THEORY OF A HEISENBERG FERROMAGNET IN THE RANDOM PHASE APPROXIMATION*

F. Englert[†]

Laboratory of Atomic and Solid State Physics and Department of Physics, Cornell University, Ithaca, New York (Received May 17, 1960)

The aim of this Letter is to present a solution of the ferromagnetic problem in the Heisenberg model in random phase approximation (RPA). This is conjectured to be the high-density limit theory. In this preliminary account we restrict ourselves to spin one-half and to a study of magnetic properties alone.

The principal result of the analysis is a magnetization curve which imitates conventional spin wave theory very closely but with the existence of renormalized spin wave frequencies according to $\omega(\mathbf{q}; T) = \omega(\mathbf{q}; 0)M(T)/M(0)$, where M(T) is the magnetization at temperature T, in accordance with an idea of Brout.¹ The theory goes over to the spherical model² at temperature higher than the Curie temperature for small static fields with the Curie point given by the spherical model value. Thus we have a consistent extrapolation formula through the whole temperature range possessing rigorously correct limiting properties for $T \rightarrow 0$ and $T \rightarrow \infty$, as well as a presumably accurate value of the Curie temperature in the limit of high density.

We write the Heisenberg Hamiltonian in the form

$$\mathcal{K} = -2 \sum_{\vec{q}} v(\vec{q}) \{ S^{Z}(\vec{q}) S^{Z}(-\vec{q}) + \frac{1}{2} [S^{+}(\vec{q}) S^{-}(-\vec{q}) + S^{-}(\vec{q}) S^{+}(-\vec{q})] \}, \quad (1)$$

where we have Fourier-analyzed the exchange potential $v(\mathbf{r})$ and the spin operators $S(\mathbf{q})$ $= N^{-1/2} \sum_i S_i \exp(i\mathbf{q} \cdot \mathbf{r}_i)$. The random phase approximation can be summarized by the simplified commutation rule which expresses the decoupling of different Fourier components:

$$[S^{\dagger}(\mathbf{\tilde{q}}), S^{-}(\mathbf{\tilde{q}}')]_{-} = \delta_{\mathbf{\tilde{q}}}, -\mathbf{\tilde{q}}' (2/\sqrt{N}) S^{\mathbb{Z}}(0),$$
$$[S^{\mathbb{Z}}(\mathbf{\tilde{q}}), S^{\pm}(\mathbf{\tilde{q}}')]_{-} = \pm \delta_{\mathbf{\tilde{q}}}, 0^{(1/\sqrt{N})} S^{\pm}(\mathbf{\tilde{q}}'), \qquad (2)$$

where N is the number of spins.

We apply to the system a finite longitudinal magnetic field H and switch on adiabatically an infinitesimal transverse rotating magnetic field of wave vector $\mathbf{\bar{q}}'$. This adds to the Hamiltonian

(1) a term,

$$\mathcal{K}' = -S^{\dagger}(-\bar{\mathbf{q}}')h_{\mathbf{q}'}, \ e^{i(\omega-i\epsilon)t} - g\mu \sum_{i} S_{i}^{z} H.$$
(3)

Denoting by $\langle O \rangle_{T, H}$ the thermal average at temperature T and external magnetic field H of the operator O, we may define the adiabatic spin susceptibility,

$$\chi_{\vec{\mathfrak{q}}'}(\omega)_{T,H} = \lim_{h_{\vec{\mathfrak{q}}'}\to 0} \left(\frac{\langle S(\vec{\mathfrak{q}'}) \rangle_{T,H}}{h_{\vec{\mathfrak{q}}'}(\omega-i\epsilon)t} \right). \quad (4)$$

Writing the Heisenberg equations of motion, one easily finds with help of (2),

$$\chi_{\vec{\mathbf{q}}}, (\omega)_{T, H} = \frac{R}{[v(0) - v(\vec{\mathbf{q}})]2R + g\mu H - \hbar\omega + i\epsilon}, \quad (5)$$

where R is the reduced magnetization, $R = 2N^{-1} \times \langle \sum_i S_i^z \rangle_{T, H}$. From the Kubo formalism,³ the appropriate form of the fluctuation-dissipation theorem is easily derived⁴:

$$\int_{-\infty}^{\infty} \frac{1}{1 - \exp(\hbar \omega / kT)} \operatorname{Im}_{\mathbf{q}} (\omega)_{T, H} d\omega$$
$$= (i\pi / \hbar) \langle S(\mathbf{q}) S^{\dagger}(-\mathbf{q}) \rangle_{T, H}, \qquad (6)$$

where χ in Eq. (6) is the adiabatic susceptibility, which in RPA is given by Eq. (5). Substituting Eq. (5) into Eq. (6), we have

$$\frac{R}{\exp\{[(v(0) - v(\mathbf{\hat{q}}))2R + g\mu H]/kT\} - 1}$$
$$= \langle S^{-}(\mathbf{\hat{q}})S^{+}(-\mathbf{\hat{q}}) \rangle_{T, H}.$$
(7)

