A precise method for visualizing dispersive features in image plots

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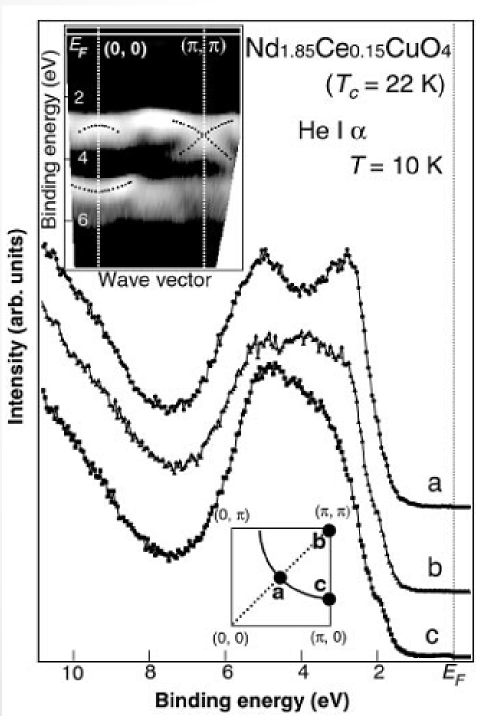
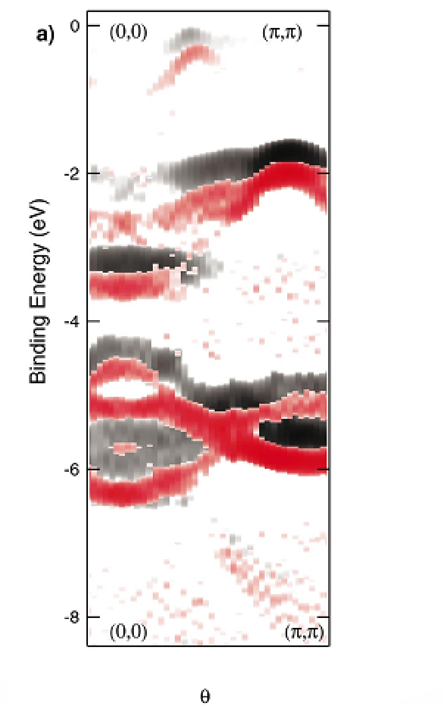
REVIEW OF SCIENTIFIC INSTRUMENTS **82**, 043712 (2011)

Introduction

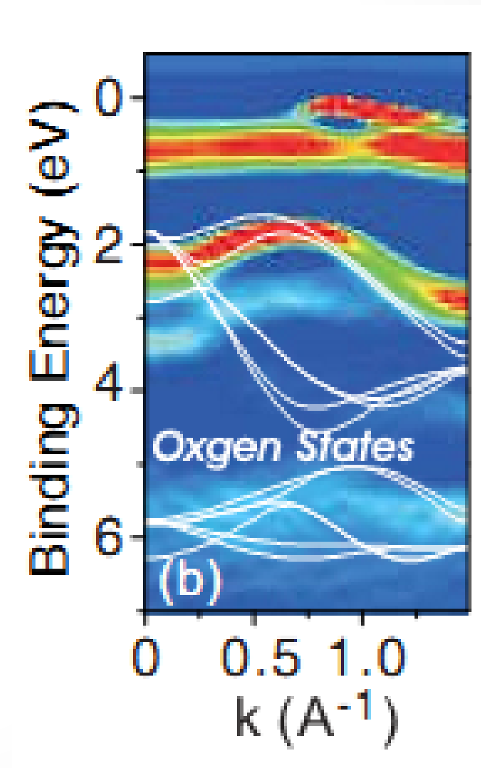
- Second derivative is widely used to get a better visualization of the band dispersions in ARPES intensity plot.



Science **291**, 1517 (2001)



PHYSICAL REVIEW B **67**, 165101 (2003)

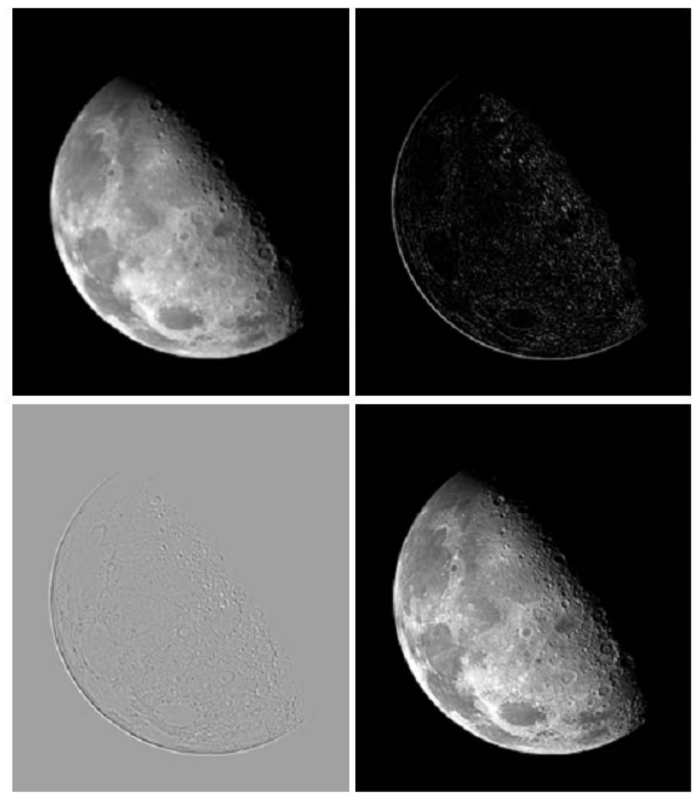


PRL **97,** 186405 (2006)

Second derivative in Digital Image Processing

- Moon picture from NASA processed by the Laplacian filter.

