



Effect of spin fluctuations on quasiparticle excitations: First-principles theory and application to sodium and lithium

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We present first-principles calculations for quasiparticle excitations in sodium and lithium, including the effects of charge and spin fluctuations. We employ the Overhauser-Kukkonen form for the electron self-energy arising from spin fluctuations and demonstrate that the coupling of electrons to spin fluctuations gives an important contribution to the quasiparticle lifetime but does not significantly reduce the occupied bandwidth. Including correlation effects beyond the random-phase approximation in the screening from charge fluctuations yields good agreement with experiment.

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Introduction. The coupling of electrons to spin fluctuations causes many fascinating phenomena: For example, it has been proposed that spin fluctuations can “glue” electrons together to form Cooper pairs, giving rise to unconventional high-temperature superconductivity [1–4]. In particular, spin fluctuations were invoked to explain superconductivity in the cuprates [1–3] and recently also in the iron pnictide and chalcogenide materials [5–7]. In addition, it is well known that the coupling of spin fluctuations to electrons can affect the electronic effective mass and consequently transport properties and the specific heat.

Theoretically, the effect of spin fluctuations on quasiparticle excitations is usually calculated using model Hamiltonians. Early studies [8–10] constructed empirical theories including spin fluctuations based on the homogeneous electron gas and simple tight-binding models. More recently, many empirical theories involving spin fluctuations were constructed to investigate superconductivity in the cuprates and pnictides. In these theories the spin susceptibility is either parametrized using experimental neutron scattering and nuclear magnetic resonance data [1,3,11] or estimated by combining density-functional theory (DFT) with interaction parameters (such as the Hubbard U) adjusted to reproduce experimental findings [6,7].

While the aforementioned theories have been very instructive, their applications have been limited by the availability of concrete experimental data needed to determine their input parameters, supporting the need for a fully first-principles theory without empirical parameters. There have been several attempts to compute the spin fluctuation–electron coupling from first principles. Notably, Winter and coworkers [12,13] calculated the spin susceptibility and the spin fluctuation–electron self-energy from DFT and evaluated the correction to the specific heat for palladium and vanadium. Later studies [14–16] employed a first-principles T -matrix approach to calculate satellites in the photoemission spectrum of nickel and quasiparticle lifetimes in metals. However, such theory requires the solution of a computationally expensive four-point equation and also a correction to account for the double counting of certain Feynman diagrams.

The alkali metals are arguably among the simplest systems in condensed matter theory. Careful comparisons between theory and experiment in these systems has guided progress in understanding electron correlation physics in the itinerant-electron limit. In particular, the Fermi surfaces of sodium and lithium are highly spherical, indicating that a description based on the homogeneous electron gas might be valid. Therefore it was surprising when angle-resolved photoemission experiments [17,18] reported a substantially smaller occupied bandwidth than was found in Hartree calculations on the homogeneous electron gas and also in DFT calculations. In addition, self-energy corrections employing the standard GW correction to the electron self energy [19,20], where the self energy is expressed as the product of the interacting Green’s function G and the screened Coulomb interaction W , could not account for the full reduction of the occupied bandwidth, indicating that electron correlation effects not included in these calculations play an essential role in these materials.

Northrup *et al.* [21,22] included vertex corrections in the dielectric matrix approximately by computing the charge susceptibility from DFT instead of employing the random-phase approximation (RPA) and found the resulting GW values to be in good agreement with experimental results for the occupied bandwidths of lithium and sodium. At the same time, Zhu and Overhauser [23] found that spin fluctuations within a paramagnon pole model could also explain the reduction of the bandwidth. This difference in the mechanism responsible for the band width reduction in the alkali metals has not yet been resolved. In particular, no first-principles calculation of the self-energy correction arising from spin fluctuations has been reported for the alkali metals.

