New York, 1963).

 ${}^{9}G$. Felcher, J. Appl. Phys. 37, 1056 (1966).

 10 J. B. Forsyth, S. J. Pickart, and P. J. Brown,

Proc. Phys. Soc. (London) 88, 333 (1969).

¹¹H. Watanabe, N. Kamaza, Y. Yamaguchi, and

M. Ohashi, J. Appl. Phys. 40, ¹¹²⁸ (1969).

 $12M$. Blume, Phys. Rev. 130 , 1670 (1963).

 $13M.$ Atoji, J. Phys. Soc. Japan 26, 1321 (1969).

¹⁴E. F. Bertaut, J. Appl. Phys. 40, 1592 (1969).

 15 A. J. Freeman and R. E. Watson, Acta Cryst. 14 , 231 (1961).

 16 C. G. Shull and Y. Yamada, J. Phys. Soc. Japan Suppl. BIII 17, 1 (1962).

 7 S. Marshall (private communication).

¹⁸S. Wakoh and J. Yamashita, J. Phys. Soc. Japan

 $\frac{21}{19}$ F. Stern, Phys. Rev. 116, 1399 (1959).

 20 R. J. Elliott and F. A. Wedgwood, Proc. Phys. Soc. (London) 84, 63 (1964).

²¹S. Takeuchi and K. Motizuki, J. Phys. Soc. Japan 24, 742 (1968).

PHYSICAL REVIEW B VOLUME 3, NUMBER 9 1 MAY 1971

Quasiclassical Spin Dynamics for the Heisenberg Model*

Y. L Chang and G. C. Summerfield

Department of Nuclear Engineering, The University of Michigan, Ann Arbor, Michigan 48105

and

D. M. Kaplan Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061

(Received 27 October 1970)

The Wigner method is employed to develop explicit relationships among quantum-mechanical and classical equations of motion and quantum-mechanical and classical pair-correlation functions of spin operators. In this method, quantum corrections to the classical theory can be accurately estimated. The formalism is applied to a spin- $\frac{1}{2}$ Heisenberg model at high temperatures. The most attractive feature of this method is that many of the results are intuitively satisfying. Finally, we make a connection between our results and the classical calculations made by several other authors.

I. INTRODUCTION

The classical theory of spin dynamics, in which the quantum-mechanical spin operators are replaced by classical vectors of fixed length, has been investigated both analytically¹ and numerical- $1y.$ ²

In particular, these authors consider the spinspin pair-correlation function

$$
\Gamma^{\alpha\alpha'}_{ii'}(t) = \frac{\operatorname{Tr}\left[S_{i\alpha} S_{i'\alpha'}(t) + S_{i'\alpha'}(t) S_{i\alpha}\right] e^{-\beta H}}{2 \operatorname{Tr} e^{-\beta H}} , \quad (1)
$$

where i and i' label the individual spins, α and α' label Cartesian components and, of course, $\hbar S_{i\alpha}(t)$ is the Heisenberg operator for the α th component of the spin operator for the *i*th spin. The "classical" approximation for the spin- j case consists of substituting vectors $j\overline{\Omega}_i$ for \overline{S}_i , where the $\bar{\Omega}_i$'s are unit vectors, and integrating over the $\bar{\Omega}_i$'s:

$$
\Gamma_{ii'}^{\alpha\alpha'}(t) \tilde{=} j^2 \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N \Omega_{i\alpha} \Omega_{i'\alpha'}(t) e^{-\beta H_{\rm cl}} / \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N e^{-\beta H_{\rm cl}} . \quad (2)
$$

The "classical" Hamiltonian $H_{c1}(\overline{\Omega}_1 \cdots \overline{\Omega}_N)$ is obtained from $H(\bar{S}_1 \cdots \bar{S}_N)$ by substituting $j \overline{\Omega}_i$ for \bar{S}_i .

