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Generalized Hedin equations and $\sigma G \sigma W$ approximation for quantum many-body systems with spin-dependent interactions

Ferdi Aryasetiawan[1,2,3] **and Silke Biermann**[3,4]

[1] Graduate School of Advanced Integration Science, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba-shi, Chiba 263-8522, Japan
[2] Research Institute for Computational Sciences, AIST, 1-1-1 Umezono, Tsukuba Central 2, Tsukuba, Ibaraki 305-8568, Japan
[3] Japan Science and Technology Agency, CREST, Japan
[4] Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France

E-mail: biermann@cpht.polytechnique.fr

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Abstract
The Hedin equations for the electron self-energy and the vertex were originally derived for a many-electron system with Coulomb interaction (Hedin 1965 *Phys. Rev.* **139** A796). Here, we present a generalized set of Hedin equations for quantum many-body systems containing spin-dependent interactions, e.g. spin–orbit and spin–spin interactions. The corresponding spin-dependent GW approximation is constructed. This work should open the way to describing the interplay of correlations and spin-dependent interactions in systems such as quantum dots or wires, as well as in interface and surface problems.

1. Introduction

During the last decades many materials with intriguing properties have been discovered. In many of these new materials the properties depend directly or indirectly on the electron spin degree of freedom. Some important examples are spintronics devices, colossal magnetoresistance materials or magnetic impurities in semiconductors. A proper description of the interplay between spin, charge and orbital degrees of freedom is crucial for understanding the electronic properties of these new materials. It is therefore timely to generalize one of the most important first-principles many-body methods used nowadays for describing electronic excitations, the Hedin equations, to spin-dependent interactions. These equations provide an iterative scheme for an expansion of the self-energy in powers of the screened interaction. In particular, the lowest-order approximation leads to the GW approximation (GWA) [1–3] which has proven very successful in studying one-particle excitation energies of real materials entirely from first-principles.

Spin-dependent interactions can be crucial, despite the tiny energy scales associated with them. To cite an example, the conduction band spin splitting in zinc blende semiconductors arising from spin–orbit coupling is only tens of meV and yet it is important for applications in spintronics: it determines the spin lifetimes and can induce a spin current in the absence of a magnetic field, the so-called Rashba effect [5]. In some cases, such as gold, spin–orbit coupling can alter the band structure rather significantly, by about an eV [4]. The spin density wave in chromium is another example where it is important to take into account spin variables. The spin-dependent interactions may arise from relativistic effects, such as spin–orbit coupling, or from an external perturbation, as in the case of a magnetic impurity in a semiconductor.

2. Spin dependence in GW calculations and models

In Hubbard-like models, it appears that the effective interaction or the Hubbard U depends on the spin variable, despite the absence of explicitly spin-dependent interactions in the Hamiltonian of the real system upon which the model is based [6]. Upon closer examination it becomes clear that the spin dependence actually arises from the basis-set expansion. Thus, the spin flip processes from one orbital to another are virtual processes, rather than real physical processes.

Consistently, in deriving the closed set of Hedin equations, starting from a many-body Hamiltonian with purely Coulombic interaction, it turns out that the screened interaction has no spin dependence when the derivation is performed in a real space representation without introducing a set of spin-dependent basis functions. Although the self-energy may depend on the spin variable, this dependence arises solely from a possible spin dependence in the Green function. Indeed it can be shown that the linear response of the self-energy with respect to the magnetic field vanishes when the many-body Hamiltonian is purely Coulombic. The magnetic-field-dependent term is only of one-particle type, giving no self-energy contribution. The dependence of the self-energy on the magnetic field arises when the many-body Hamiltonian contains terms which are explicitly spin dependent. Thus, in the following, we consider a system of electrons with *explicitly* spin-dependent interactions as described by the Hamiltonian

