

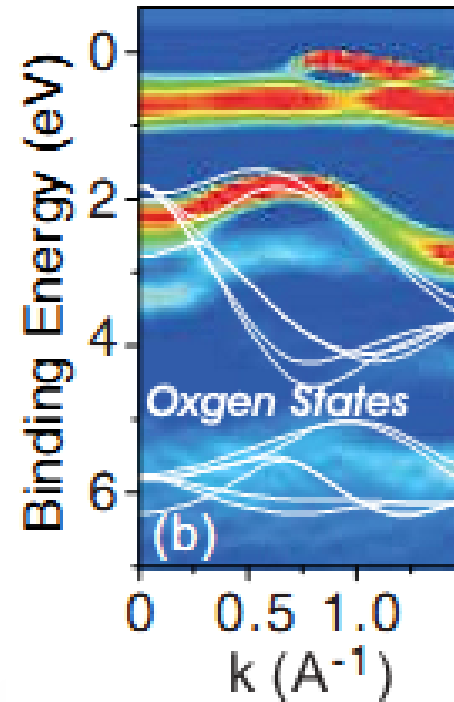
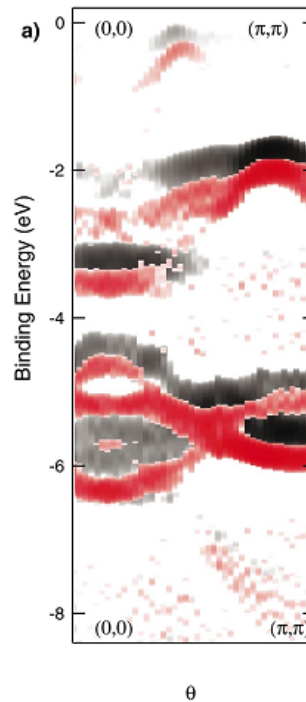
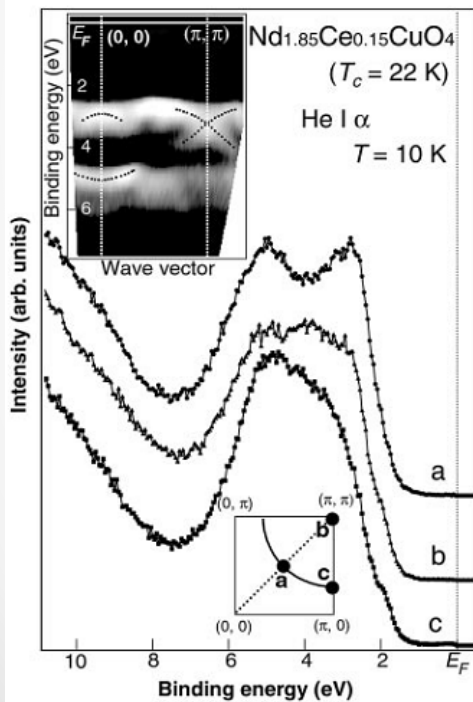
A precise method for visualizing dispersive features in image plots

Peng Zhang, P. Richard, T. Qian, Y. -M. Xu, X. Dai, and H. Ding

- Institute of Physics, Chinese Academy of Sciences
- Advanced Light Source, Lawrence Berkeley National Laboratory

Introduction

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



Science **291**, 1517 (2001)