The factor $\bar{\Omega}_i(t)$ satisfies a classical equation consistent with $H_{c1}(\vec{\Omega}_1 \cdots \vec{\Omega}_N)$. For example, if H is given by the Heisenberg model

$$
H = -\sum_{i \neq i'} J_{ii'} \vec{S}_i \cdot \vec{S}_{i'}, \qquad (3)
$$

the classical Hamiltonian is

$$
H_{c1} = -\sum_{i \neq i'} j^2 J_{ii'} \, \overline{\Omega}_i \cdot \overline{\Omega}_i.
$$
 (4)

and the classical equation of motion is

$$
\frac{d}{dt}\vec{\Omega}_i(t) = \frac{2j}{\hbar} \sum_{i' \neq i} J_{ii'} \vec{\Omega}_i(t) \times \vec{\Omega}_{i'}(t) . \tag{5}
$$

Some authors make somewhat different substitutions using $[j(j+1)]^{1/2} \overline{\Omega}_i$ rather than $j\overline{\Omega}_i$. However, in neither case is it at all clear how closely the result approximates Eq. (1).

The use of the classical approximation simplifies the computations considerably. It even makes it possible to study spin dynamics by directly solving the equation of motion for a large $($ 1000 $)$ number of coupled spins.

Before any consequential physical results are deduced from these classical calculations, it is imperative that the classical approximation be derived rigorously and systematically from the exact quantum theory and the explicit forms for the corrections to the classical approximation be evaluated in detail. Recently, the Wigner method, 3,4 in which a classical approximation emerges quite naturally from the exact quantum theory, has been formulated for spin systems. Here we employ this formalism to investigate an explicit relationship among quantum-mechanical and classical spin pair-correlation functions and quantum and classical equations of motion.

In Sec. II, a brief summary of the Wigner method and its application to the quantum equation of motion and the spin correlation functions are presented. This formulation is then applied to the spin- $\frac{1}{2}$ Heisenberg model in Sec. III, and the quantum corrections are evaluated in the high-temperature region. Finally, the validity of our formulation and other implications are discussed in Sec. IV.

II. FORMULATION

The Wigner method^{3,4} provides a technique for evaluating the trace of any function of spin operators $A(\vec{S}_i \cdots \vec{S}_N)$ by the integration of its "Wigner" equivalent" $A_w(\bar{\Omega}_1 \cdots \bar{\Omega}_N)$:

$$
\operatorname{Tr} A(\vec{\mathbf{S}}_1 \cdots \vec{\mathbf{S}}_N) = \left(\frac{2j+1}{4\pi}\right)^N
$$

$$
\times \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N A_w(\vec{\Omega}_1 \cdots \vec{\Omega}_N) . \quad (6)
$$

For a spin- j system, the Wigner equivalent of the α -component spin operator for the *i*th particle is

$$
(S_{i\alpha})_w = j\Omega_{i\alpha} \t{,} \t(7)
$$

and the Wigner equivalent of products of functions can be obtained by using a "Groenewold rule," as derived in Refs. 3 and 4,

$$
\begin{aligned} \left(A(\vec{S}_1 \cdots \vec{S}_N)B(\vec{S}_1 \cdots \vec{S}_N)\right)_w \\ &= A_w(\vec{\Omega}_1 \cdots \vec{\Omega}_N) \, G B_w(\vec{\Omega}_1 \cdots \vec{\Omega}_N) \;, \quad (8) \end{aligned}
$$

where

$$
G = \prod_{i=1}^{N} G_i , \qquad (9)
$$

$$
G_i = 1 - (1/2j) \overline{\mathbf{L}}_i \cdot \overline{\mathbf{L}}_i + (i/2j) \overline{\mathbf{L}}_i \cdot \overline{\mathbf{\Omega}}_i \times \overline{\mathbf{L}}_i , \qquad (10)
$$

for $j=\frac{1}{2}$. A backward arrow on an \overline{L}_i indicates that it operates to the left. For general values of j the expression for G_i is

$$
G_{i} = 1 + \sum_{n=1}^{2j} \frac{(2j-n)!}{(2j)!n!} (\overline{\mathbf{L}}_{i} \times \overline{\mathbf{\Omega}}_{i})_{\mu_{1}} \cdots (\overline{\mathbf{L}}_{i} \times \overline{\mathbf{\Omega}}_{i})_{\mu_{n}}
$$

$$
\times \left(\prod_{i=1}^{n} (\delta_{\mu_{i} \nu_{i}} - \Omega_{i \mu_{i}} \Omega_{i \nu_{i}} + i \epsilon_{\mu_{i} \nu_{i} \nu_{i}} \Omega_{i \nu_{i}}) \right)
$$

$$
\times (\overline{\Omega}_{i} \times \overline{\mathbf{L}}_{i})_{\nu_{n}} \cdots (\overline{\Omega}_{i} \times \overline{\mathbf{L}}_{i})_{\nu_{1}}.
$$

