to describe this system.

The Heisenberg exchange model can be written

$$H = -\sum_{\mathbf{\vec{i}} \neq \mathbf{\vec{i}}'} J_{\mathbf{\vec{i}} - \mathbf{\vec{i}}'} \vec{\mathbf{S}}_{\mathbf{\vec{i}}} \cdot \vec{\mathbf{S}}_{\mathbf{\vec{i}}}, \quad (3.1)$$

where S_{1} is the spin operator for the fermion at the \overline{I} th lattice site, and $J_{\overline{1}-\overline{1}}$ is the exchange integral, typically taken as large only when $\overline{1}-\overline{1}$ is one or two lattice spacings. (It is conventionally taken to just be a nearest-neighbor interaction.)

Using the methods of quantum field theory, we can write the spin operators in their secondquantized form in terms of fermion annihilation and creation operators. In the Pauli representation of spin our second-quantized spin operators can be written

$$S_{1}^{z} = \frac{1}{2} \left(a_{1,}^{\dagger} a_{1,}^{\dagger} - a_{1,}^{\dagger} a_{1,}^{\dagger} \right) ,$$

$$S_{1}^{y} = -\frac{1}{2} i \left(a_{1,}^{\dagger} a_{1,}^{\dagger} - a_{1,}^{\dagger} a_{1,}^{\dagger} \right) ,$$

$$S_{1}^{x} = \frac{1}{2} \left(a_{1,}^{\dagger} a_{1,}^{\dagger} + a_{1,}^{\dagger} a_{1,}^{\dagger} \right) ,$$

$$(3.2)$$

where $a_{1,+}$ destroys a fermion at lattice site 1

with spin up, $a_{1,1}^{\dagger}$ creates a fermion at lattice site \vec{l} with spin down, etc.¹⁸ The *a*'s obey anticommutation relations. We will also use the operators S_{1}^{\dagger} and $S_{\overline{1}}$ given by the definitions

$$S_{1}^{*} = S_{1}^{*} + iS_{1}^{*} ,$$

$$S_{1}^{-} = S_{1}^{*} - iS_{1}^{*} .$$
(3.3)

As is well known, the Heisenberg spin-spin form, Eq. (3.1), can be motivated by second quantizing the typical Coulomb interaction term between fermions, ¹⁹ where the exchange integral is taken as

$$J_{\vec{1},\vec{1}'} = \langle (\vec{1};\vec{1}') \mid \frac{1}{2} \sum_{i,j} \frac{e^2}{\vec{r}_i - \vec{r}_j} \mid (\vec{1};\vec{1}') \rangle \quad . \tag{3.4}$$

 $[\langle (l; l')|$ is a state specification written in the convention of ordinary quantum mechanics.] So as to be able to write H in the form to which Umezawa's self-consistent method is directly applicable, we examine Eq. (3.4) more closely, using for the matrix-element-state specifications Wannier functions which make calculations readily possible.²⁰ Expanding and simplyfying, it is easy to show that Eq. (3.4) can be written

$$J_{\vec{1},\vec{1}'} = \frac{1}{V} \sum_{\vec{q}} \frac{4\pi e^2 e^{i\vec{q}\cdot(\vec{1}-\vec{1}')}}{q^2} , \qquad (3.5)$$

where \vec{q} is a reciprocal-lattice vector. This extracts the volume dependence from the exchange integral, giving us a (1/V) factor which will be of importance later when we let $V \rightarrow \infty$, $N \rightarrow \infty$, such that $N/V = \rho$. Consequently, we will write $J_{\vec{1}\cdot\vec{l}} = (1/V)J'_{\vec{1}\cdot\vec{l}}$, where

$$J'_{\vec{1}-\vec{1}'} = \sum_{\vec{q}} \frac{4e^2 \pi e^{i\vec{q}\cdot(\vec{1}-\vec{1}')}}{q^2} \quad . \tag{3.6}$$

Therefore, using the second-quantized spin operators, Eq. (3.2), and using Eq. (3.6), we obtain the form of the model Hamiltonian Eq. (3.1) to which we will now apply the self-consistent method of Umezawa, namely, in direct lattice space,