In this paper, we describe our first-principles calculations of the contribution to the self-energy arising from spin fluctuations. In particular, we employ the spin-fluctuation self-energy formalism proposed by Kukkonen and Overhauser [24], which is simpler than the T -matrix approach since it requires neither the solution of a four-point equation nor a double counting correction. We apply the theory to sodium and lithium and find that the contribution of spin fluctuations to the reduction of the occupied bandwidth is small and, by itself, cannot explain experimental findings. We also carry out standard GW calculations and GW calculations with a

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vertex-corrected charge susceptibility, with the latter resulting in a larger reduction of the occupied bandwidth, in agreement with experiment and results in Refs. [21,22].

Methods. The properties of quasiparticles, such as their energy or lifetime, can be measured in photoemission or tunneling experiments. Mathematically, quasiparticle energies are given by the positions of the poles of the single-particle Green's function and can be determined by solving the Dyson equation

$$\left(-\frac{\nabla^2}{2} + V_{\text{ion}}(\mathbf{r}) + V_H(\mathbf{r})\right)\psi_n(\mathbf{r}) + \int d\mathbf{r}' \Sigma(\mathbf{r}, \mathbf{r}', E_n)\psi_n(\mathbf{r}') = E_n\psi_n(\mathbf{r}), \quad (1)$$

where V_{ion} and V_H denote the external potential due to the ionic cores and the Hartree potential, respectively, E_n and ψ_n are the quasiparticle energy and wave function, and Σ denotes the electron self-energy.

We approximate the self-energy using [23,25]

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega) = i \int \frac{d\omega'}{2\pi} e^{-i\delta\omega'} G(\mathbf{r}, \mathbf{r}', \omega - \omega') V_{\text{eff}}(\mathbf{r}, \mathbf{r}', \omega'), \quad (2)$$

where G and V_{eff} denote the single-particle Green's function and the effective interaction between electrons, respectively, and $\delta = 0^+$. We separate V_{eff} and subsequently Σ into three contributions: a bare Coulomb term $v(\mathbf{r}, \mathbf{r}') = 1/|\mathbf{r} - \mathbf{r}'|$ (resulting in the bare exchange contribution to the self-energy), a charge-fluctuation-mediated interaction δW_C (resulting in a correlation contribution to Σ arising from charge fluctuations), and a spin-fluctuation-mediated interaction δW_S (resulting in a spin-fluctuation contribution to Σ).

In a standard GW calculation [19,20], $\delta W_S = 0$ and $\delta W_C = v\chi_C^{\text{RPA}}v$ (suppressing all arguments and integrals for clarity) are assumed, where χ_C^{RPA} denotes the interacting charge susceptibility in the RPA. We refer to this approximation as GW_{RPA} .

Following Refs. [21,22] we include vertex corrections to the dielectric screening by calculating χ_C from DFT, i.e., by solving $\chi_C = \chi_0 + \chi_0(v + f_{xc})\chi_C$, where χ_0 denotes the noninteracting Kohn-Sham susceptibility and $f_{xc}(\mathbf{r}, \mathbf{r}') = \delta^2 E_{xc}/[\delta\rho(\mathbf{r})\delta\rho(\mathbf{r}')] with E_{xc} and $\rho(\mathbf{r})$ being the exchange-correlation energy within DFT and the electron density, respectively. Note that χ_C is exact if we know the exact E_{xc} . The simplest approximation to the exchange-correlation energy is the local density approximation (LDA) [26] and we refer to this approximation as GW_{LDA} . Inclusion of vertex corrections in χ_C leads to a better satisfaction of the Ward identity associated with particle conservation [27].$