The \overline{L}_t 's have the form of angular momentum operators

$$
\overline{\mathbf{L}}_t = -i\,\overline{\mathbf{r}}_t \times \overline{\mathbf{v}}_t \,, \tag{11}
$$

where

$$
\vec{\Omega}_t = \vec{r}_t / r_t \tag{12}
$$

With the aid of the formalism in Eqs. $(6)-(10)$. we can write the quantum correlation function, $Eq. (1), as$

$$
\Gamma_{i\,}^{\alpha\alpha'}(t) = \frac{j^2}{Z} \int d\bar{\Omega}_1 \cdots d\bar{\Omega}_N \left(e^{-\beta H}\right)_w G\left(\Omega_{i\alpha} \text{Re}G \Omega_{l\alpha'}(t)\right) ,\tag{13}
$$

where

$$
Z = \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N (e^{-\beta H})_w \ . \tag{14}
$$

Integrating Eq. (13) successively by parts, we obtain

$$
\Gamma_{ii}^{\alpha\alpha'}(t) = (j^2/Z) \int d\bar{\Omega}_1 \cdots d\bar{\Omega}_N \chi_w(\Omega_{i\alpha} \operatorname{Re} G \Omega_{i\alpha'}(t))
$$
\n(15)

where

$$
\chi_w = \overline{G} \left(e^{-\beta H} \right)_w , \tag{16}
$$

$$
\overline{G} = \prod_{i=1}^{N} \left(1 + \overline{\mathbf{L}}_i^2 \right) , \qquad (17)
$$

for the spin- $\frac{1}{2}$ case. Throughout this paper, summation is to be understood for repeated Greek indices. For the general values of j ,

$$
\overline{G} = \prod_{i=1}^N \left[1 + \sum_{n=1}^{2j} \left(\prod_{i=1}^n (\overline{L}_i^2 - l(l-1)) \right) \frac{(2j-n)!}{(2j)! \, n!} \right].
$$

For arbitrary values of j , we can write the factor in boldface parentheses in (15) as

$$
\Omega_{i\alpha} \text{Re}G \Omega_{i\alpha'}(t) = \Omega_{i\alpha} \Omega_{i\alpha'}(t) - \frac{1}{2j} \left(L_{i\gamma} \Omega_{i\alpha} \right) \left(L_{i\gamma} \Omega_{i\alpha'}(t) \right) .
$$
\n(18)

Substituting Eq. (18) into Eq. (15) and integrating by parts once more, we obtain

$$
\Gamma_{ii}^{\alpha\alpha'}(t) = (j^2/Z) \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N \chi_w \Omega_{i\alpha} \Omega_{l\alpha'}(t) + (j/2Z) \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N [\chi_w(\vec{L}_i^2 \Omega_{i\alpha}) \Omega_{l\alpha'}(t)]
$$

$$
+(L_{i\gamma}\,\chi_w)(L_{i\gamma}\Omega_{i\alpha})\Omega_{l\alpha'}(t)\,]\;.\qquad\qquad(19)
$$

Using the identity

$$
\widetilde{L}_i^2 \Omega_{i\alpha} = 2\Omega_{i\alpha} \tag{20}
$$

Eq. (19) can be rewritten as

$$
\Gamma_{i1}^{\alpha\alpha'}(t) = [j(j+1)/Z] \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N \chi_w \Omega_{i\alpha} \Omega_{l\alpha'}(t) + (j/2Z) \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N (L_{i\gamma} \chi_w) (L_{i\gamma} \Omega_{i\alpha}) \Omega_{l\alpha'}(t) . (21)
$$