Fourier transforming, we have in reciprocallattice space for H,

$$\begin{split} H &= -\frac{1}{4V} \sum_{\vec{k}} \sum_{\vec{k}_{1}} \sum_{\vec{k}_{2}} J'_{\vec{k}} \left[a_{\vec{k}_{1}-\vec{k}}^{\dagger}, a_{\vec{k}_{1}}, a_{\vec{k}_{2}+\vec{k}}^{\dagger}, a_{\vec{k}_{2}}^{\dagger}, \right. \\ &+ a_{\vec{k}_{1}-\vec{k}}^{\dagger}, a_{\vec{k}_{1}+}^{\dagger} a_{\vec{k}_{2}+\vec{k}+}^{\dagger}, a_{\vec{k}_{2}+}^{\dagger} - a_{\vec{k}_{1}-\vec{k}+}^{\dagger}, a_{\vec{k}_{1}+}^{\dagger}, a_{\vec{k}_{2}+\vec{k}}^{\dagger}, a_{\vec{k}_{2}}^{\dagger}, \\ &- a_{\vec{k}_{1}-\vec{k}}^{\dagger}, a_{\vec{k}_{1}+}^{\dagger}, a_{\vec{k}_{2}+\vec{k}+}^{\dagger}, a_{\vec{k}_{2}+}^{\dagger} + 2a_{\vec{k}_{1}-\vec{k}}^{\dagger}, a_{\vec{k}_{1}+}^{\dagger}, a_{\vec{k}_{2}+\vec{k}+}^{\dagger}, a_{\vec{k}_{2}}^{\dagger}, \end{split}$$

$$+ 2a_{\vec{k}_{1}-\vec{k}}^{\dagger}a_{\vec{k}_{1}}a_{\vec{k}_{2}+\vec{k}}a_{\vec{k}_{2}}\right] . \quad (3.8)$$

The objective will now be to show that starting from Eq. (3.7) [or Eq. (3.8)], a representation for this Hamiltonian can be found where ferromagnetism is obviously manifest. We know that the model $(\vec{S} \cdot \vec{S} \text{ form})$ is invariant in form under spin rotations generated by the unitary operators,

$$U_{\nu}(\vec{\Theta}) = e^{i\vec{\Theta}\cdot\vec{S}} = \exp\left(i\vec{\Theta}\cdot\sum_{\vec{1}}\vec{S}_{\vec{1}}\right) \quad , \qquad (3.9)$$

about the angle $\vec{\Theta}$, i.e., $UHU^{-1} = H$, and thus being totally symmetric with respect to spin orientation, there is no reason *a priori* to expect the Heisenberg exchange Hamiltonian to describe a ferromagnetic configuration (all spins aligned in a particular direction), since this represents asymmetry.

Our objective will be accomplished by the following steps, which is essentially Umezawa's self-consistent method: (i) transform to a generalized, parametrized set of variables (dynamical map); (ii) normal order the operators in H by using Wick's theorem; (iii) eliminate ($\downarrow \uparrow$), ($\uparrow \downarrow$) terms so as to determine the coefficients of the dynamical map (these are self-consistent equations); (iv) show that the higher-order (higher than second) terms have energy-conserving matrix elements in our physical Fock space *without* using the adiabatic theorem; (v) take the limit as $V \rightarrow \infty$ in order to eliminate the higher-order terms and leave us with just a Hamiltonian obviously expressing ferromagnetisms.

We first transform from the original set of operators $(a_{1,s}^*, a_{1,s}^{\dagger})$ to a generalized, parametrized set of operators $(b_{1,s}, b_{1,s}^{\dagger})$, which has the same canonical anticommutation relations as the a's. This can be written formally as

$$a_{1,s} - Tb_{1,s} T^{-1} = f(b)$$
, (3.10)

where f stands for "function of." From Von Neumann's theorem stated in Sec. I, we know that we can find a unitary T for finite volume to relate the a's and b's.

For the transformation to the b's we will use an analogous type of transformation as is used for superconducting models²¹ (a Bogoliubov-type model), where for our model we concentrate on rotating the spins in our spin Hilbert space. Thus, we try letting

$$a_{1,}^{\dagger} = u_{1} b_{1,}^{\dagger} - v_{1}^{*} b_{1,}^{\dagger} , \quad a_{1,}^{*} = u_{1}^{*} b_{1,}^{*} - v_{1}^{*} b_{1,}^{*} ,$$

$$a_{1,}^{\dagger} = v_{1}^{*} b_{1,}^{\dagger} + u_{1}^{*} b_{1,}^{\dagger} , \quad a_{1,}^{*} = v_{1}^{*} b_{1,}^{*} + u_{1}^{*} b_{1,}^{*} ,$$
(3.11)

where u_1 and v_1 are Hermitian parameters which have to be determined self-consistently, and $(u_1^2 + v_1^2) = 1$ for this to be a canonical transformation. This will take care of step (i). Then, since we are trying to bilinearize *H*, we separate it into bilinear and higher-order parts by using Wick's theorem to normal order the oper-

ators. This is step (ii). Performing these operations, using Eq. (3.11), Eq. (3.7) becomes

where : x: signifies normal ordering, i.e., annihilation operators are to operate before creation operators, and $\langle \rangle$ means a ground-state expectation value with respect to the ground state of the *a* representation. As can be seen, we have terms like $\langle \text{ground state} | Ta_1^{\dagger}, a_1^{\dagger}, T^{-1} | \text{ground state} \rangle$, and when we take the limit as $V \to \infty$ this suggests that a new set of states $\lim_{V \to \infty} (T^{-1} | \text{ground state} \rangle)$ be introduced, which depend upon the transformation parameters in *T*. This will prove to be a useful procedure. Therefore, when $V \to \infty$, which is the situation we are interested in, we will have things such as

