Electron-phonon vs. electron-impurity interactions with small electron bandwidths

F. Doğan and F. Marsiglio

Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2J1

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It is common practice to try to understand electron interactions in metals by defining a hierarchy of energy scales. Very often, the Fermi energy is considered the largest, so much so that frequently bandwidths are approximated as infinite. The reasoning is that attention should properly be focused on energy levels near the Fermi level, and details of the bands well away from the Fermi level are unimportant. However, a finite bandwidth can play an important role for low frequency properties: following a number of recent papers, we examine electron-impurity and electron-phonon interactions in bands with finite widths. In particular, we examine the behaviour of the electron self energy, spectral function, density of states, and dispersion, when the phonon spectral function is treated realistically as a broad Lorentzian function. With this phonon spectrum, impurity scattering has a significant non-linear effect.

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I. INTRODUCTION

In the last few years, a number of authors have investigated the effect of a finite Fermi energy on the properties of an interacting electron system. In the past, with the understanding that only properties near the Fermi level were important, the Fermi energy was assumed to be infinite, to facilitate integrations over electronic energies. This approximation was believed to have negligible impact on properties concerning states near the Fermi level. Alexandrov et al. first noted that accounting for a finite bandwidth leads to a significant modification of the electron density of states (EDOS) near the Fermi level; they interpreted this as a “polaronic collapse” of the electron band. From our point of view the important observation is that the EDOS actually experiences a significant alteration with electron-phonon coupling.

In this paper, following the work presented in Refs. and we wish to investigate further the impact of a finite density of states when both impurity scattering and electron-phonon coupling are present. Specifically we will examine the impact of a different bare EDOS (a Lorentzian model), and the impact of a more realistic broad phonon spectrum (previous work focused on an Einstein spectrum).

The paper is organized as follows: in the following section we briefly review the formalism to calculate the electron self energy. The formulation we use allows for several properties to be obtained explicitly and analytically. Section III deals briefly with only electron-impurity scattering. Significant changes occur at a very basic level because the bandwidth is finite. For example, the self energy acquires a real part. Section IV shows a number of results for combined electron-phonon and electron-impurity scattering, where both a delta-function and broadened Lorentzian form is used for the phonon spectrum. We also make a direct comparison with the results of Ref. to show the model dependence of the analysis. We close with a Summary of our results.

II. THE FORMALISM

The self-consistent Migdal approximation has been explained before in the cited references, so the reader is referred to them. For an arbitrary electron-phonon spectral function, , the resulting equations for the self energy, , are as follows, at zero temperature:

\[
\text{Re} \Sigma(\omega + i\delta) = \frac{1}{2\tau} \int d\epsilon \frac{N_0(\epsilon)}{N_0(0)} \text{Re} G(\epsilon, \omega + i\delta) + \\
\int_0^\infty d\nu \alpha^2 F(\nu) \left[ \left( \frac{N(\omega') - N(\omega - \nu)}{N_0(0)} \right) \frac{2\omega}{\omega^2 - (\nu + \omega')^2} + \frac{N(\omega - \nu)}{N_0(0)} \ln \frac{\omega - \nu}{\omega + \nu} \right]
\]

and

\[
\text{Im} \Sigma(\omega + i\delta) = -\frac{1}{2\tau} \frac{N(\omega)}{N_0(0)} - \pi \int_0^\infty d\nu \alpha^2 F(\nu) \left[ \frac{N(\omega - \nu)}{N_0(0)} \theta(\omega - \nu) + \frac{N(\omega + \nu)}{N_0(0)} (1 - \theta(\omega + \nu)) \right].
\]

