# Electron-Electron Interactions and the Bandwidth of Metals

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A calculation is presented of the self-energy of an electron from the screened exchange energy. Vertex corrections are included. They have a large effect upon the predictions of the width of the occupied energy bands. For aluminum the bandwidth is predicted to be 0.7 eV wider in the $GW$ approximation compared to $GW\Gamma$ which includes vertex corrections. Results using the $GW\Gamma$ approximation are similar to those of the random-phase approximation.

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There have been numerous calculations of the self-energies of electrons in metals from electron-electron interactions.[1-9] As far as we can tell, all of these calculations, except for Overhauser's,[6] make the $GW$ approximation which neglects vertex corrections. Here we include them in the calculation of the electron self-energies. This is called a $GW\Gamma$ calculation, where $\Gamma$ is the vertex function. Including $\Gamma$ changes the value of the self-energy by (5–10)%. A very sensitive test of the importance of vertex corrections, or other aspects of the screening, is in the prediction of the width of the occupied energy band. For bandwidths, including $\Gamma$ changes the predictions significantly compared to the $GW$ approximation. In fact, we find the $GW\Gamma$ results to be similar to Hedin's[4] "random-phase approximation" (RPA) results, showing the vertex effects cancel when included in both the numerator and the dielectric function.

If $\Sigma(k,\omega)$ is the self-energy, then the change in the bandwidth $W$ is

$$\Delta W = \mathrm{Re}\{\Sigma(0,0) - \Sigma(k_F,\epsilon_F)\}\,, \tag{1}$$

where $\omega=0$ is the bottom of the band and $\omega=\epsilon_F$ is the Fermi energy. This sign convention is that a positive $\Delta W$ is a narrowing of the occupied bands. We find for electron gases of high densities that vertex corrections can change $\Delta W$ by 0.7 eV. The effect is large, and should be easily measurable.

Recently there have been other calculations[7-10] and measurements[11-13] of bandwidths in metals. They provided the inspiration for the present calculation. Later we compare our results with some of these references.

For the homogeneous electron gas, the screened exchange energy is recognized as the dominant contribution to the electron self-energy. Its contribution is

$$\Sigma(k,ik) = -\frac{1}{\beta}\sum_{iq}\int \frac{d^3q}{(2\pi)^3}\frac{v_q}{\epsilon(q,iq)}\Gamma(q,iq)\frac{1}{ik+iq-\xi_{p+q}}\,, \tag{2}$$

$$\epsilon(q,iq) = 1-\chi(q,iq)\Gamma'(q,iq),\quad \Gamma'(q,iq) = 1/[1+G(q)\chi(q,iq)]\,, \tag{3}$$

where $\chi=v_qP(q,iq)$ is the susceptibility in the RPA.[14] The function $G(q)$ is a local-field correction. Many expressions for $G(q)$ have been suggested. Here we shall discuss three. If $x=q/k_F$, then the Hubbard[15] form is $G=x^2/2(1+x^2)$, Geldart and Vosko[16] (GV) have $G=x^2/2(2+x^2)$, and Vashishta and Singwi[17] (VS) have $G=A[1-\exp(-Bx^2)]$, where $A$ and $B$ are tabulated functions of the density parameter $r_s=(3/4\pi n_0)^{1/3}$.

Vertex corrections describe the correlation between the position of the electron and the positions of the other local electrons in the screening charge. The local-field factor $G(q)$ in the dielectric screening describes similar correlations between the electrons doing the screening.

The most straightforward model is RPA, where $\Gamma=\Gamma'=1$. This calculation was first done by Hedin.[4] His results have been confirmed by numerous calculations including ours. Our results for RPA are listed in Table I. The bandwidth changes are shown in Fig. 1. Since a positive value indicates band narrowing, RPA predicts a band narrowing for the range of metallic densities $1.7<r_s$. Our calculations using (2) were done at zero temperature where the discrete frequency summation over $iq$ is changed to a continuous integral. The analytic continuation of $ik\rightarrow\xi_k$ requires an additional integral, as described elsewhere.[14] Thus, we evaluate a double integral over frequency and wave vector. This complete evaluation of the integral avoids the plasmon pole approximation which is not accurate enough for the calculation of the bandwidth. Numerical accuracy is $\pm 0.0001$ Ry.

