Exact relations for the spin-correlation functions for an interacting electron gas in a nonuniform magnetic field

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Without any approximation, exact relations for the spin-density correlation functions in an interacting electron gas under an arbitrary nonuniform external magnetic field are obtained by making use of the nonperturbative canonical formulation of quantum many-body theory [T. Toyoda, Ann. Phys. (N.Y.) **173**, 226 (1987)]. The obtained results contain f-sum rules, a finite-temperature generalized Ward-Takahashi relation, as well as a finite-temperature version of the Nambu-Goldstone theorem with respect to the spontaneous symmetry breaking of the spin-rotational symmetry. [S0163-1829(98)04027-2]

I. INTRODUCTION

Quantum many-body effects in an electron gas under a magnetic field have been attracting much attention for decades.[1] The density correlation function and the spin-density correlation functions of the electrons are of vital importance in the study of the many-body effects.[2–4] While the density correlation function has been calculated for the free three- and two-dimensional electrons in a uniform external magnetic field,[1,5–11] the calculation of the many-body effects on the correlation functions seem to be extremely difficult even with the aid of powerful approximation schemes such as the random-phase approximation, quantum linked cluster expansions, etc. Therefore, in such a situation it is important to derive exact relations for correlation functions, such as frequency sum rules or Ward-Takahashi relations, which can be used to determine adjustable parameters or to examine the consistency of approximations and models. Concerning the correlation functions of an electron gas in a strong uniform magnetic field, a number of useful frequency sum rules have been given in Ref. 7. However, the f-sum rule for the spin-density correlation function of an interacting electron gas in an arbitrary magnetic field, whose magnitude and direction can be a function of the space coordinate, has not been rigorously derived to the best of the authors' knowledge.

The aim of this paper is to derive several exact relations, including the f-sum rule and Ward-Takahashi relations, for the spin-density correlation functions of the interacting electron gas under an arbitrary magnetic field without any approximational procedures. Our derivation is based on the nonperturbative canonical formulation of quantum many-body theory,[12] whose usefulness has been proved in a number of applications.[13–17] Although we consider the electrons in the three-dimensional space, the results can cover the two-dimensional case with a slight modification.

Our results are f-sum rules for the retarded density and spin-density correlation functions, a finite-temperature generalized Ward-Takahashi relation, and a set of relations for the spin-correlation functions including a finite-temperature version of the Nambu-Goldstone theorem for spontaneous breaking of the spin-rotational symmetry.

This paper is organized as follows: In the next section we define a model Hamiltonian and the correlation functions that are considered in this work. In Sec. III, an f-sum rule for the electron number-density response function is derived. An f-sum rule for the spin-density response function is also derived in Sec. IV. A finite-temperature generalized Ward-Takahashi relation is calculated in Sec. V. Exact relations for spin-correlation functions are obtained in Sec. VI. Concluding remarks and discussions are given in Sec. VII.

II. MODEL HAMILTONIAN AND RESPONSE FUNCTIONS

Let us first define a model Hamiltonian for interacting electrons in an external magnetic field. The electrons are described in terms of the second quantized field operators, i.e., the electron Schrödinger field. We therefore start with the equal-time anticommutation relations for the electron field operators,

$$[\psi_\alpha(\mathbf{x}),\psi_\beta^\dagger(\mathbf{x}')]\equiv\psi_\alpha(\mathbf{x})\psi_\beta^\dagger(\mathbf{x}')+\psi_\beta^\dagger(\mathbf{x}')\psi_\alpha(\mathbf{x}) = \delta_{\alpha\beta}\delta(\mathbf{x}-\mathbf{x}'), \tag{2.1}$$

where the Greek subscripts denote the electron-spin variables, i.e., $\alpha,\beta=\uparrow,\downarrow$. Throughout this paper we use Einstein's convention with respect to the summation over the spin variables unless there is a remark that the summation is not taken. We assume the Hamiltonian

$$H=H_A+H_S+H_{imp}+H_{\text{int}}. \tag{2.2}$$

The first term is the kinetic energy

$$H_A=\int d^3\mathbf{x}\psi_\alpha^\dagger(\mathbf{x})h_A(\nabla)\psi_\alpha(\mathbf{x}), \tag{2.3}$$

with

$$h_A(\nabla)=\frac{-\hbar^2}{2m}\sum_k\left(\partial_k+\frac{ie}{\hbar c}A_k(\mathbf{x})\right)^2-\mu, \tag{2.4}$$

where m, $-e$, μ, and A_k are the electron mass, the electron charge, the chemical potential, and the vector potential, respectively. The coupling between the electron spin and the external magnetic field is given by the Pauli spin term

$$H_S=\frac{g\mu_B}{2}\int d^3\mathbf{x}\sum_k B_k(\mathbf{x})\psi_\alpha^\dagger(\mathbf{x})\sigma_{\alpha\beta}^k\psi_\beta(\mathbf{x}), \qquad (2.5)$$

where g is the electron g factor, $\mu_B=e\hbar/2mc$ is the Bohr magneton, and σ^k $(k=1,2,3)$ are Pauli spin matrices. The interaction between impurity atoms and the electrons is assumed to be described by a c-number spin-independent potential U_{imp},

$$H_{imp}=\int d^3\mathbf{x}U_{imp}(\mathbf{x})\psi_\alpha^\dagger(\mathbf{x})\psi_\alpha(\mathbf{x}). \qquad (2.6)$$

It should be noted here that an extension of the present formulation to a spin-dependent potential is straightforward. The electron-electron interaction term is assumed to be of the form

$$H_{\rm int}=\tfrac{1}{2}\int d^3\mathbf{x}\int d^3\mathbf{x}'\,\psi_\alpha^\dagger(\mathbf{x})\psi_\beta^\dagger(\mathbf{x}')\times U_{\rm int}(\mathbf{x}-\mathbf{x}')\psi_\beta(\mathbf{x}')\psi_\alpha(\mathbf{x}). \qquad (2.7)$$

We do not specify a particular form for the interelectron potential $U_{\rm int}$. We simply assume that the potential is independent of the electron-spin variables. In Sec. VIII we shall discuss the effects of a spin-dependent electron-electron interaction on the results.

