On the extraction of the self-energy from angle-resolved photoemission spectroscopy

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Abstract. We examine a technique commonly used to extract the self-energy from angle-resolved photoemission spectroscopy data. We find that this technique works extremely well for the marginal Fermi liquid model where it follows the analytical model perfectly. Surprisingly, we find a similarly good performance in the case of a Fermi liquid. Finally, we test the influence of the energy and momentum resolution on the results. We find that while the momentum resolution plays only a minor role in the analysis (it slightly inflates the values of the imaginary part of the self-energy), the energy resolution changes the extracted functional form of the self-energy in a significant way at low binding energy.

1. Introduction

Angle-resolved photoemission spectroscopy (ARPES) plays an important role in the study of novel materials. This is, in part, due to the unique momentum resolved information it provides, since it directly measures the single-particle spectral function $A(k, \omega)$. Using data from this
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In this paper, the authors discuss the use of a technique to obtain information about various physical quantities such as band dispersion, Fermi surface, superconducting gap, pseudogap, and self-energy. This last quantity is crucial because it is closely related to the scattering rate, allowing for a comparison between ARPES and transport measurements. Systems with strong interactions cannot be described by the Fermi liquid model, where the scattering rate is proportional to the square of the binding energy. In many cases, notably high-temperature superconductors, the scattering rate is a linear function of binding energy, which led to the formulation of the marginal Fermi liquid model. Recent improvements in ARPES analysis have allowed researchers to test the validity of the MFL and other models. The spectral function is calculated in the vicinity of the Fermi momentum for a given functional dependence of the self-energy. The authors examine the applicability of the technique in the case of MFL and FL models and the influence of experimental resolution on the results. Surprisingly, both models result in an MDC lineshape that is very well approximated by a Lorenzian lineshape for a wide range of energies. This finding challenges the assumption that a Lorenzian lineshape provides definitive proof of MFL behaviour and validates the use of the extraction method in the superconducting state of cuprates, where the self-energy can be approximated by a mixture of the two models (i.e., the scattering rate is linear for higher binding energies and quadratic for low binding energies).

2. Modelling ARPES data

To verify the validity of the self-energy-extraction technique, the authors use the following approach. The spectral function is calculated in the vicinity of the Fermi momentum for a given functional dependence of the self-energy. The spectral function can generally be written as

\[ A(k, \omega) = \frac{\left| \Sigma''(k, \omega) \right|}{\left[ \omega - \nu_F k - \Sigma'(k, \omega) \right]^2 + \left( \Sigma''(k, \omega) \right)^2}, \] (1)

where, \( \nu_F \) is the bare Fermi velocity and \( \Sigma' \) and \( \Sigma'' \) are the real and imaginary parts of the self-energy. The authors assume a linear band dispersion in the vicinity of the Fermi momentum and a bare Fermi velocity of 3 eV A. This spectral function is then multiplied by the intensity plotted as a function of momentum at fixed energy. This technique, proposed by the Brookhaven group, is particularly elegant, since it can be analytically shown that with minimal assumptions, the spectral function is a simple Lorenzian in the case of a MFL. The observation of a Lorenzian lineshape in the MDC data was also treated as evidence that the underlying imaginary part of the self-energy is a linear function of binding energy. Subsequently, this technique became the method of choice for the extraction of the self-energy from ARPES data and is now widely utilized. The validity of this technique and the conditions under which it applies have not been studied methodically before. Here, we present such a study. We examine the applicability of the technique in the case of MFL and FL models and examine the influence of the experimental resolution (both energy and momentum) on the results. Surprisingly, we find that both MFL and FL models result in an MDC lineshape that is very well approximated by a Lorenzian lineshape for a wide range of energies. Commonly made assumptions that a Lorenzian lineshape provides definitive proof of MFL behaviour are therefore unfounded. This point is also significant as it validates the use of the above extraction method in the superconducting state of cuprates, where the self-energy can be approximated by a mixture of the two models (i.e., the scattering rate is linear for higher binding energies and quadratic for low binding energies).
Fermi function, \( f(\omega) \), to give the simulated ARPES intensity:

\[
I(k, \omega) = A(k, \omega) f(\omega). \tag{2}
\]

