# Green's function formalism for calculating spin-wave spectra

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(Received 4 February 1999)

We propose a formalism for calculating *ab initio* spin-wave spectra which is based on the many-body temperature Green's function. The main quantity to be calculated is the linear magnetic susceptibility from which all magnetic excitations involving the creation of an additional spin in the system can formally be obtained. The Schwinger functional derivative technique is employed in calculating the self-energy. The approach avoids both the assumption of local spins (Heisenberg model) and the use of a *local* exchange and correlation interaction (local-density approximation). Starting from the GW approximation we obtain a Bethe-Salpeter equation for the kernel describing the interaction between electrons in both spin channels. However, this kernel exhibits a *nonlocal* screened interaction. [S0163-1829(99)08933-X]

## I. INTRODUCTION

Collective spin excitations in solids are involved in many physical phenomena.[1] The energy scale of spin excitations is typically of the order of tens of meV. Spin excitations could therefore be coupled to excitations around the Fermi surface. Many physical phenomena lie in this low-energy regime. Transport and thermal phenomena such as the electronic specific heat and electrical and thermal resistivity are among the most well-known ones. Due to thermal excitations of spin waves at low temperature the magnetization in a ferromagnet obeys the Bloch law $\sim T^{3/2}$. Spin-wave excitations are also observable in the specific heat where a $T^{3/2}$ term appears in addition to the $T^3$ term due to phonon excitations. The discovery of high-temperature superconductivity has also enhanced the interest in spin excitations. There is compelling evidence to believe that spin excitations are involved in superconductivity. Like in conventional BCS (Bardeen-Cooper-Schrieffer) theory where the phonons mediate attractive interaction between electron pairs, it is proposed that spin fluctuations are the mediator of attractive interaction in the high-temperature superconductivity.[2,3]

There have been many works in the field of spin excitations or spin waves, starting from the early work of Heisenberg whose model has been very successful in explaning many phenomena involving spin fluctuations. First-principles calculations have also been performed by a number of authors. These are often based on frozen-spin approach where the excitation energy is calculated by assuming a certain spin-spiral configuration.[4–7] The system is usually mapped to the Heisenberg model and the exchange parameter $J$ is then obtained from realistic band-structure calculations. This approach is restricted to static spin excitations. It is well known that the discrepancy with experiment can be quite large. Three sources of errors are evident in this approach. The first is the use of the local-density approximation (LDA) in calculating the total energy. The second is the assumption of local spins inherent in the Heisenberg model and the third is that the assumed spin configuration may not correspond to the true eigenstate of a spin excitation.

Spin-wave spectra can also be calculated using time-dependent density-functional theory (TDFT). In the early works, severe approximations were made regarding the energy bands, wave functions, and the electron-electron interaction.[8–11] Only recently, full calculations for Fe, Ni, and Cr were made by Savrasov.[12] The spin-wave spectra are obtained from the magnetic susceptibility thus avoiding mapping to the Heisenberg Hamiltonian. The calculations successfully reproduced the spin-wave spectra of Fe but for Ni significant deviation from experiment is observed. In TDFT the response function is given exactly, so that discrepancy with experiment is mainly due to the approximate exchange-correlation functional. The local and orbital-independent nature of the local-density approximation (LDA) or its refinements appears to be the major source of the problem. Indeed, as will be shown later, the interaction between electrons responsible for the correlations determining the spectra is very nonlocal.

The purpose of this paper is to present a method to be used for practial *ab initio* calculations of the linear magnetic susceptibility. The approach is based on the Matsubara Green's function and the Schwinger functional derivative technique. The main advantage is the possibility of having a nonlocal interaction which comes out naturally from the formalism, in contrast to the LDA where a local exchange-correlation kernel is employed for describing the interaction between the electrons. Starting from the self-energy in the GW approximation (GWA), to be described later, we obtain a Bethe-Salpeter equation for the nonlocal kernel describing the interaction between electrons in both spin channels.

## II. THEORY

### A. Basic relations

We summarize some basic properties of the Matsubara Green's function in this section. More details may be found in standard textbooks on many-body theory.[13,14]

 

The Matsubara or temperature Green's function is defined by the following $2\times 2$ matrix:

$$\mathcal{G}_{\alpha\beta}(1,2) = -\langle \mathcal{T}[\hat{\psi}_\alpha(1)\hat{\psi}^\dagger_\beta(2)]\rangle. \tag{1}$$

Here, $1\equiv(\mathbf{r},\tau)$, $\alpha$ and $\beta$ denote the spin, and the symbol $\langle\ \rangle$ means grand canonical ensemble average:

$$\langle \hat{O}\rangle = \mathrm{Tr}[\hat{\rho}_0\hat{O}] \tag{2}$$

and

$$\hat{\rho}_0 = Z_0^{-1}\exp(-\beta\hat{K}_0), \quad Z_0 = \mathrm{Tr}\exp(-\beta\hat{K}_0), \tag{3}$$

$$\hat{K}_0 = \hat{H}_0 - \mu\hat{N}, \quad \beta\equiv\frac{1}{k_B T}. \tag{4}$$

The field operators are defined in the (modified) Heisenberg picture:

$$\hat{O}(\tau) = \exp(\hat{K}_0\tau)\hat{O}\exp(-\hat{K}_0\tau) \tag{5}$$

so that

$$\hat{\psi}_\alpha(\mathbf{r}\tau) = \exp(\hat{K}_0\tau)\hat{\psi}_\alpha(\mathbf{r})\exp(-\hat{K}_0\tau) \tag{6}$$

$$\hat{\psi}^\dagger_\alpha(\mathbf{r}\tau) = \exp(\hat{K}_0\tau)\hat{\psi}^\dagger_\alpha(\mathbf{r})\exp(-\hat{K}_0\tau). \tag{7}$$

*Note that $\hat{\psi}^\dagger_\alpha(\mathbf{r}\tau)$ is not the adjoint of $\hat{\psi}_\alpha(\mathbf{r}\tau)$ when $\tau$ is real.* If $\tau$ is interpreted as a complex variable, it may be analytically continued to a pure imaginary value $\tau = it$. The resulting expression $\hat{\psi}^\dagger_\alpha(\mathbf{r},it)$ is then the true adjoint of $\hat{\psi}_\alpha(\mathbf{r},it)$ and is formally identical with the usual Heisenberg picture apart from the substitution of $\hat{K}_0$ for $\hat{H}_0$.[15]

In the Matsubara formulation, the Fourier transforms are defined by

$$\mathcal{G}(i\nu_n) = \int_0^\beta d\tau\, e^{i\nu_n\tau}\mathcal{G}(\tau), \tag{8}$$

$$\mathcal{G}(\tau) = \frac{1}{\beta}\sum_n e^{-i\nu_n\tau}\mathcal{G}(i\nu_n), \tag{9}$$

where $\nu_n$ denotes the Matsubara frequency for fermion propagators. For bosons we use $\omega_n$ as a convention.

$$\nu_n = \frac{(2n+1)\pi}{\beta}, \tag{10}$$

$$\omega_n = \frac{2n\pi}{\beta}. \tag{11}$$

The Matsubara formulation is almost identical to the zero temperature one except:

- Integral over $\tau$ runs from 0 to $\beta$.
- For every diagram of order $n$, we have the factor $(-1)^n$ instead of $i^n$ as in the zero-temperature case.
- The retarded Green's function is obtained by analytic continuation:

$$G^{\mathrm{R}}(\nu) = \mathcal{G}(i\nu_n \to \nu + i\delta). \tag{12}$$

The field operator satisfies the Heisenberg equation of motion

$$\frac{\partial}{\partial\tau}\hat{\psi}_\alpha(\mathbf{r}\tau) = [\hat{K}_0, \hat{\psi}_\alpha(\mathbf{r}\tau)]. \tag{13}$$

From Eq. (13) we can easily derive the equation of motion for the Green's function:

$$\left[\frac{\partial}{\partial\tau} - \nabla^2_{\mathbf{r}}/2 - \mu\right]\mathcal{G}_{\alpha\beta}(\mathbf{r}\tau,\mathbf{r}'\tau') + \int d^3r''\int_0^\beta d\tau''\sum_\gamma \mathcal{M}_{\alpha\gamma}(\mathbf{r}\tau,\mathbf{r}''\tau'')\mathcal{G}_{\gamma\beta}(\mathbf{r}''\tau'',\mathbf{r}'\tau') = -\delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau'). \tag{14}$$