The number density of electrons with spin α is given by

$$\rho_\alpha^H(\mathbf{x},t)=\Psi_\alpha^\dagger(\mathbf{x},t)\Psi_\alpha(\mathbf{x},t) \quad (\text{no } \alpha \text{ sum}), \qquad (2.8)$$

where the superscript H means the operator is in the Heisenberg picture. We also define $\rho^H(\mathbf{x},t)=\Sigma_\alpha\rho_\alpha^H(\mathbf{x},t)$ and $\rho(\mathbf{x})=\rho^H(\mathbf{x},0)$. In terms of these electron number-density operators, the retarded density response function and its Fourier transform with respect to the time variables can be defined as[2–4]

$$D_{\alpha\beta}^R(\mathbf{x},t;\mathbf{x}',t')\equiv -i\theta(t-t')\langle[\rho_\alpha^H(\mathbf{x},t),\rho_\beta^H(\mathbf{x}',t')]\rangle, \qquad (2.9)$$

and

$$D_{\alpha\beta}^R(\mathbf{x},t;\mathbf{x}',t')=\frac{1}{2\pi}\int_{-\infty}^{\infty}D_{\alpha\beta}^R(\mathbf{x},\mathbf{x}';\omega)e^{-i(t-t')\omega}d\omega, \qquad (2.10)$$

where we have used the grand canonical ensemble expectation value

$$\langle\cdots\rangle\equiv\frac{\mathrm{Tr}\{e^{-\beta H}\cdots\}}{\mathrm{Tr}\ e^{-\beta H}}. \qquad (2.11)$$

If the external magnetic field is uniform, the density response function has translational invariance[17] and we can define the spatial Fourier transform

$$D_{\alpha\beta}^R(\mathbf{x},t;\mathbf{x}',t')=\frac{1}{(2\pi)^4}\int d^3\mathbf{k}d\omega D_{\alpha\beta}^R(\mathbf{k};\omega)\times e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')-i\omega(t-t')}. \qquad (2.12)$$

To discuss the correlations or the fluctuations in the electron spin, it is useful to define the electron spin-density operator in the Heisenberg picture

$$S_H^i(\mathbf{x},t)\equiv\Psi_\alpha^\dagger(\mathbf{x},t)\sigma_{\alpha\beta}^i\Psi_\beta(\mathbf{x},t), \qquad (2.13)$$

and also in the Schrödinger picture

$$S_i(\mathbf{x})\equiv\psi_\alpha^\dagger(\mathbf{x})\sigma_{\alpha\beta}^i\psi_\beta(\mathbf{x})=S_H^i(\mathbf{x},0), \qquad (2.14)$$

where the subscript H indicates the operator is in the Heisenberg picture. The retarded spin-density response function is defined as

$$\Lambda_{ij}^R(\mathbf{x},t;\mathbf{x}',t')\equiv -i\theta(t-t')\langle[S_H^i(\mathbf{x},t),S_H^j(\mathbf{x}',t')]\rangle, \qquad (2.15)$$

and its Fourier transform with respect to the time variables is given by

$$\Lambda_{ij}^R(\mathbf{x},t;\mathbf{x}',t')=\frac{1}{2\pi}\int_{-\infty}^{\infty}\Lambda_{ij}^R(\mathbf{x},\mathbf{x}';\omega)e^{-i(t-t')\omega}d\omega. \qquad (2.16)$$

If the external magnetic field is uniform, we can introduce the spatial Fourier transform

$$\Lambda_{ij}^R(\mathbf{x},t;\mathbf{x}',t')=\frac{1}{(2\pi)^4}\int d^3\mathbf{k}d\omega\Lambda_{ij}^R(\mathbf{k};\omega)\times e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')-i\omega(t-t')}d\omega. \qquad (2.17)$$

III. THE f-SUM RULE FOR THE DENSITY RESPONSE FUNCTION

In this section we derive the f-sum rule for the retarded density response function defined in Sec. II. There are two essential steps in the derivation. One is the integration over ω, which leads to the equal-time condition. The other is the time derivative of the field variables, which can be calculated by making use of the Heisenberg equation of motion. Consequently, the entire calculation reduces to the evaluation of various equal-time commutators. The equal-time commutators can be rigorously evaluated by virtue of the equal-time canonical anticommutation relation (2.1).

We begin with the differentiation of Eq. (2.10) with respect to t, which immediately gives

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}D_{\alpha\beta}^R(\mathbf{x},\mathbf{x}';\omega)\omega d\omega=i\left[\frac{\partial}{\partial t}D_{\alpha\beta}^R(\mathbf{x},t;\mathbf{x}',t')\right]_{t=t'}. \qquad (3.1)$$

Using the definition of the retarded response function (2.9), its time derivative can be expressed as

$$\frac{\partial}{\partial t}D_{\alpha\beta}^R(\mathbf{x},t;\mathbf{x}',t')=-i\delta(t-t')\langle[\rho_\alpha^H(\mathbf{x},t),\rho_\beta^H(\mathbf{x}',t)]\rangle -i\theta(t-t')\left\langle\left[\frac{\partial\rho_\alpha^H(\mathbf{x},t)}{\partial t},\rho_\beta^H(\mathbf{x}',t')\right]\right\rangle. \qquad (3.2)$$

The equal-time commutator in the first term on the right-hand side simply vanishes. Thus we obtain the equal-time limit of the time derivative of the response function,

$$\left[\frac{\partial}{\partial t} D^R_{\alpha\beta}(\mathbf{x},t;\mathbf{x}',t')\right]_{t=t'} = -i\theta(0)\left\langle\left[\frac{\partial\rho^H_\alpha(\mathbf{x},t)}{\partial t},\rho^H_\beta(\mathbf{x}',t)\right]\right\rangle. \tag{3.3}$$