Equation (21) is much more convenient than (15). To evaluate (15), we would have to determine the derivatives of $\Omega_{l\alpha'}(t)$ with respect to the initial unit vectors $\Omega_{\iota_{\beta}}$. This is difficult to do since we do not usually have an analytic expression for $\Omega_{1,\alpha}(t)$ in terms of the initial values. This is particularly true in the case of the numerical calculations. Of course $j\Omega_{i\alpha'}(t)$ in Eq. (21) is the Wigner equivalent of the Heisenberg operator $S_{i\alpha'}(t)$ and satisfies the Wigner equivalent of the Heisenberg equation.

$$
\frac{d}{dt} j \Omega_{t\alpha'}(t) = \frac{i}{\hbar} [H, S_{t\alpha'}(t)]_w .
$$
 (22)

For simplicity, let us consider a Heisenberg model with only nearest-neighbor exchange,

$$
H = -\sum_{i \neq i} J_{i i} \dot{\vec{S}}_i \cdot \dot{\vec{S}}_i , \qquad (23)
$$

where

$$
J_{ij} = \begin{cases} J & \text{for nearest neighbors} \\ 0 & \text{otherwise.} \end{cases}
$$
 (24)

Then

$$
\frac{d}{dt}\,\Omega_{t\,\alpha}(t) = -\frac{2\,j}{\hbar}\,\sum_{\bf l'} J_{\bf l\,l'}\,\epsilon_{\alpha\mu\,\nu}\Omega_{\bf l'\,\mu}(t)G\Omega_{\bf l\,\nu}(t) \ . \tag{25}
$$

 $(\epsilon_{\alpha\mu\nu}$ is the totally antisymmetric tensor.) It follows from Eq. (25) that

$$
\frac{d}{dt}\vec{\Omega}_1(t) = -\frac{2jJ}{\hbar}\sum_{i'}\vec{\Omega}_{i'}(t) \times \vec{\Omega}_1(t) - 2j\vec{\gamma}_1(t) , \quad (26)
$$

where the summation on l' is restricted to the nearest neighbors of l , and

$$
\gamma_{l\alpha}(t) = \frac{1}{\hbar} \sum_{l'} J_{l\,l'} \epsilon_{\alpha\mu\nu} \Omega_{l'\mu}(t) (G - 1) \Omega_{l\,\nu}(t) \quad . \tag{27}
$$

Equation (26) without $\bar{\gamma}_i(t)$ corresponds to the classical equation of motion (5) and $\bar{\gamma}_i(t)$ can be thought of as representing the quantum corrections to the classical equation of motion.

Comparing Eqs. (21) and (26), we see that we have expressed the exact quantum pair-correlation function in terms of unit vectors $\overline{\Omega}_l(t)$. The classical approximation results when we neglect the second term on the right-hand side of (19), replace χ_w with $e^{-\beta H_w}$ and neglect $\bar{\gamma}_l(t)$ in (26). This constitutes our

(19) main result. (We have given a form for the exact quantum spin pair-correlation function and the quantum equation of motion in which the classical limiting process is directly visible.)

Now expand $\Omega_{18}(t)$ in a power series in t,

$$
\Omega_{1\beta}(t) = \Omega_{1\beta} + \dot{\Omega}_{1\beta}(0)t + \cdots
$$

=
$$
\Omega_{1\beta} - \frac{2jt}{\hbar} \sum_{i'} J_{i'} \Omega_{i'} \Omega_{i'} \varepsilon_{\beta \alpha \gamma} + \cdots
$$
 (28)

This results in the expansion of $\tilde{\gamma}_t(t)$ as follows:

$$
\overline{\hat{\gamma}}_t(t) = \frac{tJ^2}{\hbar^2} \sum_{\mathbf{i}'} [\overrightarrow{\hat{\Omega}}_t(t) - \overrightarrow{\hat{\Omega}}_{\mathbf{i}'}(t)][1 - \overrightarrow{\hat{\Omega}}_t(t) \cdot \overrightarrow{\hat{\Omega}}_{\mathbf{i}'}(t)] + O(t^2) .
$$
\n(29)

