# **Derivation of the Modified Bloch Equations for Spin Systems\***

J. KORRINGAf AND J.-L. MOTCHANE

Laboratoire de Spectroscopie Hertzienne, Faculté des Sciences de Besançon, Besançon, France

P. PAPON

Laboratoire de Résonance Magnetique, Faculté des Sciences de Paris, Paris, France

AND

#### A. YOSHIMORI

## *Department of Physics, Nagoya University, Nagoya, Japan*  (Received 10 October 1963)

A new form of the equations for the time-dependent statistical matrix of a spin system is used to derive the modified Bloch equations, without considering details of the relaxation mechanism. A number of restrictive conditions are imposed on the system, most of which agree well with known limitations of the applicability of the modified Bloch equations. In order to avoid complications, only spins one-half are considered. The theory does not apply to the case where the relaxation is anisotropic but where the constant field and an applied rotating field are comparable in magnitude.

### 1. INTRODUCTION

THE motion of spin systems in liquids and in some<br>solids under influence of external fields is well<br>described by the modified Bloch equations (MBE). HE motion of spin systems in liquids and in some solids under influence of external fields is well These were obtained<sup>1</sup> as a generalization of the Bloch equations to weak fields, in which the relaxation towards thermal equilibrium in the constant external field was replaced by relaxation towards thermal equilibrium in the instantaneous total applied field. In both versions the relaxation is represented by a simple rate term in the differential equation for M, but if anisotropic, the new form assigns the instantaneous total field, and not the constant field, as the direction of anisotropy.

While these equations are plausible and well verified experimentally,<sup>2</sup> a derivation from first principles has, to our knowledge, not yet been published. As a consequence, it is not clear to which systems and under what conditions they can be expected to apply. Using a statistical method which is described in the preceding paper,<sup>3</sup> we have found a general derivation and conditions of applicability. It is presented in the following.

#### 2. STOCHASTIC EQUATIONS

The magnetization of a system with identical spins  $S^i$ is given by

$$
\mathbf{M} = \mathrm{Tr} \sum \mathbf{S}^i \rho_\theta^T / \mathrm{Tr} \rho_\theta^T. \tag{1}
$$

We use units with  $\frac{1}{2}\gamma = \hbar = k = 1$ , where  $\gamma$  is the gyromagnetic ratio of the spins and *k* is the Boltzmann con-

- 2 G. Whitfield and A. G. Redfield, Phys. Rev. 106, 918 (1957).
- 8 J. Korringa, preceding paper, Phys. Rev. 133, A1228 (1964).

stant.  $\rho_{\theta}^{T}$  is the statistical matrix of the total system, which we assume to consist of the spins in equivalent positions and a lattice.  $\theta$  is the temperature at which the system is in equilibrium before application of the timedependent fields. In Ref. 3 it was shown that Eq. (1) can be expressed in terms of a statistical matrix  $\rho_{\theta}$  which operates on the spin variables only, provided that the time-dependent fields, applied to the spins, do not disturb the thermal equilibrium of the lattice. Assuming this to be the case, we have, according to Ref. 3, Eqs. (21) and (27):

$$
\mathbf{M} = \mathrm{Tr} \sum \mathbf{S}^i \rho_\theta / \mathrm{Tr} \rho_\theta, \qquad (2)
$$

$$
\rho_{\theta} = \{ W(t - i/2\theta)W^{\dagger}(t + i/2\theta) \}_{\text{av}}, \tag{3}
$$

$$
i\partial W/\partial t = \left[\mathfrak{IC}(t) + h(t+i/2\theta)\right]W(t), \quad W(0) = 1. \quad (4)
$$

Here  $h(t)$  is the Hamiltonian of the applied timedependent fields and  $\mathcal{R}(t)$  is the Hamiltonian of the spin system.  $\mathcal{R}(t)$  includes the contribution of a constant external field  $H_0$ . It is time-dependent because it contains randomly fluctuating parameters, as explained in Ref. 3, which represent the spin-lattice interaction. "av" indicates the average over a time long compared with the correlation times of  $\mathcal{R}(t)$ .  $h(t)$  will be taken as for a rotating field:

$$
h = \sum h_i, \quad h_i(t) = H_1(S_x^i \cos \omega t + S_y^i \sin \omega t). \tag{5}
$$

The *%* axis is in the direction of the constant field.