The spin-fluctuation-mediated interaction can be approximated [23,24] using

$$\delta W_S(\mathbf{r}, \mathbf{r}', \omega) = 3 \int d\mathbf{r}_1 d\mathbf{r}_2 I_{xc}(\mathbf{r}, \mathbf{r}_1)\chi_S(\mathbf{r}_1, \mathbf{r}_2, \omega)I_{xc}(\mathbf{r}_2, \mathbf{r}'), \quad (3)$$

where $\chi_S = \chi_0 + \chi_0 I_{xc} \chi_S$ denotes the interacting spin susceptibility and $I_{xc}(\mathbf{r}, \mathbf{r}') = \delta^2 E_{xc}/[\delta m(\mathbf{r})\delta m(\mathbf{r}')] with $m(\mathbf{r})$ denoting the spin density. The factor of 3 results from the vector boson nature of the spin fluctuations.$

This intuitively appealing expression for the self-energy arising from spin fluctuations was first derived by considering the effective interaction between electrons in a homogeneous electron gas including exchange and correlation effects [24]. Later [25] it was found that the same expression may be obtained from an analysis of Feynman diagrams [42].

Computational details. We carry out DFT-LDA calculations using a plane-wave basis and norm-conserving pseudopotentials as implemented in the QUANTUM ESPRESSO program package [28]. Our plane wave cutoff is 30 Ry. For sodium we choose the unit cell corresponding to $r_s = 3.93$ and for lithium we choose it corresponding to $r_s = 3.26$ [r_s is related to the valence charge density n via $n = 3/[4\pi(r_s a_B)^3]$ with a_B being the Bohr radius]. The self-energy is calculated using the BERKELEYGW [29] program package. For the calculation of the susceptibilities and the self-energies we use $16 \times 16 \times 16$ k -point sampling of the Brillouin zone. In our first-principles calculations, we do not employ a generalized plasmon-pole model for the interacting charge and spin susceptibilities but sample these quantities along the real frequency axis. We use fine sampling with a step size of 0.1 eV up to a lower cutoff of 30 eV and then coarser sampling up to 60 eV. A broadening of 0.15 eV is used as well as 30 empty states in the calculation of the dielectric matrix and the self-energy. In this work, we employ a one-shot procedure to calculate the self-energy. The effect of self-consistency on the occupied band width of simple metals was investigated in Ref. [21] and found to be quite small.

Sodium. The occupied bandwidth of sodium in DFT is 3.19 eV. Figure 1(a) shows the self-energy correction (evaluated “on-shell,” i.e., at the mean-field energy) to the DFT-LDA band structure from charge fluctuations (including the bare exchange) and from spin fluctuations. We find a reduction of the occupied bandwidth with charge fluctuations giving a significantly larger contribution than spin fluctuations. In agreement with previous calculations [21,22], we find that vertex corrections in the charge susceptibility are very important (increasing the bandwidth reduction by a factor of two compared to the standard GW_{RPA} result): Standard GW_{RPA} theory gives a reduction of 0.31 eV, while GW_{LDA} yields a reduction of 0.63 eV, resulting in an occupied bandwidth in good agreement with the experimental findings [17,18]. See Table I. The contribution from spin fluctuations to the bandwidth reduction is very small, less than 0.1 eV.

To understand these results we observe that retaining only the bare exchange contribution to the self-energy results in a drastic *increase* of the occupied bandwidth by 3.30 eV as expected from usual Hartree-Fock theory. Inclusion of screening by charge fluctuations has the opposite effect, yielding a net reduction of the bandwidth. The RPA underestimates the screening, which explains the larger bandwidth reduction in GW_{LDA} theory [22].

Figure 1(a) also shows the result from a self-energy calculation for the homogeneous electron gas (jellium) with $r_s = 3.93$ corresponding to the valence charge density of sodium, $n = 3/(4\pi[r_s a_B]^3)$ with a_B being the Bohr radius. The occupied bandwidth in Hartree theory is 3.15 eV. This agrees very well with the *ab initio* DFT-LDA result, indicating that corrections caused by the inhomogeneity of the crystalline potential are very small. Figure 1 shows good agreement