Here, the electron Green function, , is given by the Dyson equation:

\[
G(\epsilon, \omega + i\delta) = \frac{1}{\omega + i\delta - \epsilon - \Sigma(\omega + i\delta)},
\]

where the momentum dependence is summarized by the energy . The parameter characterizes the impurity scattering strength, and has units of a scattering rate. The bare electron density of states (EDOS) is given by , while the renormalized density of states (RDOS) is given by . The former function in principle comes from a band structure calculation; we will simply model it either as a constant with finite bandwidth or a Lorentzian
The RDOS is a product of our calculation, and is given by

$$N(\omega) = \int_{-\infty}^{\infty} d\epsilon \, N_0(\epsilon) A(\epsilon, \omega),$$

where $A(\epsilon, \omega) = -\frac{i}{\pi} \text{Im} G(\epsilon, \omega + i\delta)$ is the electron spectral function. For the two simple models for the bare EDOS, $N(\omega)$ can be determined analytically in terms of the electron self energy $\Sigma$. Thus, these equations constitute a set of self-consistent equations for the electron self energy, from which all single electron properties can be calculated. As already mentioned, for the electron-impurity scattering, the process is characterized by a single number, $1/\tau$. On the other hand, the electron-phonon interaction is specified by an entire function, $\alpha^2 F(\nu)$, which we will sometimes take to be an Einstein spectrum, in which case two parameters are required, the frequency, and the “strength”, as measured by, say, the mass enhancement parameter, $\lambda \equiv 2 \int_0^\infty d\nu \, \alpha^2 F(\nu)$. To specifically examine the impact of broadened spectra, we will utilize the truncated Lorentzian shape defined in Ref. 3.

Note that an alternative formulation first determines the relevant Green function and self energy on the imaginary axis; then a set of self-consistent equations can be utilized to analytically continue the result to just above the real axis $\mathbb{R}$. This method was used in Ref. 4, and is particularly useful at finite temperature.

### III. ELECTRON-IMPURITY SCATTERING

Eqs. (1-4) require iterative self-consistent solutions. Analytic results are not possible, except in some limits. For example, with impurity scattering only, and with a bare EDOS given by a Lorentzian with half-width $D/2 \equiv \epsilon_F$, the self energy is given by

$$\Sigma(\omega + i\delta) = \frac{\omega + i\epsilon_F}{2} \left( 1 - \frac{1 - 2\epsilon_F/\tau}{(\omega + i\epsilon_F)^2} \right).$$

For an infinite bandwidth the impurity self energy is pure imaginary, $\Sigma(\omega + i\delta) = -i\epsilon_F$; finally an approximate result is obtained by using the first term in Eqs. (1) with the bare Green function on the right hand side. These results are illustrated in Fig. 1. Similar results are obtained for a constant bare EDOS with finite bandwidth (6). For the imaginary part of the self energy (which Eq. 2 indicates is proportional to the density of states when only impurity scattering is present) the main effect of the finite bandwidth is to reduce the self energy to zero beyond energies corresponding to the electronic states. The real part (Fig. 1a) experiences the biggest change, since it is zero at all frequencies if the limit of infinite bandwidth is taken first. Fig. 1b illustrates that full self-consistency impacts the low frequency behaviour in particular. Note that while the intercept of the imaginary part of the self energy retains the physical interpretation of a scattering rate, the slope of the real part is no longer related to an effective mass. This will be pertinent when both electron-impurity and electron-phonon scattering are present, as already pointed out in Ref. 4.

The renormalized EDOS is already shown (to within a minus sign and a constant factor — see Eq. (2)) in Fig. 1b. Note the renormalization at the Fermi level for the fully self-consistent results. From Eq. (2) we know that the renormalization of the EDOS is a convolution over the spectral function. Fig. 2 shows the spectral function at the Fermi level. As expected, the fully self-consistent calculation (Fig. 2a) reflects the renor-
FIG. 2: The full self consistent (a) and non-self consistent (b) electron spectral function for various values of the bandwidth, including the infinite bandwidth case. This latter result is of Lorentzian form, whereas all others deviate from this simple form. Note that the non-self consistent results (b) can be very non-Lorentzian for small bandwidths.