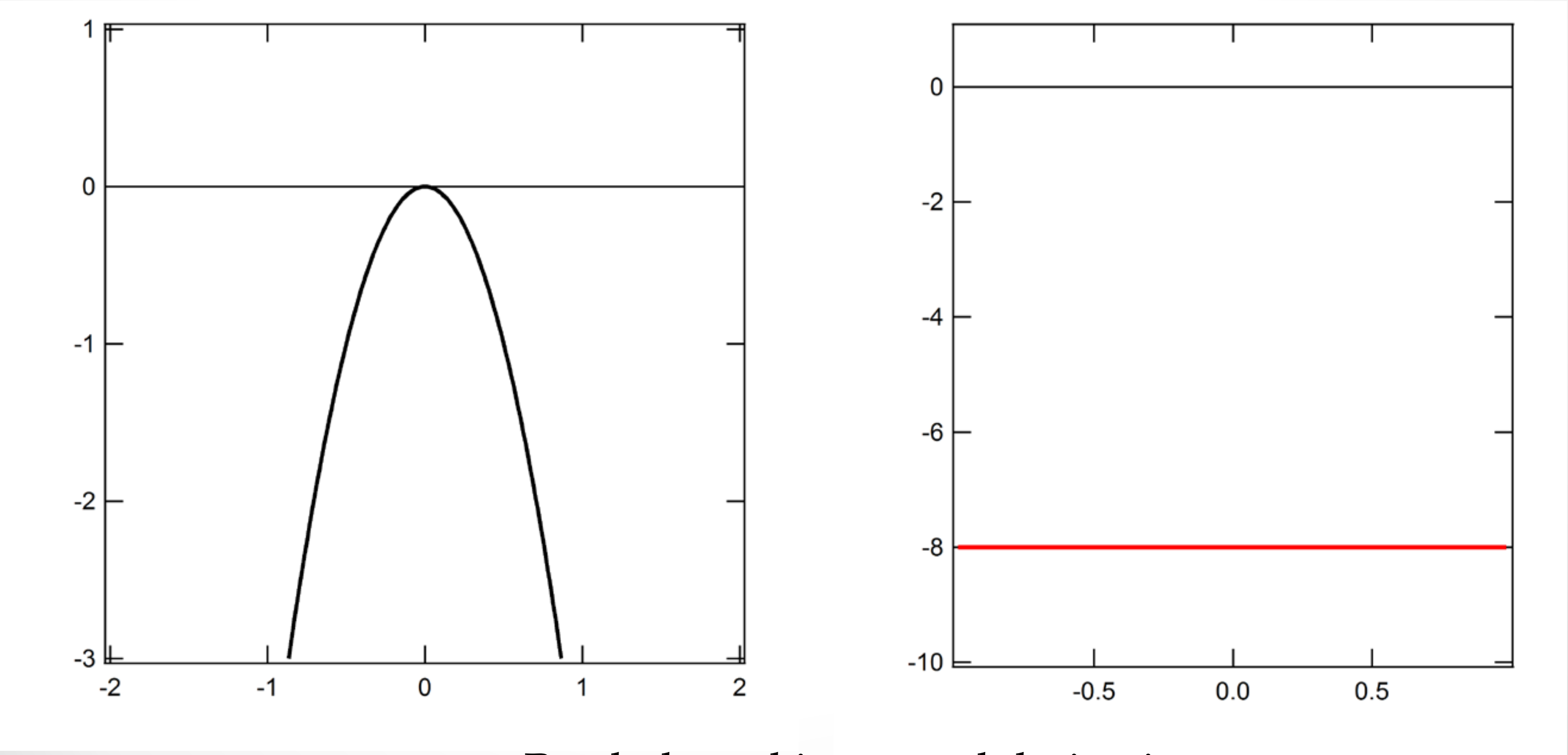
$$g(x,y) = \begin{cases} f(x,y) - \nabla^2 f(x,y) \\ f(x,y) + \nabla^2 f(x,y) \end{cases}$$



Digital Image Processing, Rafael C. Gonzalez, Richard E. Woods, Prentice Hall (2001)

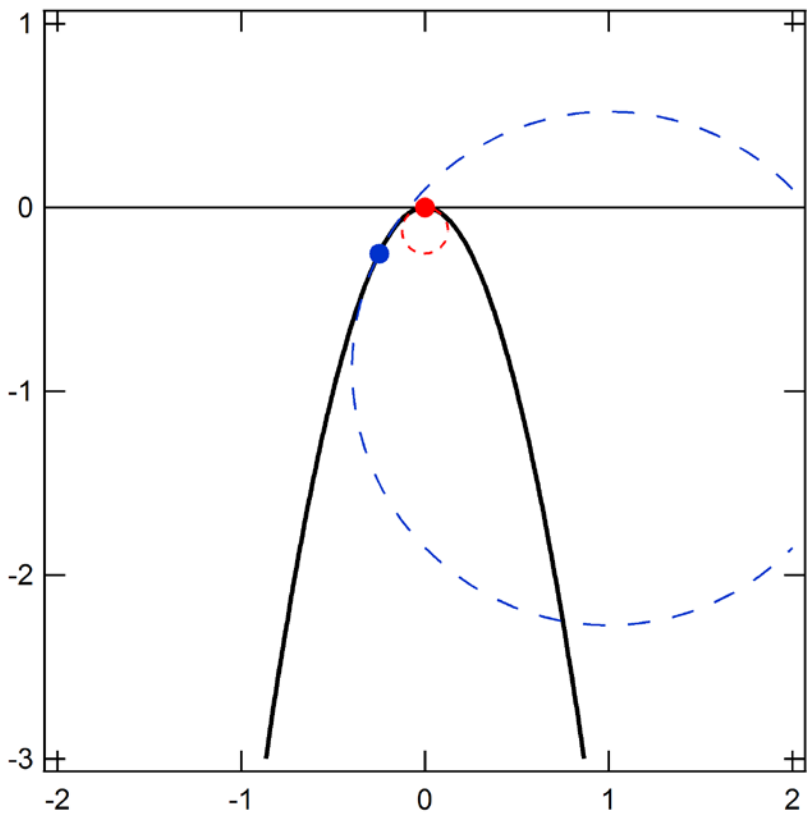
Why second derivative?