Equations (2) to (4) contain no condition other than that the lattice remains in thermal equilibrium; the form of 5C and the time dependence of the random functions it contains are, however, to be found from very complicated implicit equations, as indicated in Ref. 3. For spins  $\frac{1}{2}$ ,  $\mathcal{K}$  consists of linear and bilinear terms in  $S^i$  with random variable coefficients; for higher spin values quadratic and biquadratic expressions, etc, can occur. We now make the following assumptions;

<sup>\*</sup> This work was begun and completed during two consecutive summers at the California Research Corporation, La Habra, California.

t Guggenheim Fellow, 1962. Present address: Ohio State University, Columbus, Ohio. <sup>1</sup>R. S. Codrington, J. D. Olds, and H. C. Torrey, Phys. Rev. 95,

<sup>607 (1954).</sup> 

(A) The spins are  $\frac{1}{2}$ , so that  $\mathcal{R}(t)$  takes the form

$$
\mathcal{FC}(t) = H_0 S_s{}^i + \sum_i \mathbf{V}_i(t) \cdot \mathbf{S}^i + \sum_{i \neq j} \mathbf{S}^i \cdot \mathbf{\Phi}_{ij}{}^{(i)} \cdot \mathbf{S}^j. \tag{6}
$$

(B) All coefficients  $V_i(t)$  and  $\Phi_{ij}(t)$  are random functions of time with average value zero and with correlation times short compared to the relaxation times of the spins.

Assumption (A) avoids complicated mathematical problems, but is perhaps not necessary. Assumption (B) is very restrictive, as the systems to which it applies are only liquids and (with  $\Phi=0$ ) such solids (as, e.g., diluted paramagnetic salts) for which the spin-spin interaction can be neglected. We hope to demonstrate, however, that this restriction is necessary for the MBE to be valid.

These assumptions permit us, for the purpose of calculating  $\mathbf{M}(t)$ , to separate the system entirely into one-particle systems:

where

$$
\mathfrak{IC}(t) \longrightarrow \sum \mathfrak{IC}_i(t), \quad \rho_\theta \longrightarrow \prod \rho_{i\theta}, \qquad (7)
$$

$$
\rho_{i\theta} = \{W_i(t-i/2\theta)W_i^{\dagger}(t+i/2\theta)\}_{{\rm av}},\qquad(8)
$$

$$
i\partial W_i/\partial t = \left[\mathfrak{IC}_i(t) + h_i(t+i/2\theta)\right]W_i(t). \tag{9}
$$

The conditions for Eqs, (7) to (9) to be valid with suitably chosen  $\mathcal{R}_i(t)$  are the same as those for Eqs. (2) to (4), i.e., the random parameters in  $\mathcal{R}_i(t)$  must represent a contact of the spin *i* with a system in equilibrium at the temperature  $\theta$ . Although, on account of the rotating field  $H_1$ , the spin system is not in equilibrium, each of the spin-spin interaction terms is modulated through  $\Phi_{ij}(t)$  with the fluctuations of the lattice. As these are, by assumption (B), faster than the random reorientations of the spins, they dominate the random character of  $\mathcal{R}_i(t)$  and thus allow us to apply Eqs.  $(7)$  to  $(9)$ .

As the spins are  $\frac{1}{2}$ ,  $\mathcal{R}_i(t)$  is of the form

$$
3C_i(t) = H_0 S_z{}^i + \mathbf{H}_L{}^i(t) \cdot \mathbf{S}^i, \tag{10}
$$

where the time average of  $H_L$ <sup>*i*</sup> is zero. Suppressing the index *i,* we finally have

$$
\mathbf{M} = N \langle \mathbf{S} \rangle, \tag{11}
$$

$$
\langle S \rangle = Tr S_{\rho_{\theta}} / Tr \rho_{\theta}, \qquad (12)
$$

$$
\rho_{\theta} = \{W(t-i/2\theta)W^{\dagger}(t+i/2\theta)\}_{{\rm av}},\tag{13}
$$

$$
i\partial W/\partial t = [H_0 S_z + H_L \cdot S + H_1(S_x \cos\omega(t + i/2\theta) + S_y \sin\omega(t + i/2\theta))]W(t).
$$
 (14)

 $\mathbf{H}_{L}(t)$  is a random function of time with a correlation time short compared with the relaxation time of the spins.