The time derivative of the density operator on the right-hand side is given by the Heisenberg equation of motion,

$$\begin{aligned}\frac{\partial}{\partial t}\rho^H_\alpha(\mathbf{x},t) &= \frac{1}{i\hbar}[\rho^H_\alpha(\mathbf{x},t),H(t)]\\ &= \frac{1}{i\hbar}[\rho^H_\alpha(\mathbf{x},t),H_A(t)\\ &\quad + H_S(t)+H_{imp}(t)+H_{\text{int}}(t)]\\ &= \frac{1}{i\hbar}[\rho^H_\alpha(\mathbf{x},t),H_A(t)+H_S(t)].\end{aligned} \tag{3.4}$$

To obtain the last line we observe that the density operators commute with H_{imp} and H_{int}. That is, the explicit forms of the impurity potential U_{imp} and the electron-electron interaction potential U_{int} do not affect the derivation of the f-sum rule, as long as the two Hamiltonian terms commute with the electron number-density operator.

On the other hand, the Pauli spin term in the Hamiltonian does not commute with the number-density operator. Using the explicit form of the Pauli spin term and the basic equal-time anticommutation relation we find

$$\begin{aligned}&[\rho^H_\alpha(\mathbf{x},t),H_S(t)]\\ &= \frac{g\mu_B}{2}\int d^3\mathbf{x}'\sum_k B_k(\mathbf{x}')\\ &\quad\times[\rho^H_\alpha(\mathbf{x},t),\Psi^\dagger_\mu(\mathbf{x}',t)\sigma^k_{\mu\nu}\Psi_\nu(\mathbf{x}',t)]\\ &= i\frac{g\mu_B}{2}\operatorname{sgn}(\alpha)[\mathbf{B}(\mathbf{x})\times\Psi^\dagger_\mu(\mathbf{x},t)\boldsymbol{\sigma}_{\mu\nu}\Psi_\nu(\mathbf{x},t)]_3\\ &= i\frac{g\mu_g}{2}\operatorname{sgn}(\alpha)[\mathbf{B}(\mathbf{x})\times\mathbf{S}_H(\mathbf{x},t)]_3,\end{aligned} \tag{3.5}$$

where sgn(α) is defined as sgn($\uparrow$)=1 and sgn($\downarrow$)=−1. Similarly, the equal-time anticommutation relation and the explicit form of the kinetic energy Hamiltonian given by Eqs. (2.3) and (2.4) yield

$$\begin{aligned}[\rho^H_\alpha(\mathbf{x},t),H_A(t)] = i\hbar\sum_k \partial_k\biggl\{&\frac{-\hbar}{i2m}\Psi^\dagger_\alpha(\mathbf{x},t)(\partial_k-\overleftarrow{\partial}_k)\Psi_\alpha(\mathbf{x},t)\\ &-\frac{e}{mc}A_k(\mathbf{x})\rho^H_\alpha(\mathbf{x},t)\biggr\}\quad(\text{no }\alpha\text{ sum}).\end{aligned} \tag{3.6}$$

Now that we have obtained the time derivative of the electron number-density operator in the commutator on the right-hand side of Eq. (3.3), our next step is to evaluate the commutator with the aid of Eq. (2.1). The contribution from the spin term (3.5) can be calculated as

$$\begin{aligned}&[[\rho^H_\alpha(\mathbf{x},t),H_S(t)],\rho^H_\beta(\mathbf{x}',t)]\\ &= -\frac{g\mu_B}{2}\operatorname{sgn}(\alpha)\operatorname{sgn}(\beta)\delta(\mathbf{x}-\mathbf{x}')\\ &\quad\times[\mathbf{B}(\mathbf{x})\cdot\mathbf{S}_H(\mathbf{x},t)-B_3(\mathbf{x})S^3_H(\mathbf{x},t)].\end{aligned} \tag{3.7}$$

Note that this term vanishes if the summation over α or β is taken. The contribution from Eq. (3.6) is found to be

$$\begin{aligned}&[[\rho^H_\alpha(\mathbf{x},t),H_A(t)],\rho^H_\beta(\mathbf{x}',t)]\\ &= \frac{-\hbar^2}{m}\delta_{\alpha\beta}\biggl\{\rho^H_\alpha(\mathbf{x},t)\nabla^2\delta(\mathbf{x}-\mathbf{x}')\\ &\quad+\sum_k\partial_k\rho^H_\alpha(\mathbf{x},t)\cdot\partial_k\delta(\mathbf{x}-\mathbf{x}')\biggr\}\quad(\text{no }\alpha\text{ sum}).\end{aligned} \tag{3.8}$$

Substituting these results, Eqs. (3.7) and (3.8), into Eq. (3.3), we obtain

$$\begin{aligned}&\left[\frac{\partial}{\partial t}D^R_{\alpha\beta}(\mathbf{x},t;\mathbf{x}',t')\right]_{t=t'}\\ &= -i\theta(0)\left\langle\left[\frac{\partial\rho^H_\alpha(\mathbf{x},t)}{\partial t},\rho^H_\beta(\mathbf{x}',t)\right]\right\rangle\\ &= -\frac{i}{2}\frac{1}{i\hbar}\langle[[\rho^H_\alpha(\mathbf{x},t),H_A(t)],\rho^H_\beta(\mathbf{x}',t)]\rangle\\ &\quad-\frac{i}{2}\frac{1}{i\hbar}\langle[[\rho^H_\alpha(\mathbf{x},t),H_S(t)],\rho^H_\beta(\mathbf{x}',t)]\rangle\\ &= \frac{\hbar}{2m}\sum_k\partial_k\{\delta_{\alpha\beta}\langle\rho^H_\alpha(\mathbf{x},t)\rangle\partial_k\delta(\mathbf{x}-\mathbf{x}')\}\\ &\quad+\frac{1}{2\hbar}\frac{g\mu_B}{2}\operatorname{sgn}(\alpha)\operatorname{sgn}(\beta)\{\mathbf{B}(\mathbf{x})\cdot\langle\mathbf{S}(\mathbf{x},t)\rangle\\ &\quad-B_3(\mathbf{x})S^3_H(\mathbf{x},t)\}\quad(\text{no }\alpha\text{ sum}),\end{aligned} \tag{3.9}$$

