Point-like spin-dependent interaction in calculations of self-energy ladder diagrams

I. A. Nechaev1, I. Nagy2,1, P. M. Echenique1,3, and E. V. Chulkov1,3
1Donostia International Physics Center (DIPC), P. Manuel de Lardizabal 4, 20018 San Sebastián, Spain
2Department of Theoretical Physics, Institute of Physics, Technical University of Budapest, H-1521 Budapest, Hungary
3Departamento de Física de Materiales, Facultad de Ciencias Químicas, UPV/EHU and Centro Mixto CSIC-UPV/EHU, Apdo. 1072, 20080 San Sebastián, Spain

(Dated: March 23, 2022)

Abstract

An instantaneous and zero-range spin-dependent interaction, derived by summing an infinite number of electron-hole ladder diagrams within a local approximation, is analyzed as a function of the electron gas density and the relative spin polarization. The strength of such an interaction is defined by an integral of a statically screened Coulomb interaction with a spatially localized weighting factor. This weighting factor represents the mutually uncorrelated motion of an electron-hole pair in singlet or triplet spin states ($S^z = 0, \pm 1$). An implementation, based on a Yukawa-type interaction with a spin-polarization-dependent Thomas-Fermi screening length, is given.

PACS numbers: 71.10.-w

A rigorous study, based on quantum many-body perturbation theory as applied to excited quasiparticle states in itinerant ferromagnetic materials, requires an approach to the quasiparticle self-energy accounting for the contribution of both charge- and spin-density fluctuations. Within this approach, due to the correspondence between multiple electron-hole ($e - h$) scattering events and a spin fluctuation, the self-energy can be treated as an integral over the four-point $e - h$ scattering amplitude.

The theoretical problem, which appears already at the homogeneous electron gas level, lies in this amplitude and can be largely simplified in the following ways: (i) by using a point-like interaction with strength defined by the Hubbard $U$ parameter; (ii) by introducing a local pseudopotential obtained within some self-consistently closed procedure; (iii) by reducing an infinite set of diagrams to a local-field factor tabulated and parameterized by making use of accurate quantum Monte Carlo data for the electron gas.

Apart from the obvious theoretical interest for a prototype homogeneous system, real materials give an additional important challenge. In evaluating the quantities listed above, one should properly take into consideration the band-structure effects which surely influence calculated characteristics of excited quasiparticle states. However, the obtained results are very sensitive to an approximated form chosen for these quantities. Therefore, the question of how in ab initio calculations to sum an infinite number of diagrams, which contribute to the four-point $e - h$ scattering amplitude, is still open.

The standard formulation for excited states starts by defining a dynamical, spin-independent dielectric screening of the bare Coulomb interaction between two test charges. This concept of a polarizable medium allows a straightforward and successful implementation of the Hartree-Fock-like technique with such a screened interaction instead of the bare one (the GW method), since it is based on a complete set of single-particle states at the Hartree (mean-field) level. Thus the required approach naturally should start with the above screened interaction to consider multiple scattering effects in the important $e - h$ channel.

Here we present a theoretical study which rests on Hedin’s concept. We derive a point-like spin-dependent interaction. The foremost advantage of using the latter is that a number of many-body problems becomes more easily solvable. To achieve this goal we shall use the approach of Ref. [11] which was formulated for uniform systems in momentum space. This approach is based on a treatment of the self-energy ladder diagrams and does not contain adjustable parameters or quantities defined outside the scope of the approach. A key quantity of the approach is a local interaction $W_{\sigma}\sigma'$ that (i) ensures a simplification similar to Hubbard models, (ii) includes charge and spin fluctuations, and (iii) has a transparent connection with the exchange part of the many-body local field factor.