$$\hat{H}_0 = \sum_{\kappa} \int \mathrm{d}^3 r\ \hat{\psi}^+_\kappa(\mathbf{r}) h_0(\mathbf{r}) \hat{\psi}_\kappa(\mathbf{r}) + \tfrac{1}{2} \sum_{\kappa\beta\gamma\eta} \int \mathrm{d}^3 r\, \mathrm{d}^3 r' \times \hat{\psi}^+_\kappa(\mathbf{r}) \hat{\psi}^+_\beta(\mathbf{r}') v_{\kappa\gamma\beta\eta}(\mathbf{r}, \mathbf{r}') \hat{\psi}_\eta(\mathbf{r}') \hat{\psi}_\gamma(\mathbf{r}) \quad (1)$$

where h_0 is the one-particle Hamiltonian. The identity of the particles implies that the second term is invariant under particle interchange: $v_{\kappa\gamma\beta\eta}(\mathbf{r}, \mathbf{r}') \leftrightarrow v_{\beta\eta\kappa\gamma}(\mathbf{r}', \mathbf{r})$.

3. The Hedin equations for spin-dependent interactions

Starting from the above Hamiltonian we have derived the following closed set of Hedin equations (for a detailed derivation we refer to [7]):

$$\Sigma_{\alpha\beta}(1,2) = -\sigma^I_{\alpha\eta} \mathcal{G}_{\eta\gamma}(1,4) \Lambda^J_{\gamma\beta}(4,2,5) W_{JI}(5,1), \quad (2)$$

$$W_{IJ}(1,2) = v_{IJ}(1,2) + v_{IK}(1,3) P_{KL}(3,4) W_{LJ}(4,2), \quad (3)$$

$$P_{IJ}(1,2) = \sigma^I_{\alpha\beta} \mathcal{G}_{\beta\gamma}(1,3) \Lambda^J_{\gamma\eta}(3,4,2) \mathcal{G}_{\eta\alpha}(4,1^+), \quad (4)$$

$$\Lambda^I_{\alpha\beta}(1,2,3) = \delta(1-2)\delta(2-3)\sigma^I_{\alpha\beta} \quad (5)$$

$$+ \frac{\delta \Sigma_{\alpha\beta}(1,2)}{\delta \mathcal{G}_{\gamma\eta}(4,5)} \mathcal{G}_{\eta\eta'}(4,6) \Lambda^I_{\eta'\kappa}(6,7,3) \mathcal{G}_{\kappa\gamma}(7,5). \quad (6)$$

The Dyson equation needed to close the loop is

$$\mathcal{G}_{\alpha\beta}(1,2) = \mathcal{G}^0_{\alpha\beta}(1,2) + \mathcal{G}^0_{\alpha\gamma}(1,3) \Sigma_{\gamma\eta}(3,4) \mathcal{G}_{\eta\beta}(4,2). \quad (7)$$

Here, σ^i, $i = x, y, z$, are the Pauli spin matrices and σ^0 is defined to be a 2×2 unit matrix. Capital letter indices run over $0, x, y, z$, while Greek letters take the spin variable values ± 1. We use the following common shorthand notation: $(\mathbf{x}\tau)$ is represented by a number, repeated indices are summed and repeated variables represented by numbers are integrated, unless they appear on both sides of the equation. For clarity, we further adopt a notation that quantities with a subscript denoted by capital letter do not depend on spin, such as P_{IJ}. The spin-dependent interaction has been expanded in the Pauli and unit matrices as

$$v_{\alpha\eta\kappa\gamma}(1,2) = \sigma^I_{\alpha\eta} v_{IJ}(1,2) \sigma^J_{\kappa\gamma}. \quad (8)$$

As can be seen clearly in the above set of equations, the screened interaction expresses an interdependence between the charge and spin responses. Thus, a change in the charge density induces spin fluctuations, and vice versa. It is also clear that the self-energy is now a truly spin-dependent quantity in the sense that it is affected by the spin fluctuations as opposed to its spin dependence originating from the electron propagator or the Green function, which is already the case in the original Hedin equations. The vertex Λ is now a rather complex quantity reflecting the intricate interplay between the change of the self-energy with respect to the electric field and the change with respect to the magnetic field.