The mass operator $\mathcal{M}$ is defined by

$$\int d^3r''\int_0^\beta d\tau''\sum_\gamma \mathcal{M}_{\alpha\gamma}(\mathbf{r}\tau,\mathbf{r}''\tau'')\mathcal{G}_{\gamma\beta}(\mathbf{r}''\tau'',\mathbf{r}'\tau') = \sum_\gamma \int d^3r''\, v(\mathbf{r}-\mathbf{r}'')\mathcal{G}^{(2)}_{\alpha\beta\gamma\gamma}(\mathbf{r}\tau,\mathbf{r}'\tau',\mathbf{r}''\tau,\mathbf{r}''\tau^+), \tag{15}$$

where $\mathcal{G}^{(2)}$ is the two-particle Green's function defined as

$$\mathcal{G}^{(2)}_{\alpha\beta\eta\gamma}(1,2,3,4) \equiv (-1)^2\langle \mathcal{T}\hat{\psi}_\alpha(1)\hat{\psi}_\eta(3)\hat{\psi}^\dagger_\gamma(4)\hat{\psi}^\dagger_\beta(2)\rangle. \tag{16}$$

### B. The Schwinger functional derivative technique

We will now use Schwinger's functional derivative technique to calculate the self-energy. Since we are also interested in magnetic response, we introduce a $\tau$-varying external field which includes a magnetic field. This external field functions as a mathematical trick, similar to the principle of virtual work in classical mechanics, and it will be set to zero at the end. The coupling to the orbital motion is not considered.[16]

$$\phi(\mathbf{r}\tau) = \vec{\varphi}(\mathbf{r}\tau)\cdot\vec{\sigma}, \tag{17}$$

where

$$\vec{\varphi}(\mathbf{r}\tau) = \left[\varphi_0(\mathbf{r}\tau), \frac{1}{2}g\mu_B\mathbf{B}(\mathbf{r}\tau)\right], \tag{18}$$

$$\sigma^0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \quad \sigma^x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma^y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \sigma^z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{19}$$

For a $\tau$-dependent perturbation, it is suitable to work in the interaction (Dirac) representation where the effects of the external field are considered explicitly in contrast to the Heisenberg representation where the effects of the external field are contained implicitly in the field operators. The Dirac operator is defined by

$$\hat{O}_D(\tau) = \exp(\hat{K}_0\tau)\hat{O}\exp(-\hat{K}_0\tau). \tag{20}$$

The $\tau$-development operator which describes the dynamics of the wave function satisfies

$$-\frac{\partial}{\partial\tau}\hat{\mathcal{U}}(\tau,\tau_0)=\hat{\phi}_D(\tau)\hat{\mathcal{U}}(\tau,\tau_0) \tag{21}$$

with the formal solution

$$\hat{\mathcal{U}}(\tau,\tau_0)=\mathcal{T}\exp\left[-\int_{\tau_0}^{\tau}d\tau'\,\hat{\phi}_D(\tau')\right]. \tag{22}$$

Since $\hat{\mathcal{U}}$ consists of pairs of fermion operators, it can be commuted with a field operator without change of sign. The relationship between the operators in the Heisenberg and Dirac representations is given by

$$\hat{O}(\tau)=\hat{\mathcal{U}}(0,\tau)\hat{O}_D(\tau)\hat{\mathcal{U}}(\tau,0). \tag{23}$$

As evident from Eqs. (20) and (23) operators and states in all representations are defined to coincide at $\tau=0$.

Defining

$$\hat{\mathcal{S}}=\hat{\mathcal{U}}(\beta,0), \tag{24}$$

the Green's function can be rewritten in terms of the field operators in the Dirac representation:

$$\mathcal{G}_{\alpha\beta}(1,2)=-\frac{\langle\mathcal{T}\hat{\mathcal{S}}\hat{\psi}_{D\alpha}(1)\hat{\psi}^{\dagger}_{D\beta}(2)\rangle}{\langle\hat{\mathcal{S}}\rangle}, \tag{25}$$

where the ensemble average is taken with respect to $\hat{K}_0$, the many-body $\hat{K}$ but without the external field $\hat{\phi}$, i.e., $\hat{K}=\hat{K}_0+\hat{\phi}$.

The external field in the Dirac representation takes the form

$$\hat{\phi}_D(\tau)=\int d^3r\;\vec{\varphi}(\mathbf{r}\tau)\cdot\hat{\sigma}_D(\mathbf{r}\tau)$$

$$=\sum_{\alpha\beta}\int d^3r\;\hat{\psi}^{\dagger}_{D\alpha}(\mathbf{r}\tau)\,\phi_{\alpha\beta}(\mathbf{r}\tau)\,\hat{\psi}_{D\beta}(\mathbf{r}\tau), \tag{26}$$

where

$$\phi_{\alpha\beta}(\mathbf{r}\tau)\equiv\sum_i\;\varphi_i(\mathbf{r}\tau)\sigma^i_{\alpha\beta}. \tag{27}$$

Consider a change in the Dirac $\mathcal{G}$ upon an infinitesmal change in the external field $\phi$. We first note that

$$\frac{\delta\hat{\mathcal{S}}}{\delta\varphi_i(3)}=-\mathcal{T}[\hat{\mathcal{S}}\hat{\sigma}^i_D(3)] \tag{28}$$

and

$$\frac{\delta\mathcal{G}_{\alpha\beta}(1,2)}{\delta\varphi_i(3)}=\sum_{\gamma\eta}\;\sigma^i_{\gamma\eta}\{\mathcal{G}_{\alpha\beta}(1,2)\mathcal{G}_{\eta\gamma}(3,3^+)$$

$$-\mathcal{G}^{(2)}_{\alpha\beta\eta\gamma}(1,2,3,3^+)\}, \tag{29}$$

where $\mathcal{G}^{(2)}$ is defined in Eq. (16) and can also be written as

$$\mathcal{G}^{(2)}_{\alpha\beta\eta\gamma}(1,2,3,4)$$

$$=(-1)^2\frac{\langle\mathcal{T}\hat{\mathcal{S}}\hat{\psi}_{D\alpha}(1)\hat{\psi}_{D\eta}(3)\hat{\psi}^{\dagger}_{D\gamma}(4)\hat{\psi}^{\dagger}_{D\beta}(2)\rangle}{\langle\hat{\mathcal{S}}\rangle}. \tag{30}$$

It is also possible to define the Green's function in Eq. (25) without the denominator $\langle\hat{\mathcal{S}}\rangle$. In this case, the Hartree potential arising from the denominator corresponding to the first term in Eq. (29) has to be considered explicitly.

Defining the self-energy $\Sigma$ without the Hartree field as

$$\Sigma_{\alpha\beta}(1,2)=\mathcal{M}_{\alpha\beta}(1,2)-\delta_{\alpha\beta}\delta(1-2)V_H(1) \tag{31}$$

and using Eq. (14) with $\hat{K}_0$ replaced with $\hat{K}$ we obtain[17]

$$\mathcal{G}^{-1}_{\alpha\beta}(1,2)=-\left(\frac{\partial}{\partial\tau_1}+t_1-\mu\right)\delta_{\alpha\beta}\delta(1-2)-\phi_{\alpha\beta}(1)\,\delta(1-2)$$

$$-\Sigma_{\alpha\beta}(1,2)-\delta_{\alpha\beta}\delta(1-2)V_H(1). \tag{32}$$

In contrast to the Hartree term the external field is not diagonal in spin space. Finally using the identity

$$\frac{\delta}{\delta\phi}(\mathcal{G}^{-1}\mathcal{G})=\mathcal{G}^{-1}\frac{\delta\mathcal{G}}{\delta\phi}+\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G}=0\rightarrow\frac{\delta\mathcal{G}}{\delta\phi}=-\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G} \tag{33}$$

we extract the *exact* expressions

$$\Sigma_{\alpha\beta}(1,2)=\sum_{\eta}\int d3\;d4\;v(1-3)\mathcal{G}_{\alpha\eta}(1,4)\frac{\delta\mathcal{G}^{-1}_{\eta\beta}(4,2)}{\delta\varphi_0(3)}, \tag{34}$$

$$\frac{\delta\mathcal{G}^{-1}_{\alpha\beta}(1,2)}{\delta\varphi_0(3)}=-\delta(1-2)\,\delta_{\alpha\beta}\left[\delta(1-3)+\frac{\delta V_H(1)}{\delta\varphi_0(3)}\right]$$

$$-\frac{\delta\Sigma_{\alpha\beta}(1,2)}{\delta\varphi_0(3)}. \tag{35}$$

It is interesting to note that only a change in the electric field $\varphi_0$ has to be considered when calculating the electron self-energy. Keeping only the first term in Eq. (35) we obtain the exchange contribution to the self-energy and including the next term generates the well-known GWA. Since $1-\delta V_H/\delta\varphi_0$ is the inverse dielectric function $\epsilon^{-1}$, the GWA is then given by $\Sigma=\mathcal{G}\mathcal{W}$ where $\mathcal{W}$ is the screened Coulomb interaction $\mathcal{W}=v\epsilon^{-1}$. Thus the GWA takes into account only the change in the Hartree potential. The response function in the GWA corresponds therefore to that in the random-phase approximation (RPA). Qualitatively we may regard the GWA as the Hartree-Fock approximation but with the bare interaction replaced with a screened one. The last term in Eq. (35) is referred to as the vertex correction which will be needed in calculating the spin-wave spectra.