Past calculations usually have set $\Gamma=1$ in the numera-

TABLE I. Electron self-energies $-\mathrm{Re}\Sigma(k,\xi_k)$ in rydbergs. Accuracy is $\pm 0.0001$. (a) Calculations with $\Gamma=1$. (b) Calculations with $\Gamma=(1+\chi G)^{-1}$. GV is Geldart-Vosko (Ref. 16) and VS is Vashishta-Singwi (Ref. 17) form for $G(q)$.

| | $r_s=1$ | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| | | | (a) $\Gamma=1$ | | | |
| RPA | | | | | | |
| $k=0$ | 1.5220 | 0.7364 | 0.4993 | 0.3854 | 0.3180 | 0.2730 |
| $k=k_F$ | 1.3965 | 0.7499 | 0.5270 | 0.4123 | 0.3419 | 0.2938 |
| GV | | | | | | |
| $k=0$ | 1.4920 | 0.7126 | 0.4814 | 0.3721 | 0.3080 | 0.2654 |
| $k=k_F$ | 1.4013 | 0.7558 | 0.5335 | 0.4191 | 0.3488 | 0.3007 |
| VS | | | | | | |
| $k=0$ | 1.4879 | 0.7068 | 0.4764 | 0.3686 | 0.3066 | 0.2660 |
| $k=k_F$ | 1.4028 | 0.7591 | 0.5383 | 0.4253 | 0.3564 | 0.3096 |
| | | | (b) $\Gamma=(1+\chi G)^{-1}$ | | | |
| GV | | | | | | |
| $k=0$ | 1.5196 | 0.7217 | 0.4820 | 0.3679 | 0.3011 | 0.2567 |
| $k=k_F$ | 1.3693 | 0.7270 | 0.5068 | 0.3941 | 0.3250 | 0.2780 |
| VS | | | | | | |
| $k=0$ | 1.5104 | 0.7059 | 0.4619 | 0.3452 | 0.2766 | 0.2311 |
| $k=k_F$ | 1.3549 | 0.7087 | 0.4859 | 0.3714 | 0.3011 | 0.2532 |

tor of (2), while keeping $\Gamma'$ in the dielectric function. Our results for this type of approximation are shown in Table I in part (a) labeled "$\Gamma=1$." Results for GV and VS local-field factors are numerically similar. Their differences are accentuated when calculating the change in bandwidth. The top dashed line in Fig. 1 is the VS prediction which has more band narrowing than RPA.

Here we report calculations using vertex corrections with $\Gamma=\Gamma'$. This choice has been shown by Ting, Lee, and Quinn[18] to be correct for dielectric functions of the Hubbard type. They also show that only one power of $\Gamma$ belongs in the numerator of (2).

Numerical results are shown in part (b) of Table I. Vertex corrections change the self-energies by (5–10)%. While these differences are not large, they have an important effect upon the predicted bandwidths. Using the VS choice for $G(q)$ gives the solid line shown in Fig. 1. Indeed, almost any choice for $G(q)$ yields this same curve. The result is also quite similar to RPA. Our conclusion is that the effects of $\Gamma(q)$ nearly cancel when added to both the vertex function and the dielectric function. This cancellation was predicted by Rice.[5] Similar cancellation occurs in the calculation of many other self-energies, where the effects of vertex corrections are largely cancelled by dressing internal Green's functions.