(new ground state $|a_{1,a_{1}}^{\dagger}|$ new ground state). (3.13)

As has been illustrated in the literature cited in Sec. I, T^{-1} |ground state \rangle in general is in a different representation than |ground state \rangle .

Imposing the condition that the coefficient of b_{1}^{\dagger} , b_{1}^{\bullet} , and of b_{1}^{\dagger} , b_{1}^{\bullet} , vanish, and using the canonical condition $(u_{1}^{2} + v_{1}^{2}) = 1$, self-consistent equations can then be determined for u_{1} and v_{1} . From Eq. (3.12) the equations to be solved are

 $2C_{1}^{(1)}u_{1}^{*}v_{1}^{*}+u_{1}^{2}C_{1}^{(2)}-v_{1}^{2}C_{1}^{(2)\dagger}=0$

 $2C_{1}^{(1)}u_{1}^{*}v_{1}^{*}+u_{1}^{2}C_{1}^{(2)\dagger}-v_{1}^{2}C_{1}^{(2)}=0 ,$

where

and

$$C_{\vec{1}}^{(1)} = \sum_{\vec{1}'} J_{\vec{1}-\vec{1}'} \langle a_{\vec{1}'}^{\dagger}, a_{\vec{1}'}, -a_{\vec{1}'}^{\dagger}, a_{\vec{1}'} \rangle ,$$

$$C_{\vec{1}}^{(2)} = \sum_{\vec{1}'} -2 J_{\vec{1}-\vec{1}'} \langle a_{\vec{1}'}^{\dagger}, a_{\vec{1}'} \rangle , \qquad (3.15)$$

$$C_{\vec{1}}^{(2)\dagger} = \sum_{\vec{1}'} -2J_{\vec{1}-\vec{1}'} \langle a_{\vec{1}'}^{\dagger} a_{\vec{1}'} \rangle ,$$

where now $|\rangle = T^{-1}|$ ground state \rangle . Solving Eq. (3.14) using the quadratic formula, we obtain

$$u_{1}^{2} = \frac{1}{2} \left(1 \pm C_{1}^{(1)} B_{1}^{-1} \right) , \qquad (3.16)$$

$$v_{1}^{2} = \frac{1}{2} \left[1 \pm (-) C_{1}^{(1)} B_{1}^{-1} \right], \qquad (3.17)$$

$$u_{\vec{1}}v_{\vec{1}} = \pm \frac{1}{4} \left(C_{\vec{1}}^{(2)} + C_{\vec{1}}^{(2)} \right) B_{\vec{1}}^{-1} , \qquad (3.18)$$

where $|C_{\bar{1}}|^2 = C_{\bar{1}}^{(2)} C_{\bar{1}}^{(2)\dagger}$, and the upper sign of $u_{\bar{1}}^2$ is taken at the same time as the upper signs of $v_{\bar{1}}^2$ and $u_{\bar{1}}v_{\bar{1}}$, and likewise for the lower signs.

Then the bilinear part of H from Eq. (3.12) becomes

$$H_{bi} = -\sum_{\vec{1}} \frac{1}{2} \left[\left(u_{\vec{1}}^2 - v_{\vec{1}}^2 \right) C_{\vec{1}}^{(1)} - u_{\vec{1}} v_{\vec{1}}^* (C_{\vec{1}}^{(2)} + C_{\vec{1}}^{(2)\dagger}) \right] \\ \times \left(b_{\vec{1}}^{\dagger}, b_{\vec{1}}, - b_{\vec{1}}^{\dagger}, b_{\vec{1}}, \right) \quad . \quad (3.19)$$

If we take the upper signs in Eqs. (3.16)-(3.18), then

$$H_{\rm bi} = -\sum_{\vec{1}} \frac{1}{2} B_{\vec{1}} (b_{\vec{1}}^{\dagger}, b_{\vec{1}}, - b_{\vec{1}}^{\dagger}, b_{\vec{1}},) \quad , \qquad (3.20)$$

where

(3.14)

$$B_{1}^{*} = \left[\left(C_{1}^{(1)} \right)^{2} + \left| C_{1}^{(2)} \right|^{2} \right]^{1/2} > 0 \quad . \tag{3.21}$$