Accomplishing our goal, first, we perform a real-space analysis of the approach of Ref. [11]. Such an analysis allows one to derive basic equations of the approach to be applied to a broader spectrum of materials. Unless stated otherwise, atomic units, $e^2 = h = m = 1$, are used throughout this work. By applying standard notation for the coordinate, $\bar{1} \equiv (\sigma_1, r_1, \epsilon_1)$, in which the quasiparticle spin is denoted as $\sigma_1$, the Bethe-Salpeter equation defining the $e - h$ scattering amplitude (the $T$ matrix) can be written as

$$T(\bar{1}, \bar{2}|\bar{3}, \bar{4}) = T^0(\bar{1}, \bar{2}|\bar{1}', \bar{2}') \delta(\bar{1}' - \bar{3})\delta(\bar{2}' - \bar{4})$$
$$+ K^0(\bar{1}', \bar{2}'|\bar{3}', \bar{4}') T(\bar{3}', \bar{4}'|\bar{3}, \bar{4})$$

(1)

where $T^0(\bar{1}, \bar{2}|\bar{1}', \bar{2}')$ is the irreducible $e - h$ vertex and the free propagator for $e - h$ pair is given by the product of
the Green functions as $K^0(1, 2|1', 2') = iG(1, 1')G(2', 2)$. In Eq. (1), an integral over space-time coordinates and a sum over spin are implied for repeated variables. To perform a selective summation of ladder diagrams along the line of Hedin’s expansion for the self-energy in terms of a dynamically screened Coulomb interaction $W$, the irreducible $e - h$ vertex can be chosen as

$$T^0(1, 2|3, 4) = W(1, 2)\delta(1 - 3)\delta(2 - 4)\delta_{\sigma\sigma'}\delta_{\sigma\sigma'},$$

where in the right-hand side the spin variables are explicitly written out and space-time coordinates are abbreviated as $1 \equiv (r_1, t_1)$. As a result, the $T$ matrix is defined by the ladder approximation to the Bethe-Salpeter equation as

$$T_{\sigma\sigma'}(1, 2|3, 4) = W(1, 2)[\delta(1 - 3)\delta(2 - 4) + \int d1'd2'K^0_{\sigma\sigma'}(1, 2|1', 2') \times T_{\sigma\sigma'}(1', 2'|3, 4)],$$

(2)

where the $e - h$ propagator expressed in terms of the Green functions diagonal in spin space. In Eq. (2), there is no sum over spin implied and all integrals are written explicitly. The $T$ matrix describes propagation of a mutually correlated $e - h$ pair carrying spin $S^z = 0, \pm 1$. This correlation is realized by repeatedly interacting pair-constituents via $W(1, 2)$ in the intermediate state.

In real space, the approximation done in Ref. [11] results in the $T$ matrix given by

$$T_{\sigma\sigma'}(1, 2|3, 4) = \tilde{\Gamma}_{\sigma\sigma'}(1|4)\delta(1 - 2)\delta(3 - 4),$$

(3)

where

$$\tilde{\Gamma}_{\sigma\sigma'}(1|4) = \tilde{\Gamma}(1, 4) + \int d1'd2'\tilde{\Gamma}(1', 1') \times K^0_{\sigma\sigma'}(1', 1'|2', 2') \tilde{\Gamma}(2', 4).$$

(4)

The interaction $\tilde{\Gamma}_{\sigma\sigma'}(1, 4)$ is defined by the equation

$$\int d1'd2'K^0_{\sigma\sigma'}(1, 1|1', 1')\tilde{\Gamma}(1', 2')K^0_{\sigma\sigma'}(2', 2'|4, 4) = \int d1'd2'K^0_{\sigma\sigma'}(1, 1|1', 2')W(1', 2')K^0_{\sigma\sigma'}(1', 2'|4, 4).$$

(5)

The obtained $T$ matrix is a local one describing scattering processes in which the coordinates of the $e - h$ pair both for initial states and for final states coincide. This locality essentially simplifies the self-energy evaluation as an integral over the $T$ matrix. Actually, owing to Eqs. (5) and (4), the $T$-matrix contribution as an additional term to the GW self-energy $\Sigma_{GW}(1, 2) = iG_{\sigma}(1, 2)W(1, 2)$ can be cast into the $GW$-like form given by

$$\Sigma_{\sigma}(1, 2) = -i \sum_{\sigma'}G_{\sigma}(1, 2)T_{\sigma\sigma'}(1|2),$$

(6)

where

$$T_{\sigma\sigma'}(1|2) = \int d1'd2'\tilde{\Gamma}(1', 1')K^0_{\sigma\sigma'}(1', 1'|2', 2') \times \tilde{\Gamma}(2', 2) - \tilde{\Gamma}(2', 2).$$

(7)

Thus, in real space we have obtained the $T$-matrix contribution by exploiting the local approximation which seems to be reasonable for the corrections to the $GW$ term (see, e.g., Ref. [11]).