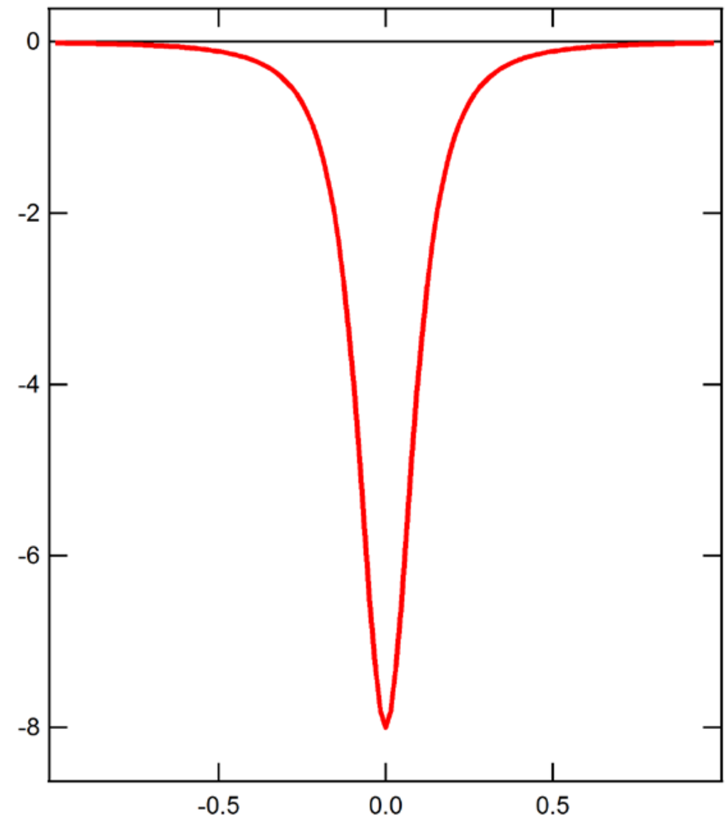
- There is no theory claiming that second derivatives will recover the peak features.



Parabola and its second derivative

Curvature and curve peaks





Curvature is a measure of the amount of curving.

$$C(x) = \frac{f''(x)}{(1 + f'(x)^2)^{\frac{3}{2}}}$$

1D curvature

- Definition

$$C(x) = \frac{f''(x)}{(1+f'(x)^2)^{\frac{3}{2}}}$$

- For linear transformation, $f(x) \rightarrow I_0 f(x)$

$$C(x) = \frac{I_0 f''(x)}{(1+I_0^{\,2} f'(x)^2)^{\frac{3}{2}}} \sim \frac{f''(x)}{(I_0^{\,-2} + f'(x)^2)^{\frac{3}{2}}} \sim \boxed{\frac{f''(x)}{(C_0 + f'(x)^2)^{\frac{3}{2}}}}$$

There is an extra constant, which makes the curvature more flexible to get the band dispersions.

The arbitrary constant

- When C_0 goes to infinity

$$C(x) \sim \frac{f''(x)}{\left(C_0 + f'(x)^2\right)^{3/2}} \sim f''(x),$$

Curvature is the same as second derivative.

- When C_0 goes to 0

$$C(x) \sim \frac{f''(x)}{\left(C_0 + f'(x)^2\right)^{3/2}} \sim \frac{f''(x)}{f'(x)^3}.$$

f'(x) is 0 at peak positions

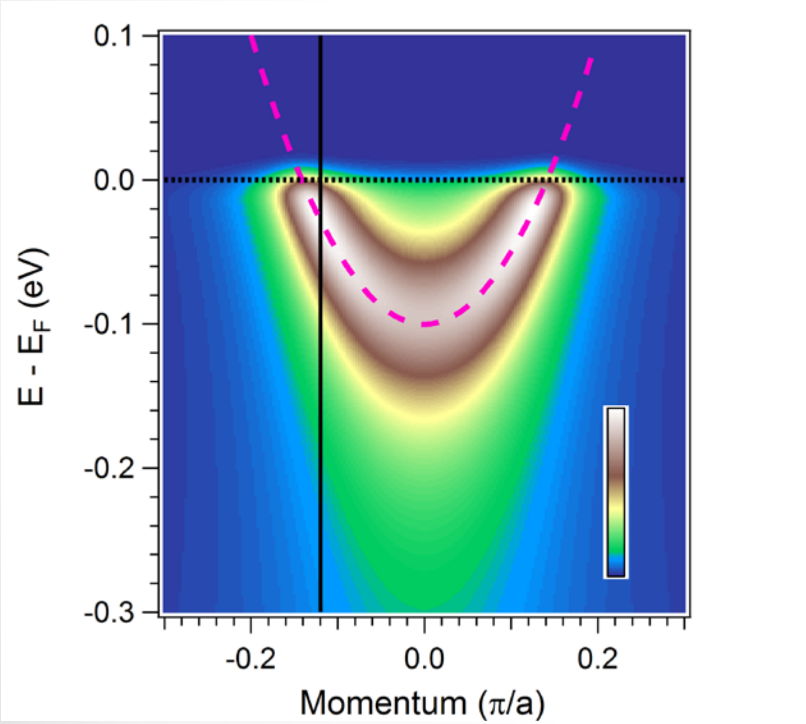
Curvature peaks approach the original peaks.