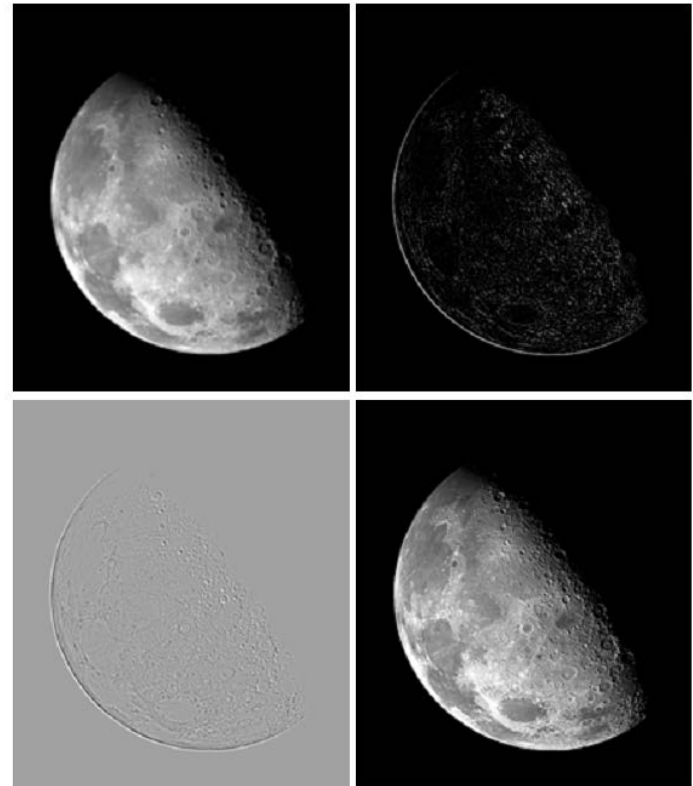
PHYSICAL REVIEW B **67**, 165101 (2003)

PRL **97**, 186405 (2006)

Second derivative in Digital Image Processing

- Moon picture from NASA processed by the Laplacian filter.

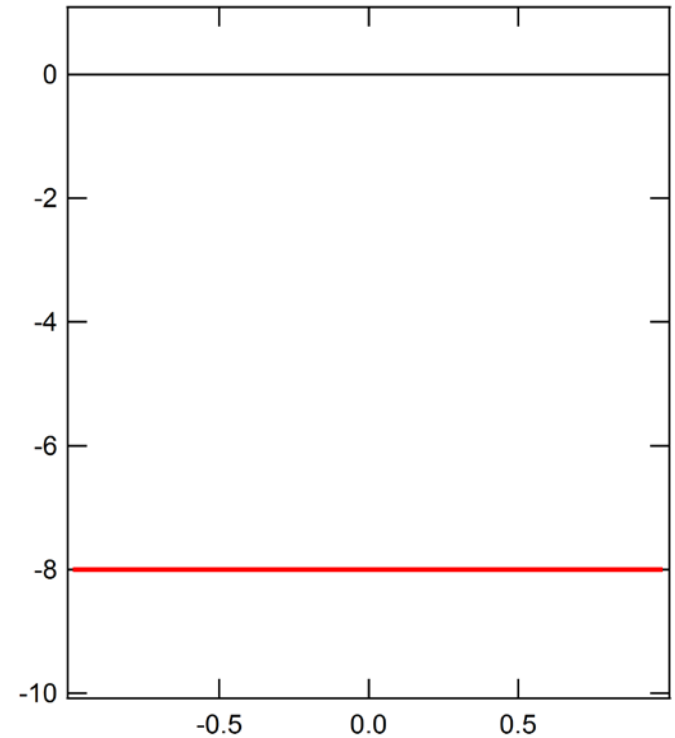
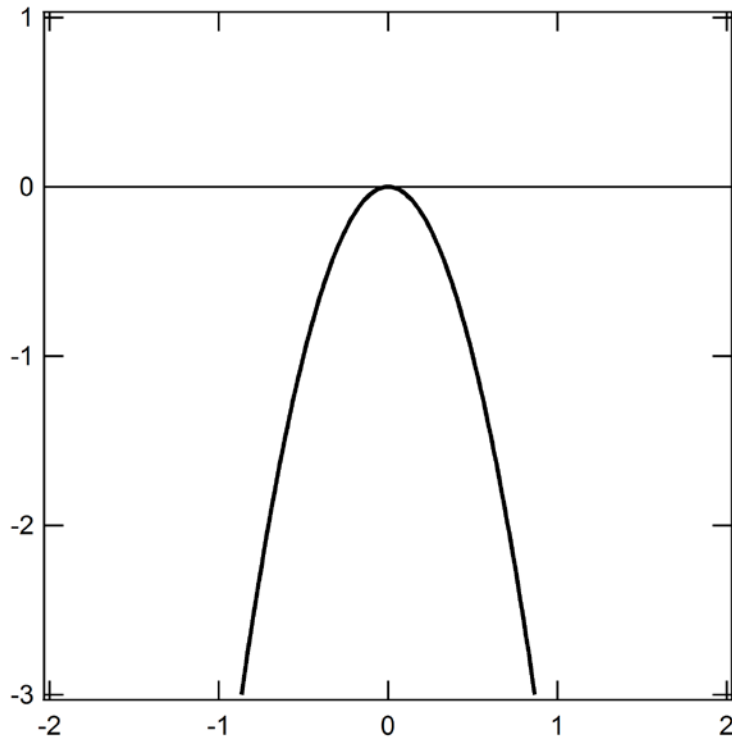
$$g(x, y) = \begin{cases} f(x, y) - \nabla^2 f(x, y) \\ f(x, y) + \nabla^2 f(x, y) \end{cases}$$