Now we can address to our main goal, deriving an instantaneous and zero-range potential

$$\tilde{W}_{\sigma\sigma'}(1, 2) = V^0_{\sigma\sigma'}(1 - 2).$$

(8)

It is obvious that in this case the irreducible $e - h$ vertex becomes highly local as in Hubbard models. Further, we will be guided by the results of Ref. [11], where for a uniform system and at small four-momentum transfer along the $e - h$ channel the local interaction $\tilde{W}_{\sigma\sigma'}$ was obtained to be constant in momentum space. Consequently, its real space equivalent corresponds to a $\delta$-function interaction we need: the resulting $T$ matrix has the form which can be obtained from Eq. (4) by using the zero-range spin-dependent interaction $\tilde{\Gamma}$ instead of $W(1, 2)$.

In terms of the noninteracting $e - h$ Green function

$$G^0_{\sigma\sigma'}(q, \omega) = \left[1 - n_F(\epsilon_{\sigma\sigma'})\right]n_F(\epsilon_{\sigma\sigma'}) \rho(\omega - \epsilon_{\sigma\sigma'}^T + i\eta)$$

$$- \frac{n_F(\epsilon_{\sigma\sigma'})\left[1 - n_F(\epsilon_{\sigma\sigma'})\right]}{\omega - \epsilon_{\sigma\sigma'}^T + i\eta},$$

where $n_F$ is the Fermi distribution function and the energy $\epsilon_{\sigma\sigma'}$ is measured from the Fermi energy $\epsilon_F$, the free $e - h$ propagator is given by

$$K^0_{\sigma\sigma'}(q, \omega) = \int \frac{dk}{(2\pi)^3} G^0_{\sigma\sigma'}(q, \omega).$$

We introduce a quantity which characterize the mutually uncorrelated motion of the $e - h$ pair as

$$\xi_{\sigma\sigma'}(r) = \frac{1}{K^0_{\sigma\sigma'}(0, 0)} \int \frac{dk}{(2\pi)^3} e^{ikr} \lim_{q \to 0} G^0_{\sigma\sigma'}(q, 0).$$

(9)

This quantity is unity at $r = 0$ and tends to zero as $\sim 1/r$ at $r \to \infty$. Thus, we can write the point-like interaction strength in real space as

$$V^0_{\sigma\sigma'} = \int dr\left|\xi_{\sigma\sigma'}(r)\right|^2 V(r),$$

(10)

with a statically screened Coulomb interaction denoted as $V(r) = W(r, \omega = 0)$. In this expression, $\left|\xi_{\sigma\sigma'}(r)\right|^2$ can be considered as a spatially localized weighting factor.

In models based on the underlying Hartree approach, the interaction in Eq. (10) can be approximated by a simple Yukawa form $(1/r)\exp(-\lambda r)$, where $\lambda$ specifies a characteristic length of the screening in the system [e.g., in Thomas-Fermi approximation $\lambda = \lambda_{TF} = (4k_F/\pi)^{1/2}$]. For completeness, we have to note that in Hartree-Fock-type approximations for electron-electron interactions the screening length can differ ($\lambda \sim k_F$) from the Thomas-Fermi one. Hedin’s expansion, being our basic frame in the present work, rests on $W(1, 2)$
which corresponds to the dielectric (Hartree) screening between two test charges.

In order to highlight the physical meaning of the quantities $\xi_{\sigma\sigma'}(r)$ and $V_{\sigma\sigma'}^0$ entering Eq. (10), first, we consider the homogenous electron gas (HEG) in the paramagnetic state. In this case $\xi_{\sigma\sigma}(r)$ [denoted as $\xi_p(r)$] can be easily found as $\xi_p(r) = j_0(k_F r)$, where $j_0$ is the spherical Bessel function of order 0 and $k_F$ is the Fermi wave vector. Thus, the point-like interaction of strength $V_p^0$ can be identified with the pseudopotential

$$V_p^0 = \frac{\pi}{k_F^2} \ln \left(1 + 4k_F^2/\lambda_{TF}^2\right), \quad (11)$$

that in a weak scattering regime reproduces the well-known expression for the interaction energy of the quasiparticles both of which are on the Fermi surface. This $V_p^0$ is inversely proportional to $k_F^2$, showing an expected behavior since the scattering has vanishing effect by growing density.