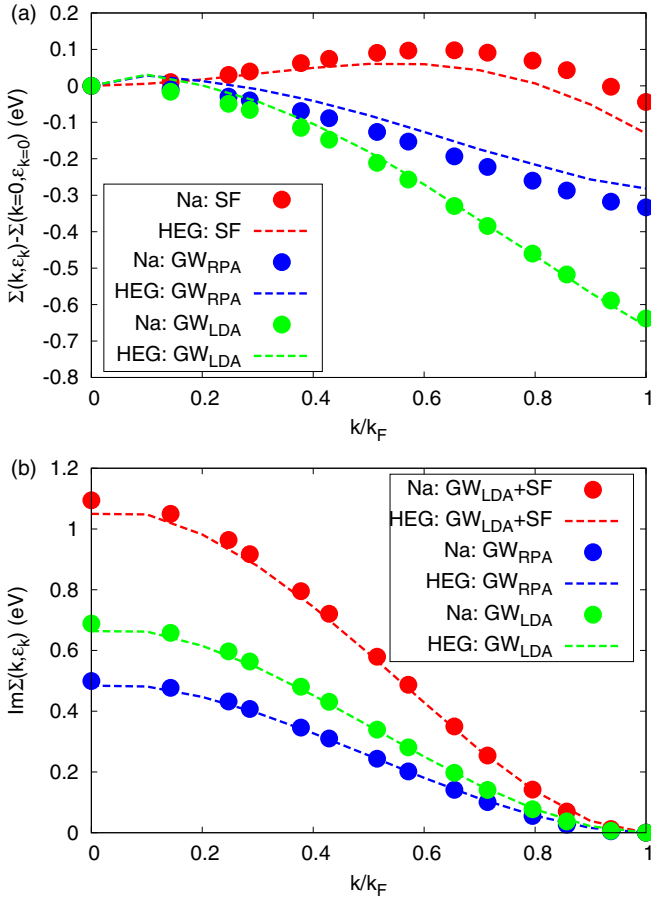


FIG. 1. (Color online) (a) On-shell self-energy corrections for the occupied states in sodium. The dashed curves are results for the homogeneous electron gas (HEG) with $r_s = 3.93$, while the circles are results from *ab initio* calculations. The GW_{RPA} theory (blue [dark gray]), GW_{LDA} theory (green [light gray]), and the spin-fluctuation self energy (red [gray]) are shown. (b) Imaginary part of the on-shell self-energy for the occupied states in sodium. The labels are the same as in panel (a).

between the on-shell self energies from the *ab initio* calculation and jellium.

If the exact self-energy was known, quasiparticle properties should be calculated “off-shell”; i.e., the quasiparticle equation, Eq. (1), should be solved and the self-energy should be evaluated at the quasiparticle energy. It has been argued [30,31], however, that for approximate self-energies quasiparticle properties should be determined by evaluating the self-energy “on the shell” to avoid mixing different orders of perturbation theory. Table I shows that off-shell calculations result in a larger occupied bandwidth than on-shell calculations. The ratio of the bandwidth reductions in off-shell and on-shell calculations is approximately equal to the renormalization constant $Z_k = [1 - \partial \Sigma_k(E_k^{qp}) / \partial \omega]^{-1}$, which is about 0.6 for the occupied states of sodium.

According to Eq. (2), the self-energy should be calculated using the interacting Green’s function. To approximately account for this self-consistency requirement we have shifted all mean-field energies such that the resulting quasiparticle energy agrees with the shifted mean-field energy [32] at the

TABLE I. Occupied bandwidth of sodium obtained from on-shell and off-shell evaluations of the self-energy. We also give results with approximate self-consistency (sc) achieved by shifting the mean-field energies. All energies are given in electron volts.

	On-shell	Off-shell	Off-shell + sc
GW_{RPA}	2.86	3.00	2.98
GW_{LDA}	2.55	2.83	2.80
$\text{GW}_{\text{LDA}} + \text{SF}$	2.51	2.85	2.78
Exp. [17]	2.5		
Exp. [18]	2.65		
DFT-LDA	3.19		

Fermi level. Table I shows that self-consistency leads to only very small changes in the occupied bandwidth.