For simplicity, we neglect the matrix elements. The simulated ARPES intensity is convoluted with the momentum and energy resolutions, thus yielding model data with a known self-energy. We then attempt to extract the self-energy from the model data and compare it to the original assumptions. This process is repeated for the FL and MFL models and for different values of the momentum and energy resolution. The self-energy, \( \Sigma \), is calculated in the following way. Firstly, we make an assumption about the imaginary part of the self-energy for the FL and MFL liquid models, respectively:

\[
\Sigma''_{FL} = a + \omega^2 + T^2, \tag{3}
\]

\[
\Sigma''_{MFL} = \sqrt{(a + b\omega)^2 + T^2}. \tag{4}
\]

The square root in the last equation serves as a good approximation for the \( \text{Max}(\omega, T) \) expression that was originally proposed in the MFL model and is easier to implement numerically [13]. The impurity scattering coefficient \( a = 10 \text{ meV} \) and the coefficient \( b = 1 \). We then calculate the real part of the self-energy using the Kramers–Kronig transformation, as described previously [9].

The momentum resolution is taken into account by summing the spectra within a given momentum window. Such a procedure is justified, as the data in a real angle multiplexing analyser are usually electronically summed within a momentum range larger than the angular resolution of the lens and therefore a ‘window’ function is a better approximation than a Gaussian. The energy resolution is taken into account by convoluting the result with a one-dimensional Gaussian function of a defined width. A typical result from this procedure for the MFL model is shown in figure 1. In panel (a) the imaginary and real parts of the self-energy are plotted, while in panel (b) the simulated MDC data and Lorenzian fits are shown. The good quality of the fits is gratifying and expected, since in the case of an MFL the MDCs are Lorenzian, as discussed in section 1. We plot the corresponding results for the FL model in figure 2. Surprisingly, it can be seen that the MDC curves are equally represented using a Lorenzian lineshape for most energies.

3. Results and discussion

To obtain a more accurate comparison, we now compare the assumed self-energy to the one extracted from the model data. To do this we first fit Lorenzians to the MDCs obtained from the MFL model and plot their half-width at half-maximum, \( \Delta k \), multiplied by the bare Fermi velocity versus the binding energy. This result corresponds to the extracted values of the imaginary part of the self-energy:

\[
\Sigma'' = \Delta k v_F^0. \tag{5}
\]

We repeat this procedure for several sets of data, broadened by different momentum and energy resolutions. The resulting curves are plotted in figure 3(a), along with the imaginary part of the self-energy initially used to generate the model data. The extracted self-energy values agree
almost perfectly at higher binding energies. Both the absolute values as well as the linear dependence on the binding energy are well reflected in the extracted self-energy data. The differences between the model and extracted $\Sigma''$ are visible only at low energies (shown in the inset of figure 3(a), where we magnify the region around the chemical potential). The differences due to momentum resolution are not very significant—they slightly increase the value of $\Sigma''$ at
Figure 2. Simulated ARPES data for an FL. (a) Imaginary (red) and real (blue) parts of the self-energy. (b) Momentum distribution curves (red) with Lorenzian fits (blue).

low energies. The energy resolution has a more profound effect in the sense that it moves the minimum of $\Sigma''$ towards positive binding energies, which one could mistakenly interpret as a violation of particle–hole symmetry. It is not so, as in this study we have started with a $\Sigma''$ that was symmetric and the extracted data are much more symmetric at higher energy resolutions. The exact mechanism of this shift is explained later in the text when we discuss figure 5. Next, in figure 3(b) we compare the band dispersion (obtained from the MDC peak position) extracted...
Figure 3. Results for the fitting of simulated ARPES data for an MFL. (a) Extraction of the imaginary part of the self-energy. The inset shows the magnified region close to the chemical potential. (b) Influence of the momentum and energy resolution on the extraction of the band dispersion. (c) Magnified region close to the chemical potential from panel (b).
Figure 4. Results for the fitting of simulated ARPES data for the MFL model. (a) Extraction of the imaginary part of the self-energy. The inset shows the magnified region close to the chemical potential. (b) Influence of the momentum and energy resolution on the extraction of the band dispersion. (c) Magnified region close to the chemical potential from (b).