The spin-Hedin equations can be applied, for example, to Hamiltonians containing interactions of the following form:

$$v_{\alpha\gamma\beta\eta}(\mathbf{r}, \mathbf{r}') = \begin{cases} \sigma^0_{\alpha\gamma} \sigma^0_{\beta\eta} / |\mathbf{r} - \mathbf{r}'|, \\ \sigma^i_{\alpha\gamma} J_{ij}(\mathbf{r}, \mathbf{r}') \sigma^j_{\beta\eta}, \\ \sigma^i_{\alpha\gamma} \mu_i(\mathbf{r}, \mathbf{r}') \sigma^0_{\beta\eta} \end{cases} \quad (9)$$

where the first is the usual Coulomb interaction, the second a spin–spin interaction and the third a spin–orbit interaction, which contains the angular momentum operator.

4. The $\sigma G \sigma W$ approximation and its interpretation

To appreciate the significance of the new set of Hedin equation it is constructive to consider a generalization of the Hedin GWA, by approximating the vertex functions by

$$\Lambda^I_{\alpha\beta}(1,2,3) = \delta(1-2)\delta(2-3)\sigma^I_{\alpha\beta}. \quad (10)$$

The polarization then becomes

$$P_{IJ}(1,2) = \sigma^I_{\alpha\beta} \mathcal{G}_{\beta\gamma}(1,2) \sigma^J_{\gamma\eta} \mathcal{G}_{\eta\alpha}(2,1^+) \quad (11)$$

yielding the self-energy

$$\Sigma^{\mathrm{GW}}_{\alpha\beta}(1,2) = -\sigma^I_{\alpha\eta} \mathcal{G}_{\eta\gamma}(1,2) \sigma^J_{\gamma\beta} W_{JI}(2,1). \quad (12)$$

To assess the physical meaning of these equations we first consider the special case of spin-independent interactions. Many materials in fact possess an inherent spin structure, such as a spin-spiral structure arising from exchange interaction but without an explicit spin-dependent interaction. In this case, the Green function acquires non-diagonal spin components and for a non-interacting Green function we have explicitly

$$\mathcal{G}^0_{\alpha\beta}(\mathbf{r}, \mathbf{r}'; \mathrm{i}\omega) = \sum_n \frac{\phi^*_{n\alpha}(\mathbf{r}) \phi_{n\beta}(\mathbf{r}')}{\mathrm{i}\omega - \varepsilon_n} \quad (13)$$

where $\phi_{n\alpha}$ and ε_n are some one-particle wavefunction and eigenenergy, respectively. The polarization is computed according to (11) but since the interaction is purely Coulombic, $v_{IJ} = v_{00}\delta_{IJ}\delta_{I0}$ and only the charge component P_{00} is needed:

$$P_{00}(1,2) = \mathcal{G}_{\alpha\gamma}(1,2) \mathcal{G}_{\gamma\alpha}(2,1^+). \quad (14)$$

The screened interaction is given by (3), which consequently only retains the charge channel:

$$W_{00}(1,2) = v_{00}(1,2) + v_{00}(1,3) P_{00}(3,4) W_{00}(4,2). \quad (15)$$

This is then used in (12) to construct the self-energy, which naturally acquires non-diagonal components in the spin space and we obtain a generalization of the original Hedin equations to a spin-dependent Green function and self-energy with purely Coulombic interaction:

$$\Sigma^{\mathrm{GW}}_{\alpha\beta}(1,2) = -\mathcal{G}_{\alpha\beta}(1,2)W_{00}(2,1). \tag{16}$$