where we have used $\theta(0)=\frac{1}{2}$ in accordance with its Fourier transform. From this equation we find the final form of the f-sum rule:

$$\begin{aligned}&\frac{1}{2\pi}\int_{-\infty}^{\infty}\omega D^R_{\alpha\beta}(\mathbf{x},\mathbf{x}';\omega)d\omega\\ &= \frac{i\hbar}{2m}\delta_{\alpha\beta}\{\langle\rho_\alpha(\mathbf{x})\rangle\nabla^2\delta(\mathbf{x}-\mathbf{x}')\\ &\quad+\boldsymbol{\nabla}\delta(\mathbf{x}-\mathbf{x}')\cdot\boldsymbol{\nabla}\langle\rho_\alpha(\mathbf{x})\rangle\}\\ &\quad+\frac{ig\mu_B}{4\hbar}\operatorname{sgn}(\alpha)\operatorname{sgn}(\beta)\delta(\mathbf{x}-\mathbf{x}')\\ &\quad\times\{\mathbf{B}(\mathbf{x})\cdot\langle\mathbf{S}(\mathbf{x})\rangle-B_3(\mathbf{x})\langle S_3(\mathbf{x})\rangle\}\quad(\text{no }\alpha\text{ sum}).\end{aligned} \tag{3.10}$$

This is the new f-sum rule for the electron number-density response function for the interacting electron gas in an arbitrary magnetic field. If one takes summation over α or β, the last term vanishes due to the sign functions, recovering the well-known f-sum rule for the electron-density response function.[4] The **B**-field dependent second term is our new result.

If the external magnetic field is uniform, the above sum rule can be written as

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\omega D^{R}_{\alpha\beta}(\mathbf{k};\omega)d\omega = \frac{-i\hbar}{2m}\,\delta_{\alpha\beta}k^2\langle\rho_\alpha\rangle+\frac{ig\mu_B}{4\hbar}\,\mathrm{sgn}(\alpha)\times\mathrm{sgn}(\beta)\{\mathbf{B}\cdot\langle\mathbf{S}\rangle-B_3\langle S_3\rangle\}\quad(\text{no }\alpha\text{ sum}),\tag{3.11}$$

where the function $D^{R}_{\alpha\beta}(\mathbf{k};\omega)$ has been defined in Eq. (2.12).

IV. THE f-SUM RULE FOR THE SPIN-DENSITY RESPONSE FUNCTION

Following the previous section, we now consider the retarded spin-density response function and derive the corresponding f-sum rule. The derivation is similar to that given in the previous section. The basic ingredients in the derivation are various equal-time commutators, which are almost equivalent to the commutators appeared in the previous section.

From the Fourier transform of the spin-response function, Eq. (2.16), similarly to Eq. (3.1), we have

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\Lambda^{R}_{ii}(\mathbf{x},\mathbf{x}';\omega)\,\omega d\omega = i\left[\frac{\partial}{\partial t}\,\Lambda^{R}_{ii}(\mathbf{x},t;\mathbf{x}',t')\right]_{t=t'}.\tag{4.1}$$

By virtue of the definition of the spin-response function (2.15), the right-hand side can be expressed in terms of equal-time commutators,

$$\lim_{t'\to t}\frac{\partial}{\partial t}\,\Lambda^{R}_{ii}(\mathbf{x},t;\mathbf{x}',t') = -i\lim_{t'\to t}\delta(t-t')\langle[S^i_H(\mathbf{x},t),S^i_H(\mathbf{x}',t)]\rangle - i\lim_{t'\to t}\theta(t-t')\left\langle\left[\frac{\partial S^i_H(\mathbf{x},t)}{\partial t},S^i_H(\mathbf{x}',t')\right]\right\rangle.\tag{4.2}$$

The commutator in the first term on the right-hand can be evaluated with the aid of Eq. (2.1),

$$[S^i_H(\mathbf{x},t),S^j_H(\mathbf{x}',t)] = i2\,\delta(\mathbf{x}-\mathbf{x}')\sum_k\,\varepsilon_{ijk}S^k_H(\mathbf{x},t),\tag{4.3}$$

where ε_{ijk} is the antisymmetric tensor. Because $\varepsilon_{iik}=0$ in the present case, the commutator in the first term on the right-hand side of Eq. (4.2) vanishes. Consequently, Eq. (4.2) reduces to

$$\lim_{t'\to t}\frac{\partial}{\partial t}\,\Lambda^{R}_{ii}(\mathbf{x},t;\mathbf{x}',t') = -i\,\theta(0)\left\langle\left[\frac{\partial S^i_H(\mathbf{x},t)}{\partial t},S^i_H(\mathbf{x}',t)\right]\right\rangle.\tag{4.4}$$

The time derivative of the spin-density operator on the right-hand side can be calculated by making use of the Heisenberg equation of motion,

$$i\hbar\,\frac{\partial}{\partial t}\,S^i_H(\mathbf{x},t) = [S^i_H(\mathbf{x},t),H_A(t)+H_S(t)+H_{imp}(t)+H_{\mathrm{int}}(t)].\tag{4.5}$$

Because of Eq. (4.3) the following two commutators simply vanish,

$$[S^i_H(\mathbf{x},t),H_{imp}(t)]=0,\tag{4.6}$$

$$[S^i_H(\mathbf{x},t),H_{\mathrm{int}}(t)]=0,\tag{4.7}$$

and the right-hand side of Eq. (4.5) reduces to

$$i\hbar\,\frac{\partial}{\partial t}\,S^i_H(\mathbf{x},t) = [S^i_H(\mathbf{x},t),H_A(t)]+[S^i_H(\mathbf{x},t),H_S(t)].\tag{4.8}$$