We employed the jellium model to investigate the effect of additional approximations to the self-energy. In standard first-principles GW_{RPA} calculations, one sometimes employs a generalized plasmon-pole model [19] to extend the static inverse dielectric matrix to finite frequencies. In this model the imaginary part of the inverse dielectric function for each \mathbf{G} and \mathbf{G}' component is assumed to be a simple δ function, i.e., $\text{Im}\epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega) \propto \delta[\omega - \omega_{\mathbf{G}\mathbf{G}'}(\mathbf{q})]$ with $\omega_{\mathbf{G}\mathbf{G}'}(\mathbf{q})$ denoting the effective plasmon frequency. Figure 2(a) shows that the plasmon-pole model reproduces the self-energy shifts arising from charge fluctuations quite well. Zhu and Overhauser [23] employed a similar *paramagnon-pole model* to simplify the calculation of the spin-fluctuation self-energy: They assumed that the imaginary part of the interacting spin susceptibility can be represented by a single mode, the paramagnon. However, in contrast to the plasmon, which cannot decay into particle-hole pairs for small wave vectors, the paramagnon has a linear acoustic-like dispersion (as determined by the f -sum rule [23]) and can decay into particle-hole pairs: Fig. 2(b) shows the imaginary part of the spin, charge, and noninteracting susceptibilities at $q/q_F = 0.6$. The charge susceptibility has a sharp plasmon peak at ~ 7 eV that lies outside the particle-hole continuum given by the noninteracting susceptibility. The spin susceptibility has significant overlap with the noninteracting susceptibility and exhibits a broad structure. In contrast to the charge susceptibility, the spin susceptibility is not well represented by a single sharp mode.

As a consequence, the spin-fluctuation self energy with a paramagnon-pole model gives very different results from the theory without this approximation; see Fig. 2(a). It results in a drastic narrowing of the occupied bandwidth by ~ 1.4 eV. While Zhu and Overhauser [23] empirically correct for the finite lifetimes of the paramagnon, it is likely that their predicted bandwidth narrowing of 0.7 eV is also spuriously large and caused by the paramagnon-pole approximation.

Figure 2 also shows that for the GW_{LDA} theory the plasmon-pole approximation leads to a further reduction of the occupied bandwidth by ~ 0.2 eV. The resulting bandwidth (calculated “off-shell”) agrees well with previous first-principles results [21,22].

Figure 1(b) on the other hand shows that spin fluctuations contribute significantly to the line width [$2\text{Im}\Sigma_k(\epsilon_k)$] of quasiparticles. In particular, at the bottom of the band, $k = 0$, the