Theoretical development of the self-energy in condensed-matter physics has been conventionally based on Feynman's diagrammatic expansion. In quantum electrodynamics, where this approach was first introduced, such an expansion is well justified by the fact that the expansion parameter describing the coupling of the electromagnetic field to the electrons is small, in the sense that a perturbation expansion

leads to a convergent result. In condensed-matter physics, the expansion parameter is the Coulomb potential which by no means can be regarded as ''small.'' Nevertheless the Feynman diagrammatic approach has been used routinely without much justification which has led to many fundamental problems. It is known, for example, that a straightforward expansion of the self-energy in powers of the screened Coulomb interaction $\mathcal{W}$ yields negative spectral functions, which are unphysical.[18,19] Another fundamental problem is double counting. When summing two or more sets of diagrams to infinite order, the lower-order diagrams (second-order) are usually double counted simply from the fact that the number of second-order diagrams is very limited so that they are bound to be included in both sets. Furthermore, there is no prescription which sets of diagrams that should be summed. So far, the choice of diagrams is based on physical intuition.

The problems associated with the Feynman diagrammatic approach discussed in the previous paragraph do not seem to arise in the Schwinger approach. In the latter, the basic quantity is the response function which is directly related to $\delta\mathcal{G}^{-1}/\delta\varphi$ as in Eq. (48). This is in contrast to the diagrammatic approach where the (screened) Coulomb interaction is regarded as an expansion parameter for the self-energy. It is reasonable to expect that the self-energy expressed in terms of the response function, which is a physical quantity, would yield physically sensible results such as positive definite spectra. While we have no proof, we might argue that if we calculate the self-energy at different time steps, i.e., we regard the perturbing potential $\phi$ as static at a given time step, the self-energy $\Sigma$ in the GWA certainly has the correct analytic properties. We are, however, interested in the change of $\Sigma$ with respect to $\phi$. The fact that $\Sigma$ has the correct analytic properties for all $\phi$ corresponding to different time steps does not necessarily guarantee that its variation with respect to $\phi$ (the vertex) has the correct analytic properties as well. Nevertheless it is reasonable to expect that this is the case.

A further advantage is that the problem with double counting does not arise since the formulation is not based on diagrammatic expansion in the first place. Even if we do interpret the integral equation for the response function in the Schwinger approach in terms of diagrams, there is still no double counting. Furthermore, the approach provides a systematic way of improving the self-energy at least theoretically.

It is also possible to use the Schwinger approach to develop a perturbation expansion in powers of the screened interaction $\mathcal{W}$ which would then be equivalent to the conventional diagrammatic approach. Thus it is important to note that we should always solve for the *response function* or $\delta\mathcal{G}^{-1}/\delta\varphi$ and use this in the self-energy expression in Eq. (34), i.e., we do not wish to make a term-by-term expansion in powers of $\mathcal{W}$ since such an expansion is known to give unphysical results.

In our definition of the Green's function in Eq. (25), the ensemble average is taken with respect to the *interacting* system but without the external field $\phi$. This is different from the conventional definition in the interaction picture where the ensemble average is taken with respect to the noninteracting system without the Coulomb interaction. In real time, $\tau \to it$, and for zero temperature, our definition does not make any assumption about the so-called adiabatic connection where a noninteracting ground state is adiabatically connected to the interacting one by means of a slow switching of the Coulomb interaction from $t=\pm\infty$ to $t=0$. It has been pointed out that such an assumption may not be valid.[20]

### C. Magnetic response

Let an interacting many-electron system be perturbed by a time-dependent external field as in Eq. (17) which includes a magnetic field. We work now with real time. To first order in $\hat{\phi}$ the solution to the time-development operator in Eq. (22) is

$$\hat{U}(t,t_0)=1-i\int_{t_0}^{t}dt'\,\hat{\phi}_D(t'). \tag{36}$$

Assume that the external field is switched on at time $t_0=0$. Note that $\Psi_D(0)=\Psi_S(0)=\Psi$. The Dirac state at time $t$ is

$$|\Psi_D(t)\rangle=|\Psi\rangle-i\int_0^t dt'\,\hat{\phi}_D(t')|\Psi\rangle \tag{37}$$

and the expectation value of an operator in this state reads

$$\begin{aligned}&\langle\Psi_D(t)|\hat{O}_D(t)|\Psi_D(t)\rangle\\&\quad=\langle\Psi|\hat{O}|\Psi\rangle-i\int_0^t dt'\langle\Psi|[\hat{O}_D(t),\hat{\phi}_D(t')]|\Psi\rangle.\end{aligned} \tag{38}$$

Following convention, we replace the operators in the Dirac representation by the operators in the Heisenberg representation since the Dirac representation is equivalent to the Heisenberg representation without the external field. Thus it is understood that the Heisenberg operators are defined below with respect to the full *unperturbed* Hamiltonian $\hat{K}_0$. We are interested in the spin density response, i.e.,

$$\hat{O}(t)\to\hat{\sigma}(\mathbf{r}t)=\sum_{\alpha\beta}\hat{\psi}^{\dagger}_{\alpha}(\mathbf{r}t)\vec{\sigma}_{\alpha\beta}\hat{\psi}_{\beta}(\mathbf{r}t). \tag{39}$$

Thus

$$\delta\langle\hat{\sigma}(\mathbf{r}t)\rangle=\int d^3r'\int_0^t dt'\,R^r(\mathbf{r}t,\mathbf{r}'t')\cdot\vec{\varphi}(\mathbf{r}'t'), \tag{40}$$

where we have defined the retarded response function

$$R^r(\mathbf{r}t,\mathbf{r}'t')\equiv -i\,\mathrm{Tr}\{\hat{\rho}[\hat{\sigma}(\mathbf{r}t),\hat{\sigma}(\mathbf{r}'t')]\}\theta(t-t'). \tag{41}$$

The dot product refers to the primed coordinate. The Matsubara response function is defined as

$$\mathcal{R}(\mathbf{r}\tau,\mathbf{r}'\tau')=-\mathrm{Tr}\{\hat{\rho}\mathcal{T}[\hat{\sigma}(\mathbf{r}\tau)\hat{\sigma}(\mathbf{r}'\tau')]\}. \tag{42}$$

By inserting a complete set of states in between the spin operators, it is well known[13,14] that the two response functions share exactly the same spectral function $S^r$:

$$R^r(\mathbf{r},\mathbf{r}',\omega)=\int_{-\infty}^{\infty}d\omega'\frac{S^r(\mathbf{r},\mathbf{r}',\omega')}{\omega-\omega'+i\delta}, \tag{43}$$

$$\mathcal{R}(\mathbf{r},\mathbf{r}';i\omega_n)=\int_{-\infty}^{\infty}d\omega'\frac{S^r(\mathbf{r},\mathbf{r}',\omega')}{i\omega_n-\omega'},\tag{44}$$

where[21]

$$S^r(\mathbf{r},\mathbf{r}',\omega)\equiv Z_0^{-1}\sum_{jk}\ e^{-\beta(E_j-\mu N)}(1-e^{-\beta\omega})\langle j|\hat{\sigma}(\mathbf{r})|k\rangle \times\langle k|\hat{\sigma}(\mathbf{r}')|j\rangle\,\delta(\omega-E_k+E_j).\tag{45}$$