The first commutator on the right-hand side of Eq. (4.8) can be evaluated using the basic equal-time anticommutation relation,

$$[S^i_H(\mathbf{x},t),H_A(t)] = \frac{-\hbar^2}{2m}\sum_k\,\partial_k\left\{I^{ik}_H(\mathbf{x},t)+\frac{i2e}{\hbar c}\,A_k(\mathbf{x})S^i_H(\mathbf{x},t)\right\},\tag{4.9}$$

where we have defined

$$I^{ik}_H(\mathbf{x},t)\equiv\Psi^\dagger_\alpha(\mathbf{x},t)\sigma^i_{\alpha\beta}\overleftrightarrow{\partial}_k\Psi_\beta(\mathbf{x},t).\tag{4.10}$$

Using formula (4.3), we also find

$$[S^i_H(\mathbf{x},t),H_S(t)] = ig\mu_B\sum_k\,\varepsilon_{ijk}B_j(\mathbf{x})S^k_H(\mathbf{x},t).\tag{4.11}$$

Substituting these results, Eqs. (4.9) and (4.11), into (4.8) we obtain the equation of motion for the spin-density operator,

$$i\hbar\,\frac{\partial}{\partial t}\,S^i_H(\mathbf{x},t) = \frac{-\hbar^2}{2m}\sum_k\,\partial_k\left\{I^{ik}_H(\mathbf{x},t)+\frac{i2e}{\hbar c}\,A_k(\mathbf{x})S^i_H(\mathbf{x},t)\right\} + ig\mu_B\sum_k\sum_j\,\varepsilon_{ijk}B_j(\mathbf{x})S^k_H(\mathbf{x},t).\tag{4.12}$$

Note that the equation does not contain the electron-impurity or the electron-electron interaction terms, because they are assumed to be spin independent. If they have spin dependence, additional terms emerge on the right-hand side.

Now the commutator in Eq. (4.4) can be written as

$$i\hbar\left[\frac{\partial}{\partial t}S^i_H(\mathbf{x},t),S^i_H(\mathbf{x}',t)\right]$$
$$=\frac{-\hbar^2}{2m}\sum_k \partial_k\left\{[I^{ik}_H(\mathbf{x},t),S^i_H(\mathbf{x}',t)]+\frac{i2e}{\hbar c}A_k(\mathbf{x})\right.$$
$$\left.\times[S^i_H(\mathbf{x},t),S^i_H(\mathbf{x}',t)]\right\}+ig\mu_B\sum_{m,n}\varepsilon_{imn}B_m(\mathbf{x})$$
$$\times[S^n_H(\mathbf{x},t),S^i_H(\mathbf{x}',t)]. \tag{4.13}$$

The commutator in the first term on the right-hand side can be evaluated by making use of Eq. (4.3),

$$[I^{ik}_H(\mathbf{x},t),S^j_H(\mathbf{x}',t)]=2\delta_{ij}\Psi^\dagger_\alpha(\mathbf{x},t)\Psi_\alpha(\mathbf{x},t)\partial_k\delta(\mathbf{x}-\mathbf{x}')$$
$$+i2\sum_l \varepsilon_{ijl}\delta(\mathbf{x}-\mathbf{x}')I^{lk}_H(\mathbf{x},t). \tag{4.14}$$

Substituting Eqs. (4.3) and (4.14) into Eq. (4.13), we find

$$i\hbar\left[\frac{\partial}{\partial t}S^i_H(\mathbf{x},t),S^i_H(\mathbf{x}',t)\right]$$
$$=\frac{-\hbar^2}{m}\rho_H(\mathbf{x},t)\nabla^2\delta(\mathbf{x}-\mathbf{x}')+\frac{-\hbar^2}{m}$$
$$\times\nabla\delta(\mathbf{x}-\mathbf{x}')\cdot\nabla\rho_H(\mathbf{x},t)-2g\mu_B\delta(\mathbf{x}-\mathbf{x}')$$
$$\times\{\mathbf{B}(\mathbf{x})\cdot\mathbf{S}_H(\mathbf{x},t)-B_i(\mathbf{x})S^i_H(\mathbf{x},t)\}. \tag{4.15}$$

This is still an operator relation. Taking the ensemble average we obtain the final result

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\omega\Lambda^R_{ii}(\mathbf{x},\mathbf{x}';\omega)d\omega$$
$$=\frac{i\hbar}{2m}\langle\rho(\mathbf{x})\rangle\nabla^2\delta(\mathbf{x}-\mathbf{x}')+\frac{i\hbar}{2m}\nabla\delta(\mathbf{x}-\mathbf{x}')\cdot\nabla\langle\rho(\mathbf{x})\rangle$$
$$+\frac{ig\mu_B}{\hbar}\delta(\mathbf{x}-\mathbf{x}')\{\mathbf{B}(\mathbf{x})\cdot\langle\mathbf{S}(\mathbf{x})\rangle-B_i(\mathbf{x})\langle S_i(\mathbf{x})\rangle\}, \tag{4.16}$$

which is the f-sum rule for the retarded spin-density response function. If the external field is uniform, this sum rule reduces to

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\omega\Lambda^R_{ii}(\mathbf{k},\omega)d\omega$$
$$=\frac{-i\hbar k^2}{2m}\langle\rho\rangle+\frac{ig\mu_B}{\hbar}\{\mathbf{B}\cdot\langle\mathbf{S}\rangle-B_i\langle S_i\rangle\}. \tag{4.17}$$

