PERTURBATION THEORY FOR SPIN GREEN’ S FUNCTIONS

PHYSICS

1969

SovietRxiv

Abstract

Full Text

UDC 538.113

PHYSICS

D. I. KADYROV

PERTURBATION THEORY FOR SPIN GREEN' S FUNCTIONS

(Presented by Academician S. V. Vonsovskii, 28 IV 1969)

1. In paper (^{1}), integro-differential equations were derived for finding the macroscopic magnetic moment of a paramagnet placed in a prescribed magnetic field. In the present work the kernels of these equations are calculated in the following approximations: both magnetic temperatures are regarded as high, the lattice temperature as unchanged, the Hamiltonian as not explicitly time-dependent, and the gyromagnetic tensor as having the form $\overline{\overline{g}} = \gamma\overline{\overline{1}}$. It turns out that, in the indicated approximations, the problem of calculating the kernels is the problem of calculating two-time retarded Green' s functions composed of spin operators (as well as phonon creation and annihilation operators), in which the averaging is performed with respect to the equilibrium statistical operator of the lattice. The calculation of such (we shall call them spin) Green' s functions is carried out with the aid of a perturbation theory constructed specially for this purpose, which, unlike the standard one (^{2}), operates not with the unperturbed energies of the particles, but with their exact complex "energies," including damping, and therefore does not lead to divergences.

2. We specify here the Hamiltonians of the Zeeman subsystem, the interaction subsystem, and the lattice as follows:

$$-\mathbf{H}\cdot\mathbf{M} = -\Omega^{\alpha} I_{0\alpha}, \tag{1}$$

$$u = \frac{1}{2n}\sum_{q} v^{\alpha\beta}(q) I_{q\alpha} I_{-q\beta} + \frac{1}{n}\sum_{qp} W_p^{\alpha\beta}(q, q+p)(b_p - b_{-p}^{+}) I_{q+p\alpha} I_{-q\beta}, \tag{2}$$

$$\mathcal{H}_L = \sum_{p} \omega_p b_p^{+} b_p. \tag{3}$$

Here $\Omega^{\alpha} \equiv \delta_0^{\alpha}\Omega$ with $\Omega \equiv \gamma|\mathbf{H}|$; $W_p^{\alpha\beta}(q, q+p) \equiv w_p^{\alpha\beta}(q) - w_p^{\alpha\beta}(q+p)$;

$$w_p^{\alpha\beta}(q) \equiv \frac{i}{\sqrt{2n\omega_p}}\, e_p q\, v^{\alpha\beta}(q);$$

b_p and b_p^+ are the annihilation and creation operators of a phonon with wave vector p; ω_p is the energy of such a phonon; e_p is a unit vector directed along p; $I_{q\alpha}$ (q is a reciprocal-lattice vector, $\alpha = +, -, 0$) are mechanical angular-momentum operators satisfying the commutation relations

$$[I_{q\alpha}, I_{q'\alpha'}] = e_{\alpha\alpha'}^{\alpha''} I_{q+q'\alpha''}, \tag{4}$$

and tensor indices are lowered and raised with the aid of the metric tensor $\lambda_{\alpha\beta} = \lambda^{\alpha\beta} = 1$ for $\alpha + \beta = 0$ and 0 for $\alpha + \beta \neq 0$.

We introduce Green' s functions defined by the relations

$$\langle I_{Q\alpha} \mid I_{-Q}^{\bar{\alpha}} \rangle_t = -i\theta(t) \operatorname{Sp} I_{Q\alpha} \exp\{-itL\} \sigma_L I_{-Q}^{\bar{\alpha}} [{}^{1/3} nj(j+1)]^{-1}, \tag{5}$$

$$\begin{pmatrix} b_p & b_p^+ \\ b_p^+ & b_p \end{pmatrix}_t = -i\theta(t) \operatorname{Sp} \begin{pmatrix} b_p \\ b_p^+ \end{pmatrix} \exp\{-itL\} \sigma_L \begin{pmatrix} b_p^+ & \left[n_p^{-1} \right] \\ b_p & \left[(1+n_p)^{-1} \right] \end{pmatrix}, \tag{6}$$

$$\sigma_L = (\operatorname{Sp} \exp\{-\beta_L \mathscr{H}_L\})^{-1} \exp\{-\beta_L \mathscr{H}_L\}, \qquad n_p = (\exp\{\beta_L \omega_p\} - 1)^{-1}. \tag{7}$$