### D. RPA magnetic response

The charge and magnetic $\tau$-ordered response function is defined by

$$\mathcal{R}_{ij}(1,2)\equiv\frac{\delta\langle\hat{\sigma}^i(1)\rangle}{\delta\varphi_j(2)},\tag{46}$$

where $i,j=0,x,y,z$. The external scalar field corresponds to $j=0$ and $j=x,y,z$ to the magnetic fields. The spin density is given by[22]

$$\langle\hat{\sigma}^i(1)\rangle=\sum_{\alpha\beta}\ \sigma^i_{\beta\alpha}\mathcal{G}_{\alpha\beta}(1,1^+).\tag{47}$$

It is convenient from now on to use a convention where *a repeated index or variable implies a summation or integration provided the index or variable does not appear on the other side of the equation*. We write the sum explicitly when necessary. From Eq. (32) we obtain

$$\frac{\delta\mathcal{G}^{-1}_{\mu\nu}(1,2)}{\delta\varphi_j(3)}=-\sigma^j_{\mu\nu}\delta(1-2)\,\delta(1-3)-\delta_{\mu\nu}\delta(1-2)\frac{\delta V_H(1)}{\delta\varphi_j(3)}-\frac{\delta\Sigma_{\mu\nu}(1,2)}{\delta\varphi_j(3)}\tag{48}$$

so that using the identity in Eq. (33),

$$\frac{\delta\mathcal{G}_{\alpha\beta}(1,2)}{\delta\varphi_j(3)}=\mathcal{G}_{\alpha\mu}(1,4)\,\epsilon^{-1}_{j,\mu\nu}(4,3)\mathcal{G}_{\nu\beta}(4,2)+\mathcal{G}_{\alpha\mu}(1,4)\frac{\delta\Sigma_{\mu\nu}(4,5)}{\delta\varphi_j(3)}\mathcal{G}_{\nu\beta}(5,2),\tag{49}$$

where we have defined

$$\epsilon^{-1}_{j,\alpha\beta}(1,2)\equiv\left[\sigma^j_{\alpha\beta}\delta(1-2)+\sigma^0_{\alpha\beta}\frac{\delta V_H(1)}{\delta\varphi_j(2)}\right].\tag{50}$$

We note that $\epsilon^{-1}_{j,\alpha\beta}(1,2)$ acts as a spin-flip centra for $j=x,y$. From Eqs. (46), (47), and (49) the exact expression for the response function reads

$$\mathcal{R}_{ij}(1,2)=\sigma^i_{\beta\alpha}\mathcal{G}_{\alpha\mu}(1,4)\left[\delta(4-5)\,\epsilon^{-1}_{j,\mu\nu}(4,2)+\frac{\delta\Sigma_{\mu\nu}(4,5)}{\delta\varphi_j(2)}\right]\mathcal{G}_{\nu\beta}(5,1^+).\tag{51}$$

Diagrammatically, the response function consists of a closed electron-hole diagram (bubble) with a spin-flip centra at one end and an electron-hole diagram with the nonlocal vertex inserted. In the simplest possible model, where the interaction between electron-hole pairs is taken to be a constant $U$ (see, e.g., Ref. 23) and free propagators are used, the transverse response function exhibits a pole when $[1-U\chi_0(\mathbf{q},\omega(\mathbf{q}))]=0$, where $\chi_0$ is the Pauli susceptibility. This pole corresponds to a spin-wave excitation. For the charge response, we can go beyond the usual RPA expression and include also the vertex contribution using the present formalism.

Let us investigate the consequences of neglecting the last vertex term; i.e., focus on

$$\mathcal{R}_{ij}(1,2)=\sigma^i_{\beta\alpha}\mathcal{G}_{\alpha\mu}(1,3)\left[\sigma^j_{\mu\nu}\delta(3-2)+\sigma^0_{\mu\nu}\frac{\delta V_H(3)}{\delta\varphi_j(2)}\right]\mathcal{G}_{\nu\beta}(3,1^+).\tag{52}$$

The problem is to evaluate $\delta\langle n\rangle/\delta\varphi_j$ since $V_H(3)=v(3-4)\langle n(4)\rangle$.

$$\begin{aligned}\frac{\delta\langle n(1)\rangle}{\delta\varphi_j(2)}&=\frac{\delta}{\delta\varphi_j(2)}[\sigma^0_{\alpha\beta}\mathcal{G}_{\beta\alpha}(1,1^+)]\\&=\frac{\delta\mathcal{G}_{\gamma\gamma}(1,1^+)}{\delta\varphi_j(2)}\\&=-\mathcal{G}_{\gamma\lambda}(1,3)\frac{\delta\mathcal{G}^{-1}_{\lambda\eta}(3,4)}{\delta\varphi_j(2)}\mathcal{G}_{\eta\gamma}(4,1^+)\\&=\mathcal{G}_{\gamma\lambda}(1,3)\,\delta(3-4)\left[\delta(3-2)\sigma^j_{\lambda\eta}+\sigma^0_{\lambda\eta}\frac{\delta V_H(3)}{\delta\varphi_j(2)}\right]\mathcal{G}_{\eta\gamma}(4,1^+)\\&=\mathcal{G}_{\gamma\lambda}(1,3)\left[\delta(3-2)\sigma^j_{\lambda\eta}+\sigma^0_{\lambda\eta}\frac{\delta V_H(3)}{\delta\varphi_j(2)}\right]\mathcal{G}_{\eta\gamma}(3,1^+).\end{aligned}\tag{53}$$

Rearranging the equation yields

$$[\delta(1-4)-\mathcal{P}^0(1,3)v(3-4)]\frac{\delta\langle n(4)\rangle}{\delta\varphi_j(2)}=\mathcal{P}^j(1,2),\tag{54}$$

where we have defined the polarization

$$\mathcal{P}^j_{\alpha\beta}(1,2)\equiv\mathcal{G}_{\alpha\gamma}(1,2)\sigma^j_{\gamma\eta}\mathcal{G}_{\eta\beta}(2,1^+),\tag{55}$$

$$\mathcal{P}^j(1,2)\equiv\mathcal{P}^j_{\alpha\alpha}(1,2).\tag{56}$$

*If $\mathcal{G}$ is diagonal in spin space then*[24]

$$\mathcal{P}^j=0,\quad \mathcal{R}_{0j}\equiv\frac{\delta\langle n\rangle}{\delta\varphi_j}=0\quad\text{if}\quad j=x,y\quad\text{and}\quad\mathcal{G}_{\alpha\beta}=\mathcal{G}_{\alpha\alpha}\delta_{\alpha\beta}.\tag{57}$$

Consequently, the diagonal Hartree contribution to $\epsilon^{-1}_{j,\alpha\beta}$ vanishes for $j=x,y$. We may define the charge dielectric function as

$$\epsilon(1,2)\equiv\delta(1-2)-\mathcal{P}^0(1,3)v(3-2).\tag{58}$$

Note that $\mathcal{P}^0$ means charge polarization rather than zeroth-order polarization. Thus from Eq. (52)

$$\mathcal{R}_{ij}(1,2)=\sigma^i_{\beta\alpha}\{\mathcal{P}^j_{\alpha\beta}(1,2)+\mathcal{P}^0_{\alpha\beta}(1,3)v(3-4)\mathcal{R}_{0j}(4,2)\}, \tag{59}$$

$$\mathcal{R}_{0j}(1,2)=\epsilon^{-1}(1,3)\mathcal{P}^j(3,2). \tag{60}$$

For charge-density response we have the usual RPA result:

$$\mathcal{R}_{00}(1,2)=\mathcal{P}^0(1,2)+\mathcal{P}^0(1,3)v(3-4)\mathcal{R}_{00}(4,2). \tag{61}$$

Schematically,

$$\mathcal{R}_{00}=(1+\mathcal{R}_{00}v)\mathcal{P}^0=(1-\mathcal{P}^0v)^{-1}\mathcal{P}^0 \tag{62}$$

which implies

$$\epsilon^{-1}=1+\mathcal{R}_{00}v. \tag{63}$$

We have used the fact that the response function is symmetric.

It is worthwhile to digress and discuss briefly the well-known GWA from the point of view of the Schwinger functional derivative technique. The GWA can be readily obtained by inserting $\delta\mathcal{G}^{-1}/\delta\varphi$ in Eq. (48) into Eq. (34), neglecting the last vertex term. $\delta V_H/\delta\varphi_j$ is obtained by solving the RPA equation in Eq. (54). The GWA self-energy may thus be regarded as arising from the response of the Hartree potential to an external perturbation. As emphasized in Sec. II B, it is not necessary to employ diagrammatic expansion of the self-energy. Rather, the self-energy can be expressed in terms of the response function which is a physical quantity. It is always possible to translate the Schwinger approach to the Feynman approach in order to find the corresponding diagrams when necessary.