But now what about the fourth-order terms in Eq. (3.12)? We will proceed to show that they give no contribution as $V \rightarrow \infty$. Using the anticommutation relations of the *b*'s, namely,

$$\{ b_{1,s}^{\dagger}, b_{1,s}^{\dagger}, b_{1,s}^{\dagger} \} = b_{1,s}^{\dagger}, b_{1,s}^{\dagger}, b_{1,s}^{\dagger}, b_{1,s}^{\dagger}, b_{1,s}^{\dagger} = \delta_{1,1}^{\dagger}, \delta_{s,s}^{\prime}, \\ \{ b_{1,s}^{\dagger}, b_{1,s}^{\dagger}, b_{1,s}^{\dagger} \} = \{ b_{1,s}^{\dagger}, b_{1,s}^{\dagger}, b_{1,s}^{\dagger} \} = 0 ,$$
(3.22)

we find after some tedious algebra that the commutator of H_{bi} [in Eq. (3.20)] with the quadrilinear terms in Eq. (3.12) is

$$\begin{split} [H_{\text{quad}}, H_{\text{bi}}] = &\sum_{\vec{1}} \sum_{\vec{1}'} J_{\vec{1}-\vec{1}'} : \{ (4u_{\vec{1}}v_{\vec{1}}u_{\vec{1}'}v_{\vec{1}'} - 2u_{\vec{1}}^2v_{\vec{1}}^2 - 2u_{\vec{1}}^2v_{\vec{1}'}^2) B \\ &\times (b_{\vec{1}}^{\dagger}, b_{\vec{1}}, b_{\vec{1}'}^{\dagger}, b_{\vec{1}'}, b_{\vec{1}'}, b_{\vec{1}'}, b_{\vec{1}'}, b_{\vec{1}'}) \\ &+ (4u_{\vec{1}}v_{\vec{1}}u_{\vec{1}'}v_{\vec{1}'} + 2u_{\vec{1}}^2u_{\vec{1}'}^2 + 2v_{\vec{1}}^2v_{\vec{1}'}^2) \\ &\times (B_{\vec{1}} - B_{\vec{1}'})(b_{\vec{1}'}^{\dagger}, b_{\vec{1}'}, b_{\vec{1}'}, b_{\vec{1}'}) \} : , \quad l \neq l' . \end{split}$$

$$(3.23)$$

However, we have using Eqs. (3.15)-(3.18) and (3.21) that this commutator vanishes *if* we take the typical case where the exchange integral *J* depends only on the relative distance between lattice sites and, in particular, we take this to be a nearest-neighbor interaction. Thus,

$$[H_{\text{quady}} H_{\text{bi}}] = 0 \quad . \tag{3.24}$$

Therefore, if Eq. (3.24) is satisfied, then sandwiching $[H_{quad}, H_{bi}]$ between eigenstates of H_{bi} gives us

$$\langle s' | H_{quad} H_{bi} | s \rangle = \langle s' | H_{bi} H_{quad} | s \rangle$$
 (3.25)

or

$$\langle s' | H_{quad} | s \rangle = \frac{E_{s'}}{E_s} \langle s' | H_{quad} | s \rangle$$
, (3.26)

where

$$|s\rangle = \Pi \quad b_k^{\dagger} |0\rangle \quad , \qquad (3.27)$$

and E_s is the eigenvalue of H_{bi} operating on $|s\rangle$; $|0\rangle$ stands for the Fock ground state of the b's. This means that the matrix elements of H_{quad} must be energy conserving, $E_{s'} = E_s$, with respect to the eigenstates of H_{bi} if there is to be any contribution from them in our "b" Hilbert space.

Now let us consider these energy-conserving terms. As is the case so many times when dealing with interacting systems, it is convenient to use Fourier-transformed quantities. At this point, this will prove useful to us. Fourier transforming H_{quad} in Eq. (3.12), we have as a typical term