The values of $\Delta W$ are positive for $r_s>2$, which predicts that the occupied bands are narrower. For aluminum at $r_s=2.07$, the bands are predicted to be narrower by 0.05 eV when calculated with $\Gamma=\Gamma'$. This value should be compared to a narrowing of 0.74 eV calculated with $\Gamma=1$. An error of 0.7 eV is made in the bandwidth prediction when vertex corrections are made in the dielectric function but not in the numerator. Other recent calculations[9,12] have made this approximation, and probably have these kind of errors. For sodium at $r_s=3.96$ we predict a band narrowing of 0.36 eV which is also the RPA prediction. Since occupied bandwidths can be measured, these predictions can be tested experimentally.

Metallic aluminum provides an excellent test case. A free-electron gas of aluminum density has an occupied bandwidth of 11.7 eV. One must also consider the band narrowing caused by the scattering from the crystal potential. Singhal and Callaway[19] and Szmulowicz and Segall[20] predict that the one-electron bands are narrowed by 0.7 eV. Thus one-electron theory predicts the bands have a width of 11.0 eV. Recent measurements[12,21] give a bandwidth of 10.6 eV, which suggests an experimental narrowing of 0.4 eV from electron-electron interactions. These experiments are discussed below. Using $\Gamma=\Gamma'$ we predict a band narrowing of 0.05 eV, or that the total width of the occupied bands is 10.9 eV.

X-ray emission spectra have been the traditional method of measuring bandwidth. Neddemeyer [22] analyzed a variety of x-ray emission data[22–24] and concluded that the bandwidth of aluminum is $11.67\pm0.14$ eV. Recently Livins and Schnatterly[21] measured the $L$ emission spectra and concluded that the bandwidth is 10.6 eV. This difference from Neddermeyer is due to a more sophisticated analysis of the low-energy tail caused by shakeup. Better analyses of shakeup will undoubtedly

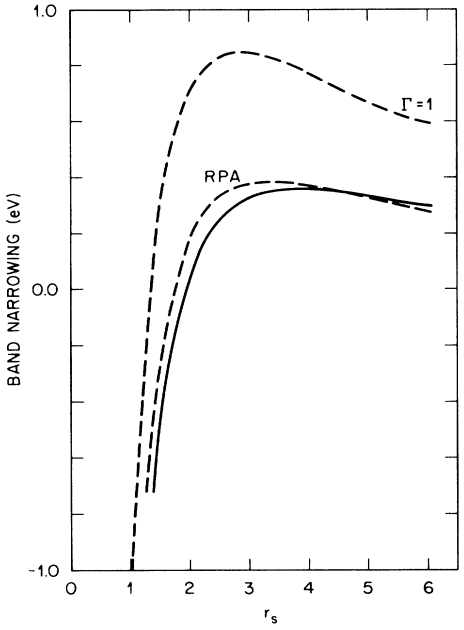


FIG. 1. Band narrowing vs density ($r_s$) for several calculations of the electron self-energy. RPA is the random-phase approximation which has $G=0$. The other choice of $G$ is that of Vashishta and Singwi (VS) in Ref. 17. The dashed line on top is the VS prediction with $\Gamma=1$, while the solid line is the VS prediction with $\Gamma=(1+\chi G)^{-1}$. The solid line is a universal result which is predicted by many choices for $\Gamma(q)$.

cause further refinements of the experimental value.

The photoemission data of Refs. 11 and 12 show a bandwidth of 10.6 eV. Elsewhere[25] we have shown that photoemission data are distorted by surface effects. In Ref. 10 we used self-energies calculated with $\Gamma(q)$, and surface effects, to reproduce the photoemission data for sodium. We expect that similar phenomena is occurring in aluminum. Recently it has been argued that metallic sodium has narrower bands in x-ray absorption.[13] Our calculations show a band narrowing of 11% which is similar to that observed.[13,26]

In conclusion, we have included vertex corrections in the calculation of the self-energies of electrons from electron-electron interactions. We find that including the same vertex term $\Gamma(q)$ as is used in the dielectric function causes the net bandwidth predictions to be similar to RPA. Very large bandwidth changes, although not as large as reported in Ref. 12, are found when $\Gamma(q)$ is used in the dielectric function but not in the numerator.

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