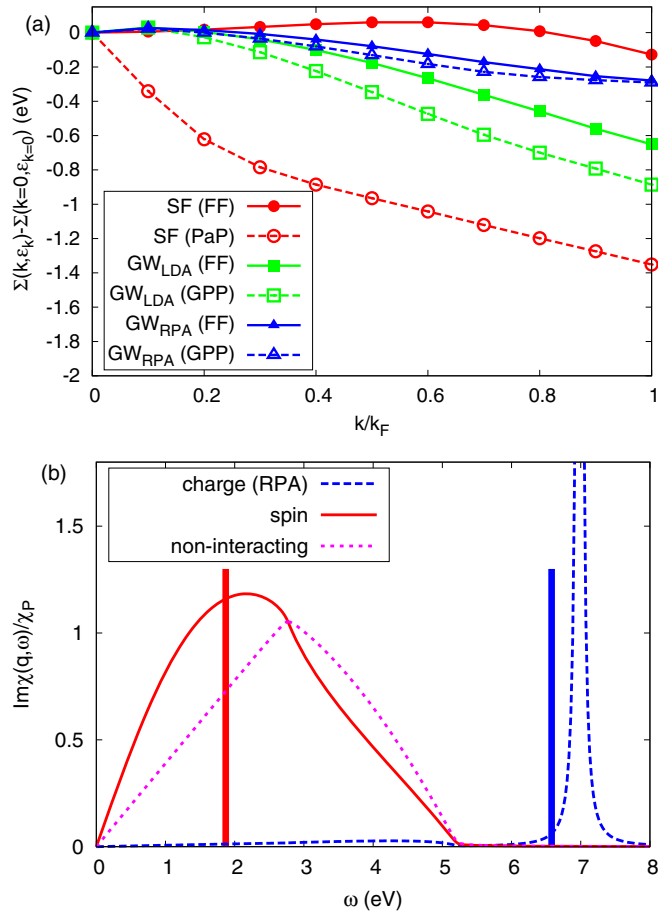


FIG. 2. (Color online) (a) Comparison of the on-shell self-energy corrections for the occupied states of jellium with $r_s = 3.93$ (corresponding to sodium) from full-frequency and simplified calculations using the generalized plasmon-pole (GPP) and paramagnon-pole (PaP) models for the GW_{RPA} self-energy (blue [dark gray]), GW_{LDA} self-energy (green [light gray]), and spin-fluctuation self-energy (red [gray]). (b) Frequency-dependent imaginary parts of the charge (blue [dark gray] dashed curve), spin (red [gray] solid curve), and non-interacting (magenta [gray] dotted curve) susceptibilities for jellium at $q/q_F = 0.6$. The susceptibilities are divided by the Pauli susceptibility $\chi_P = -k_F/\pi^2$. The vertical lines denote the locations of the δ -function peaks in a plasmon-pole model (blue [dark gray]) [33] and a paramagnon-pole model (red [light gray]) [23].

quasiparticle line width is a factor of 2 larger than the GW_{RPA} value when vertex corrections in χ_C and spin fluctuations are included. This agrees well with the experimental findings [16,34–35].

Lithium. In contrast to sodium, the occupied bandwidth resulting from Hartree theory applied to the homogeneous electron gas, 4.65 eV, is much larger than the value obtained

TABLE II. Occupied bandwidth of lithium obtained from on-shell and off-shell evaluations of the self-energy. We also give results with approximate self-consistency (sc) achieved by shifting the mean-field energies. All energies are given in electron volts.

	On-shell	Off-shell	Off-shell + sc
GW_{RPA}	3.19	3.29	3.30
GW_{LDA}	2.83	3.09	3.10
$\text{GW}_{\text{LDA}} + \text{SF}$	2.87	3.24	3.08
Exp. [37]	2.86		
DFT-LDA	3.45		

in a DFT-LDA calculation including the crystalline potential, 3.45 eV. This shows that—even though the Fermi surface is spherical to a high degree [36]—crystal effects are very important in lithium.

Table II shows our results for the occupied bandwidth of lithium. Again, the occupied bandwidth reduction in GW_{RPA} theory is too small to explain the experimental finding. Adding vertex correction in χ_C yields good agreement with experiment [37], while spin fluctuations lead only to a small change in the occupied bandwidth.

Conclusions. We have calculated the effect of spin and charge fluctuations on quasiparticle excitations in alkali metals from first principles. In contrast to previous calculations [23], we find that spin fluctuations contribute little to the observed bandwidth reduction compared to mean-field results. Instead, as observed in Refs. [21,22] inclusion of vertex corrections in the dielectric screening gives agreement with experimental bandwidths. Previous studies which included vertex corrections in both the dielectric screening and the self-energy found that agreement with experiment worsens [38,39]. Other studies reported cancellations between self-energy vertex corrections and self-consistency effects [40,41]. Further work is necessary to clarify this issue. We also find that spin fluctuations give an important contribution to the line width and lifetime of the quasiparticle excitations. We note that the first-principles framework presented here can be applied to materials with d electrons, where spin fluctuations are expected to play an essential role, such as pnictide superconductors and ferromagnetic metals.

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