$$H_{\text{quad}} = \frac{1}{4V} \sum_{\vec{k}} \sum_{\vec{k}_1} \sum_{\vec{k}_2} -J'_{\vec{k}} (u_{\vec{k}_1 - \vec{k}} v_{\vec{k}} v_{\vec{k}_2 + \vec{k}} v_{\vec{k}_2} + v_{\vec{k}_1} - \vec{k} u_{\vec{k}_1} v_{\vec{k}_2 + \vec{k}} v_{\vec{k}_2} - v_{\vec{k}_1 - \vec{k}} u_{\vec{k}_1} u_{\vec{k}_2 + \vec{k}} u_{\vec{k}_2} - u_{\vec{k}_1 - \vec{k}} v_{\vec{k}_1} u_{\vec{k}_2 + \vec{k}} u_{\vec{k}_2} + 2u_{\vec{k}_1 - \vec{k}} u_{\vec{k}_1} u_{\vec{k}_2 + \vec{k}} v_{\vec{k}_2} - 2v_{\vec{k}_1 - \vec{k}} v_{\vec{k}_1} v_{\vec{k}_2 + \vec{k}} u_{\vec{k}_2}): b_{\vec{k}_1 - \vec{k}_1} b_{\vec{k}_1}, b_{\vec{k}_2 + \vec{k}} b_{\vec{k}_2}, : (3.28)$$

There are a number of other terms similar in form to Eq. (3.28), but this will suffice for our purposes.

Now, at this point, we need to recall from Eq. (3.22) that

$$\{b_{\vec{k},s}^{*}, b_{\vec{k}',s'}^{\dagger}\} = \delta_{\vec{k},\vec{k}'}\delta_{s,s'} \quad . \tag{3.29}$$

However, in the limit as $V \rightarrow \infty$, the momentum spectrum becomes continuous (since $\Delta \mathbf{k} \propto \mathbf{1}/V$), so that to be mathematically correct, Eq. (3.29) should be given by

$$\{b_{\vec{k},s}, b_{\vec{k}',s'}^{\mathsf{T}}\} = \delta(\vec{k} - \vec{k}')\delta_{s,s'}, \qquad (3.30)$$

where $\delta(\vec{k} - \vec{k}')$ is the Dirac δ function. Therefore, it is useful to introduce some new operators (volume normalized b's) $d_{\vec{k},s'}^*$ $d_{\vec{k},s}^{\dagger}$ given by

$$d_{\vec{k},s} = (V)^{1/2} (2\pi)^{-3/2} b_{\vec{k},s} ,$$

$$d_{\vec{k},s}^{\dagger} = (V)^{1/2} (2\pi)^{-3/2} b_{\vec{k},s}^{\dagger} ,$$
(3.31)

so that for finite volume our anticommutation relations are

$$\{ d_{\vec{k},s}^{\dagger}, d_{\vec{k}',s'}^{\dagger} \} = [V/(2\pi)^3] \delta_{\vec{k},\vec{k}'}^{\dagger} \delta_{s,s'} , \{ d_{\vec{k},s}^{\dagger}, d_{\vec{k}',s'}^{\dagger} \} = \{ d_{\vec{k},s}^{\dagger}, d_{\vec{k}',s'}^{\dagger} \} = 0 .$$

$$(3.32)$$

Then for the situation we are interested in, $V \rightarrow \infty$, Eq. (3.32) gives the desired results²²

$$\{ d_{\vec{k},s}, d_{\vec{k}',s'}^{\dagger} \} = \delta(\vec{k} - \vec{k}') \delta_{s,s'} ,$$

$$\{ d_{\vec{k},s}, d_{\vec{k}',s'}^{\dagger} \} = \{ d_{\vec{k},s}^{\dagger}, d_{\vec{k}',s'}^{\dagger} \} = 0 .$$

$$(3.33)$$

For further mathematical preciseness, as pointed out in some of the references cited in Sec. I on inequivalent representations, we smear out our annihilation and creation operators with an orthonormal set of square-integrable functions, $f_J(k)$, by defining our fermion annihilation operators as ²³

$$d_{s}(f_{J}) = (2\pi)^{3}(V)^{-1} \sum_{\vec{k}} f_{J}(\vec{k}) d_{\vec{k},s} \quad (J = 1, 2, ...) \quad .$$
(3.34)

Then the basis states in Eq. (3.27) are defined as

$$\begin{aligned} |1\rangle &= d_s^{\dagger}(f_J) |0'\rangle , \\ |2\rangle &= d_s^{\dagger}(f_J) d_{s'}^{\dagger}(f_{J'}) |0'\rangle , \end{aligned}$$

$$(3.35)$$

etc., where $|1\rangle$ stands for a one-particle state, $|2\rangle$ for a two-particle state, and $|0'\rangle$ for the Fock ground state of the d's. These states are normalizable and allow us to construct a well-behaved Hilbert space, whereas the states obtained by operating on the Fock ground state of the d's by the $d_{\vec{k},s}$'s are not. However, for most practical calculations the $b_{\vec{k},s}$ or $d_{\vec{k},s}$ can still be used, but if problems are encountered, the $d_s(f_J)$'s should be used.