A bar over a tensor index means that summation over it is not carried out. In the equations for the functions (5), (6) and other Green' s functions,

necessary for finding (5), (6), the correlation functions of the spin and phonon operators taken at one and the same instant of time are computed exactly. We shall seek the Fourier components of the functions (5), (6) in the form

$$\langle I_{Q\alpha} \mid I_{-Q}^{\bar{\alpha}} \rangle_E = (E - E_{Q\alpha})^{-1}, \qquad \left(\begin{matrix} b_p \\ b_p^+ \end{matrix} \middle| \begin{matrix} b_p^+ \\ b_p \end{matrix} \right)_E = (E - E_p^{\mp})^{-1}. \tag{8}$$

Here $E_{Q\alpha}$ and $E_p^{\mp}$ are complex functions of E to be determined. Substitution of (8) into the equations of motion for the Fourier components of the functions (5), (6) leads to the following equations for $E_{Q\alpha}$ and $E_p^{\mp}$:

$$0 = E_{Q\alpha} - \alpha\Omega - \left[e_{\alpha\beta}^{\gamma} \frac{1}{n} \sum_q v^{\beta\delta}(q) \langle I_{q+Q\gamma} I_{-q\delta} \mid I_{-Q}^{\bar{\alpha}} \rangle_E + 2 e_{\alpha\beta}^{\gamma} \frac{1}{n} \sum_{qp} W_p^{\beta\delta}(q, q+p) \langle (b_p - b_{-p}^+) I_{q+p+Q\gamma} I_{-q\delta} \mid I_{-Q}^{\bar{\alpha}} \rangle_E \right] \tag{9}$$

$$0 = E_p^{\mp} \mp \omega_p \mp \frac{1}{n} \sum_q W_p^{\alpha\beta}(q, q \mp p) \left(I_{q\mp p\alpha} I_{-q\beta} \middle| \begin{matrix} b_p^+ \\ b_p \end{matrix} \right)_E (E - E_p^{\mp}). \tag{10}$$

The Green' s functions entering (9), (10) will be sought in the form of expansions in powers of the spin-spin and spin-lattice interactions and of the quantities $E_{Q\alpha}$ and $E_p^{\mp}$. These functions obey a system of coupled equations, which we write in the form

$$\begin{aligned}
&(E - E_{Q\alpha}) \left\langle \begin{matrix} b_p \\ b^+_{-p} \end{matrix} \; I_{q+p+Q\gamma} I_{-q\delta} \mid I^{\bar{\alpha}}_{-Q} \right\rangle_E = - e^{\alpha\alpha'}_{\gamma} \frac{1}{n} \sum_{q'} v_{\beta'\delta'}(q') \times \\
&\times \left\langle \begin{matrix} b_p \\ b^+_{-p} \end{matrix} \; I_{q+p+Q\gamma} I_{-q\delta} \mid I^{\gamma'}_{q'-Q} I^{\delta'}_{-q'} \right\rangle_E - 2e^{\alpha\beta'}_{\gamma'} \frac{1}{n} \sum_{q'p'} W^{\beta'\delta'}_{p'}(q', q'+p') \times \\
&\times \left\langle \begin{matrix} b_p \\ b^+_{-p} \end{matrix} \; I_{q+p+Q\gamma} I_{-q\delta} \mid (b_{p'} - b^+_{-p'}) I^{\gamma'}_{q'+p'-Q} I^{\delta'}_{-q'} \right\rangle_E - (E_{Q\alpha} - \alpha\Omega) \times \\
&\times \left\langle \begin{matrix} b_p \\ b^+_{-p} \end{matrix} \; I_{q+p+Q\gamma} I_{-q\delta} \mid I^{\bar{\alpha}}_{-Q} \right\rangle_E ,
\end{aligned} \tag{11}$$