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

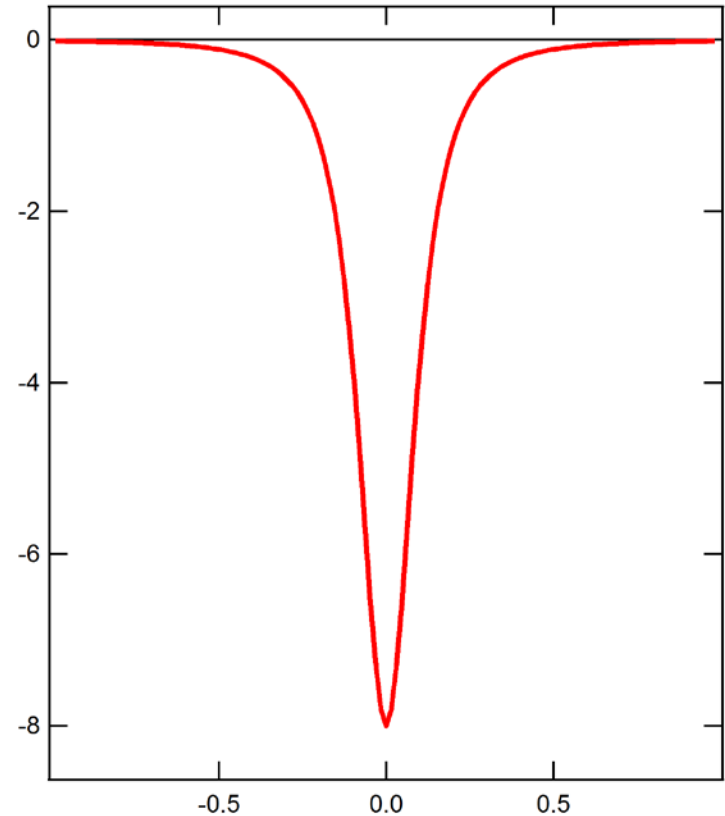
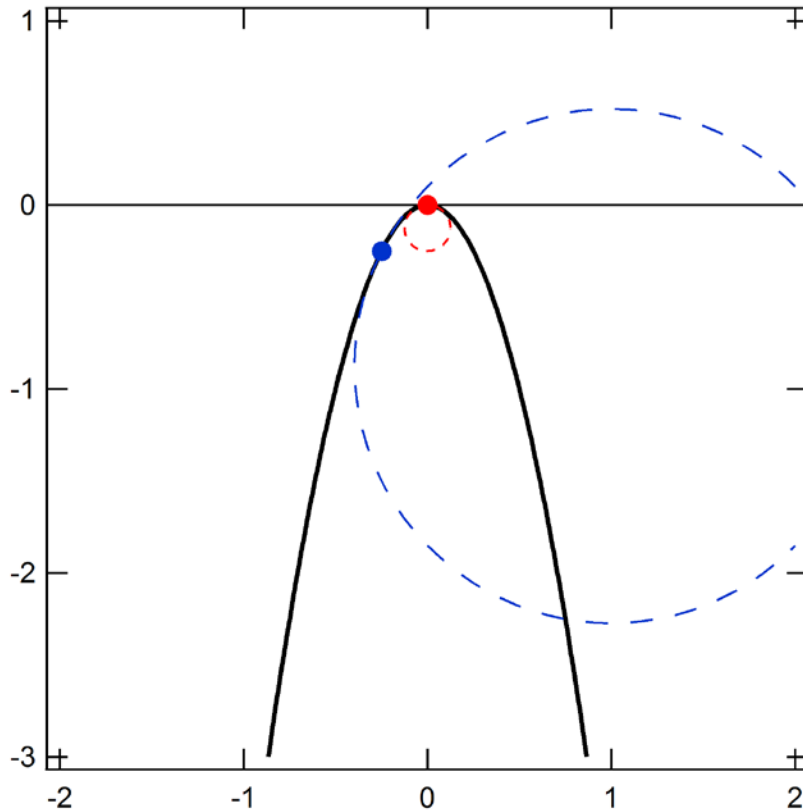
Why second derivative?