Now, having the mathematical machinery, if we look at the matrix elements of the Fourier transform of H_{quad} with respect to the states in Eq. (3.35), recalling from Eq. (3.26) that they must be energy-conserving, we have for the representative term in Eq. (3.28),

$$\begin{pmatrix} -\langle s' | (2\pi)^{6} (4V^{3})^{-1} \sum_{\vec{k}} \sum_{\vec{k}_{1}} \sum_{\vec{k}_{2}} F(\vec{k}, \vec{k}_{1}, \vec{k}_{2}) \\ : d^{\dagger}_{\vec{k}_{1} - \vec{k}} d_{\vec{k}_{1}} d^{\dagger}_{\vec{k}_{2} + \vec{k}} d_{\vec{k}_{2}} : |s\rangle \end{pmatrix}_{\text{EC}} , \quad (3.36)$$

where

$$\begin{split} F(\vec{k}, \vec{k}_{1}, \vec{k}_{2}) = J'_{\vec{k}} (u_{\vec{k}_{1} - \vec{k}} v_{\vec{k}_{1}} v_{\vec{k}_{2} + \vec{k}} v_{\vec{k}_{2}} + v_{\vec{k}_{1} - \vec{k}} u_{\vec{k}_{1}} v_{\vec{k}_{2} + \vec{k}} v_{\vec{k}_{2}} \\ &- v_{\vec{k}_{1} - \vec{k}} u_{\vec{k}_{1}} u_{\vec{k}_{2} + \vec{k}} u_{\vec{k}_{2}} - u_{\vec{k}_{1} - \vec{k}} v_{\vec{k}_{1}} u_{\vec{k}_{2} + \vec{k}} u_{\vec{k}_{2}} \\ &+ 2 u_{\vec{k}_{1} - \vec{k}} u_{\vec{k}_{1}} u_{\vec{k}_{2} + \vec{k}} v_{\vec{k}_{2}} - 2 v_{\vec{k}_{1} - \vec{k}} \\ &\times v_{\vec{k}_{1}} v_{\vec{k}_{2} + \vec{k}} u_{\vec{k}_{2}}) \quad , \quad (3.37) \end{split}$$

and (EC) means energy conserving, i.e., for Eq. (3.36),

$$E_{\vec{k}_1 - \vec{k}} + E_{\vec{k}_2 + \vec{k}} = E_{\vec{k}_1} + E_{\vec{k}_2} \quad . \tag{3.38}$$

Taking, for example, two-particle states in Eq. (3.36) and using Eqs. (3.26) and (3.31)-(3.35), we can reduce Eq. (3.36) to

$$\begin{split} \left| (2\pi)^{6} (4V^{3})^{-1} \langle 0 \left| 0 \right\rangle \left(\sum_{\vec{k}} \sum_{\vec{k}_{1}} \sum_{\vec{k}_{2}} f_{1}^{*}(\vec{k}_{1} - \vec{k}) \right. \\ \left. \times f_{J_{2}}^{*}(\vec{k}_{2} + \vec{k}) F(\vec{k}, \vec{k}_{1}, \vec{k}_{2}) \left\{ f_{J_{3}}(\vec{k}_{1}) f_{J_{4}}(\vec{k}_{2}) \right. \\ \left. - f_{J_{3}}(\vec{k}_{2}) f_{J_{4}}(\vec{k}_{1}) \right\} \right]_{EC} \,. \quad (3.39) \end{split}$$

Now what is important is the energy-conservation requirement imposed on Eq. (3.39). Equation (3.38) could be solved for the x component k^x of \vec{k} as a function of \vec{k}_1 , \vec{k}_2 , k^y , k^z . Then Eq. (3.39) becomes in the limit as $V \rightarrow \infty$,

$$\begin{split} \lim_{V \to \infty} \left((4\pi)^{-2} (V)^{-1/3} \int d\vec{\mathbf{k}}_1 \int d\vec{\mathbf{k}}_2 \int dk^y \int dk^x \\ & \times \left\{ f_{J_1}^* [\vec{\mathbf{k}}_1 - g(\vec{\mathbf{k}}_1, \vec{\mathbf{k}}_2, k^y, k^g) \\ & \times \hat{\imath} + k^y \hat{\jmath} + k^x \hat{k} \right\} f_{J_2}^* [\vec{\mathbf{k}}_2 + g(\vec{\mathbf{k}}_1, \vec{\mathbf{k}}_2, k^y, k^g) \hat{\imath} + k^y \hat{\jmath} + k^z \hat{k}] \\ & \times \left[f_{J_3}(\vec{\mathbf{k}}_2) f_{J_4}(\vec{\mathbf{k}}_1) - f_{J_3}(\vec{\mathbf{k}}_1) f_{J_4}(\vec{\mathbf{k}}_2) \right] \\ & \times F[\{g(\vec{\mathbf{k}}_1, \vec{\mathbf{k}}_2, k^y, k^z) \hat{\imath} \\ & + k^y \hat{\jmath} + k^z \hat{k} \}, \vec{\mathbf{k}}_1, \vec{\mathbf{k}}_2] \} \right) \quad, (3.40) \end{split}$$

where g represents "function of" and the $(V)^{-1/3}$ factor coming as a result of energy conservation makes the matrix element vanish when $V \rightarrow \infty$. In precisely the same manner as Eq. (3.40) was obtained, it can be shown that all the matrix elements for H_{quad} vanish in the limit as $V \rightarrow \infty$.