For a spin-polarized HEG, when the electron and the hole belong to the same $\sigma$ subsystem ($S^z = 0$), $\xi_{\sigma\sigma}(r) = j_0(k_F^s r)$, where the Fermi wave vector $k_F^s$ for spin $\sigma$ is expressed as $k_F^s = k_F(1 - \sigma \zeta) + \frac{1}{\sqrt{3}}$ with the paramagnetic value of $k_F$. Here $\sigma = +1$ for spin-up ($\uparrow$) and $\sigma = -1$ for spin-down ($\downarrow$), respectively. The relative spin polarization (SP) $\zeta$ is given by $\zeta = |n_\uparrow - n_\downarrow|/n$, where $n_\sigma$ is the spin $\sigma$ electron density, $n = n_\uparrow + n_\downarrow$ being the total electron density.

In addition to $\xi_{\sigma\sigma}(r)$, the $\zeta$ dependence of the strength $V_p^0$ comes from $\lambda_{TF}(\zeta) = \lambda_{TF} \sqrt{\frac{1}{2} \sum_{\sigma} (1 - \sigma \zeta)^{1/3}}$ obtained at the long-wave limit from the standard expression for the irreducible polarizability in the spin-polarized case. As a net result, $V_p^0$ has the same form as Eq. (11) but with $k_F^s$ and $\lambda_{TF}(\zeta)$ instead of $k_F$ and $\lambda_{TF}$, respectively.

Fig. 2 illustrates the spin-diagonal part of the interaction strength $V_{\sigma\sigma}^0$ over its value in the paramagnetic state as a function of $r_s$ at the SP $\zeta = 0.33, 0.67$, and 1.0. Inset: the ratio $\lambda_{TF}(\zeta)/\lambda_{TF}$ as a function of $\zeta$. 

FIG. 1: The spin-diagonal part of the point-like interaction strength $V_{\sigma\sigma}^0$ over its value in the paramagnetic state as a function of $r_s$ at the SP $\zeta = 0.33, 0.67$, and 1.0.

FIG. 2: The spin-non-diagonal part of $\xi_{\sigma\sigma'}$ as a function of $r$ at different values of the SP $\zeta$.

FIG. 3: The spin-diagonal part of the point-like interaction strength $V_{\sigma\sigma}^0$ over its value in the paramagnetic state as a function of $r_s$ at the SP $\zeta = 0.33, 0.67$, and 1.0. Inset: the ratio $\lambda_{TF}(\zeta)/\lambda_{TF}$ as a function of $\zeta$. 

Using the Yukawa form for $V(r)$, one obtains the following expression for the strength

$$V_p^0 = \frac{\pi}{k_F^2} \ln \left(1 + 4k_F^2/\lambda_{TF}^2\right), \quad (11)$$

that in a weak scattering regime reproduces the well-known expression for the interaction energy of the quasiparticles both of which are on the Fermi surface. This $V_p^0$ is inversely proportional to $k_F^2$, showing an expected behavior since the scattering has vanishing effect by growing density.

For a spin-polarized HEG, when the electron and the hole belong to the same $\sigma$ subsystem ($S^z = 0$), $\xi_{\sigma\sigma}(r) = j_0(k_F^s r)$, where the Fermi wave vector $k_F^s$ for spin $\sigma$ is expressed as $k_F^s = k_F(1 - \sigma \zeta) + \frac{1}{\sqrt{3}}$ with the paramagnetic value of $k_F$. Here $\sigma = +1$ for spin-up ($\uparrow$) and $\sigma = -1$ for spin-down ($\downarrow$), respectively. The relative spin polarization (SP) $\zeta$ is given by $\zeta = |n_\uparrow - n_\downarrow|/n$, where $n_\sigma$ is the spin $\sigma$ electron density, $n = n_\uparrow + n_\downarrow$ being the total electron density.