Consider now the vertex contribution $\delta\Sigma/\delta\phi_0$. From Eq. (35) we have

$$\begin{aligned}\frac{\delta\mathcal{G}^{-1}_{\alpha\beta}(1,2)}{\delta\varphi_0(3)}&=-\delta(1-2)\,\delta_{\alpha\beta}\left[\delta(1-3)+\frac{\delta V_H(1)}{\delta\varphi_0(3)}\right]\\&\quad-\frac{\delta\Sigma_{\alpha\beta}(1,2)}{\delta\varphi_0(3)}\\&=-\delta(1-2)\,\delta_{\alpha\beta}\epsilon^{-1}(1,3)-\frac{\delta\Sigma_{\alpha\beta}(1,2)}{\delta\varphi_0(3)}.\end{aligned} \tag{64}$$

From Eq. (34) the self-energy without the last vertex term is

$$\Sigma_{\alpha\beta}(1,2)=-\mathcal{G}_{\alpha\beta}(1,2)\mathcal{W}(1,2) \tag{65}$$

which is the GW approximation (GWA).[25] It is necessary to allow the Green's function to have nondiagonal components in the spin space, for otherwise there would be no spin fluctuations in the $xy$ directions. We now take into account the vertex within the GWA and only consider the change in $\mathcal{G}$ for the moment.

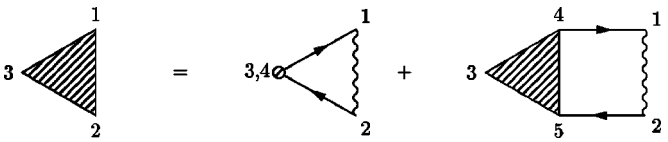


FIG. 1. Feynman diagrams for the vertex in Eq. (66). The solid line represents the Green's function, the wiggly line the screened interaction $\mathcal{W}$, and the small circle $\epsilon^{-1}_j$.

$$\begin{aligned}\frac{\delta\Sigma_{\alpha\beta}(1,2)}{\delta\varphi_j(3)}&=-\frac{\delta\mathcal{G}_{\alpha\beta}(1,2)}{\delta\varphi_j(3)}\mathcal{W}(1,2)\\&=-\mathcal{W}(1,2)\mathcal{G}_{\alpha\mu}(1,4)\left\{\epsilon^{-1}_{j,\mu\nu}(4,3)\mathcal{G}_{\nu\beta}(4,2)\right.\\&\quad\left.+\frac{\delta\Sigma_{\mu\nu}(4,5)}{\delta\varphi_j(3)}\mathcal{G}_{\nu\beta}(5,2)\right\}.\end{aligned} \tag{66}$$

This is an integral equation for the vertex which can be solved as follows:

$$\begin{aligned}&\{\delta_{\mu\alpha}\delta_{\nu\beta}\delta(4-1)\,\delta(5-2)\\&\quad+\mathcal{W}(1,2)\mathcal{G}_{\alpha\mu}(1,4)\mathcal{G}_{\nu\beta}(5,2)\}\frac{\delta\Sigma_{\mu\nu}(4,5)}{\delta\varphi_j(3)}\\&=-\mathcal{W}(1,2)\mathcal{G}_{\alpha\mu}(1,4)\epsilon^{-1}_{j,\mu\nu}(4,3)\mathcal{G}_{\nu\beta}(4,2).\end{aligned} \tag{67}$$

Defining

$$\begin{aligned}\mathcal{D}_{\alpha\beta,\mu\nu}(1,2|3,4)&\equiv\delta_{\mu\alpha}\delta_{\nu\beta}\delta(3-1)\,\delta(4-2)\\&\quad+\mathcal{W}(1,2)\mathcal{G}_{\alpha\mu}(1,3)\mathcal{G}_{\nu\beta}(4,2),\end{aligned} \tag{68}$$

$$\Pi_{j,\alpha\beta}(1,2|3)\equiv\mathcal{G}_{\alpha\mu}(1,4)\epsilon^{-1}_{j,\mu\nu}(4,3)\mathcal{G}_{\nu\beta}(4,2), \tag{69}$$

$$\mathcal{N}_{j,\alpha\beta}(1,2|3)\equiv-\mathcal{W}(1,2)\Pi_{j,\alpha\beta}(1,2|3), \tag{70}$$

the vertex is given by (diagrammatically in Fig. 1)

$$\Lambda_{j,\alpha\beta}(1,2|3)\equiv\frac{\delta\Sigma_{\alpha\beta}(1,2)}{\delta\varphi_j(3)}=\mathcal{D}^{-1}_{\alpha\beta,\mu\nu}(1,2|4,5)\mathcal{N}_{j,\mu\nu}(4,5|3). \tag{71}$$

When substituted into Eq. (51) this vertex correction results in ladder diagrams.

Let us go further and consider the $\mathcal{W}$ term. The Bethe-Salpeter equation for the screened interaction $\mathcal{W}$ is

$$\mathcal{W}=v+v\mathcal{P}^0\mathcal{W}, \tag{72}$$

$$\begin{aligned}\frac{\delta\mathcal{W}}{\delta\varphi}&=v\frac{\delta\mathcal{P}^0}{\delta\varphi}\mathcal{W}+v\mathcal{P}^0\frac{\delta\mathcal{W}}{\delta\varphi}=(1-v\mathcal{P}^0)^{-1}v\frac{\delta\mathcal{P}^0}{\delta\varphi}\mathcal{W}\\&=\mathcal{W}\frac{\delta\mathcal{P}^0}{\delta\varphi}\mathcal{W}.\end{aligned} \tag{73}$$

We therefore must evaluate

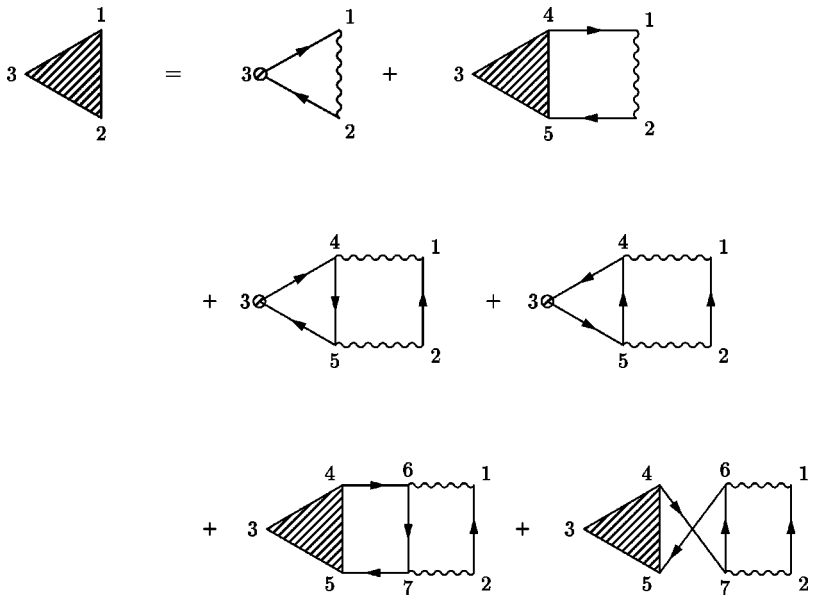

FIG. 2. Feynman diagrams for the full vertex starting from the GWA. The solid line represents the Green's function, the wiggly line the screened interaction $\mathcal{W}$, and the small circle $\epsilon_j^{-1}$.

$$\frac{\delta \mathcal{P}^0(1,2)}{\delta \varphi_j(3)} = \left\{ \frac{\delta \mathcal{G}_{\gamma\gamma}(1,2)}{\delta \varphi_j(3)} \mathcal{G}_{\gamma\gamma}(2,1^+) + \mathcal{G}_{\gamma\gamma}(1,2) \frac{\delta \mathcal{G}_{\gamma\gamma}(2,1^+)}{\delta \varphi_j(3)} \right\}$$
$$= \{ \Pi_{j,\gamma\gamma}(1,2|3) + \mathcal{G}_{\gamma\mu}(1,4) \Lambda_{j,\mu\nu}(4,5|3) \mathcal{G}_{\nu\gamma}(5,2) \} \mathcal{G}_{\gamma\gamma}(2,1^+) + \mathcal{G}_{\gamma\gamma}(1,2) \{ \Pi_{j,\gamma\gamma}(2,1^+|3) + \mathcal{G}_{\gamma\mu}(2,4) \Lambda_{j,\mu\nu}(4,5|3) \mathcal{G}_{\nu\gamma}(5,1^+) \}. \quad (74)$$