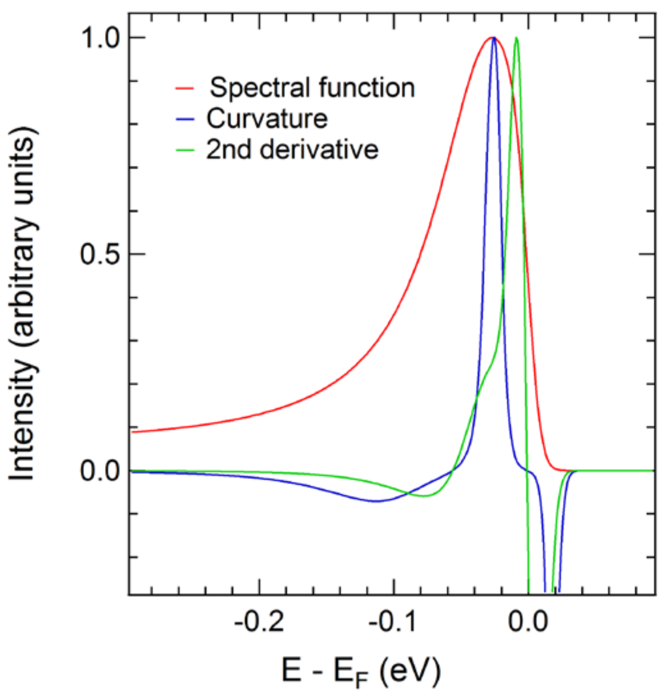
A computting tip

$$C(x) \sim \frac{f''(x)}{(C_0 + f'(x)^2)^{\frac{3}{2}}} \sim \frac{f''(x)}{(a_0 + f'(x)^2 / |f'(x)|_{\max}{}^2)^{\frac{3}{2}}}$$

- f'(x) can be in a very wide range depending on data. To make the constant more robust, it is better to normalize f'(x) by its maximum.
- The reasonable range of a_0 is about 10 ~ 0.001. (However, you can go further, depending on the data.)

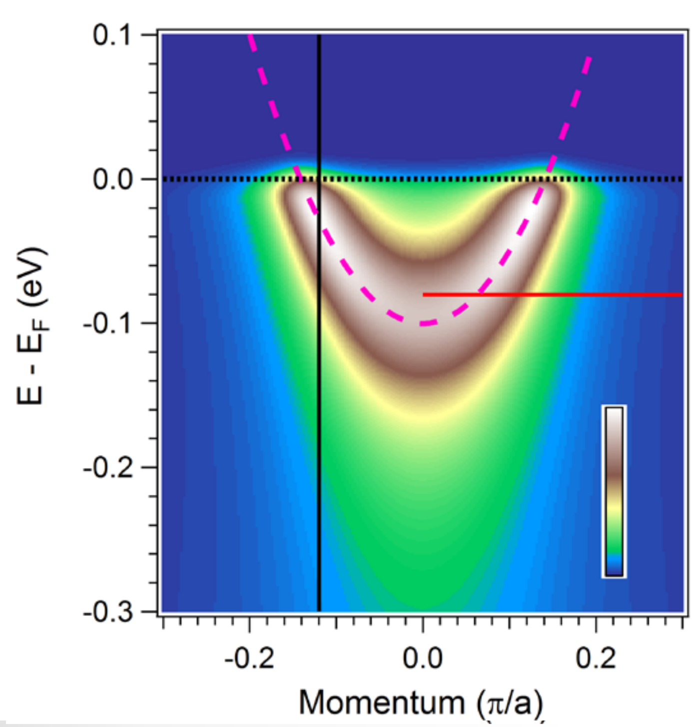
Curvature Application

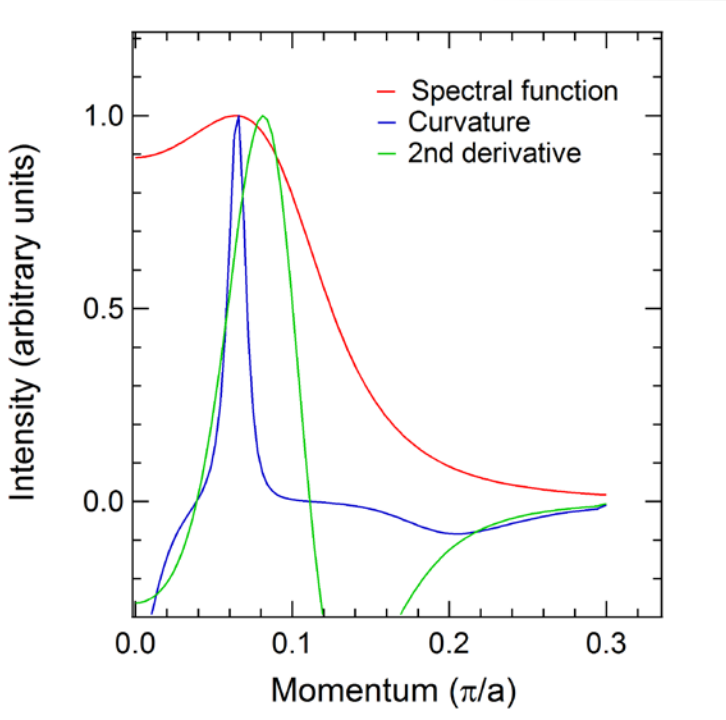




- More accurate peaks;
  Sharper bands.