V. FINITE TEMPERATURE GENERALIZED W-T RELATIONS

In the previous two sections we have used the Heisenberg picture for the electron Schrödinger field operator. In this and the following sections we use the τ-Heisenberg picture in order to derive the finite-temperature generalized Ward-Takahashi relations[12] (FTGWTR) within the framework of the Matsubara's finite-temperature Green's function theory. The τ-Heisenberg picture is defined as

$$\psi_\alpha(\mathbf{x},\tau)\equiv e^{(1/\hbar)H\tau}\psi_\alpha(\mathbf{x})e^{-(1/\hbar)H\tau}\equiv\psi_\alpha(x). \tag{5.1}$$

Throughout this and the following sections we use the notation $x\equiv(\mathbf{x},\tau)$. We assume the same model Hamiltonian defined in Sec. II,

$$H=H_A(\tau)+H_S(\tau)+H_{imp}(\tau)+H_{\rm int}(\tau). \tag{5.2}$$

All the terms in the Hamiltonian are the same as those given in Eqs. (2.2)–(2.7) except the operators are defined in the τ-Heisenberg picture. We start with the identity for the time-ordered product of the field operators[12]

$$\frac{\partial}{\partial\tau}T_\tau\{\rho_\alpha(x)\psi_\mu(x')\psi^\dagger_\nu(x'')\}$$
$$=\delta(\tau-\tau')T_\tau\{[\rho_\alpha(x),\psi_\mu(x')]\psi^\dagger_\nu(x'')\}$$
$$+\delta(\tau-\tau'')T_\tau\{\psi_\mu(x')[\rho_\alpha(x),\psi^\dagger_\nu(x'')]\}$$
$$+T_\tau\left\{\frac{\partial\rho_\alpha(x)}{\partial\tau}\psi_\mu(x')\psi^\dagger_\nu(x'')\right\}, \tag{5.3}$$

where the notation $T_\tau\{\cdots\}$ stands for the time-ordered product with respect to τ. With the aid of Eq. (2.1), the commutators in the first and the second terms on the right-hand side can be calculated. Then, the above identity reduces to

$$\frac{\partial}{\partial\tau}T_\tau\{\rho_\alpha(x)\psi_\mu(x')\psi^\dagger_\nu(x'')\}$$
$$=-\delta_{\alpha\mu}\delta(x-x')T_\tau\{\psi_\mu(x')\psi^\dagger_\nu(x'')\}+\delta_{\alpha\nu}\delta(x-x'')$$
$$\times T_\tau\{\psi_\mu(x')\psi^\dagger_\nu(x'')\}+T_\tau\left\{\frac{\partial\rho_\alpha(x)}{\partial\tau}\psi_\mu(x')\psi^\dagger_\nu(x'')\right\}. \tag{5.4}$$

The τ derivative of the number-density operator in the third term can be obtained by making use of the Heisenberg equation of ''motion''

$$\frac{\partial}{\partial\tau}\rho_\alpha(x)=\frac{-1}{\hbar}[\rho_\alpha(x),H]=\frac{-1}{\hbar}[\rho_\alpha(x),H_A(\tau)$$
$$+H_S(\tau)+H_{imp}(\tau)+H_{\rm int}(\tau)]. \tag{5.5}$$

As the commutator calculations are essentially same as those carried out in the previous sections in the derivation of the f-sum rules, we immediately obtain

$$\frac{\partial\rho_\alpha(x)}{\partial\tau}=\frac{-1}{\hbar}\lim_{x'''\to x}\{h_A(\nabla)-h_A(-\nabla''')\}\psi^\dagger_\alpha(x''')\psi_\alpha(x)$$
$$-i\frac{g\mu_B}{2\hbar}\,\mathrm{sgn}(\alpha)\sum_{ij}\varepsilon_{ij3}B_i(\mathbf{x})\psi^\dagger_\xi(x)\sigma^j_{\xi\zeta}\psi_\zeta(x), \tag{5.6}$$

which corresponds to Eq. (4.12). By virtue of this result, the operator relation (5.6) yields

$$\lim_{x'''\to x}\left[\delta_{\xi\alpha}\delta_{\zeta\alpha}\left\{\frac{\partial}{\partial\tau}+\frac{1}{\hbar}\,h_A(\nabla)+\frac{\partial}{\partial\tau'''}-\frac{1}{\hbar}\,h_A(-\nabla''')\right\}+i\,\frac{g\mu_B}{2\hbar}\,\mathrm{sgn}(\alpha)[\mathbf{B}(\mathbf{x})\times\boldsymbol{\sigma}_{\xi\zeta}]_3\right]\times T_\tau\{\psi_\xi^\dagger(x''')\psi_\zeta(x)\psi_\mu(x')\psi_\nu^\dagger(x'')\}$$
$$=-\delta_{\alpha\mu}\delta(x-x')T_\tau\{\psi_\alpha(x)\psi_\nu^\dagger(x'')\}+\delta_{\alpha\nu}\delta(x-x'')T_\tau\{\psi_\mu(x')\psi_\alpha^\dagger(x)\}$$
$$(\text{no }\alpha\text{ sum}).\quad(5.7)$$

In order to rewrite this operator relation as a finite-temperature generalized Ward-Takahashi relation, we introduce the temperature Green's functions

$$-\langle T_\tau\{\psi_\alpha(x)\psi_\nu^\dagger(x'')\}\rangle=G_{\alpha\nu}(x,x''),\quad(5.8)$$

and

$$\langle T_\tau\{\psi_\alpha^\dagger(x''')\psi_\alpha(x)\psi_\mu(x')\psi_\nu^\dagger(x'')\}\rangle$$
$$=-\langle T_\tau\{\psi_\alpha(x)\psi_\mu(x')\psi_\nu^\dagger(x'')\psi_\alpha^\dagger(x''')\}\rangle$$
$$=-G^{\mathrm{II}}_{\alpha\mu;\nu\alpha}(x,x';x'',x''')\quad(\text{no }\alpha\text{ sum}).\quad(5.9)$$