FIG. 3: Real (a) and imaginary (b) parts of the electron self-energy, for a moderate electron-phonon coupling strength, $\lambda = 1$. The phonon spectrum is a delta function at frequency $\nu_E = 10$ meV. Results are shown for one bandwidth, $D = 10\nu_E$, and for various electron-impurity scattering strengths, as shown. Note that the logarithmic singularity in (a) remains for all impurity scattering strengths. Overall, the “sharp” features due to the Einstein oscillator remain throughout, independent of the impurity scattering rate.

IV. ELECTRON-PHONON PLUS ELECTRON-IMPURITY SCATTERING

(A) EINSTEIN PHONON

Results with just the electron-phonon interaction have already been presented, so we will focus on the two effects in combination. Figs. 3a and 3b show the real and imaginary parts of the self energy as the electron-impurity scattering strength is varied. For the electron-phonon scattering, we have used an Einstein spectrum with frequency $\nu_E = 10$ meV, and strength $\lambda = 1$. Our results are similar to those of Ref. 4 except that our real part has much sharper features than theirs, presumably
because ours is at $T = 0$ (theirs is at a small non-zero temperature). It is also evident from our method of solution (see Eqs. [12]) that a logarithmic singularity at $\omega = \nu_E$ persists no matter what strength of impurity scattering is present. Thus, somewhat counterintuitively, impurity scattering does not smear out the singularity at $\omega = \nu_E$. As will be evident below, the singularity at $\omega = \nu_E$ results in a collapse of the renormalized EDOS at that frequency. The phonon contribution to the imaginary part of the self-energy is zero until $\omega = \nu_E$, and the impurity contribution is also zero at $\omega = \nu_E$, due to the collapse of the electron band at this frequency. This combination ensures that the overall imaginary part of the self energy drops to zero at this frequency, as Fig. 3b shows. However, at $\omega = 2\nu_E$, the result is in general non-zero: while the electron-phonon contribution is zero, since it depends on the EDOS with frequency shifted by $\nu_E$, the impurity contribution is not zero since the renormalized EDOS at that frequency is non-zero. Therefore the total function is non-zero for $\omega = 2\nu_E$.

As Cappelluti and Pietronero pointed out already in Ref. [4], the slope of the real part of the self energy at the Fermi energy ($\omega = 0$) changes systematically with impurity scattering. This makes inference of the electron-phonon coupling strength from the self energy a very difficult problem. Moreover, the “kink” observed in photoemission spectroscopy [10] will be affected. However, for an Einstein spectrum, the “kink” actually becomes more pronounced with increasing impurity scattering, as shown in Fig. 4. This is because the logarithmic singularity remains in the real part of the self energy, but impurity scattering makes this singularity sharper, as Fig. 4 illustrates. As shown below, with a more realistic electron phonon coupling spectrum the conclusion of Ref. [4] applies, namely that the “kink” becomes smeared with increasing electron-impurity scattering.

In Fig. 5a and 5b we show the spectral function at the Fermi energy and the renormalized density of states for the parameters of Fig. 3, for various degrees of impurity scattering. Note that in (b) the “collapse” of the band evident at $\omega = \nu_E$ remains for all strengths of impurity scattering. Spectral weight is pushed to higher energies as the impurity scattering increases. In (a) when no impurity scattering is present (solid curve) the spectral function is given by a delta function at the origin (indicated by the vertical line with the arrow), followed by an incoherent piece that starts at $\omega = \nu_E = 10 \text{ meV}$.
FIG. 6: Real (a) and imaginary (b) parts of the electron self energy, calculated using an interaction with phonons described by a Lorentzian spectrum centered at $\omega = 10$ meV with $\lambda = 1$. The Lorentzian describing the phonons has broadening parameter, $\delta = 3$ meV. Note that overall trends are the same as for the Einstein phonon (Fig. 3) except everything is smooth. In the real part the degree of the dip (near $\omega \approx \nu_E = 10$ meV) is strongly altered by the impurity scattering (in the Einstein phonon case it remains singular).