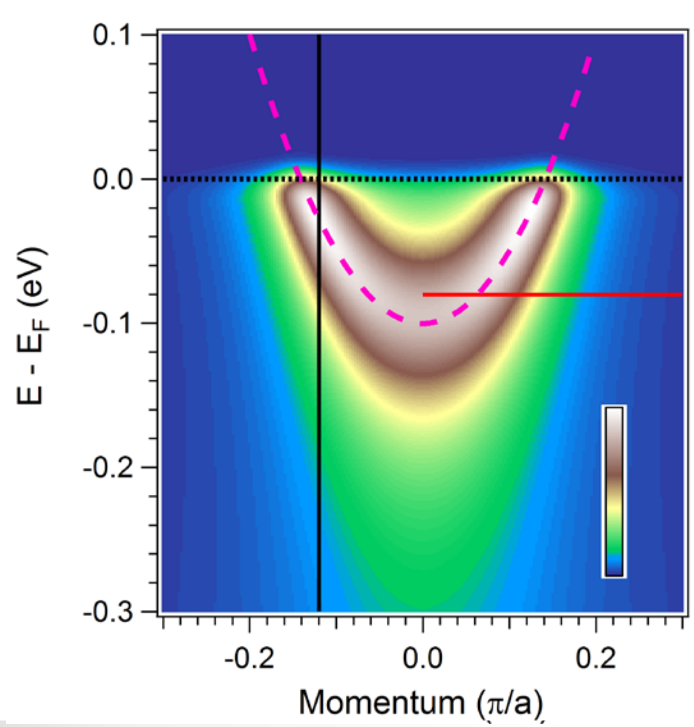
Curvature Application

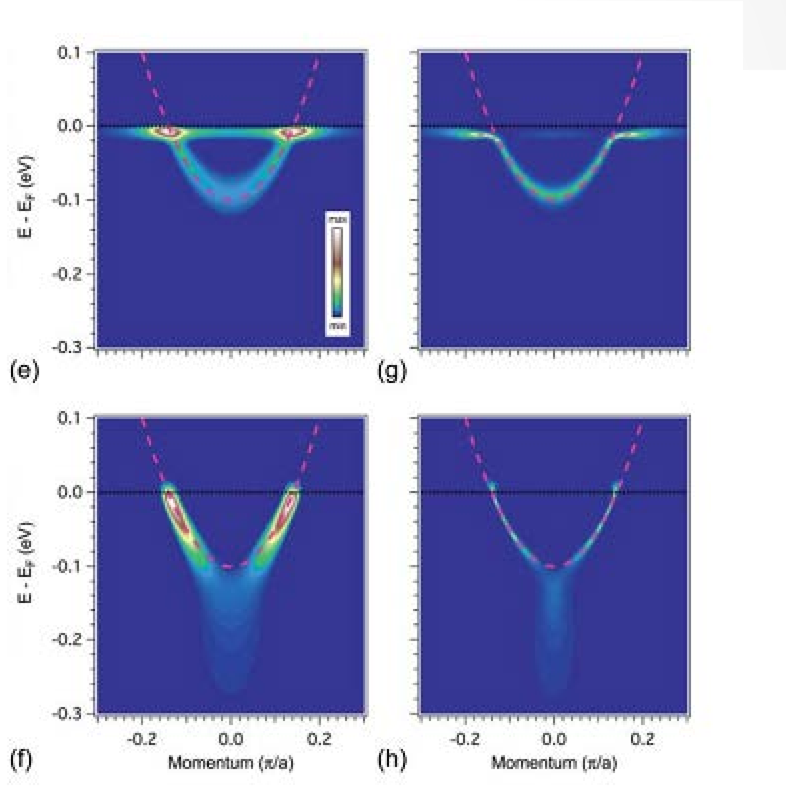




More accurate peaks;
Sharper bands.