Then Eq. (5.7) can be written as

$$\lim_{x'''\to x}\left[\delta_{\xi\alpha}\delta_{\zeta\alpha}\left\{\frac{\partial}{\partial\tau}+\frac{1}{\hbar}\,h_A(\nabla)+\frac{\partial}{\partial\tau'''}-\frac{1}{\hbar}\,h_A(-\nabla''')\right\}+i\,\frac{g\mu_B}{2\hbar}\,\mathrm{sgn}(\alpha)[\mathbf{B}(\mathbf{x})\times\boldsymbol{\sigma}_{\xi\zeta}]_3G^{\mathrm{II}}_{\zeta\mu;\nu\xi}(x,x';x'',x''')\right]$$
$$=-\delta_{\alpha\mu}\delta(x-x')G_{\alpha\nu}(x,x'')+\delta_{\alpha\nu}\delta(x-x'')G_{\mu\alpha}(x',x)$$
$$(\text{no }\alpha\text{ sum}).\quad(5.10)$$

This is the FTGWTR for the electrons under an arbitrary magnetic field.

VI. EXACT RELATIONS FOR THE SPIN-DENSITY CORRELATION FUNCTIONS

The derivation of the finite-temperature generalized Ward-Takahashi relation in the previous section can be straightforwardly applied to obtain more physically direct relations, i.e., some exact relations between the spin-density correlation functions. We first define the spin-density operator in the τ-Heisenberg picture,

$$S_i(x)\equiv\psi_\alpha^\dagger(x)\sigma^i_{\alpha\beta}\psi_\beta(x).\quad(6.1)$$

Then the identity corresponding to Eq. (5.4) is

$$\frac{\partial}{\partial\tau}\,T_\tau\{S_i(x)S_j(x')\}=\delta(\tau-\tau')[S_i(x),S_j(x')]+T_\tau\left\{\frac{\partial S_i(x)}{\partial\tau}\,S_j(x')\right\}.\quad(6.2)$$

The commutator in the first term is essentially the same as that given by Eq. (4.3). The only difference is that here the operators are in the τ-Heisenberg picture. The τ derivative of the spin-density operator in the second term is given by Eq. (4.8) by changing the picture from the Heisenberg picture to the τ-Heisenberg picture. The contributions from the impurity term and the electron-electron interaction term vanish. The remaining two terms correspond to Eqs. (4.9) and (4.11), respectively. The τ integration of the left-hand side of Eq. (6.2) gives

$$\int_0^{\beta\hbar}d\tau\,\frac{\partial}{\partial\tau}\,T_\tau\{S_i(x)S_j(x')\}$$
$$=S_i(\mathbf{x},\beta\hbar)S_j(\mathbf{x}',\tau')-S_j(\mathbf{x}',\tau')S_i(\mathbf{x},0).\quad(6.3)$$

Therefore, if we make the τ integration of Eq. (6.2) and take the grand canonical ensemble average, the left-hand side vanishes due to the cyclic invariance of the trace,[12]

$$\int_0^{\beta\hbar}d\tau\,\frac{\partial}{\partial\tau}\,\langle T_\tau\{S_i(x)S_j(x')\}\rangle=0.\quad(6.4)$$

The next step is to integrate both sides of Eq. (6.2) over the entire $\mathbf{x}$ space. Then, the first term on the right-hand side of Eq. (6.2) yields

$$\int d^3\mathbf{x}\int_0^{\beta\hbar}d\tau\,\delta(\tau-\tau')\langle[S_i(x),S_j(x')]\rangle$$
$$=2i\sum_k\,\varepsilon_{ijk}\langle S_k(x')\rangle,\quad(6.5)$$

and the second term gives

$$\int d^3\mathbf{x}\int_0^{\beta\hbar}d\tau\left\langle T_\tau\left\{\frac{\partial S_i(x)}{\partial\tau}\,S_j(x')\right\}\right\rangle$$
$$=\frac{-ig\mu_B}{\hbar}\sum_k\sum_l\,\varepsilon_{ikl}\int d^3\mathbf{x}\int_0^{\beta\hbar}d\tau B_k(\mathbf{x})\times\langle T_\tau\{S_l(x)S_j(x')\}\rangle.\quad(6.6)$$

Thus we obtain the following exact relation:

$$\sum_k\,\varepsilon_{ijk}\langle S_k(x)\rangle=\frac{g\mu_B}{2\hbar}\sum_k\sum_l\,\varepsilon_{ikl}\int d^3\mathbf{x}'\int_0^{\beta\hbar}d\tau' B_k(\mathbf{x}')\times\langle T_\tau\{S_l(x')S_j(x)\}\rangle.\quad(6.7)$$

This can also be written as

$$\langle S_i(x)\rangle=\frac{g\mu_B}{4\hbar}\int d^3\mathbf{x}'\int_0^{\beta\hbar}d\tau'\left\{-B_i(\mathbf{x}')\sum_k\times\langle T_\tau\{S_k(x')S_k(x)\}\rangle+\sum_k\,B_k(\mathbf{x}')\times\langle T_\tau\{S_i(x')S_k(x)\}\rangle\right\}.\quad(6.8)$$

It is straightforward to extend this result to higher order correlation functions. Starting with the identity[12]

$$\frac{\partial}{\partial\tau}T_\tau\{S_i(x)S_j(x')S_k(x'')\}$$
$$=\delta(\tau-\tau')T_\tau\{[S_i(x),S_j(x')]S_k(x'')\}$$
$$+\delta(\tau-\tau'')T_\tau\{S_j(x')[S_i(x),S_k(x'')]\}$$
$$+T_\tau\left\{\frac{\partial S_i(x)}{\partial\tau}S_j(x')S_k(x'')\right\}, \tag{6.9}$$

we can similarly obtain

$$\sum_l \{\varepsilon_{ijl}\langle T_\tau\{S_l(x')S_k(x'')\}\rangle+\varepsilon_{ikl}\langle T_\tau\{S_j(x')S_l(x'')\}\rangle\}$$
$$=\frac{g\mu_B}{2\hbar}\int d^3\mathbf{x}\int_0^{\beta\hbar}d\tau\sum_l\sum_m \varepsilon_{ilm}B_l(\mathbf{x})$$
$$\times\langle T_\tau\{S_m(x)S_j(x')S_k(x'')\}\rangle. \tag{6.10}$$