$$\begin{aligned}
&(E - E^{\mp}_p) \left(I_{q\mp p\alpha} I_{-q\beta} \middle| \begin{matrix} b^+_p \\ b_p \end{matrix} \right)_E = \pm \frac{1}{n} \sum_{q'} W_{p\alpha'\beta'}(q', q' \pm p) \times \\
&\times \left(I_{q\mp p\alpha} I_{-q\beta} \mid I^{\alpha'}_{q'\pm p} I^{\beta'}_{-q'} \right)_E - (E^{\mp}_p \mp \omega_p) \left(I_{q\mp p\alpha} I_{-q\beta} \middle| \begin{matrix} b^+_p \\ b_p \end{matrix} \right)_E ,
\end{aligned} \tag{12}$$

$$\begin{aligned}
&(E - E_{q+Q\gamma} - E_{-q\delta}) \langle I_{q+Q\gamma} I_{-q\delta} \mid I^{\gamma'}_{q'-Q} I^{\delta'}_{-q'} \rangle_E \\
&\quad = \frac{1}{3} nj(j+1) \, [\delta^{\gamma'}_{\gamma} \delta^{\delta'}_{\delta} \delta(q+q') + \delta^{\delta'}_{\gamma} \delta^{\gamma'}_{\delta} \delta(q+Q-q')] + \ldots \\
&\quad\quad - (E_{q+Q\gamma} - \gamma\Omega + E_{-q\delta} - \delta\Omega) \times \\
&\quad \times \langle I_{q+Q\gamma} I_{-q\delta} \mid I^{\gamma'}_{q'-Q} I^{\delta'}_{-q'} \rangle_E ,
\end{aligned} \tag{13}$$

$$\begin{aligned}
&(E - E^{\mp}_{\mp p} - E_{q+p+Q\gamma} - E_{-q\delta}) \left\langle \begin{matrix} b_p \\ b^+_{-p} \end{matrix} \; I_{q+p+Q\gamma} I_{-q\delta} \mid (b_{p'} - b^+_{-p'}) I^{\gamma'}_{q'+p'-Q} I^{\delta'}_{-q'} \right\rangle_E = \\
&= \left[\begin{matrix} -n_p \\ 1 + n_p \end{matrix} \right] \frac{1}{3} nj(j+1) \delta(p+p') [\delta^{\gamma'}_{\gamma} \delta^{\delta'}_{\delta} \delta(q+q') + \delta^{\delta'}_{\gamma} \delta^{\gamma'}_{\delta} \times \\
&\times \delta(q - q' + p + Q)] + \ldots - (E^{\mp}_{\mp p} \mp \omega_p + E_{q+p+Q\gamma} - \gamma\Omega + E_{-q\delta} - \delta\Omega) \times \\
&\times \left\langle \begin{matrix} b_p \\ b^+_{-p} \end{matrix} \; I_{q+p+Q\gamma} I_{-q\delta} \mid (b_{p'} - b^+_{-p'}) I^{\gamma'}_{q'+p'-Q} I^{\delta'}_{-q'} \right\rangle_E .
\end{aligned} \tag{14}$$