Curvature Application





Second derivative

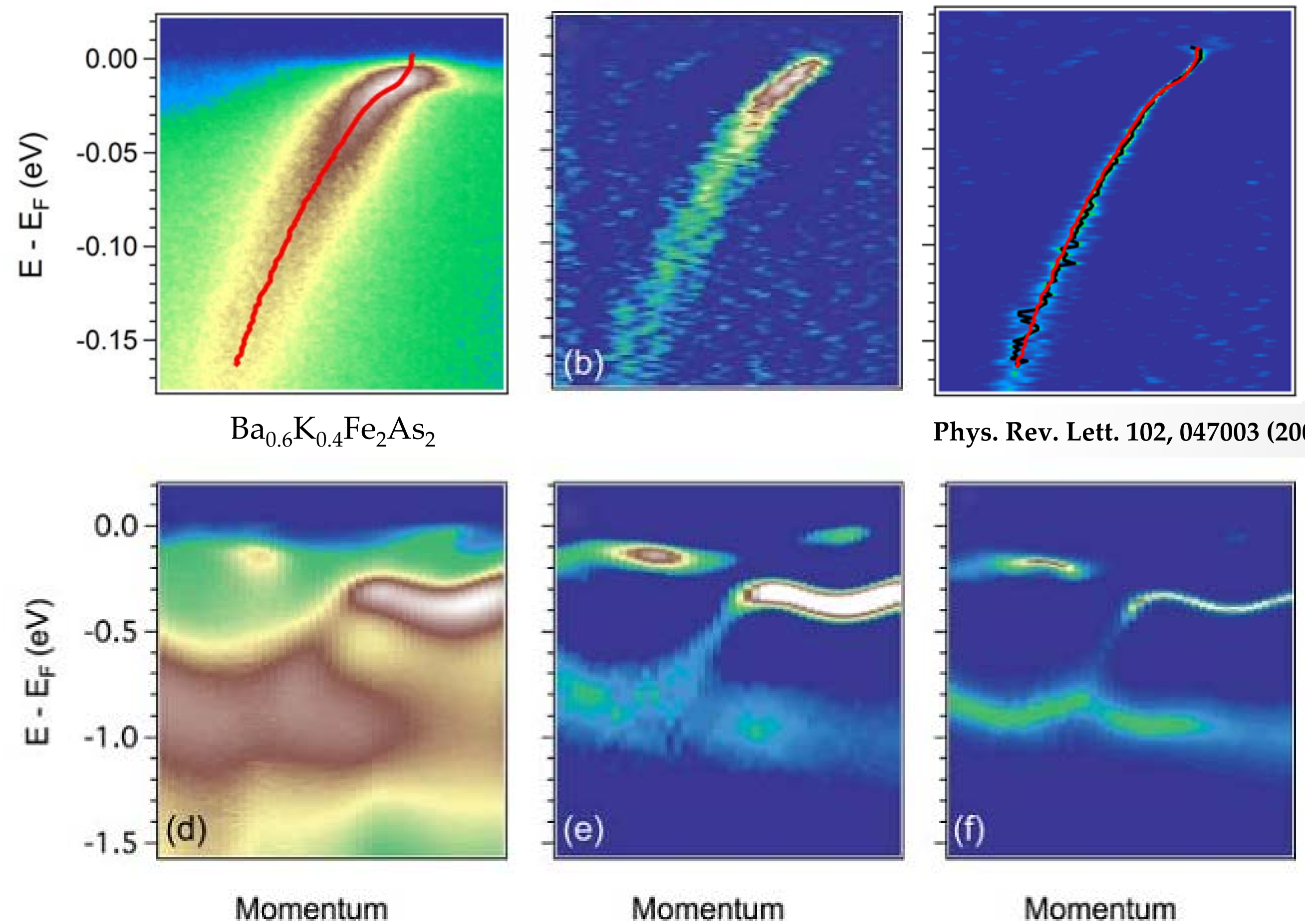
Curvature

More accurate peaks;
Sharper bands.

Curvature Application

Advantages:

- More accurate peaks;
- Sharper bands.
-



$Sr_4V_2O_6Fe_2As_2$

Physical Review B 83, 140513(R) (2011)

Raw data Second derivative Curvature

2D Lapalace Operator

- In ARPES data, we cannot use Laplacian filter since the dimensions of the two terms are different.

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$$

- We can start from the Taylor expansion

$$f(x_0+\Delta x, y_0+\Delta y) = f(x_0, y_0) + (\frac{\partial f(x_0,y_0)}{\partial x}\Delta x + \frac{\partial^2 f(x_0,y_0)}{\partial y^2}\Delta y) + (\underbrace{\frac{\partial^2 f(x_0,y_0)}{\partial x^2}(\Delta x)^2 + \frac{\partial^2 f(x_0,y_0)}{\partial y^2}(\Delta y)^2}_{} + 2\frac{\partial^2 f(x_0,y_0)}{\partial x \partial y}(\Delta x \Delta y)) + \ldots$$

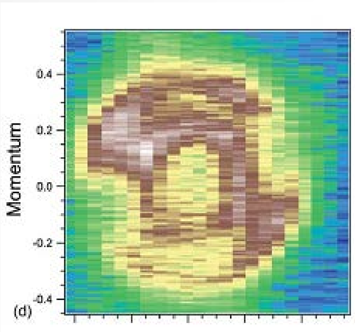
- Using the second order terms

$$\Delta f = \frac{\partial^2 f}{\partial x^2}(\Delta x)^2 + \frac{\partial^2 f}{\partial y^2}(\Delta y)^2$$

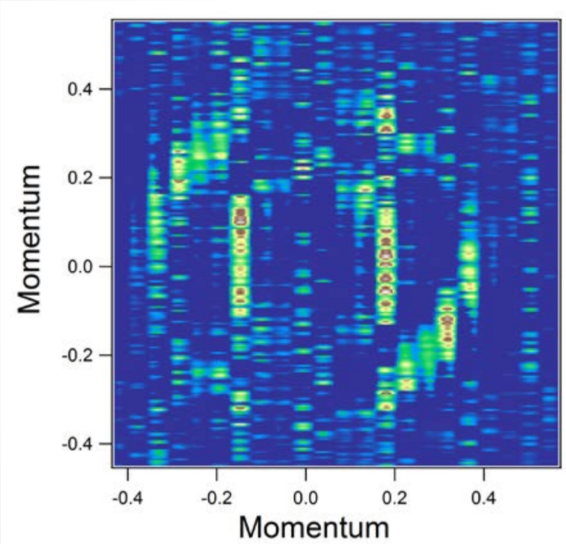
- We got

$$\Delta f \sim \frac{\Delta f}{(\Delta y)^2} = \frac{\partial^2 f}{\partial x^2}(\frac{\Delta x}{\Delta y})^2 + \frac{\partial^2 f}{\partial y^2}$$