In a completely similar way, we obtain

$$\frac{R}{1 - \exp\{-[(v(0) - v(\mathbf{\bar{q}}))2R + g\mu H]/kT\}} = \langle S^{+}(\mathbf{\bar{q}})S^{-}(-\mathbf{\bar{q}}) \rangle_{T, H}.$$
(8)

Using the sum rule,

$$\sum_{\mathbf{\vec{q}}} [S^{\dagger}(\mathbf{\vec{q}})S^{\dagger}(-\mathbf{\vec{q}}) + S^{\dagger}(\mathbf{\vec{q}})S^{\dagger}(-\mathbf{\vec{q}})] = N, \qquad (9)$$

we obtain the following equation for the magneti-

zation:

$$N = R \sum_{\vec{q}} \operatorname{coth}\left(\frac{[v(0) - v(\vec{q})]2R + g\mu H}{2kT}\right).$$
(10)

Equation (10) has two classes of solutions in the limit $H \rightarrow 0$.

(a) $H \rightarrow 0$, $R \neq 0$, or the ferromagnetic region. The physical interpretation of (10) in the ferromagnetic region is best seen by writing (10) (as $H \rightarrow 0$) in "spin wave" form:

$$n = \sum_{\vec{q}} \frac{R}{\exp\{[v(0) - v(\vec{q})]2R/kT\} - 1},$$
 (11)

where n is the number of "spin deviations"; $n = \frac{1}{2}N(1 - R)$. Thus the magnetization curve (11) appears as a consequence of the existence of collective spin motions generalizing at finite temperature the well-known spin waves by renormalizing their frequency by a factor R. This concept of renormalized spin waves, which leads to a T^3 correction to the usual spin-wave theory for the magnetization curve at low temperature, seems to be in contradiction with Dyson's theory,⁵ and this discrepancy will be studied in detail in the future. This concept and the T^3 law which results has been already introduced by Brout and Haken¹ from a physical point of view. The magnetization curve obtained in reference 1, however, is not the same as the present one. A detailed study has been made of this discrepancy by Brout. It has turned out that the reasoning in reference 1 contained an inconsistency in the evaluation of traces in RPA. In a subsequent publication it will be shown how the final result [Eq. (10)] can be obtained by a consistent RPA in the partition function.

The Curie point determined from (10) or (11) is obtained by taking the limit $R \rightarrow 0$, $H \rightarrow 0$:

$$1/kT_c = F(1)/v(0),$$
 (12)

with

$$F(1) = \frac{1}{N} \sum_{\vec{q}} \frac{1}{1 - [v(\vec{q})/v(9)]}$$

which is the Curie point of the spherical model.² (b) $H \rightarrow 0$, $R \rightarrow 0$, or the paramagnetic region.

The susceptibility being defined by $\chi = \frac{1}{2}g \,\mu R / H$ as $H \rightarrow 0$, one finds immediately from (10)

$$1 = \frac{1}{N} \sum_{\vec{q}} \frac{1}{\beta [v(0) - v(\vec{q})] + \beta (g\mu/2)^2 / \chi}.$$
 (13)

If we write

$$\chi = \left(\frac{g\mu}{2}\right)^2 \beta \frac{1}{1 - \beta [v(0) - \delta]}, \qquad (14)$$

one sees from (13) that δ is determined by

$$1 = \frac{1}{N} \sum_{\vec{q}} \frac{1}{1 - \beta [v(\vec{q}) - \delta]}, \qquad (15)$$

which shows the equivalence of our paramagnetic curve with that obtained from the spherical model.² Because of the work of Brout,⁶ we speculate on the present theory as the high-density limit theory.

A complete discussion of these results, as well as the thermodynamic and nonequilibrium properties, will be published in a forthcoming paper.

We should like to thank R. Brout for his help in this study as well as for many very interesting discussions.

- ¹R. Brout (private communication); see also R. Brout and H. Haken, Bull. Am. Phys. Soc. 5, 148 (1960).
 - ²T. Berlin and M. Kac, Phys. Rev. 86, 821 (1952).
 - ³R. Kubo, J. Phys. Soc. (Japan) <u>12</u>, 570 (1957).
- ⁴L. D. Landau and E. M. Lifshitz, <u>Statistical Phys-</u> <u>ics</u> (Pergamon Press, New York, 1958), p. 401.
- ⁵F. J. Dyson, Phys. Rev. <u>102</u>, 1217, 1230 (1956).
 ⁶R. Brout, Phys. Rev. <u>118</u>, 1009 (1960).

^{*}This work has been supported in part by the Office of Naval Research.

[†]On leave of absence from Université Libre de Bruxelles, Bruxelles, Belgium.