## 3. SOLUTION OF THE STOCHASTIC EQUATIONS

The solution of Eq. (14) for the special case  $H_1=0$  was discussed in a previous publication.<sup>4</sup> In a frame rotating with the Larmor frequency  $H_0$  one finds a random rotation, expressible in three Euler angles *(xix2xz)*   $=(\vartheta,\varphi,\psi)$ , which are random functions of time. The probability  $P(x, x_0, t)$  that the angles change, in the time  $\overline{t}$ , from the values  $x_0$  to  $x$  satisfies the diffusion equation

$$
\frac{\partial P}{\partial t} = \mathfrak{F}_0 P \,, \tag{15}
$$

$$
\mathfrak{F}_0 = (1/2\tau_1)(K_x^2 + K_y^2) + (1/2\tau_0)K_z^2. \tag{16}
$$

The operators  $\bf{K}$  are *i* times the operators of angular momentum

$$
K_x \pm iK_y = \exp(\pm i\psi) [\partial/\partial \vartheta \mp i(\sin \vartheta)^{-1} \times (\partial/\partial \varphi - \cos \vartheta \partial/\partial \psi)], \quad (17)
$$

$$
K_z = \partial/\partial \psi. \tag{18}
$$

 $\tau_1$  and  $\tau_0$  are expressible in terms of the square average of the components of  $\mathbf{H}_L$  (assumed here to be isotropic) and their correlation time  $\sigma$ 

$$
1/\tau_1 = \sigma \langle H_{Lx}^2 \rangle_{\rm av} (1 + H_0^2 \sigma^2)^{-1}, \tag{19}
$$

$$
1/\tau_0 = \sigma \langle H_{Lz}^2 \rangle_{\rm av}.\tag{20}
$$

In order to solve Eq. (14), we go to a rotating frame by applying the transformation

$$
W(t) = \exp(-i\omega S_z t)W'/t.
$$
 (21)

This gives

$$
i\partial W'/\partial t = \left[\Delta HS_z + H_1 \cosh(\omega/2\theta)S_x + iH_1 \sinh(\omega/2\theta)S_y + H_L'(t) \cdot S\right]W'(t), \quad (22)
$$

where  $\Delta H = H_0 - \omega$ , and where  $H_L'(t)$  is the local field seen on the rotating frame.

We first consider the high-temperature limit  $1/\theta \rightarrow 0$ . The transformation to a frame precessing around the effective field

$$
W'(t) = \exp[-i(\Delta H S_z + H_1 S_x)t]W''(t), \qquad (23)
$$

removes the external field terms and replaces  $H_L'$  with  $H_L''$ , the random field seen on these axes. The procedure used in Ref. 4 gives

$$
\frac{\partial P}{\partial t} = \mathfrak{F}P,\tag{24}
$$

$$
\mathfrak{F} = \sum G_{\alpha\beta} K_{\alpha} K_{\beta},\tag{25}
$$

$$
G_{\alpha\beta} = \Delta t \langle \bar{H}_{L\alpha}^{\prime\prime} \bar{H}_{L\beta}^{\prime\prime} \rangle_{\text{av}} , \qquad (26)
$$

where  $\bar{H}_{L}$ <sup>"</sup> is the average of  $H_{L}$ <sup>"</sup> over a time  $\Delta t$ satisfying

$$
\sigma \ll \Delta t \ll T. \tag{27}
$$

*T* is a relaxation time of the spins, expressible in terms of  $G_{\alpha\beta}$ . The averages in Eq. (26) are calculated on the assumption that the components of  $H_L(t)$  in the resting frame are statistically independent. The short-time average must be taken in order to obtain a random-walk problem. A simple calculation shows, however, that the coefficients  $G_{\alpha\beta}$  depend explicitly on  $\Delta t$  unless the effective field  $H_e = (\Delta H^2 + H_1^2)^{1/2}$  and the correlation

<sup>4</sup> A. Yoshimori and J. Korringa, Phys. Rev. 128, 1054 (1962),

times  $\sigma$  satisfy

$$
H_{\epsilon}\sigma \ll 1. \tag{28}
$$

We will assume in the following that this inequality is obeyed. In view of assumption (B), this is hardly a restriction except for the fact that it excludes frequencies very far from resonance and exceedingly large values of  $H_1$ .