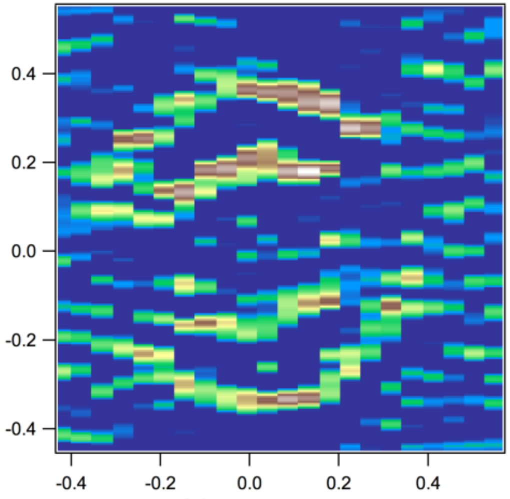
Application



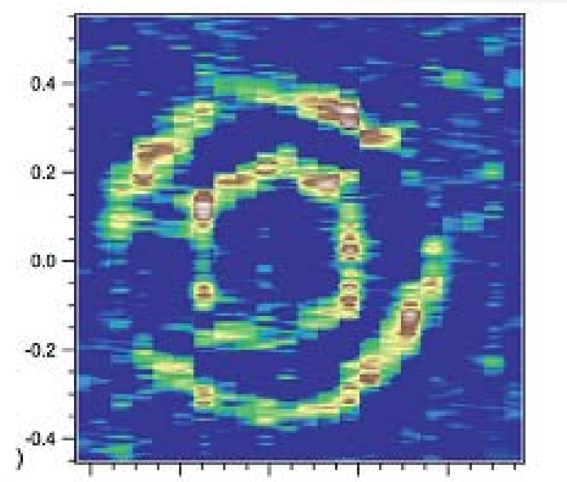
Raw data



Horizontal
second derivative



Vertical
second derivative



2D
second derivative

2D curvature

- Mean curvature in 2D

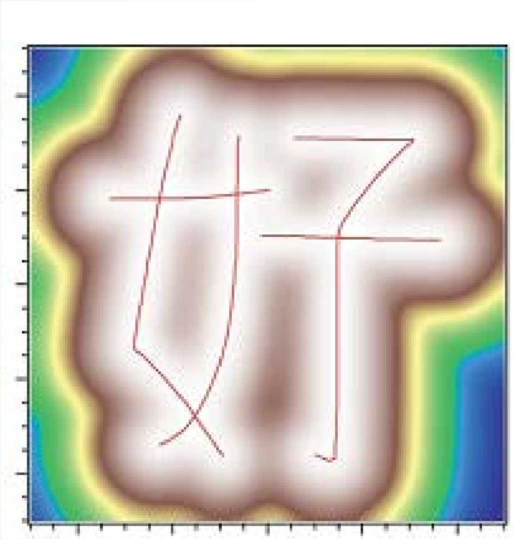
$$C(x,y)=\frac{[1+(\frac{\partial f}{\partial x})^2]\frac{\partial^2 f}{\partial y^2}-2\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\frac{\partial^2 f}{\partial x\partial y}+[1+(\frac{\partial f}{\partial y})^2]\frac{\partial^2 f}{\partial x^2}}{[1+(\frac{\partial f}{\partial x})^2+(\frac{\partial f}{\partial y})^2]^{\frac{3}{2}}}$$

- Making replacements: $\frac{\partial f}{\partial x}\to\frac{\partial f}{\partial x}I_0\Delta x\,,\frac{\partial f}{\partial y}\to\frac{\partial f}{\partial y}I_0\Delta y$

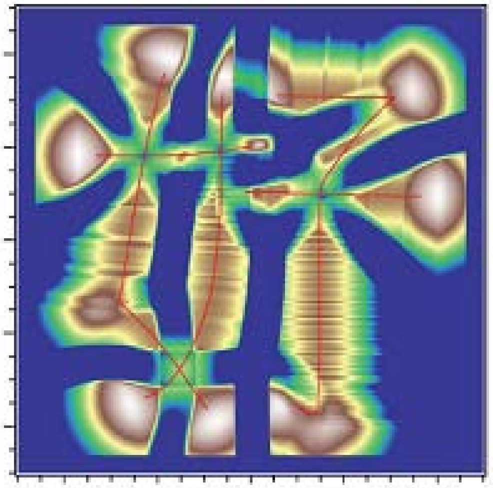
$$C(x,y)\sim\frac{\left[1+C_x\left(\frac{\partial f}{\partial x}\right)^2\right]C_y\frac{\partial^2 f}{\partial y^2}-2C_xC_y\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\frac{\partial^2 f}{\partial x\partial y}+\left[1+C_y\left(\frac{\partial f}{\partial y}\right)^2\right]C_x\frac{\partial^2 f}{\partial x^2}}{\left[1+C_x\left(\frac{\partial f}{\partial x}\right)^2+C_y\left(\frac{\partial f}{\partial y}\right)^2\right]^{3/2}},$$

