Fitting of the effective mass

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In solid state physcis, the effective mass is defined as follows:

$$\frac{1}{m^*_{\alpha\beta}} = \frac{1}{\hbar^2}\frac{d^2E(\mathbf{k})}{dk_\alpha dk_\beta} \tag{1}$$

where m^* is effective mass, and $E(k)$ is the band dispersion relation between energy E and k. And the effective mass reflects the band curvature, the flatter of band, the larger effective mass.

In this report, I will fit the effective mass around the Γ point for the semiconductor material $CuInSe_2$ by taking advantage of least-squares fitting in Python.
Energy E is as follows:

$$E = \frac{\hbar^2}{2m^*_{xy}}(k_x^2 + k_y^2) + \frac{\hbar^2}{2m^*_z}(k_z^2) \tag{2}$$

which means that we want to know the value m^*_{xy} and m^*_z by given the value of E and k_x, k_y and k_z.

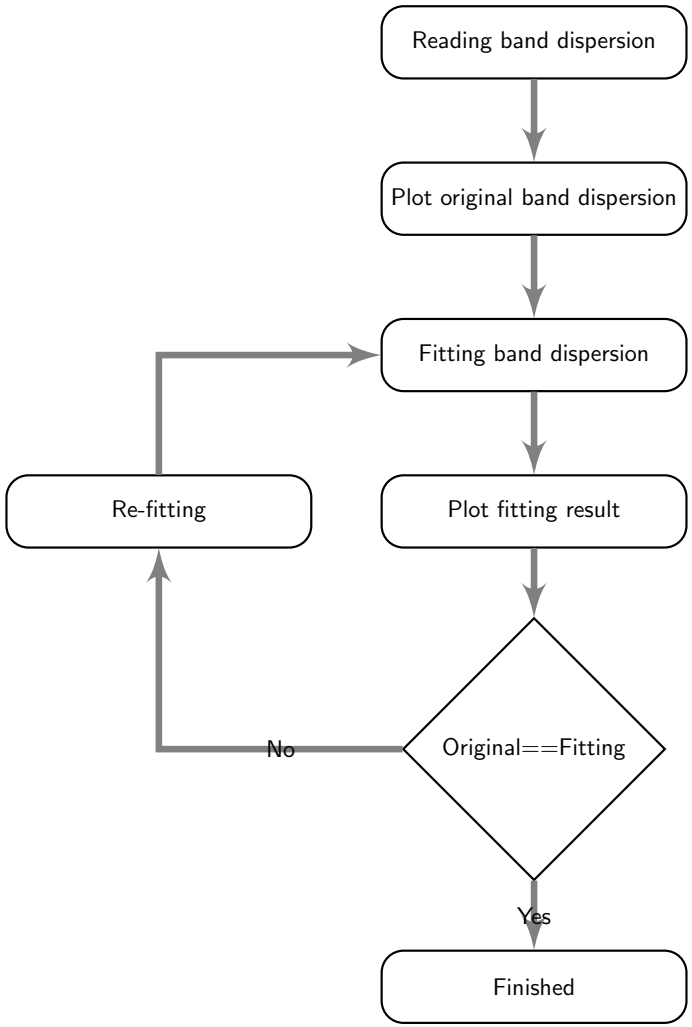

Figure: Flow chart of fitting energy band dispersion

Here are the results from fitting, I compare my fitting results (value inside the parentheses in red color) with the paper [C. Persson, Appl. Phys. Lett. 93, 072106 (2008)], where I find out there are quite similar, so the code is reliable to be used.

Table: Effective mass for $CuInSe_2$

	$c1$	$v1$	$v2$	$v3$
m_{xy}	0.08 (0.08)	0.14 (0.13)	0.25 (0.25)	0.27 (0.26)
m_z	0.09 (0.09)	0.66 (0.65)	0.12 (0.12)	0.28 (0.28)

And following figures are the fitting result from $v1$ as one example, also with testing results.