In equations (13), (14) the terms containing the interactions explicitly have not been written out. The equation for the function $\langle I_{q+Q\gamma} I_{-q\delta} \mid I^{\alpha}_{-Q} \rangle_E$ is obtained from (11) if one sets there $p = 0$,

$$\begin{matrix} b_p \\ b^+_{-p} \end{matrix} \quad = 1.$$

The equation for $(I_{q\mp p\alpha} I_{-q\beta} \mid I^{\alpha'}_{q'\pm p} I^{\beta'}_{-q'})_E$

follows from equation (13), if in it one makes the replacement $\langle|\rangle \to (|)$, $Q \to \mp p$, $\gamma \to \alpha$, $\gamma' \to \alpha'$, $\delta \to \beta$, $\delta' \to \beta'$. In doing so it is necessary to take into account that the replacement of angle brackets by round ones entails, in the free term of (13), the replacement

$${}^1\!/_3 nj(j+1) \to [{}^1\!/_3 nj(j+1)^2] \begin{bmatrix} n_p^{-1} \\ (1+n_p)^{-1} \end{bmatrix}.$$

As is seen from (9) and (10), the quantities $E_{Q\alpha} - \alpha\Omega$ and $E^{\mp}_p \mp \omega_p$ are at least of first order in the interactions. Therefore, wishing to obtain the solutions of equations (11), (12) in the zeroth approximation, we must neglect not only those of their terms which contain the interactions explicitly, but also terms proportional to $E_{Q\alpha} - \alpha\Omega$ and $E^{\mp}_p \mp \omega_p$. Having done this, we note that equations (11), (12) in the zeroth approximation have only zero solutions. Hence it immediately follows that $E_{Q\alpha} - \alpha\Omega$ and $E^{\mp}_p \mp \omega_p$ are in fact quantities of second order of smallness. In order to find the solutions of (11), (12) in the first approximation, it is necessary, in the right-hand sides of these equations, to cross out the terms containing $E_{Q\alpha} - \alpha\Omega$ and $E^{\mp}_p \mp \omega_p$. The calculation of the remaining terms on the right can be carried out with the help of the solutions of equations (13), (14) in the zeroth approximation. In obtaining the latter, only the free terms must be taken into account in the right-hand sides of equations (13), (14). Substituting the solutions of (11), (12) in the first approximation into equations (9) and (10), we obtain for $E_{Q\alpha}$ and $E^{\mp}_p$ the following equations, valid up to and including the second order in the interactions:

$$\begin{aligned} 0 = E_{Q\alpha} - \alpha\Omega + \frac{j(j+1)}{3n} \sum_{q\gamma\delta} \frac{e^{\delta\delta}_{\alpha\beta}(q)\{v_{\beta'\delta}(q) e^{\overline{\alpha\beta'}} \underset{q\to q+Q}{\gamma\delta \to \gamma}\}}{E - E_{q+Q\gamma} - E_{-q\delta}} - \frac{4j(j+1)}{3n} \times \\ \times \sum_{q\gamma\delta} e^{\gamma\delta}_{\alpha\beta} W^{\beta\delta}_p (q, q+p) \left[W_{p\beta'\delta}(q, q+p) e^{\overline{\alpha\beta'}} \underset{q\to q+Q}{\gamma\delta \to \gamma} \right] \times \\ \times \left[\frac{n_p}{E - E^-_p - E_{q+p,Q\gamma} - E_{-q\delta}} + \frac{n_p \to 1 + n_p}{E^-_p \to E^+_{-p}} \right], \end{aligned} \tag{15}$$

$$0 = E^{\mp}_p \mp \omega_p + 2 \left[\frac{j(j+1)}{3} \right]^2 \begin{bmatrix} n_p^{-1} \\ (1+n_p)^{-1} \end{bmatrix} \sum_{q\alpha\beta} \frac{|W^{\alpha\beta}_p (q, q\mp p)|^2}{E - E_{q\mp p\,\alpha} - E_{-q\beta}}. \tag{16}$$

The method for obtaining fourth- and higher-order corrections to (15), (16) is obvious.