Where $C_x=(I_0\Delta x)^2$, $C_y=(I_0\Delta y)^2$

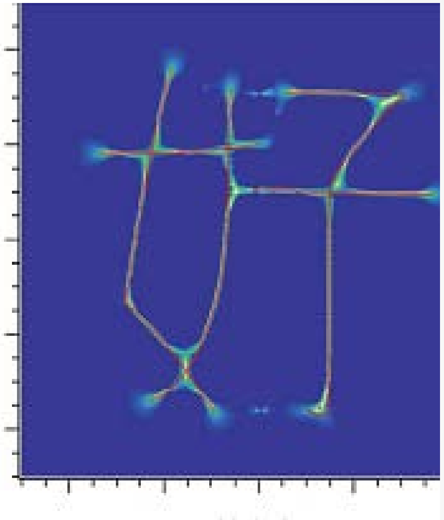
2D Curvature Application



Raw data



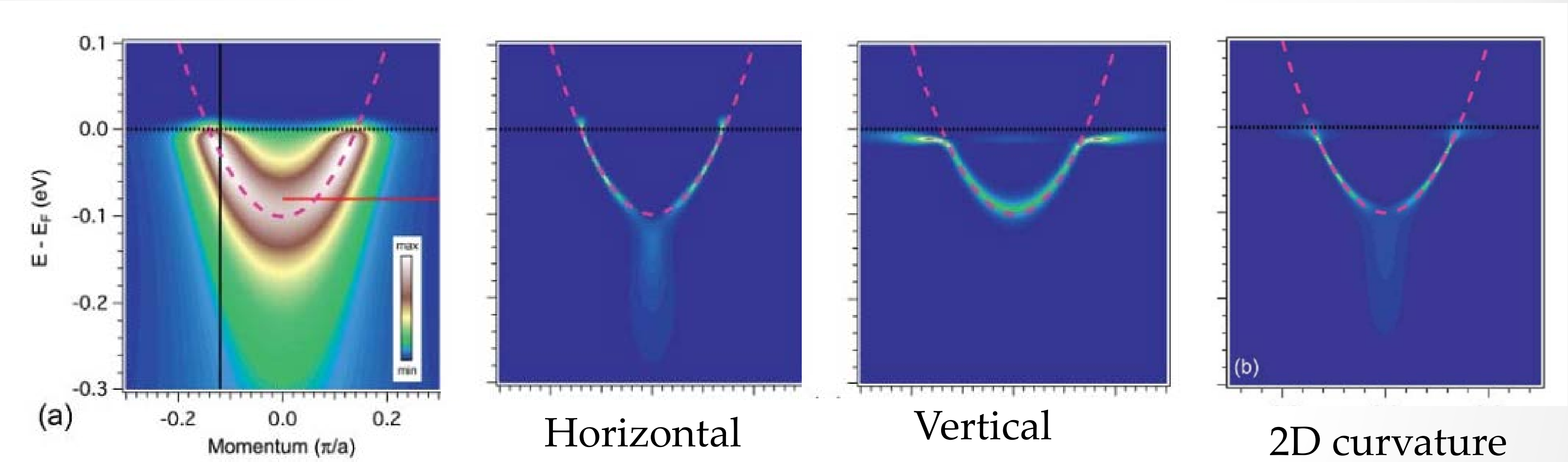
2D second derivative



2D curvature

- 2D curvature method gives a much better representation of the original character, with very sharp strokes.
- Only little distortion can be observed near stroke intersections and near the beginning and the end of each stroke.

2D Curvature Application



Horizontal curvature

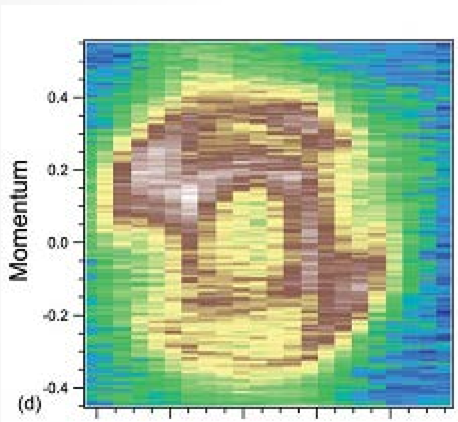
Vertical curvature

2D curvature

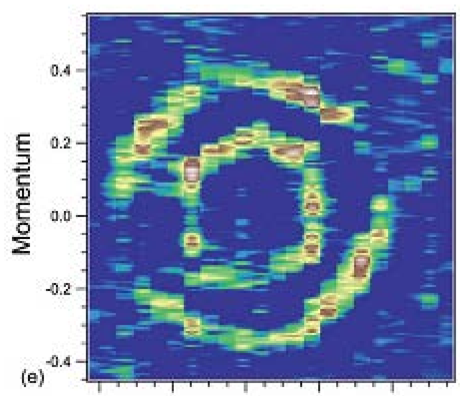
- 2D curvature method tracks the original band dispersion with higher accuracy over the whole range of energy.

2D Curvature Application

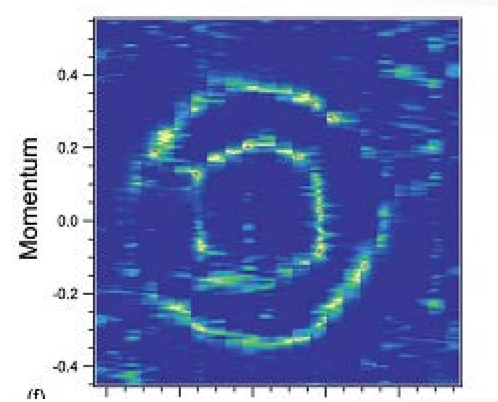
- Fermi surface contour of $Ba_{0.6}K_{0.4}Fe_2As_2$



Raw data



2D second derivative



2D curvature

Conclusions

- 1D curvature

$$f''(x) \longrightarrow \boxed{C(x) \sim \frac{f''(x)}{\left(C_0 + f'(x)^2\right)^{3/2}}}$$

- 2D curvature

$$C(x,y) \sim \frac{\left[1 + C_x\left(\frac{\partial f}{\partial x}\right)^2\right] C_y \frac{\partial^2 f}{\partial y^2} - 2C_x C_y \frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\frac{\partial^2 f}{\partial x \partial y} + \left[1 + C_y\left(\frac{\partial f}{\partial y}\right)^2\right] C_x \frac{\partial^2 f}{\partial x^2}}{\left[1 + C_x\left(\frac{\partial f}{\partial x}\right)^2 + C_y\left(\frac{\partial f}{\partial y}\right)^2\right]^{3/2}},$$

Where $C_x=(l_0\Delta x)^2$, $C_y=(l_0\Delta y)^2$

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