We have used Eq. (49) in the second line. Thus the complete ''denominator'' $\mathcal{D}$ and ''numerator'' $\mathcal{N}$ are

$$\mathcal{D}_{\alpha\beta,\mu\nu}(1,2|4,5) \equiv \delta_{\mu\alpha}\delta_{\nu\beta}\delta(4-1)\delta(5-2) + \mathcal{W}(1,2)\mathcal{G}_{\alpha\mu}(1,4)\mathcal{G}_{\nu\beta}(5,2) + \mathcal{G}_{\alpha\beta}(1,2)\mathcal{W}(1,6)\mathcal{G}_{\gamma\mu}(6,4)\mathcal{G}_{\nu\gamma}(5,7) \times \mathcal{G}_{\gamma\gamma}(7,6^+)\mathcal{W}(7,2) + \mathcal{G}_{\alpha\beta}(1,2)\mathcal{W}(1,6) \times \mathcal{G}_{\gamma\gamma}(6,7)\mathcal{G}_{\gamma\mu}(7,4)\mathcal{G}_{\nu\gamma}(5,6^+)\mathcal{W}(7,2), \quad (75)$$

$$\mathcal{N}_{j,\alpha\beta}(1,2|3) \equiv -\mathcal{W}(1,2)\Pi_{j,\alpha\beta}(1,2|3) - \mathcal{G}_{\alpha\beta}(1,2)\mathcal{W}(1,4) \times \{ \Pi_{j,\gamma\gamma}(4,5|3)\mathcal{G}_{\gamma\gamma}(5,4^+) + \mathcal{G}_{\gamma\gamma}(4,5)\Pi_{j,\gamma\gamma}(5,4^+|3) \}\mathcal{W}(5,2). \quad (76)$$

In general we have to solve for the vertex $\Lambda$ (diagrammatically in Fig. 2) and then calculate the response from Eq. (51).

## III. THE VERTEX EQUATION IN FREQUENCY SPACE

For practical calculations, it is suitable to transform the vertex equation into Fourier space and to use basis functions for the space variables. We define the vertex to be

$$\Lambda^j_{\alpha\beta}(1,2,3) = \frac{\delta \Sigma_{\alpha\beta}(1,2)}{\delta \varphi_j(3)}. \quad (77)$$

After taking the functional derivative with respect to $\phi$ we assume that the Green's function is now diagonal in spin space. From Eqs. (66) and (50) we obtain

$$\Lambda^j_{\alpha\beta}(1,2,3) = -\mathcal{W}(1,2)\mathcal{G}_{\alpha\mu}(1,4)\{ \epsilon^{-1}_{j,\mu\nu}(4,3)\mathcal{G}_{\nu\beta}(4,2) + \Lambda^j_{\mu\nu}(4,5,3)\mathcal{G}_{\nu\beta}(5,2) \}$$
$$= -\mathcal{W}(1,2)\mathcal{G}_{\alpha}(1,4)\{ \epsilon^{-1}_{j,\alpha\beta}(4,3)\mathcal{G}_{\beta}(4,2) + \Lambda^j_{\alpha\beta}(4,5,3)\mathcal{G}_{\beta}(5,2) \}$$
$$= -\mathcal{W}(1,2)\mathcal{G}_{\alpha}(1,4)\{ \sigma^j_{\alpha\beta}\delta(3-4)\mathcal{G}_{\beta}(4,2) + \Lambda^j_{\alpha\beta}(4,5,3)\mathcal{G}_{\beta}(5,2) \}. \quad (78)$$

In the last line we have assumed that $\alpha \neq \beta$ since this is the case of interest. This equation should depend on relative time only, not on absolute time. We therefore have

$$\Lambda^j_{\alpha\beta}(1,2,3) = \Lambda^j_{\alpha\beta}(1,2,3;\tau_1-\tau_3,\tau_3-\tau_2)$$
$$= \frac{1}{\beta^2} e^{-i\nu_m(\tau_1-\tau_3)} e^{i\nu_n(\tau_2-\tau_3)} \Lambda^j_{\alpha\beta}(1,2,3;\nu_m,\nu_n)$$
$$= \frac{1}{\beta^2} e^{-i\nu_m\tau_1} e^{i\nu_n\tau_2} \Lambda^j_{\alpha\beta}(1,2,3;\nu_m,\nu_n). \quad (79)$$

We have set $\tau_3 = 0$ in the last line since we can choose $\tau_3$ as a reference point. Similarly, we have

$$\mathcal{G}_{\alpha}(1,4) = \frac{1}{\beta} e^{-i\nu_n(\tau_1-\tau_4)} \mathcal{G}_{\alpha}(1,4;\nu_n), \quad (80)$$

$$\mathcal{W}(1,2) = \frac{1}{\beta} e^{-i\omega_m(\tau_1-\tau_2)} \mathcal{W}(1,2;\omega_m), \quad (81)$$

Since $\mathcal{W}$ is bosonic, the frequency is even as in Eq. (11). At this point we should keep in mind that repeated indices or variables are to be summed or integrated.

Using these Fourier expansions in Eq. (78), multiplying both sides by $\exp(i\nu_m\tau_1)$ and $\exp(-i\nu_n\tau_2)$ and integrating over $\tau_1$ and $\tau_2$ we obtain

$$\Lambda^j_{\alpha\beta}(1,2,3;\nu_m,\nu_n)+\frac{1}{\beta}\mathcal{W}(1,2;\omega_k)\mathcal{G}_\alpha(1,4;\nu_m-\omega_k)\times\mathcal{G}_\beta(5,2;\nu_n-\omega_k)\Lambda^j_{\alpha\beta}(4,5,3;\nu_m-\omega_k,\nu_n-\omega_k)=-\frac{1}{\beta}\mathcal{W}(1,2;\omega_k)\mathcal{G}_\alpha(1,3;\nu_m-\omega_k)\sigma^j_{\alpha\beta}\mathcal{G}_\beta(3,2;\nu_n-\omega_k). \tag{82}$$

The frequency dependence of the screened interaction $\mathcal{W}$ makes the equation very difficult to solve. Much simplification is achieved when we assumed that $\mathcal{W}$ is static:

$$\mathcal{W}(1,2;\tau_1-\tau_2)\approx\mathcal{W}(1,2)\,\delta(\tau_1-\tau_2), \tag{83}$$

where

$$\mathcal{W}(1,2)=\int d\tau\,\mathcal{W}(1,2;\tau). \tag{84}$$

With this static approximation, the vertex $\Lambda$ depends only on one frequency and the vertex equation becomes

$$[\delta(1-4)\delta(2-5)-\mathcal{W}(1,2)\mathcal{K}_{\alpha\beta}(12,45;\omega_m)]\Lambda^j_{\alpha\beta}(4,5,3;\omega_m)=\frac{1}{\beta}\mathcal{W}(1,2)\sigma^j_{\alpha\beta}\mathcal{K}_{\alpha\beta}(12,33;\omega_m), \tag{85}$$

where we have defined the kernel $\mathcal{K}$ as

$$\mathcal{K}_{\alpha\beta}(12,45;\omega_m)=-\frac{1}{\beta}\mathcal{G}_\alpha(1,4;\omega_m+\nu_k)\mathcal{G}_\beta(5,2;\nu_k). \tag{86}$$

Using a noninteracting Green's function,

$$\mathcal{G}_\alpha(1,2;\nu_m)=\frac{\psi_{\mathbf{k}n\alpha}(1)\psi^*_{\mathbf{k}n\alpha}(2)}{i\nu_m-\varepsilon_{\mathbf{k}n\alpha}}, \tag{87}$$

the sum over frequencies in the kernel can be performed analytically (see, e.g., p. 272 of Ref. 13) which gives

$$\mathcal{K}_{\alpha\beta}(12,45;\omega_m)=\psi_{\mathbf{k}n\alpha}(1)\psi^*_{\mathbf{k}'n'\beta}(2)\psi^*_{\mathbf{k}n\alpha}(4)\psi_{\mathbf{k}'n'\beta}(5)\times\frac{f(\varepsilon_{\mathbf{k}n\alpha})-f(\varepsilon_{\mathbf{k}'n'\beta})}{i\omega_m+\varepsilon_{\mathbf{k}'n'\beta}-\varepsilon_{\mathbf{k}n\alpha}}. \tag{88}$$