The solutions of equations (15), (16) can be obtained by constructing an iterative process in which, as the zeroth approximation, one takes $\operatorname{Re} E_{Q\alpha}^{(0)} = \alpha\Omega$, $\operatorname{Im} E_{Q\alpha}^{(0)} = 0$, $\operatorname{Re} E_p^{\mp(0)} = \pm\omega_p$, $\operatorname{Im} E_p^{\mp(0)} = 0$. When substituting into (15), (16) $\operatorname{Re} E_{Q\alpha} = \alpha\Omega$ and $\operatorname{Re} E_p^{\mp} = \pm\omega_p$, the quantities $\operatorname{Im} E_{Q\alpha}$ and $\operatorname{Im} E_p^{\mp}$ must be equated to zero only after the result has been obtained.

The perturbation theory formulated above can be generalized to the case of Green' s functions usually used in many-particle theory.

3. Let us use the perturbation theory formulated in Sec. 2 to calculate the kernels discussed in Sec. 1. These kernels can be represented in the form of expansions in powers of the interactions and of the Heisenberg operator of natural time evolution. The Fourier components of the principal terms of such expansions can be written in the form

$$K_{ff'}(E) = -{}^1\!/_3\, inj(j+1)\{\langle [f,u] \mid [f',\tilde{u}]\rangle_E - \langle [f,u] \mid \tilde{u}\rangle_E (\langle u \mid \tilde{u}\rangle_E)^{-1} \langle u \mid [f',\tilde{u}]\rangle_E\}, \tag{17}$$

where f and f' denote M or $\mathcal{H}_L$, and

$$\tilde{u} = \beta_L^{-1} \int_0^{\beta_L} d\lambda\, \exp\{\lambda \mathcal{H}_L\}\, u\, \exp\{-\lambda \mathcal{H}_L\}.$$

The calculation of the Green' s functions constituting $K_{ff'}(E)$ is completely reduced to the calculation of the spin Green' s functions already found by us in the zeroth approximation in Sec. 2 when solving equations (13), (14). Therefore we shall restrict ourselves to giving explicit expressions for a pair of fragments of $K_{ff'}(E)$ in the zeroth approximation:

$$\begin{aligned} \langle [I_{0\alpha}, u] \mid \tilde{u}\rangle_E = &-\frac{j(j+1)}{3n} \sum_{q\gamma\delta} \frac{v^{\beta\delta}(q) e^{\eta}_{\alpha\beta} v^{\eta}_{\gamma\delta}(q)}{E - E_{q\eta} - E_{-q\delta}} \\ &- \frac{4j(j+1)}{3n} \sum_{qp\gamma\delta} (\beta_L \omega_p)^{-1}\, W_p^{\beta\delta}(q, q+p) e^{\eta}_{\alpha\beta} W^{\eta}_{p\gamma\delta}(q, q+p) \\ &\times \left[\frac{1}{E - E_p^- - E_{q+p\gamma} - E_{-q\delta}} + E_p^- \to E_{-p}^+ \right], \end{aligned} \tag{18}$$

$$\langle u([I_{0\alpha}, \tilde{u}])\rangle_E = \langle [I_{0\alpha}, u] \mid \tilde{u}\rangle_E. \tag{19}$$

Equalities of the type (19) ensure the fulfillment of the Onsager relations for the nuclei $K_{ff'}(E)$.

The author is grateful to I. G. Shaposhnikov for the topic and for discussions.

Perm State University
named after A. M. Gorky

Received
15 IV 1969

References

1. D. I. Kadyrov, I. G. Shaposhnikov, *DAN*, **189**, No. 1 (1969).
2. S. V. Tyablikov, V. L. Bonch-Bruevich, *Perturbation Theory for Two-Time Temperature Green' s Functions.* Rotaprint, V. A. Steklov Mathematical Institute, Academy of Sciences of the USSR, T-7, 1962.

Note: Figure translations are in progress. See original paper for figures.

Source: Math-Net.Ru and CyberLeninka. Machine translation. Verify with the original.