- 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, $f(x) \rightarrow I_0 f(x)$

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

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

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

Curvature is the same as second derivative.

- When C_0 goes to 0

$$C(x) \sim \frac{f''(x)}{(C_0 + f'(x)^2)^{3/2}} \sim \frac{f''(x)}{f'(x)^3} \rightarrow f'(x) \text{ is 0 at peak positions}$$

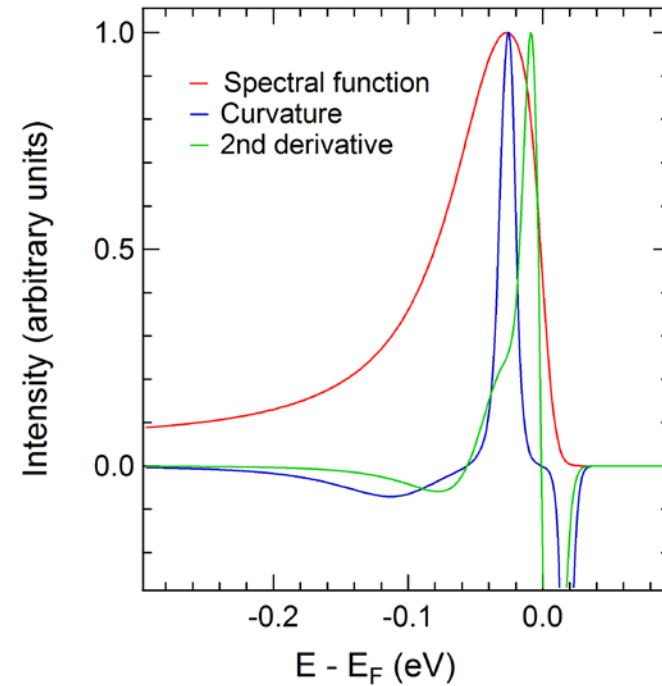
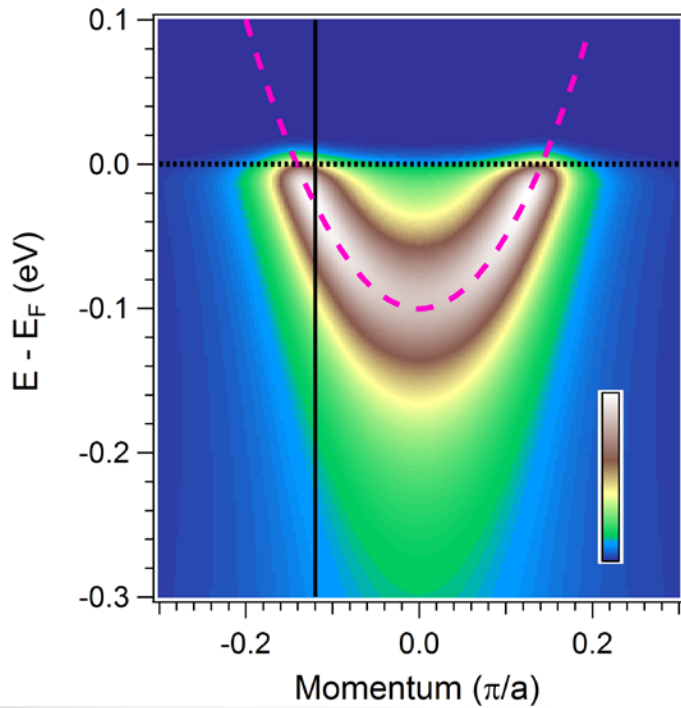
Curvature peaks approach the original peaks.