In addition to $\xi_{\sigma\sigma}(r)$, the $\zeta$ dependence of the strength $V_p^0$ comes from $\lambda_{TF}(\zeta) = \lambda_{TF} \sqrt{\frac{1}{2} \sum_{\sigma} (1 - \sigma \zeta)^{1/3}}$ obtained at the long-wave limit from the standard expression for the irreducible polarizability in the spin-polarized case. As a net result, $V_p^0$ has the same form as Eq. (11) but with $k_F^s$ and $\lambda_{TF}(\zeta)$ instead of $k_F$ and $\lambda_{TF}$, respectively.

Fig. 2 illustrates the spin-diagonal part of the interaction strength plotted as the ratio $V_{\sigma\sigma}^0/V_p^0$ for $r_s$ ranging from 2 to 6 (the metallic density range) at different $\zeta$ parameters. Due to the nontrivial $\zeta$ dependence resulting from $\xi_{\downarrow\downarrow}(r)$ and $V(r)$ with $\lambda_{TF}(\zeta)$ in the basic Eq. (10), as the SP increases $V_{\downarrow\downarrow}^0$ becomes greater or smaller than its value in the paramagnetic state at fixed $r_s$. On the other hand, the results for $V_{\downarrow\uparrow}/V_p^0$ show that at fixed $r_s$ the ratio demonstrates a monotonic increase with increasing $\zeta$. This increase becomes smaller as $r_s$ increases. However, at $\zeta \to 1$ limit this monotonic behavior together with decreasing $n_\uparrow$ can lead to a nontrivial
\[ \xi_{\parallel}(r) = \frac{1}{2} \sum_{\sigma} \left( 1 - \frac{\alpha}{\zeta} \right) \left[ j_0(k_F r) + j_2(k_F^2 r) \right]. \tag{12} \]

Note that \( \xi_{\parallel}(r) = \xi_{\parallel}(r) \) and at \( \alpha = 0, \xi_{\parallel}(r) = \xi_{\parallel}(r) \).

At the \( \alpha \rightarrow 1 \) limit, \( \xi_{\parallel}(r) \) tends to \( j_0(k_F r) + j_2(k_F^2 r) \).

Fig. 2 gives insight into the detailed (radial) behavior of the screening length \( \lambda_F(\zeta) \). As is evident from the figure, for \( r \) from zero to the mentioned node.

A comparison of Figs. 1 and 2 unambiguously shows that it is \( V_0^0 \) in the spin-diagonal part of the point-like interaction strength which exhibits the most strong changes as a function of the SP in the itinerant many-body system.

In conclusion, we have determined the real-space \( e-h \) scattering amplitude and its contribution to the quasiparticle self-energy within a local approximation by using, as a background, a variational momentum-space approach. We have shown that for low-energy quasiparticle excitations this amplitude can be expressed in terms of an instantaneous and zero-range spin-dependent pseudopotential. The strength \( V_0^0 \) of such a pseudopotential is defined by the volume integral of the screening Coulomb interaction with a weighting factor concerned with the mutually uncorrelated motion of the \( e-h \) pair carrying spin \( S^z = 0, \pm 1 \). The analysis carried out for the strength shows that the obtained results, due to the transparent dependencies on those physical variables which are based on Hedin's polarization concept, could be useful in attempts to go beyond the GW method in an \textit{ab initio} study on itinerant ferromagnets.

We thank V.V. Tugusheva for a critical reading of the manuscript and useful discussions. This work was partially supported by Departamento de Educación del Gobierno Vasco and MCyT (Grant No. FIS 2004-06490-C03-01). The work of I.N. was supported partly by the Hungarian OTKA (Grant Nos. T046868 and T049571).

---

\* Also at: Theoretical Physics Department, Kostroma State University, st. 1-st of May, 14, 156961 Kostroma, Russia.