from the model data for various resolutions. In a similar way to the imaginary part of the self-energy, the dispersion is not affected significantly by the momentum resolution, while the energy resolution again leads to a significant difference. This is evident from figure 3(c), where the region close to the chemical potential is shown magnified. The dispersion of the curve with worse energy resolution diverges close to $\omega = 0$. This is again due to the interplay of the energy resolution with the Fermi function, where the MDC peak position is weighted towards the occupied portion of...
Figure 5. Illustration of the effects of the energy resolution on the extraction of the self-energy. (a) Effects of the energy resolution on the width. The three MDCs for negative \( \omega \) are equally weighted, but the MDCs for positive \( \omega \) are weighted mainly by the MDC at \( \omega = 2 \text{ meV} \), which is narrowest. This leads to the MDC at \( \omega = 0 \) being broader than the MDC at \( \omega > 0 \). (b) Effects on dispersion. The black curve is the MDC at \( \omega = 0 \) (\( \Delta E = 1 \text{ meV} \)), the green curve is the sum of the three upper MDCs—an equivalent of \( \Delta E = 4 \text{ meV} \). The green curve is shifted towards negative \( k \), since it is heavily weighted by the MDC at \( \omega = -2 \text{ meV} \) due to Fermi function.

We now examine the accuracy of the extraction method in the case of a FL. The overall functional dependence of the imaginary part of the self-energy extracted from the model data is very close to the assumed one, as evident from figure 4(a). These data are affected by the momentum and energy resolution in a very similar way to the previous MFL. However, at low energy
resolutions, we observe an additional feature—a dip at positive binding energy. In figure 4(b), we plot the dispersion extracted from the data for various resolutions. We note that the dispersion in this model is almost linear, with a small deviation caused by a high-frequency cut-off. We also note that the extracted dispersion is affected by the momentum and energy resolution in the same way as it was for the MFL.

To gain insights into the effects of the energy resolution on the extracted values of the self-energy, we plot in figure 5(a) three MDCs on either side of the chemical potential. While the weight of the curves for $\omega < 0$ do not change significantly, dramatic changes occur for $\omega > 0$ due to the Fermi cut-off. This is a well-known fact since for sharp spectral peaks, the chemical potential lies at about 80% of the leading edge, instead of 50% for the Fermi function alone [14]. This means that the spectral weight of the MDC changes more rapidly for $\omega > 0$. The bottom two curves in (a), are normalized sums of the three MDCs for $\omega < 0$ (blue curve) and $\omega > 0$ (red curve). The first curve is clearly broader because it is weighted almost equally by all three MDCs, while the second curve, due to Fermi function is heavily weighted by the MDC at $\omega = 0$ (which has the smallest width). This explains the asymmetry observed in figures 3 and 4. We now consider the influence of the energy resolution on the dispersion. In figure 5(b), we compare the position of the MDC obtained with a 1 meV energy resolution (black curve) with the sum of the three MDCs around the chemical potential, whose sum simulates a worsened energy resolution (green curve). Here again, since the green curve is heavily weighted by the MDC at more negative energies (due to the Fermi function), it will therefore be shifted towards negative values of momenta. This is exactly what we observed earlier when discussing figures 3 and 4.

4. Conclusions

In summary, we have examined the accuracy of a technique commonly used to extract the self-energy from ARPES data by using data modelling. We find that the technique of fitting the MDC with a Lorenzian yields good results not only in case of MFL, but also in FL. This is particularly important as it means this simple technique can be applied in the superconducting state, where signatures of both models are present. We also find that inadequate energy resolution can lead to artificial features in the extracted functional dependence of both the self-energy and dispersion for low values of the binding energy.

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