The problem is then to invert the expression in the bracket on the left-hand side of Eq. (85). The space variable 3 is not involved in the inversion and may therefore be fixed. The vertex is expected to be short-range but nevertheless nonlocal (orbital dependent). A suitable basis for this problem is the LMTO (linear muffin-tin orbital)[26] basis. The Bloch wave functions in the LMTO method is expanded as follows:

$$\psi_{\mathbf{k}n\alpha}=\chi^{\mathbf{k}}_{RL\alpha}b_{RL}(\mathbf{k}n\alpha). \tag{89}$$

$R$ labels the atoms in the unit cell. The basis functions have the form

$$\chi^{\mathbf{k}}_{RL\alpha}=\phi_{RL\alpha}+\dot\phi_{R'L'\alpha}h_{R'L',RL}(\mathbf{k}), \tag{90}$$

where $\dot\phi_{RL\alpha}$ is the energy derivative of $\phi_{RL\alpha}$ calculated at some energy usually chosen to be the center gravity of the band. In the LMTO basis the kernel $\mathcal{K}$ is then given by

$$\mathcal{K}_{\alpha\beta}(12,45;\omega_m)=\chi^{\mathbf{k}}_{R_1L_1\alpha}(1)\chi^{\mathbf{k}'*}_{R_2L_2\beta}(2)\chi^{\mathbf{k}*}_{R_4L_4\alpha}(4)\chi^{\mathbf{k}'}_{R_5L_5\beta}(5)\times b_{R_1L_1}(\mathbf{k}n\alpha)b^*_{R_2L_2}(\mathbf{k}'n'\beta)\times b^*_{R_4L_4}(\mathbf{k}n\alpha)b_{R_5L_5}(\mathbf{k}'n'\beta)\times\frac{f(\varepsilon_{\mathbf{k}n\alpha})-f(\varepsilon_{\mathbf{k}'n'\beta})}{i\omega_m+\varepsilon_{\mathbf{k}'n'\beta}-\varepsilon_{\mathbf{k}n\alpha}}. \tag{91}$$

The $\mathbf{k}$ dependence of the basis functions makes the inversion of the vertex equation very difficult to perform. In most cases, the $\dot\phi_{RL}$ term is much smaller than the $\phi_{RL}$ term and we may neglect the $\dot\phi_{RL}$ term. Furthermore, we make an onsite approximation where $R_1=R_2=R_3=R_4=R$. With these approximations, the kernel becomes

$$\mathcal{K}_{\alpha\beta}(12,45;\omega_m)=\phi_{RL_1\alpha}(1)\phi^*_{RL_2\beta}(2)\times\mathcal{K}^R_{\alpha\beta}(L_1L_2,L_4L_5;\omega_m)\times\phi^*_{RL_4\alpha}(4)\phi_{RL_5\beta}(5), \tag{92}$$

where

$$\mathcal{K}^R_{\alpha\beta}(L_1L_2,L_4L_5;\omega_m)=b_{RL_1}(\mathbf{k}n\alpha)b^*_{RL_2}(\mathbf{k}'n'\beta)b^*_{RL_4}(\mathbf{k}n\alpha)b_{RL_5}(\mathbf{k}'n'\beta)\times\frac{f(\varepsilon_{\mathbf{k}n\alpha})-f(\varepsilon_{\mathbf{k}'n'\beta})}{i\omega_m+\varepsilon_{\mathbf{k}'n'\beta}-\varepsilon_{\mathbf{k}n\alpha}}. \tag{93}$$

Although the $\mathbf{k}$ dependence of the basis function is neglected, the $\mathbf{k}$ dependence of the eigenvalues and the eigenvectors are retained in the kernel $\mathcal{K}$.

Using the above expression for the kernel in Eq. (85), multiplying both sides by $\phi^*_{RL\alpha}(1)\phi_{RL'\beta}(2)$ and integrating over space variables 1 and 2 we obtain for a given $\omega_m$, $R$ and space variable 3

$$[\delta_{LL_4}\delta_{L'L_5}-\mathcal{W}^R_{\alpha\beta}(LL',L_1L_2)\times\mathcal{K}^R_{\alpha\beta}(L_1L_2,L_4L_5;\omega_m)]\Lambda^{jR}_{\alpha\beta}(L_4L_5,3;\omega_m)=\mathcal{Q}^{jR}_{\alpha\beta}(LL',3;\omega_m), \tag{94}$$

where

$$\Lambda^{jR}_{\alpha\beta}(LL',3;\omega_m)=\phi^*_{RL\alpha}(1)\Lambda^j_{\alpha\beta}(1,2,3;\omega_m)\phi_{RL'\beta}(2), \tag{95}$$

$$\mathcal{W}^R_{\alpha\beta}(L_1L_2,L_3L_4)=\phi^*_{RL_1\alpha}(1)\phi_{RL_2\beta}(2)\mathcal{W}(1,2)\times\phi_{RL_3\alpha}(1)\phi^*_{RL_4\beta}(2), \tag{96}$$

$$\mathcal{Q}^{jR}_{\alpha\beta}(LL',3;\omega_m)=\sigma^j_{\alpha\beta}\mathcal{W}^R_{\alpha\beta}(LL',L_1L_2)\times\mathcal{K}^R_{\alpha\beta}(L_1L_2,L_4L_5;\omega_m)\times\phi^*_{RL_4\alpha}(3)\phi_{RL_5\beta}(3). \tag{97}$$

Equation (94) is now readily used in practical calculations and can be straightforwardly solved by inverting the expression in the bracket on the left-hand side. When solving for $\Lambda$

the relevant quantity on the right-hand side is $\mathcal{W}_{\alpha\beta}$. The other quantities are not involved in the inversion process. The problem is very similar to solving the Bethe-Salpeter equation in the $T$-matrix approach[27] or in excitonic problems.[28,29]

It is straightforward to calculate the Fourier component of the full response function in Eq. (51) by multiplying the equation with $\exp[i\omega_n(\tau_1-\tau_2)]$ and integrating over $\tau=\tau_1-\tau_2$:

$$\mathcal{R}_{ij}(1,2;\omega_n)=-\sigma^i_{\beta\alpha}\sigma^j_{\alpha\beta}\mathcal{K}_{\alpha\beta}(11,22;\omega_n) - \sigma^i_{\beta\alpha}\mathcal{K}_{\alpha\beta}(11,45;\omega_n)\Lambda^j_{\alpha\beta}(4,5,2;\omega_n). \tag{98}$$

The $\mathbf{q}$ component of the response function is obtained by taking the matrix element

$$\begin{aligned}\mathcal{R}_{ij}(\mathbf{q},\omega_n)&=\int d^3r\, d^3r' \times\exp(-i\mathbf{q}\cdot\mathbf{r})\mathcal{R}_{ij}(\mathbf{r},\mathbf{r}';\omega_n)\exp(i\mathbf{q}\cdot\mathbf{r}')\\ &=-\sigma^i_{\beta\alpha}\sigma^j_{\alpha\beta}\langle\mathbf{q}|\phi_{RL_1\alpha}\phi^*_{RL_2\beta}\rangle \times[\mathcal{K}^R_{\alpha\beta}(L_1L_2,L_3L_4;\omega_n) + \mathcal{T}^R_{\alpha\beta}(L_1L_2,L_3L_4;\omega_n)]\langle\phi^*_{RL_3\alpha}\phi_{RL_4\beta}|\mathbf{q}\rangle,\end{aligned} \tag{99}$$

where

$$\langle\mathbf{q}|\phi_{RL_1\alpha}\phi^*_{RL_2\beta}\rangle=\int d^3r\exp(-i\mathbf{q}\cdot\mathbf{r})\phi_{RL_1\alpha}(\mathbf{r})\phi^*_{RL_2\beta}(\mathbf{r}) \tag{100}$$

and schematically

$$\mathcal{T}=\mathcal{K}[1-\mathcal{W}K]^{-1}\mathcal{W}\mathcal{K}. \tag{101}$$

The response function is then continued analytically to real frequencies $\omega_n\rightarrow\omega+i\delta$ and the imaginary part gives the spin-wave spectrum.