1 A.L. Fetter and J.D. Walecka, Quantum Theory of Many-Particle Systems (McGraw-Hill, New York, 1971).

2 See, e.g. R. Knorren, K.H. Bennemann, R. Burgermeister, and M. Aeschlimann, Phys. Rev. B 61, 9427 (2000); V.P. Zhukov, E.V. Chulkov, and P.M. Echenique, Phys. Rev. Lett. 93, 096401 (2004); J. Schäfer, M. Hoinik, E. Rotenberg, P. Blaha, and R. Claessen, Phys. Rev. B 72, 155115 (2005); M. Cinchetti, M. Sánchez Albañeda, D. Hoffmann, T. Roth, J.-P. Wüstenberg, M. Krauß, O. Andrei, Y. Yoshimoto, and S. Tsuneyuki,, cond-mat/0510425 (unpublished); F. Aryasetiawan, K. Karlsson, O. Jepsen, and U. Schönberger, cond-mat/0603138 (unpublished).

3 S. Domiani and S. Engelsberg, Phys. Rev. Lett. 17, 750 (1966); W.F. Brinkman and S. Engelsberg, Phys. Rev. 169, 417 (1968).

4 C.J. Pethick and G.M. Carneiro, Phys. Rev. A 7, 304 (1973).

5 N.E. Bickers, in Theoretical Methods for Strongly Correlated Electrons, edited by D. Sénéchal, A.-M. Tremblay, and C. Bourbonnais (Springer, New York, 2004).

6 G.F. Giuliani and G. Vignale, Quantum Theory of the Electron Liquid (Cambridge University Press, Cambridge, England, 2005).

7 A. Liebsch, Phys. Rev. B 23, 5203 (1981); F. Manghi, V. Bellini, and C. Arcangeli, Phys. Rev. B 56, 7149 (1997).

8 See, e.g., F. Sottile, V. Olevano, and L. Reining, Phys. Rev. Lett. 91, 056402 (2003); G. Adragna, R. Del Sole, and A. Marini, Phys. Rev. B 68, 165108 (2003); S. Botti, F. Sottile, N. Vast, V. Olevano, L. Reining, H.-C. Weissker, A. Rubio, G. Onida, R. Del Sole, R. W. Godby, Phys. Rev. B 69, 155112 (2004).

9 See, e.g., F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A.I. Lichtenstein, Phys. Rev. B 70, 195104 (2004); I.V. Solovyev and M. Imada, ibid. 71, 045103 (2005); I.V. Solovyev, ibid. 73, 155117 (2006); K. Nakamura, R. Arita, Y. Yoshimoto, and S. Tsuneyuki,, cond-mat/0510425 (unpublished); F. Aryasetiawan, K. Karlsson, O. Jepsen, and U. Schönberger, cond-mat/0603138 (unpublished).

10 L. Hedin, Phys. Rev. 139, A796 (1965).

11 I.A. Nechaev and E.V. Chulkov, Phys. Rev. B 71, 115104 (2005).

12 Here \( S^z \) is an extra spin projection caused by exciting the \( e-h \) pair in the system and assigned to this pair.

13 N.E. Zein, S.Y. Savrasov, and G. Kotliar, Phys. Rev. Lett. 96, 226403 (2006).

14 I.A. Nechaev and E.V. Chulkov, Phys. Rev. B 73, 165112 (2006).

15 G.E. Engel, Phys. Rev. Lett. 78, 3515 (1997).

16 I. Nagy, J.I. Juaristi, R. Díez Muñoz, and P.M. Echenique, Phys. Rev. B 67, 073102 (2003).

17 M. Corona, P. Gori-Giorgi, and J.P. Perdew, Phys. Rev. B 69, 045108 (2004).

18 I. Nagy, R. Díez Muñoz, J.I. Juaristi, and P.M. Echenique, Phys. Rev. B 69, 233105 (2004).

19 K. Huang and C.N. Yang, Phys. Rev. 105, 767 (1957); A. Derevianko, Phys. Rev. A 72, 044701 (2005); Z. Idziaszek
and T. Calarco, Phys. Rev. Lett. 96, 013201 (2006).
20 T.L. Ainsworth and K.S. Bedell, Phys. Rev. B 35, 8425 (1987).
21 T. Moriya, Spin Fluctuations in Itinerant Electron Magnetism (Springer, Berlin, 1985).
22 Y. Zhang and S. Das Sarma, Phys. Rev. Lett. 95, 256603 (2005).