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TUTORIAL
Simulations of ARPES spectra for basic many-body interactions

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The aim of this tutorial is two-fold : first, to have a glance at how interactions affect the standard Bloch band structure of a solid, and second, to get familiar with a software (IGOR), widely used in the photoemission community, that is both user-friendly and powerful for data analysis (and even for interfacing experiments).

For simplicity, we will work only along one momentum direction, hence using $\mathbf{k} = k$, and will take the lattice constant as 1 Å, hence the edges of the Brillouin zone at $k = \pm\pi$.

Numerical constants : If, as usual in ARPES, the energies are expressed in eV, the momenta in Å^{-1}, and the rest in SI units, then one has, in the appropriate units : $\hbar^2/2m_e = (1/0.512)^2 = 3.815$, where m_e is the bare electron mass. Additionally, 1 eV$/k_B = 11604$ K.

Energy reference : We define the Fermi level as the zero of binding energy. At zero Kelvin, negative energies correspond to occupied states, and positive energies to non-occupied states.

For electrons photo-emitted from a many-body state of energy ε and momentum k, the ARPES intensity is given by :

$$I(\varepsilon, k) = I_0 \times A(\varepsilon, k) \times f(\varepsilon, T), \tag{1}$$

where I_0 is the "dipole matrix element", that we will consider henceforth constant and equal to 1 (in reality, I_0 can depend on electron momentum and photon energy and polarization !), $f(\varepsilon, T)$ is the Fermi-Dirac distribution at temperature T, and $A(\varepsilon, k)$ is the *many-body* spectral function. The last is given by :

$$A(\varepsilon, k) = \frac{1}{\pi} \frac{\Sigma_2(\varepsilon, k)}{[\varepsilon - \varepsilon_0(k) - \Sigma_1(\varepsilon, k)]^2 + \Sigma_2(\varepsilon, k)^2}, \tag{2}$$

where $\Sigma_1(\varepsilon, k)$ and $\Sigma_2(\varepsilon, k)$ are the real and imaginary parts of the electron self-energy (*and are Hilbert transforms of each other !*), and $\varepsilon_0(k)$ is the *bare* electron dispersion, i.e., the Bloch band of a free independent electron in the ionic periodic lattice.

From now on, to simplify the calculations, we will assume that the carriers are electrons, and their density is small, so that $\varepsilon_0(k) \approx -E_0 + (\hbar^2/2m_e)k^2$ (i.e., the periodic variation of the energy is neglected), with $(-E_0) < 0$ the energy of the bottom of the band. Additionally, we assume that the self-energy is k-independent : $\Sigma(\varepsilon, k) = \Sigma(\varepsilon)\ \forall k$.

1 Free electron with constant scattering rate

1. To familiarize yourself with IGOR's vectors of data (called "waves"), plot $f(\varepsilon, T)$ versus ε for several temperatures. Be mindful of using a *meaningful* energy scale (eV or meV) for the horizontal axis !
2. We assume that the electron scattering rate is constant (i.e., energy-independent), for instance due to impurity scattering. Hence, $\Sigma_2(\varepsilon) = \Gamma_0 = 0.02$ eV. In this case, causality imposes that $\Sigma_1(\varepsilon) = 0\ \forall \varepsilon$ (can you show it ?). Plot, *using color scales*, the electron spectral function, then the ARPES intensity (spectral function times the Fermi-Dirac distribution at temperature T). Play using different band-bottom energies and different temperatures.

2 Interaction with an Einstein phonon

The interaction of an electron with an Einstein phonon (a single phonon at an energy $\hbar\Omega_0 > 0$) is characterized by :

$$\Sigma_2^{\mathrm{E}}(-\hbar\Omega_0 < \varepsilon < \hbar\Omega_0) = 0 \tag{3}$$

$$\Sigma_2^{\mathrm{E}}(\varepsilon < -\hbar\Omega_0) = (\pi/2)\lambda\hbar\Omega_0 \tag{4}$$

$$\Sigma_2^{\mathrm{E}}(\varepsilon > \hbar\Omega_0) = (\pi/2)\lambda\hbar\Omega_0, \tag{5}$$

where $\lambda > 0$ is the (unitless) electron-phonon coupling constant. Thus, the *total* electron self-energy is :

$$\Sigma_2(\varepsilon) = \Gamma_0 + \Sigma_2^{\mathrm{E}}(\varepsilon). \tag{6}$$

The real part of the self-energy of an Einstein phonon is (can you show it ?) :

$$\Sigma_1^{\mathrm{E}}(\varepsilon) = -\frac{\lambda\hbar\Omega_0}{2} \log\left|\frac{\varepsilon + \hbar\Omega_0}{\varepsilon + \hbar\Omega_0}\right|, \tag{7}$$

1. Plot, *using color scales*, the electron spectral function, then the ARPES intensity. Play using different phonon energies, relative to the band-bottom, and different coupling constants. Choose a low temperature (e.g., 10 K) and a small impurity scattering rate (e.g., $\Gamma_0 = 0.02$ eV) to avoid a too large extrinsic (temperature + scattering) broadening and better see the effects of varying the other parameters.

3 Fermi liquid

For a 3D Fermi liquid of band-bottom $-E_0$ (hence "Fermi energy E_0"), the imaginary part of the self-energy is :

$$\Sigma_2(\varepsilon)^{\mathrm{FL}} = \alpha_{3D} \frac{\pi}{8E_0} \frac{\varepsilon^2 + (\pi k_B T)^2}{1 + e^{-\varepsilon/k_B T}}, \tag{8}$$

where, for most densities in the metallic range, the constant $\alpha_{3D} \approx 1$. (G. Giulani and G. Vignale, *The Quantum Theory of the Electron Liquid*, Cambridge University Press 2005).

1. Calculate numerically the real part of the Fermi-liquid self-energy.
2. Plot the ARPES intensity for a Fermi liquid. Play using different temperatures and values for α_{3D}.

4 To play at home : Resolution broadening

Write a procedure to convolute the above-calculated ARPES intensities with a 2D Gaussian representing the instrumental energy and momentum resolutions (typical values are $1 - 100$ meV and $0.001 - 0.1$ Å^{-1}). Analyze the effect of resolution broadening on the different spectral features.