Consequently, since an operator is determined by its matrix elements in the Hilbert space, our original Hamiltonian written now in terms of the b's just reduces to

$$H = H_{bi} + C = -\sum_{\vec{1}} \frac{1}{2} B_{\vec{1}} (b_{\vec{1}}^{\dagger}, b_{\vec{1}}, -b_{\vec{1}}^{\dagger}, b_{\vec{1}}) + C \quad .$$
(3.41)

From Eqs. (3.2) and (3.11) we have for our second-quantized spin operators in terms of the b's, denoting these by s_{1} in order to distinguish them from the original S_{1} ,

$$S_{\vec{1}}^{\vec{z}} = \frac{1}{2} (b_{\vec{1}}^{\dagger}, b_{\vec{1}}, - b_{\vec{1}}^{\dagger}, b_{\vec{1}})$$
,

$$\begin{split} & \hat{s}_{1}^{2} = \frac{i}{2} \left(b_{1}^{\dagger}, b_{1}^{\dagger}, + b_{1}^{\dagger}, b_{1}^{\dagger}, b_{1}^{\dagger} \right) , \\ & \hat{s}_{1}^{y} = -i \frac{i}{2} \left(b_{1}^{\dagger}, b_{1}^{\dagger}, - b_{1}^{\dagger}, b_{1}^{\dagger}, b_{1}^{\dagger} \right) , \\ & \hat{s}_{1}^{*} = \hat{s}_{1}^{x} + i \hat{s}_{1}^{y} = b_{1}^{\dagger}, b_{1}^{\dagger}, \\ & \hat{s}_{1}^{*} = \hat{s}_{1}^{x} - i \hat{s}_{1}^{y} = b_{1}^{\dagger}, b_{1}^{\dagger}, \\ \end{split}$$
(3.42)

Therefore, Eq. (3.41) can be written

$$H = -\sum_{\vec{1}} B_{\vec{1}} \otimes \hat{\vec{1}} + C \quad . \tag{3.43}$$

(The constant will be determined by setting our lowest-energy eigenvalue at zero.)

Equation (3.43) is just what we had hoped for at the outset. It describes an assembly of independent spin- $\frac{1}{2}$ particules. Obviously, $B_{\mathbf{i}}$ can be interpreted as an internal magnetic field produced by the interactions between the Fermions, and all spins are aligned in some manner by this field. For $B_{\mathbf{i}} > 0$ the state of lowest energy is that of parallel alignment of the physical particle spins in the +z direction [and for $B_{\mathbf{i}} < 0$, in the (-z)direction]. The ground state of Eq. (3.43) can then be written

$$|\sigma\rangle_{phys} = |0\rangle_{phys} = |\uparrow\uparrow\ldots\uparrow\ldots\rangle = \prod_{\vec{1}} (b_{\vec{1}}^{\dagger})|0\rangle , \qquad (3.44)$$

where $|\sigma\rangle_{phys}$ stands for the physical ground state. [Then from Eq. (3.43),

$$C = {}_{\text{phys}} \langle 0 \left| \sum_{\vec{1}} B_{\vec{1}} S_{\vec{1}}^{\sharp} \right| 0 \rangle_{\text{phys}} , \qquad (3.45)$$

and we will not be concerned with this term in further work, other than to remember that it sets the minimum energy at zero.] Thus, using the five steps at the beginning of this section, we have indeed found a ferromagnetic representation for the Heisenberg exchange model.