With Eq. (28) satisfied, it is easier to solve Eq. (22)  $(1/\theta=0)$  directly, as one can take the short-time average of the equations of motion of the Euler angles in that frame with *At* satisfying

$$
\sigma \ll \Delta t \ll T \quad \text{and} \quad H_e \Delta t \ll 1. \tag{29}
$$

These inequalities guarantee that the change in the Euler angles in the rotating frame due to the random field and the effective field, respectively, is small. A simple calculation gives

$$
\frac{\partial P}{\partial t} = \mathfrak{F}P, \quad \mathfrak{F} = \mathfrak{F}_0 + \mathfrak{F}_1,\tag{30}
$$

$$
\mathfrak{F}_1 = -\Delta H K_z - H_1 K_x, \qquad (31)
$$

as was to be expected.

At finite temperatures, the imaginary term in Eq. (22) offers a new problem. Equation (22) is still solved by a rotation, but the Euler angles will take nonreal values. One can, however, follow the same procedure by considering x and its complex conjugate  $\bar{x}$  to be independent variables, and by using correspondingly a probability  $P(x, \bar{x}; x_0, \bar{x}_0, t)$  of six variables. We find

$$
\frac{\partial P}{\partial t} = \mathfrak{F}P, \quad \mathfrak{F} = \mathfrak{F}_0 + \mathfrak{F}_1 + \mathfrak{F}_2,\tag{32}
$$

$$
\mathfrak{F}_0 = (1/2\tau_1)[(K_x + K_x)^2 + (K_y + K_y)^2] + (1/2\tau_0)(K_x + \bar{K}_z)^2, \quad (33)
$$

$$
\mathfrak{F}_1 = -\Delta H(K_z + \bar{K}_z) \n-H_1 \cosh(\omega/2\theta)(K_x + \bar{K}_x), \quad (34)
$$

$$
\mathfrak{F}_2 = -iH_1 \sinh(\omega/2\theta)(K_y - \bar{K}_y). \tag{35}
$$

Here the barred vector  $K$  has the same form as  $K$ , Eqs. (17) and (18), but with  $\vartheta$ ,  $\varphi$ ,  $\psi$  changed to  $\bar{\vartheta}$ ,  $\bar{\varphi}$ ,  $\bar{\psi}$ .

### **4. THE MACROSCOPIC EQUATIONS**

The equations of motion for  $\langle S(t) \rangle$  will now be obtained in the "high" temperature approximation, i.e., up to and including terms in  $1/\theta$ . On the rotating frame one has

$$
\langle S' \rangle = Tr S \rho_{\theta} / Tr \rho_{\theta}', \qquad (36)
$$

$$
\rho_{\theta}' = \exp(i\omega S_z t) \rho_{\theta} \exp(-i\omega S_z t). \tag{37}
$$

From Eqs. (13), (21), and (22) one finds, to first order in  $1/\theta$ :

$$
\exp(i\omega S_z t)W(t-i/2\theta) \n= \exp(-S_z\omega/2\theta)W'(t-i/2\theta) \n= [1 - (H_0S_z + H_1S_z)/2\theta]W'(t).
$$
 (38)

We now write Eq. *(36)* as

$$
\langle S_{\alpha}^{\prime} \rangle = R_{\alpha}^{\prime} / R_{0}^{\prime}, \qquad (39)
$$

$$
R_i' = \mathrm{Tr} S_i \rho_\theta',\tag{40}
$$

 $i=x, y, z, 0, S_0=1$ . Using the invariance of a trace for cyclic permutation, Eq. (38) gives

$$
R_{\mathbf{z}}' = \text{Tr}(R_{\mathbf{z}}'' - R_0''H_1/2\theta),
$$
  
\n
$$
R_{\mathbf{y}}' = \text{Tr}(R_{\mathbf{y}}''), \qquad (41)
$$
  
\n
$$
R_{\mathbf{z}}' = \text{Tr}(R_{\mathbf{z}}'' - R_0''H_0/2\theta),
$$
  
\n
$$
R_0' = \text{Tr}(R_0'' - R_{\mathbf{z}}''H_1/2\theta - R_{\mathbf{z}}''H_0/2\theta),
$$