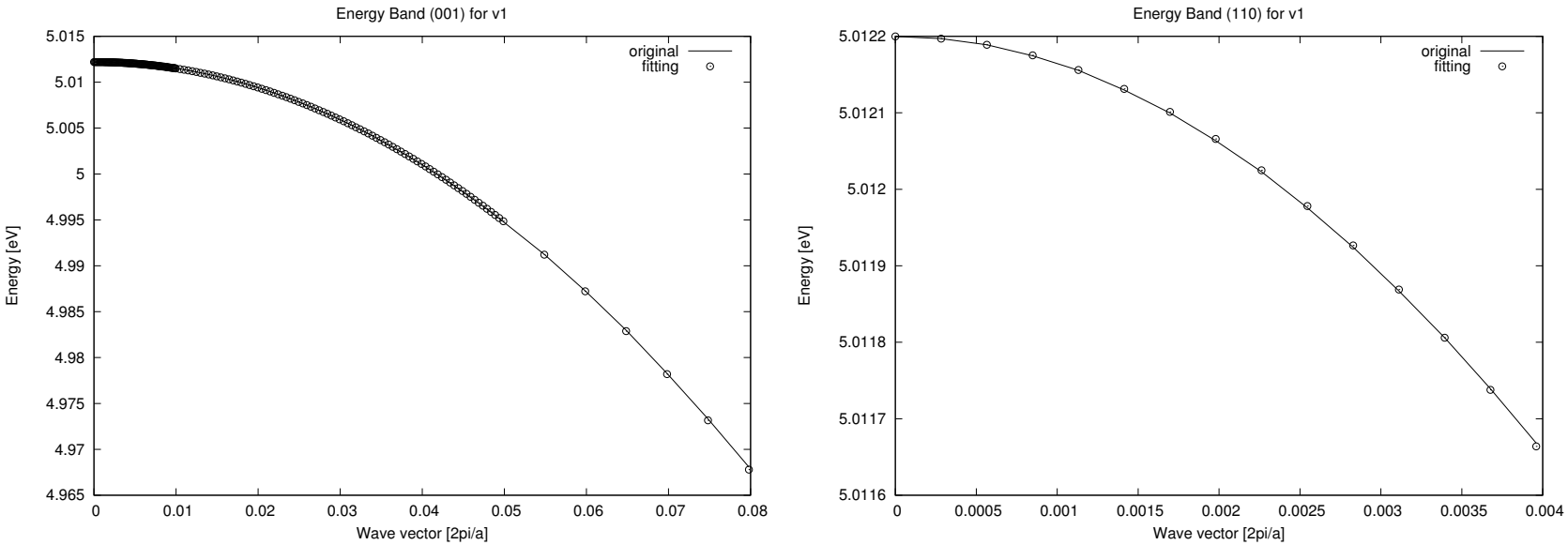

Figure: Fitting results for band $v1$

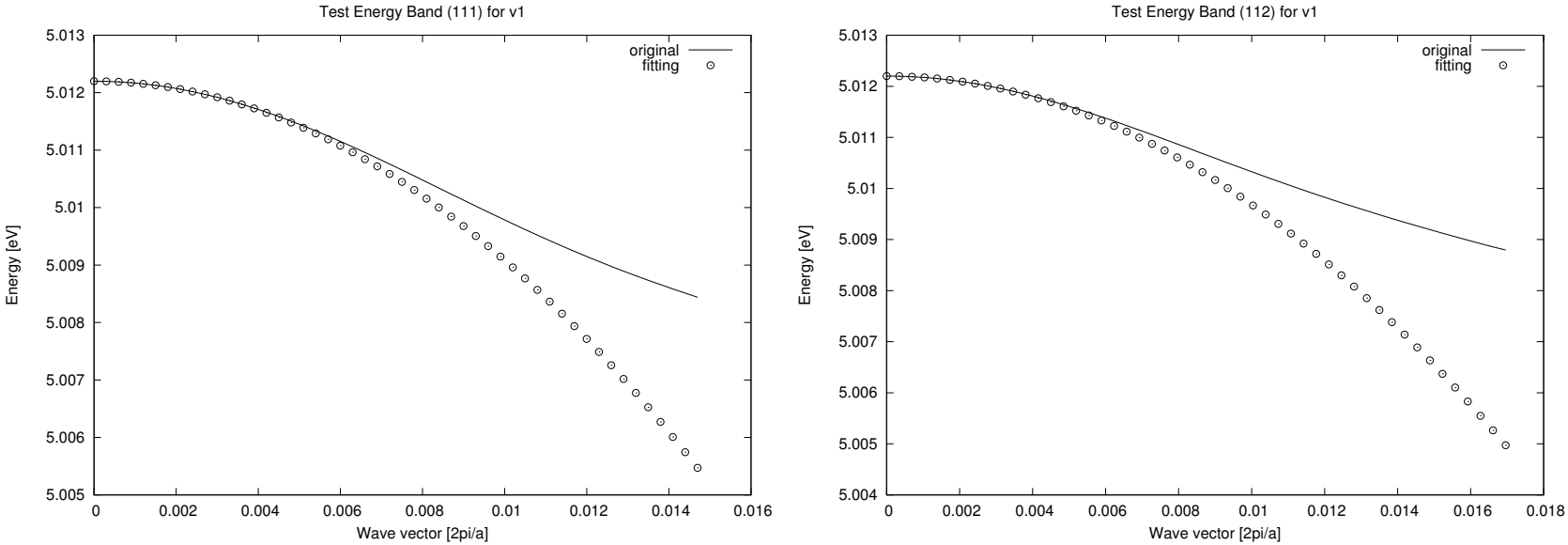

Figure: Testing results for band $v1$

There are several places I can improve this code, for example, I can creat a graphical user interface to convenient user, or make this code more flexible, or find the maximum valence band index automatically.

Thank you for your time!