As we will now indicate, this ferromagnetic representation is inequivalent to the original a representation. From the dynamical map, Eq. (3.11), we formally have for the operator connecting b's and a's,

$$T = \exp\left(\sum_{\vec{k}} (b_{\vec{k}}^{\dagger}, b_{\vec{k}}, - b_{\vec{k}}^{\dagger}, b_{\vec{k}}) \Theta_{\vec{k}}\right) , \qquad (3.46)$$

where $u_{\mathbf{k}}^{*} = \cos\Theta_{\mathbf{k}}^{*}$, $v_{\mathbf{k}}^{*} = \sin\Theta_{\mathbf{k}}^{*}$. Then from $b = T^{-1}aT$ and $|\sigma\rangle_{\operatorname{orig}} = |0\rangle_{\operatorname{orig}} = T|0\rangle_{\operatorname{phys}}$, we have

$$|0\rangle_{\rm phys} = T^{-1}|0\rangle_{\rm orig} \quad . \tag{3.47}$$

Thus, letting $V \rightarrow \infty$, we obtain

$$\operatorname{orig} \langle 0 | 0 \rangle_{\text{phys}} = \operatorname{phys} \langle 0 | T | 0 \rangle_{\text{phys}} = \lim_{V \to \infty} \{ \exp[-V(2\pi)^{-3} \times \int d\vec{k} | \ln \cos\Theta_{\vec{k}} |] \} = 0 \quad . \quad (3.48)$$

From the references cited in Sec. I on inequivalent representations this means that T is not unitarily implementable (subjectively) into our physical Fock space (b space).

Now, of course, there are infinitely many pos-

sible z directions along which the spins could be aligned. We now proceed to indicate that all of these ferromagnetic representations are inequivalent. First of all, the ground state degenerate with $|0\rangle_{phys}$, i.e., have different directions of spin alignments, are obtained from

$$\left[\exp\left(i\vec{\Theta}\cdot\sum_{\vec{1}}\vec{s}_{\vec{1}}\right)\right]|0\rangle_{\text{phys}} \quad . \tag{3.49}$$

If we consider the scalar product

$$_{\mathrm{phys}}\langle 0 | \exp\left(i\vec{\Theta}\cdot\sum_{\vec{1}}\vec{s}_{\vec{1}}\right) | 0 \rangle_{\mathrm{phys}}$$

and use the Euler-angle representation (ϕ, Θ, ψ) for $\vec{\Theta}$, then in the limit as $N \rightarrow \infty$, $V \rightarrow \infty$, $N/V \rightarrow \rho$, we have

$$\lim_{\substack{N \to \infty \\ V \neq \infty \\ N/V \neq \rho}} \left[phys \langle 0 | \exp\left(i\vec{\Theta} \cdot \sum_{\vec{I}} \vec{S}_{\vec{I}} \right) | 0 \rangle_{phys} \right] \\ \propto \lim_{\substack{N \to \infty \\ V \neq \infty \\ N/V \neq \rho}} (\cos\frac{1}{2}\Theta)^N = 0 \quad . \quad (3.50)$$

Therefore, the degenerate ground states of our ferromagnetic Hamiltonian, Eq. (3.43), are not connected by unitary operators and belong to different Hilbert spaces.

At this point, it may also be beneficial to note that the original-variable Hamiltonian, Eq. (3.7), has more than one representation description in the limit as $V \rightarrow \infty$. If we explicitly normal order Eq. (3.7) [or Eq. (3.8)] without transforming to generalized parametrized variables, we then find immediately that

$$[H_{\rm bi}, H_{\rm quad}] = 0 \quad . \tag{3.51}$$

Then in exactly the same manner as we found Eq.

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(3.43), we find for this case in the limit as $V \rightarrow \infty$ that *H* reduces to

$$H = -\frac{3}{4}J_0\sum_{\mathbf{i}} (a_{\mathbf{i}}^{\dagger}, a_{\mathbf{i}}, + a_{\mathbf{i}}^{\dagger}, a_{\mathbf{i}}, - (3.52)$$

For this representation, \bigstar spins are just as favored for the ground state as \bigstar spins at any site and with respect to any axis. This could be interpreted as a "paramagnetic" representation.

IV. CONCLUSION

In conclusion, applying Umezawa's methods of quantum field theory to solid-state systems, we have shown explicitly that the Heisenberg magnetic-exchange model does describe a ferromagnetic system when one is in the appropriate representation. All the higher-order terms were definitely accounted for, and this was accomplished without using the adiabatic theorem. The method used to eliminate these terms certainly adds validity to taking the exchange integral to depend only on relative distance between lattice sites and, in particular, on nearest neighbors; because by doing this, we were then led directly to the ferromagnetic Hamiltonian in Eq. (3.43).

It is important to point out that Eq. (3.43) can be obtained just by letting V become very large, and not necessarily going to ∞ , as can be seen from Eq. (3.40). How large depends on the order of magnitude of the other factors in Eq. (3.40).

Thus, the Heisenberg exchange Hamiltonian can properly be called the Heisenberg ferromagnetic Hamiltonian.

In a future paper, the physical implications involved in picking out the ferromagnetic representation for the Heisenberg exchange model will be discussed.

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