We are evaluating the $\overline{\Omega}_i$'s at t rather than t=0. This gives the same series to order t . We will retain only the first term in (29). Substituting (29) into (26), we obtain

$$
\frac{d}{dt}\vec{\Omega}_t(t) = -\frac{2jJ}{\hbar} \sum_{\mathbf{r}}' \vec{\Omega}_{\mathbf{r}}(t) \times \vec{\Omega}_{\mathbf{r}}(t)
$$

$$
-\frac{2j t J^2}{\hbar^2} \sum_{\mathbf{r}}' [\vec{\Omega}_{\mathbf{r}}(t) - \vec{\Omega}_{\mathbf{r}'}(t)][1 - \vec{\Omega}_{\mathbf{r}}(t) \cdot \vec{\Omega}_{\mathbf{r}'}(t)].
$$
(30)

We note that the first term in the right-hand side of Eq. (30) gives rise to precessions of $\overline{\Omega}_t$, about the axis parallel to its nearest neighbor. The second term gives rise to torques which tend to rotate $\tilde{\Omega}_l$ in the plane of $\overline{\Omega}_t$ and its nearest neighbor. The magnitude of this force vanishes for either aligned or antialigned $\vec{\Omega}_i$'s, and hence will tend to bring the system into its ordered state. The first precessional terms do not tend to align or antialign the spins. Obviously, the last term in (30) will give rise to damping of the precessional motion of $\Omega_1(t)$. The contribution of this term to the spin-wave damping will be discussed in a subsequent paper.

III. APPLICATION AT HIGH TEMPERATURE

We now wish to apply the formalism embodied in (21) to obtaining the corrections to the classical correlation function $[cf. Eq. (2)]$. We restrict ourselves to the high-temperature region. In the hightemperature region, we can obtain an explicit expression for the Wigner equivalent of the density operator (see Appendix)-for simplicity in this section, we will consider only spin- $\frac{1}{2}$:

$$
(e^{-\beta H})_w = e^{A(\beta)} \t{,} \t(31)
$$

where

$$
A(\beta) = -\beta H_w + \beta^2 \left(\frac{1}{2} J H_w + \frac{3}{16} \sum_{i \neq 1} J_{i1}^2 + \frac{1}{8} \sum_{i \neq 1} J_{i1}^2 J_{i1}^2 \sqrt{3} I_{i2}^2 + \frac{1}{8} \sum_{i \neq 1} J_{i1}^2 (\sqrt{3} I_i + \sqrt{3} I_i^2) \right)
$$

3054

Using Eq. (17) , we can write

$$
\chi_w = 1 - 9\beta H_w + \frac{1}{2}\beta^2 \left(\frac{1}{8}\sum_{i\neq l} J_{i\,l}^2 (3 - 18\vec{\Omega}_i \cdot \vec{\Omega}_l) + \frac{9}{4}\sum_{i\neq l\neq l'} J_{i\,l} J_{l\,l} \vec{\Omega}_i \cdot \vec{\Omega}_{l'} + \frac{81}{16}\sum_{i\neq l\neq m\neq n} J_{i\,l} J_{mn} (\vec{\Omega}_i \cdot \vec{\Omega}_l) (\vec{\Omega}_m \cdot \vec{\Omega}_n) + \cdots \right)
$$
 (33)

Some straightforward manipulation yields

$$
\chi_w = e^{A(\beta)} \left(1 + (-8\beta + 4\beta^2 J) H_w
$$

+ $\beta^2 \sum_{i \neq i \neq l'} J_{i l} J_{l l'} \overrightarrow{\Omega}_i \cdot \overrightarrow{\Omega}_{l'} + O(\overrightarrow{\Omega}^4) + O(\beta^3) \right)$. (34)

We insert (34) into (21). Then we expand this result in a series of correlations of increasing order in the $\overline{\Omega}_i$'s. Including only terms of second order, this results in

$$
\Gamma_{i\,t}^{\alpha\alpha'} = \frac{1}{Z} \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N e^{A(\beta)} \Big(j(j+1)\Omega_{i\,\alpha}\Omega_{I\alpha'}(t) - \frac{2}{16} (2\beta J - \beta^2 J^2) \sum_{i'} \Omega_{i'\,\alpha}\Omega_{I\alpha'}(t) - \frac{9}{16} \beta^2 J^2 \sum_{i'': (i')} \Omega_{i'\,\alpha}\Omega_{I\,\alpha'}(t) \Big). \tag{35}
$$

Of course Z can be written as

$$
Z = \int d\vec{\Omega}_1 \cdot \cdot \cdot d\vec{\Omega}_N \, e^{A\langle \beta \rangle} \,. \tag{36}
$$

In Eq. (35), the summation on i' is restricted to the nearest neighbors of i , and the summatic on $i^{\prime}{}'$ is restricted to the nearest neighbors of i such that $i'' \neq i$.