where

$$
R_i'' = \{W'^{\dagger}(t)S_iW'(t)\}_{{\rm av}}.\tag{42}
$$

The time derivative of these quantities can be found by expressing the average in terms of the probability *P:* 

$$
R_i^{\prime\prime} = \int P(x\bar{x}t)W^{\dagger}(\bar{x})S_iW(x)\rho(x)\rho(\bar{x})d^3x d^3\bar{x}, \quad (43)
$$

where  $W(x)$  is the familiar expression of a rotation matrix for spin  $\frac{1}{2}$  in Euler angles and  $\rho(x) = \sin \theta$ . Therefore,

$$
dR_i''/dt = \int (\mathfrak{T}P)W^{\dagger}S_iW = \int P\mathfrak{T}^{\dagger}(W^{\dagger}S_iW), \quad (44)
$$

where  $\mathfrak{F}^{\dagger}$  is the Hermitian conjugate of  $\mathfrak{F}$ , obtained by changing the sign of  $\mathfrak{F}_1$  and  $\mathfrak{F}_2$ . Carrying out the differentiations, we find

$$
dR_i''/dt = \sum T_{ij}^{\prime\prime} R_j^{\prime\prime},\qquad(45)
$$

$$
T_{ij}^{\prime\prime} = \begin{bmatrix} -1/T_2 & -\Delta H & 0 & 0\\ \Delta H & -1/T_2 & -H_1 & -\omega H_1/2\theta\\ 0 & H_1 & -1/T_1 & 0\\ 0 & -\omega H_1/2\theta & 0 & 0 \end{bmatrix}, (46)
$$

with

$$
1/T_1 = 1/\tau_1, 1/T_2 = \frac{1}{2}(1/\tau_0 + 1/\tau_1).
$$
 (47)

Taking the trace, and inserting in Eq. (41), one obtains

$$
dR_i'/dt = \sum T_{ij'}R_j',\qquad(48)
$$

$$
T_{ij} = \begin{bmatrix} -1/T_2 & -\Delta H & 0 & H_1/2\theta T_2 \\ \Delta H & -1/T_2 & -H_1 & 0 \\ 0 & H_1 & -1/T_1 & H_0/2\theta T_1 \\ H_1/2\theta T_2 & 0 & H_0/2\theta T_1 & 0 \end{bmatrix} . \quad (49)
$$

Substituting in

$$
d\langle S_{\alpha}\rangle/dt = (dR_{\alpha}/dt)/R_0' - R_{\alpha}'(dR_0'/dt)/R_0'^2, (50)
$$

one sees that the last term is of third order in  $1/\theta$ , because  $R_{\alpha}$ '( $\alpha = x, y, z$ ) are small of first order. One

therefore has

$$
d\langle S_x'\rangle/dt = -(\langle S_x'\rangle - H_1/2\theta)/T_2 - \Delta H \langle S_y'\rangle,
$$
  
\n
$$
d\langle S_y'\rangle/dt = -\langle S_y'\rangle/T_2 + \Delta H \langle S_x'\rangle - H_1 \langle S_x'\rangle,
$$
 (51)  
\n
$$
d\langle S_z'\rangle/dt = -(\langle S_z'\rangle - H_0/2\theta)/T_1 + H_1 \langle S_y'\rangle,
$$

which, but for an unimportant difference to be discussed below, are the MBE.

## 5. ALTERNATIVE INTERPRETATION

This derivation of the MBE can be given a different and intuitively more appealing interpretation which has guided us in the beginning stage of this work. We will briefly sketch our original approach, and show that it goes completely parallel with that given above.

The idea was to obtain the ensemble average for a large number of spins from the time average over the motion of a single spin. Any spin experiences the external fields and a fluctuating field, representing its interaction with the other spins and with the lattice. It "senses" the value of  $\theta$  only through the latter interaction. This field must therefore be such that, in the time average, it tends to produce a Boltzmann distribution, in the direction of the instantaneous total field. The rotating field will, of course, prevent this equilibrium state from being realized. The fluctuating field must therefore be complex, as it must produce transitions between the two spin states (quantized in the direction of the total field) with *a priori* probabilities  $p_{\pm\mp}$  satisfying

$$
n_{+}p_{+-} = n_{-}p_{-+}, \quad n_{-}/n_{+} = 1 + H_{\text{tot}}/\theta. \tag{52}
$$

A real field gives  $p_{+-} = p_{-+}$ ; the fluctuating field must therefore have rotating components in  $+$  and  $-$  direction of different intensity.