## IV. SPIN WAVES

The energy needed to flip a spin of a particular electron is given by the exchange interaction. For a ferromagnet of delocalized electrons, this means an interband transition of an electron into the corresponding exchange-shifted band (Stoner excitations). Thus the minimum energy necessary for a spin flip is given by the energy separation between the upper edge of the majority spin band and the Fermi level. However, there exists also a collective excitation state, in which one spin is reversed, but only as an average over the whole solid. This so called spin wave can, similar to plasmons, decay into single-particle excitations. Neutron scattering allows an experimental determination of the dispersion curve $\omega(\mathbf{q})$, where $\mathbf{q}$ is the difference between the incident and scattered neutron wave vectors, respectively, and $\omega$ is the energy loss.

The spin-wave excitation spectrum is given by the spectral function of the following spin-spin density correlation function:

$$\mathcal{R}^{-+}(1,2)=-\frac{\langle\mathcal{T}\hat{\mathcal{S}}\hat{\sigma}^-(1)\hat{\sigma}^+(2)\rangle}{\langle\hat{\mathcal{S}}\rangle}, \tag{102}$$

where

$$\hat{\sigma}^+\equiv\hat{\sigma}^x+i\hat{\sigma}^y,\quad \hat{\sigma}^-\equiv\hat{\sigma}^x-i\hat{\sigma}^y. \tag{103}$$

Following the same analysis leading to Eq. (45), the spectral function $S^{-+}=|\mathrm{Im}\,R^{-+}|/\pi$ is given by

$$S^{-+}(\mathbf{r},\mathbf{r}',\omega)\equiv Z_0^{-1}\sum_{jk}e^{-\beta(E_j-\mu N)}(1-e^{-\beta\omega})\langle j|\hat{\sigma}^-(\mathbf{r})|k\rangle \times\langle k|\hat{\sigma}^+(\mathbf{r}')|j\rangle\delta(\omega-E_k+E_j). \tag{104}$$

The physical meaning of $\hat{\sigma}^+(\mathbf{r})$ is that it increases the spin of an electron at $\mathbf{r}$ by 1. The spin of the states $|k\rangle$ must therefore be larger by 1 than that of the states $|j\rangle$, i.e., the states $|k\rangle$ contain a spin-wave excitation. Thus a peak in $S^{-+}$ may be identified with a spin-wave excitation.

The quantity $R^{-+}$ is related to the response functions. The spin-density response is given by ($\hat{\sigma}^i\equiv\hat{\sigma}^i_D$)

$$\begin{aligned}\frac{\delta\langle\hat{\sigma}^i(1)\rangle}{\delta\varphi_j(2)}&=\frac{\delta}{\delta\varphi_j(2)}[\sigma^i_{\beta\alpha}\mathcal{G}_{\alpha\beta}(1,1^+)]\\ &=\frac{\delta}{\delta\varphi_j(2)}\frac{\langle\mathcal{T}\hat{\mathcal{S}}\hat{\sigma}^i(1)\rangle}{\langle\hat{\mathcal{S}}\rangle}\\ &=-\frac{\langle\mathcal{T}\hat{\mathcal{S}}\hat{\sigma}^i(1)\hat{\sigma}^j(2)\rangle}{\langle\hat{\mathcal{S}}\rangle}+\frac{\langle\mathcal{T}\hat{\mathcal{S}}\hat{\sigma}^i(1)\rangle\langle\mathcal{T}\hat{\mathcal{S}}\hat{\sigma}^j(2)\rangle}{\langle\hat{\mathcal{S}}\rangle^2}\\ &=-\frac{\langle\mathcal{T}\hat{\mathcal{S}}\tilde{\sigma}^i(1)\tilde{\sigma}^j(2)\rangle}{\langle\hat{\mathcal{S}}\rangle},\end{aligned} \tag{105}$$

where

$$\tilde{\sigma}^i=\hat{\sigma}^i-\langle\hat{\sigma}^i\rangle. \tag{106}$$

We can write

$$\hat{\sigma}^-\hat{\sigma}^+=(\hat{\sigma}^x-i\hat{\sigma}^y)\hat{\sigma}^x+(\hat{\sigma}^y+i\hat{\sigma}^x)\hat{\sigma}^y. \tag{107}$$

Defining

$$\frac{\delta}{\delta\varphi^+}\equiv\frac{\delta}{\delta\varphi^x}+i\frac{\delta}{\delta\varphi^y}, \tag{108}$$

$$\frac{\delta}{\delta\varphi^-}\equiv\frac{\delta}{\delta\varphi^x}-i\frac{\delta}{\delta\varphi^y}, \tag{109}$$

the quantity $\mathcal{R}^{-+}$ can then be written as

$$\mathcal{R}^{-+}(1,2)=\frac{\delta\langle\hat{\sigma}^-(1)\rangle}{\delta\varphi^+(2)} \tag{110}$$

or schematically

$$\mathcal{R}^{-+}=\mathcal{R}_{xx}+\mathcal{R}_{yy}+i[\mathcal{R}_{xy}-\mathcal{R}_{yx}]. \tag{111}$$

*We have assumed that* $\langle \hat{\sigma}^x \rangle = \langle \hat{\sigma}^y \rangle = 0$, i.e., the initial state has no spin component along the *x* and *y* directions.

## V. CONCLUDING REMARKS

In conclusion, we have presented a scheme for performing *ab initio* calculations of the linear magnetic susceptibility. The method is based on the Matsubara Green's function and the Schwinger functional derivative technique. The kernel describing multiple-scattering events between electron-hole pairs is given by the solution to a Bethe-Salpeter equation. The screened interaction $W(\mathbf{r}\tau,\mathbf{r}'\tau')$ between electron and hole propagators can be obtained, at least within RPA.[30]

We discuss the advantages of the Schwinger approach over the conventional diagrammatic approach. For condensed matter problems involving large or infinite systems, the Schwinger approach seems to provide a natural way of calculating the self-energy where the main quantity is the physical response function. It is reasonable to expect that the approach overcomes some of the problems associated with the straightforward expansion of the self-energy in powers of the screened interaction as is commonly done in the conventional diagrammatic approach. We would like to point out also that our definition of the Green's function in Eq. (25) for zero temperature does not require the usual assumption about adiabatic connection.

The results for the transverse susceptibility presented by Savrasov[12] are very promising. However, the spin-wave dispersion curve for Ni deviates significantly at higher energies, compared to experimental data. The observed discrepancies were attributed to the LDA exchange-correlation interaction. Thus it is tempting to investigate if a *nonlocal* interaction can cure these problems. Application of the present formalism to some transition metals is currently in progress.


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$$\hat{H}_0 = \sum_\alpha \int d^3r\, \hat{\psi}^\dagger_\alpha(\mathbf{r})(-\nabla^2_{\mathbf{r}}/2)\hat{\psi}_\alpha(\mathbf{r}) + \frac{1}{2}\sum_{\alpha\beta}\int d^3r\, d^3r'\, \hat{\psi}^\dagger_\alpha(\mathbf{r})\hat{\psi}^\dagger_\beta(\mathbf{r}')v(\mathbf{r}-\mathbf{r}')\hat{\psi}_\beta(\mathbf{r}')\hat{\psi}_\alpha(\mathbf{r}).$$

[16] The spin-orbit contribution $\Sigma_{\alpha\beta}\int d^3r\, \hat{\psi}^\dagger_\alpha(\mathbf{r})[\mathbf{E}(\mathbf{r})\cdot(\mathbf{p}\times\vec{\sigma})]_{\alpha\beta}\hat{\psi}_\beta(\mathbf{r})$ is not included in the Hamiltonian. $\mathbf{E}(\mathbf{r})$ is the periodic electrostatic field from the ions and $\mathbf{p} = -i\nabla_{\mathbf{r}}$.

[17] The left-hand side of Eq. (14) will contain the term $\Sigma_\gamma \phi_{\alpha\gamma}(1)\mathcal{G}_{\gamma\beta}(1,2)$. The Heisenberg field operators in the Green function now have a time dependence given by $\hat{\psi}_\alpha(\mathbf{r},\tau) = \hat{\mathcal{U}}^\dagger_s(\tau,\tau_0)\hat{\psi}_\alpha(\mathbf{r})\hat{\mathcal{U}}_s(\tau,\tau_0)$ where $\hat{\mathcal{U}}_s(\tau,\tau_0) = \mathcal{T}\exp[-\int_{\tau_0}^{\tau} d\tau' \hat{K}(\tau')]$.

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[22] It means that the total charge is $\langle\sigma^0(1)\rangle$, $\langle\sigma^x(1)\rangle = \langle\sigma^y(1)\rangle = 0$ and the magnetization $\langle\sigma^z(1)\rangle = m(1)$. The transverse response function corresponds to magnetic field in *xy* plane and the longitudinal response to a field in *z* direction.

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