(B) LORENTZIAN PHONON SPECTRUM

Many of these results contain anomalously sharp features because of the use of an Einstein model for the phonon spectral function. It was already shown in Ref. 3 that these features are considerably smoothened when a more realistic spectrum is used. Here we use the broadened Lorentzian spectrum of Ref. 3 with $\delta = 3$ meV. Results are shown in Fig. 6 for (a) the real and (b) imaginary parts of the self energy. Clearly the singularity in the real part is absent even without impurity scattering; in contrast to the Einstein mode case, however, impurity scattering alters the nature of the dip near $\nu_E$ considerably. The rest of the frequency dependence for both real and imaginary parts is also affected considerably, as was the case with the Einstein spectrum. In particular, the high frequency portion of the real part remains enhanced due to impurity scattering, and, as remarked in Ref. 4, this will affect the interpretation of the high frequency extrapolation of the dispersion relation as measured in photoemission [10]. Of special note here, however, is the definite reduction of the magnitude of the slope of the real part of the self energy near $\omega = 0$. The way this would appear for the dispersion relation is shown in Fig. 7. Note the ambiguity which impurity scattering causes for the extraction of an electron-phonon coupling strength from such a measurement [4].

Examining the entire spectral function and/or EDOS may be a more promising way to proceed. Of course some experimental challenges concerning background and resolution would have to be overcome in the meantime. In Fig. 8 we show the spectral function for (a) $\epsilon_k = 0$ and (b) $\epsilon_k = -5$ meV. Clearly once impurity scattering is included the separation of the quasiparticle contribution (normally a delta-function without impurities) from the incoherent part (normally with weight $\lambda/(1+\lambda)$ when the Fermi energy is infinite) will become very difficult. This is especially true for a broad electron-phonon spectrum, particularly one that goes to zero at zero frequency (the one used here is cut off before zero frequency is achieved, at $\omega = 0.05$ meV).

In Fig. 9, we show the renormalized EDOS, for various impurity scattering strengths. Even if the underlying electron band structure were known with absolute certainty it would be very difficult to disentangle electron-phonon effects from electron-impurity effects.

All of the results presented so far utilized a Lorentzian-shaped bare EDOS to represent the “bare” electron spec-
FIG. 8: The spectral function at (a) the Fermi level and (b) -5 meV for the same parameters as in Fig. 6. Note that a delta function occurs only at the Fermi level (indicated by the arrow in (a)) when no impurity scattering is used. Increasing the impurity scattering strength immediately broadens the delta function into a Lorentzian-like piece; the incoherent part is already broad, and changes only quantitatively.

The structure near the phonon frequencies is smoothed considerably by the impurity scattering. The latter also accounts for a considerable shift of spectral weight to higher frequency.

V. SUMMARY

In summary, we have examined the effect of both electron-phonon and single impurity scattering on the electron self energy and Green function under special circumstances. These include the presence of a finite bandwidth and phonons which are not infinitely sharp in energy. The broadened nature of the phonon spectrum can be due to intrinsic effects on a single phonon (anharmonicity, interactions, etc.) that give rise to a broadened lineshape; on the other hand they may arise from simply accounting for the dispersion displayed by phonons in real materials. We found that the “smearing” effect expected from impurity scattering is much more pronounced when such a realistic phonon spectrum is used. Otherwise many single electron properties retain sharp features in frequency space when an Einstein spectrum is used. Unfortunately, this combination of finite bandwidth (usually with unknown band structure) and uncertain degree of impurity scattering hinders the ability to infer details concerning the electron-phonon interaction.

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FIG. 10: A comparison of the (a) real, and (b) imaginary part of the self energy, and (c) the dispersion, for a Lorentzian (solid curve) vs. constant (dashed curve) bare EDOS. Mostly high frequency parts change quantitatively. This means that a full inversion of such curves to determine the underlying microscopic interactions would in practice be very difficult.

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