A computing tip

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

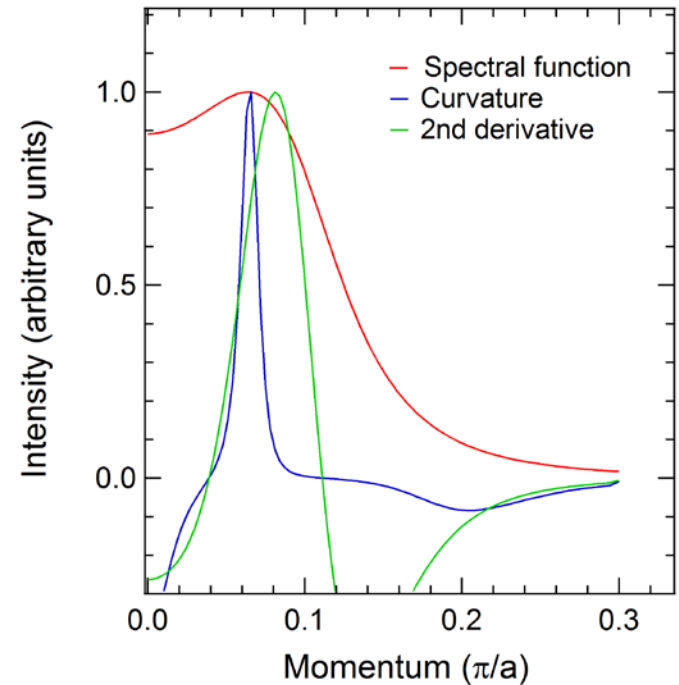
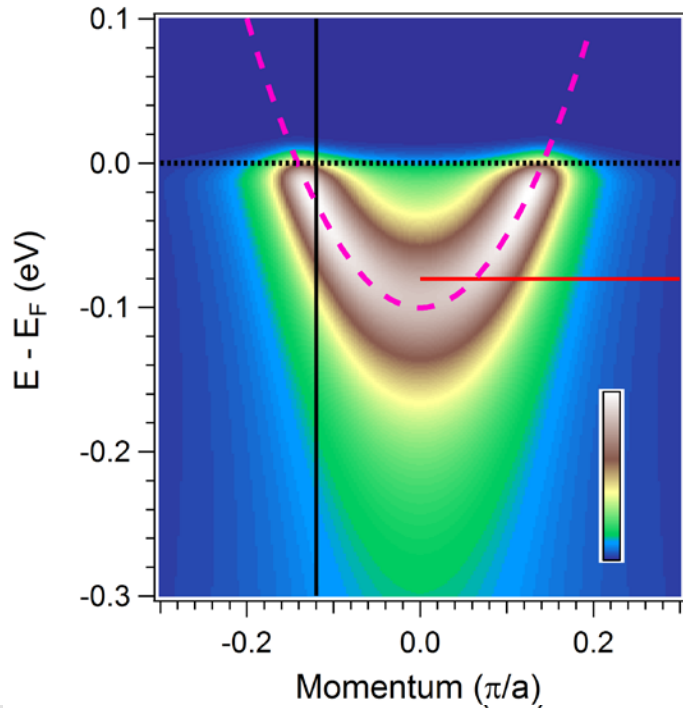
- $f'(x)$ can be in a very wide range depending on data. To make the constant more robust, it is better to normalize $f'(x)$ by its maximum.
- The reasonable range of a_0 is about $10 \sim 0.001$. (However, you can go further, depending on the data.)