Now we wish to expand (35) in a series of classical correlation functions of increasing order, and

we shall again keep only the terms of second order
\n
$$
\Gamma_{ii}^{\alpha\alpha'}(t) = j(j+1)\langle \Omega_{i\alpha}\Omega_{i\alpha'}(t) \rangle_{c1}
$$
\n
$$
-\frac{9}{16}(2\beta J - \beta^2 J^2) \sum_{i'} \langle \Omega_{i'\alpha}\Omega_{i\alpha'}(t) \rangle_{c1}
$$
\n
$$
-\frac{9}{16}\beta^2 J^2 \sum_{i'\alpha' \alpha'} \langle \Omega_{i'\alpha}\Omega_{i\alpha'}(t) \rangle_{c1}, \qquad (37)
$$

where $\langle \cdots \rangle_{c1}$ is defined to be

$$
\langle \cdots \rangle_{c1} = \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N \, e^{-\beta H_w} \cdots / \int d\vec{\Omega}_1 \cdots d\vec{\Omega}_N e^{-\beta H_w} \,. \tag{38}
$$

The difference between the first term of Eq. (37) and Eq. (2) is that in the latter, $\Omega_{i',\alpha'}(t)$ is taken to obey the classical equation of motion, i. e. , Eq. (5); in Eq. (37), $\Omega_{l\alpha'}(t)$ obeys Eq. (26). The ordinary classical approximation is retrieved in Eq. (3V) if (i) all terms in the right-hand side after the first are ignored and (ii) $\bar{\gamma}_1(t) \rightarrow 0$ in Eq. (26).

We see that the higher-order contributions to (37) [including those from $A(\beta)$] will contribute to higher-order classical correlations. It might seem that the constant term in (32), $\frac{3}{16}\sum_{i\neq l}J_{i l}^2$, will contribute extra second-order correlations. This term in $e^{A\langle 6\rangle}$ appears in both the numerator and denominator in (35) and just cancels.

IV. DISCUSSION

In the deviation of (37) we have ignored higherorder correlations. For example, the next-order corrections are of the general form

$$
\langle \Omega_{i\alpha} \Omega_{i'\beta} \Omega_{l'\gamma} \Omega_{l'\nu}(t) \rangle_{c1} . \tag{39}
$$

Also, from Z, there are terms,

$$
\langle \Omega_{i\alpha} \Omega_{i'\beta} \rangle_{c1} \langle \Omega_{i\gamma} \Omega_{i'\nu}(t) \rangle_{c1} .
$$

We would expect this term to be very small unless, say, $i=i'$. Such a term actually occurs, however, and it is multiplied by a factor $(\beta J)^m$ with m at least unity. The other fourth-order correlations should go roughly as the square of the secondorder correlation which is already small in the disordered phase.

To use (37), we can simply use the numerical results of, say, Ref. 2 for the correlation functions. In doing this, we would be ignoring an essential quantum feature of the spin problem. That is, we would be approximating $\dot{\gamma}_i(t)$ in (26) by zero. We have already pointed out that $\bar{\gamma}_l(t)$ is the factor which provides both a torque tending to align the spins and a term tending to damp out the spin-wave modes. Both of these effects are essentially quantum mechanical in nature.

An alternative approach would be to use $Eq. (30)$ as the equation of motion, compute the pair correlations, and substitute these results into (37). This program would not involve any more difficult a numerical computation than was required in Ref. 2. It would provide an estimate of the quantum effects in the equation of motion.

In summary, we have, employing the Wigner method, exhibited the exact quantum spin pair-correlation functions and equations of motion in a form which allows the quantum corrections to classical results to be accurately estimated. This has been applied to the high-temperature spin- $\frac{1}{2}$ pair-cor relation function to obtain various pair-correlation additions to the classical results.