If  $H_c'(t)$  is this complex<sup> $\mathbb{F}_1$ field, seen in the rotating</sup> frame, we would have, for the operator  $S'(t)$  in the Heisenberg representation

$$
\mathbf{S}'(t) = W_c'^{\dagger}(t)\mathbf{S}W_c'(t)\,,\tag{53}
$$

$$
i\partial W_c'/\partial t = (\Delta H S_z + H_1 S_x + H_c'(t) \cdot S)W_c'(t). \quad (54)
$$

The simplest way to obtain a field of this type is to assume that it becomes a real field  $H_L'(t)$  after a nonunitary transformation  $\exp[-(H_0S_z + H_1S_x)/2\theta]$ , by which the occupation numbers  $n<sub>±</sub>$  are absorbed in the normalization of the wave function. Writing

$$
W_c'(t) = \exp[-\left(H_0 S_z + H_1 S_x\right)/2\theta\right]W'(t),\qquad(55)
$$

one has

$$
i\partial W'/\partial t = (\Delta H S_z + H_1 S_z + i H_1 S_y \omega/2\theta + H_L' \cdot S)W'(t).
$$
 (56)

Comparing with Eqs. *(38)* and (22) one sees that, to first order in  $1/\theta$ ,  $W_c' = \exp(iS_z\omega t)W(t-i/2\theta)$ . Therefore, one can find the long-time average of  $dS_a(t)/dt$  by using the same diffusion equation. This gives the Eqs. (48) and

(49) as operator equations. Taking the trace gives the MBE.

#### **6. CONCLUDING REMARKS**

The limiting conditions under which the above derivation of the MBE applies can be summarized as follows: (1) All spins are equivalent; (2) the spins have value  $\frac{1}{2}$ ; (3) the system is a liquid or a gas, or a solid in which spin-spin interaction can be neglected compared with spin-lattice interaction; (4) the important correlation times  $\sigma$  of the lattice motion are short compared with the relaxation time of the spins; (5) the applied rotating field satisfies  $H_1 \propto (6)$  the lattice is in thermal equilibrium. It would be of interest to know if these conditions, which are sufficient for the validity of the MBE, are also necessary.

With higher spin values and possibly quadrupole interactions, one expects in general to find several relaxation times, corresponding to different transitions between the spin levels. A discussion, under which conditions the MBE are valid in the average, falls outside the scope of this paper. With respect to conditions (3), it is well known that spin systems not satisfying it have in general a non-Lorentzian line shape, i.e., nonexponential relaxation. In the light of the present approach, this can best be understood in conjunction with assumption (4). The part of the local field  $H_L$  caused by neighbor spins owes its time dependence to liquid or lattice motion and to random reorientation of the spins. This last source of time dependence has correlation times comparable with the relaxation time of the spins. In the light of the present theory, this gives a non-Markoffian system for which the diffusion equation is far more complicated than Eq. (15) and does not lead to exponential relaxation. Therefore, unless the liquid motion completely averages out the spin-spin interaction in times  $\sigma \ll T$ , one can have the MBE only if the spin-spin contribution to  $H<sub>L</sub>(t)$  is negligible. Although certain qualitative aspects of the MBE may remain valid, it is precisely to systems not obeying these conditions that the theory of Redfield<sup>5</sup> applies and for which it predicts deviations from the MBE.

Condition (5), although not serious from a practical point of view, is responsible for the fact that our formalism does not apply to the most general case considered in Ref. 1, i.e., when  $T_1 \neq T_2$  and  $H_1 \approx H_0$ . This comes from the fact that these two relations are incompatible with  $H_1 \subset \ll 1$ , because a difference between  $T_1$  and  $T_2$ can be traced to large denominators of the form  $1 + H_0^2 \sigma^2$ , appearing differently in the expressions for  $T_1$ and  $T_2$ . Therefore, in the framework of the present theory,  $T_1 \neq T_2$  implies  $H_0 \gg H_1$ , and the question whether the axis of anisotropy of the relaxation is along *Ho* or *Htot,* as suggested in Ref. 1, becomes immaterial. This leaves the general case undecided, although it

<sup>5</sup> A. G. Redfield, Phys. Rev. 98, 1787 (1955).

seems doubtful that one will find a simple result as suggested in Ref. 1.