This emerges naturally in the present formulation as a special case where explicitly spin-dependent interactions are absent. As can be seen in the above equation, the dependence of the self-energy on the spin variable arises entirely from the Green function rather than the screened interaction. Using this self-energy one solves the Dyson equation (7) to obtain a new Green function or one can also solve the quasiparticle equation

$$[h^0(1)\sigma^0_{\alpha\beta} + V^{\mathrm{H}}_{\alpha\beta}(1)]\psi_{n\beta}(1) + \Sigma^{\mathrm{GW}}_{\alpha\beta}(1,2;E_n)\psi_{n\beta}(2) = E_n\psi_{n\alpha}(1) \tag{17}$$

where $V^{\mathrm{H}}_{\alpha\beta} = V^{\mathrm{H}}_I\sigma^I_{\alpha\beta}$ is the generalized spin-dependent Hartree potential where

$$V^{\mathrm{H}}_I(1) = \rho_J(3)v_{JI}(3,1) \tag{18}$$

with the charge and spin density given by

$$\rho_I(1) = \mathcal{G}_{\gamma\kappa}(1,1^+)\sigma^I_{\kappa\gamma}. \tag{19}$$

Self-consistency may be reached by using the new Green function to calculate a new P, W and Σ. The cycle is continued until self-consistency is achieved, and in the case of spin–orbit coupling one obtains a self-consistent screened μ. Correlation effects on orbital moments and spin densities can then be accessed including life-time effects.

Let us now consider the case when the interaction is spin dependent, which may arise from purely spin–spin interaction or spin–orbit coupling, among other possibilities. A particle of up spin $\mathcal{G}^0_{\uparrow\uparrow}$ enters the self-energy $\Sigma_{\uparrow\uparrow}$. Upon entering the self-energy the electron spin is flipped to down spin by a spin operator $\sigma^i_{\uparrow\downarrow}$ and a magnon represented by W_{ij} is emitted. Upon leaving the self-energy the spin operator $\sigma^j_{\downarrow\uparrow}$ causes the electron to reabsorb the magnon and return to its original up spin configuration. This process is analogous to the original Hedin GWA whereby an electron emits and absorbs a plasmon but without the possibility of spin flip (upper panel of figure 1).

5. Conclusions

In conclusion, we have extended the original set of Hedin equations for many-electron systems with purely Coulombic interaction to systems with explicitly spin-dependent interactions. The charge and spin degrees of freedom are coupled through the equations: a change in the charge density induces a change in the spin density, and vice versa. The first-order self-energy term (in the spin-dependent screened interaction) leads to a generalized σGσW approximation. These equations allow for a truly first-principles study of a wide range of problems where correlation effects induced by spin interactions and the interplay between the charge and spin degrees of freedom play a crucial role in determining physical properties. We envisage applications to nanoscale magnetic systems ranging from quantum dots and quantum wires to magnetic impurities in semiconductors or nanoparticles, as well as to crystals with inherent spin structure and to film, surface and interface problems [8, 9]. From a theoretical point of view, the recently proposed GW + DMFT scheme [10] can also be extended to systems with explicitly spin-dependent interactions.

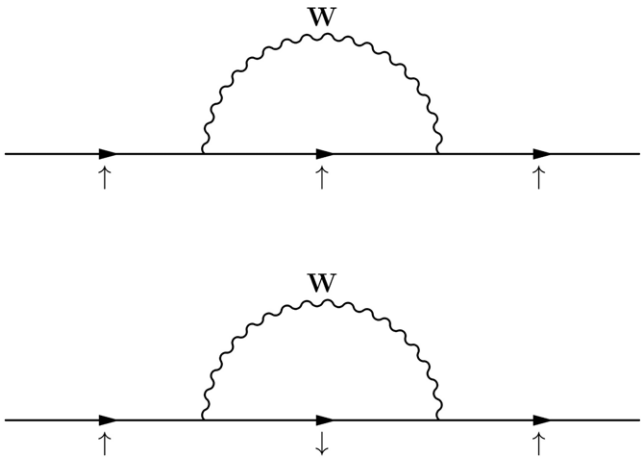

Figure 1. In the usual GWA only the diagram of the upper panel appears. The new σGσW approximation also includes the possibility of spin flips at the interaction vertices (see the diagram in the lower panel).

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