This can be readily generalized to

$$\sum_{k=1}^{N}\sum_l \varepsilon_{ij_kl}\langle T_\tau\{S_{j_1}(x_1)\cdots S_{j_{k-1}}(x_{k-1})S_l(x_k)$$
$$\times S_{j_{k+1}}(x_{k+1})\cdots S_{j_N}(x_N)\}\rangle$$
$$=\frac{g\mu_B}{2\hbar}\int d^3\mathbf{x}\int_0^{\beta\hbar}d\tau\sum_l\sum_m \varepsilon_{ilm}B_l(\mathbf{x})$$
$$\times\langle T_\tau\{S_m(x)S_{j_1}(x_1)\cdots S_{j_N}(x_N)\}\rangle. \tag{6.11}$$

To the best of the authors' knowledge, the results (6.7), (6.8), (6.10), and (6.11) are new. It should be also noted that these relations have been derived without any approximations.

VII. DISCUSSIONS AND CONCLUDING REMARKS

We have derived sum rules, a FTGWTR, and a set of exact relations for the spin-density correlation functions. Among these results, the exact relations obtained in the last section provide a direct physical interpretation. Evidently the relation (6.8) illustrates the response of the spin density of the system of interacting electrons to an arbitrary external magnetic field that is coupled with the electron spin via the interaction Hamiltonian H_s given by Eq. (2.5). The correlation functions express the response of the electron spin to the perturbation caused by the external magnetic field. These correlation functions depend on the magnetic field.

The relation (6.8) can be regarded as a finite-temperature version of Nambu-Goldstone's theorem. In order to realize a spontaneous breaking of the spin-rotational symmetry, it is necessary to include a spin-dependent electron-electron interaction. Then, as a consequence of cooperative phenomena, it may be possible to have a spin-ordered state that breaks the spin-rotational symmetry of the original Hamiltonian at sufficiently low temperature.[18]

Here we show that the results (6.8), (6.10), and (6.11) are unchanged at the presence of a spin-dependent electron-electron interaction in the Hamiltonian,

$$H_{\rm int}(\tau)=\tfrac{1}{2}\int d^3\mathbf{x}'\int d^3\mathbf{x}''U_S(|\mathbf{x}'-\mathbf{x}''|)\mathbf{S}(\mathbf{x}',\tau)\cdot\mathbf{S}(\mathbf{x}'',\tau). \tag{7.1}$$

Due to such a spin dependence, the τ derivative of the spin-density operator now has the new term

$$[S_i(x),H_{\rm int}(\tau)]=\tfrac{1}{2}\int d^3\mathbf{x}'\int d^3\mathbf{x}''U_S(|\mathbf{x}'-\mathbf{x}''|)$$
$$\times\sum_k [S_i(\mathbf{x},\tau),S_k(\mathbf{x}',\tau)S_k(\mathbf{x}'',\tau)]. \tag{7.2}$$

It is straightforward to calculate the commutator on the right-hand side of Eq. (7.2) and to find that the commutator vanishes after the integration over the entire $\mathbf{x}$ space,

$$\int d^3\mathbf{x}\sum_k [S_i(\mathbf{x},\tau),S_k(\mathbf{x}',\tau)S_k(\mathbf{x}'',\tau)]$$
$$=i2\sum_k\sum_l \varepsilon_{ilk}\left\{\int d^3\mathbf{x}\,\delta(\mathbf{x}-\mathbf{x}')-\int d^3\mathbf{x}\,\delta(\mathbf{x}-\mathbf{x}'')\right\}$$
$$\times S_l(\mathbf{x}',\tau)S_k(\mathbf{x}'',\tau)$$
$$=0. \tag{7.3}$$

Hence we find

$$\int d^3\mathbf{x}[S_i(x),H_{\rm int}(\tau)]=0. \tag{7.4}$$

Consequently, because of the $\mathbf{x}$ integration in Eqs. (6.5) and (6.6), the final result (6.7) is not affected by the spin-dependent interaction (7.1) added to the Hamiltonian.

To see the relation between Eq. (6.7) and the Nambu-Goldstone theorem, it is sufficient to observe that

$$M_i(x)\equiv\lim_{B\to 0}\langle S_i(x)\rangle \tag{7.5}$$

can be regarded as the order parameter for the spontaneous broken spin-rotational symmetry.[18] If the system is symmetric under spin rotation, $M_i(x)$ must vanish. Therefore, if $M_i(x)$ does not vanish in the zero magnetic field limit, $M_i(x)$ is nothing else but the order parameter of the spontaneous symmetry breaking. The nonvanishing $M_i(x)$ also means that the right-hand side of Eq. (6.8) does not vanish,

$$\lim_{B\to 0}\frac{g\mu_B}{4\hbar}\int d^3\mathbf{x}'\int_0^{\beta\hbar}d\tau'\left\{-B_i(\mathbf{x}')\sum_k\langle T_\tau\{S_k(x')S_k(x)\}\rangle\right.$$
$$\left.+\sum_k B_k(\mathbf{x}')\langle T_\tau\{S_i(x')S_k(x)\}\rangle\right\}\neq 0. \tag{7.6}$$

This is the finite-temperature version of the Nambu-Goldstone theorem.[11,18,19] In order to relate the singularity of the spin-correlation functions, $\langle T_\tau\{S_i(x')S_k(x)\}\rangle$ or $\langle T_\tau\{S_k(x')S_k(x)\}\rangle$, to Nambu-Goldstone bosons, one can perform analytic continuation with respect to the frequency to obtain the real-time response functions.[20] In such a case, the poles of the response functions may be expected to show the excitation spectrums of magnons.[18] Further detailed discussions will be given in a forthcoming paper.

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