The last condition, finally, depends on the value of  $H_1$ and of  $T_1$ , and also on the lattice-lattice relaxation times which will become a factor of importance in paramagnetic salts at low temperatures.

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# Energy of the Many-Fermion Normal System\*

KLEBER S. MASTERSON, jR.,f AND KATURO SAWADA *University of California, San Diego, La Jolla, California*  (Received 20 September 1963)

Perturbation theoretic equations for several properties of the zero-temperature many-fermion normal system are rederived from general considerations. Though none of the equations are new, some of the derivations are, and taken together they form a brief and simple summary of many-fermion relations and a basis for further investigation of the basic perturbation description of the many-fermion normal system: the Brueckner-Goldstone expansion. A "change-of-parameter" technique is then developed and employed to investigate the possible use of the true momentum density instead of the unperturbed Fermi distribution in the Brueckner-Goldstone expansion and in the Brueckner  $K$ -matrix approximation. The result is a simpler, approximate perturbation series for the interaction energy, whose accuracy for nuclear matter is estimated to be approximately  $\pm 2$  MeV. The new approximation is exact to the fourth order.

## **I. INTRODUCTION**

THE theory of the many-fermion system has been<br>the object of intense study for many years.<br>This paper is limited to a small portion of the over-all HE theory of the many-fermion system has been the object of intense study for many years. field, the study of the perturbation theory of the zerotemperature "normal" state—that state in which there is no binding which would lead to a phenomenon such as superconductivity. The basic theory for the perturbation treatment has been developed, and is presented briefly in the next section as the basic tool on which the remainder of this investigation depends. This basic tool is the Brueckner-Goldstone linked-cluster expansion<sup>1</sup> (BG expansion), the perturbation theoretic expression for the ground-state energy of the system described above. With the BG expansion as a basis, the properties of a many-fermion system are then analyzed and several general relations are developed. These have previously been derived with the framework of Green's function theory, but the equations developed here are expressed as explicit perturbation series in contrast to some of the original derivations.

A "change-of-parameter" technique is then developed and employed to derive an approximation to the BG

expansion in terms of the true momentum densities instead of the Fermi step function unperturbed distribution. It is shown that the above replacement, coupled with the neglect of the "self-energy" terms in the expansion, yields an approximation which is exact through fourth order and whose accuracy is estimated to be approximately  $\pm 2$  MeV for nuclear matter. This approximation further leads to a modified form of the Brueckner *K* matrix approximation in which the selfconsistent energy denominators are replaced by free kinetic energies and the Fermi distributions by the (self-consistent) momentum densities. An application to nuclear matter calculations in which the momentum densities are calculated to low order in perturbation theory, avoiding the self-consistency restriction, is discussed in another paper.<sup>2</sup>

#### **II. THE BRUECKNER-GOLDSTONE LINKED-CLUSTER EXPANSION**

The heart of the perturbation theory of the normal state of zero-temperature many-fermion systems is the Brueckner-Goldstone linked-cluster expansion (BG expansion).<sup>1</sup> It is briefly reviewed in this section because of its importance in the following sections and in order to establish notation.

The Schrödinger equation for the system is

$$
(H_0+H_I)\Psi = E\Psi = (E_0+\Delta E)\Psi, \qquad (2.1)
$$

<sup>\*</sup> Based in part on a thesis submitted by K. S. Masterson to the Faculty of the University of California, La Jolla, in partial fulfill-<br>ment of the requirements for the degree of Doctor of Philosophy.<br>† Present address: U. S. S. Wright (CC-2), % F.P.O., New York, N. Y.

<sup>!</sup>K. A. Brueckner, Phys. Rev. 97, 1353 (1955); **100,** 36 (1955); *The Many-Body Problem* (John Wiley, & Sons, Inc., New York, 1959); J. Goldstone, Proc. Roy. Soc. (London) **A239,**  267 (1957).

<sup>2</sup> K. S. Masterson, Jr. (to be published).