ACKNOWLEDGMENT

We wish to thank Professor P. F. Zweifel for a number of suggestions which clarified several points in the manuscript.

APPENDIX: DERIVATION OF EOS. (25) AND (26)

Consider

$$
D_w \equiv (e^{-\beta H})_w \quad . \tag{A1}
$$

Then,

$$
\frac{d}{d\beta}D_w = -H_wGD_w \t{A2}
$$

where

$$
H_w = -\frac{1}{4} \sum_{i \neq i} J_{ii} \overrightarrow{\Omega}_i \cdot \overrightarrow{\Omega}_i .
$$
 (A3)

*Work supported in part by the National Science Foundation.

 1 H. A. Brown and J. M. Luttinger, Phys. Rev. 100. 685 (1955); M. E. Fisher, Am. J. Phys. 32, 343 (1964); G. 8. Joyce, Phys. Rev. 155, 478 (1967).

 2 R. E. Watson, M. Blume, and G. H. Vineyard, Phys.

PHYSICAL REVIEW B VOLUME 3, NUMBER 9

Try the form

$$
D_w = e^{A(\beta)}, \quad A(\beta) = \sum_{n=1}^{\infty} a_n \beta^n.
$$
 (A4)

Then, substituting $(A4)$ into $(A2)$ and equating the coefficients of β^n in both sides, we obtain

$$
a_1 = -H_w, \quad a_2 = \frac{1}{2} \left[(H^2)_w - H_w^2 \right],
$$

$$
a_3 = -\frac{1}{3!} \left[(H^3)_w - H_w^3 \right] + a_2 H_w,
$$
 (A5)

and Eq. (26) follows straightforwardly.

Rev. 181, 811 (1969); Phys. Rev. B 2, 684 (1970); C. G. Windsor, in Neutron Inelastic Scattering (IAEA, Vienna, 1968).

~D. M. Kaplan and G. C. Summerfield, Phys. Rev. 187, 639 (1968).

4D. M. Kaplan (unpublished}.

1 MAY 1971

Field Dependence of the Anomalous Hall Coefficient in Dilute Magnetic Alloys*

M. T. Béal-Monod
Physique des Solides, [†] Faculté des Sciences, 91 Orsay, France

and

R. A. Weiner \ddagger

Physics Department, University of California-San Diego, La Jolla, California 92037 (Received 12 June 1970)

The anomalous Hall coefficient R of dilute magnetic alloys exhibiting the Kondo effect is calculated in the second Born approximation using the $s-d$ exchange model. The variation of R as a function of the magnetic field, for fixed temperature, is studied. Comparisons are made with other theories and recent experimental data.

I. INTRODUCTION

The effect of an external magnetic field on the Kondo¹ behavior of the electrical resistivity in dilute magnetic alloys has been studied theoretically from two different approaches: The 8-matrix theory of More and Suhl² and a second-Born-approximation calculation by the authors.³ The first approach is in principle correct at all temperatures and fields, but because of its complexity and the amount of computer calculation needed, it cannot easily be fitted to the experimental results. The second one gives explicit formulas which can readily be compared with experiment, but it is only a rough approximation, and the limits of its validity can only be fixed through the exact theory. Both papers contained calculations of the conduction-electron relaxation times for spin up (τ_*) and spin down (τ_{-}) . Recently, More has used the S-matrix life-

times to compute the Hall coefficient as a function of the magnetic field $R(H)$ for fixed temperatures.⁴ He obtains curves of $R(H)$ increasing more or less rapidly with H , which he compared with the experimental data on impure gold due to Gaidukov.⁵ However, the physical explanation of this behavior could not be obtained from this calculation. In the present paper we shall calculate $R(H)$ using the expressions for τ_{+} and τ_{-} obtained in third-order perturbation theory. 3 We show that the field dependence of R is essentially explained in terms of the square of the impurity spin magnetization⁶ for low fields $g\mu_B H/kT$ <1. We compare this result with More's and with the recent data.⁷ We also obtain the very high-field $(g\mu_B H/k T > 10)$ behavior of $R(H)$. This last case is discussed more extensively elsewhere. 8 The behavior of R is compared with the similar behavior of the magnetoresistivity, and suggestions are made for further experiments.

 $\overline{\mathbf{3}}$