Curvature Application



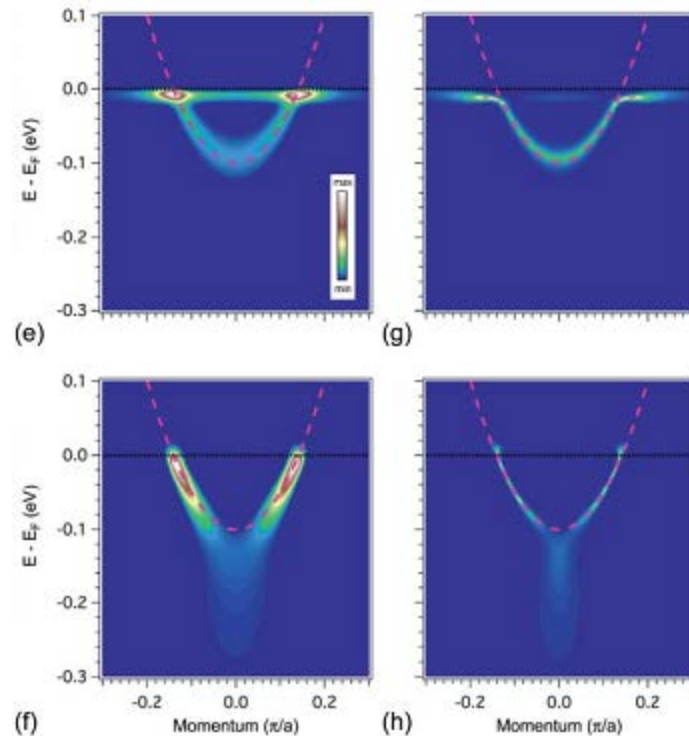
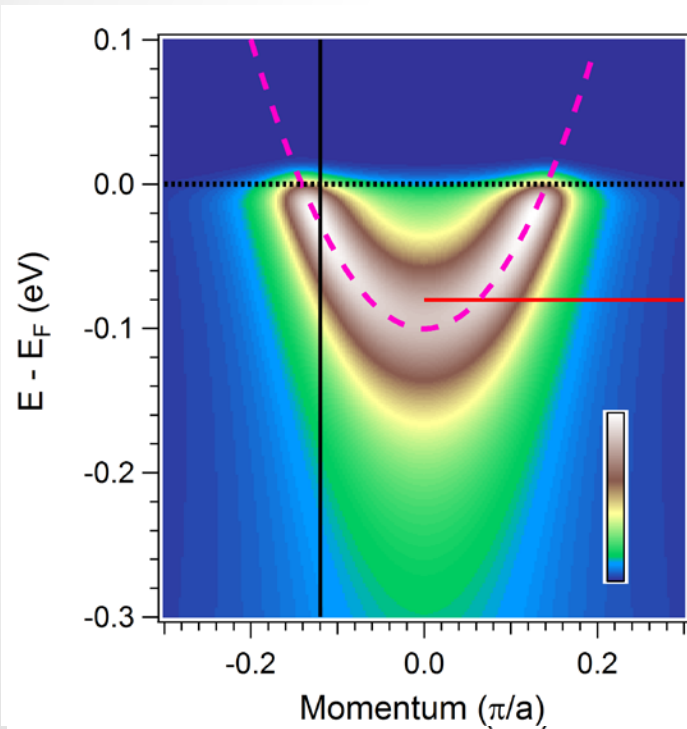
- More accurate peaks;
- Sharper bands.

Curvature Application



- More accurate peaks;
- Sharper bands.

Curvature Application



Second
derivative

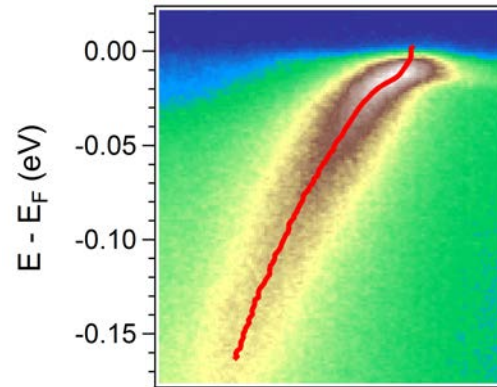
Curvature

- More accurate peaks;
- Sharper bands.

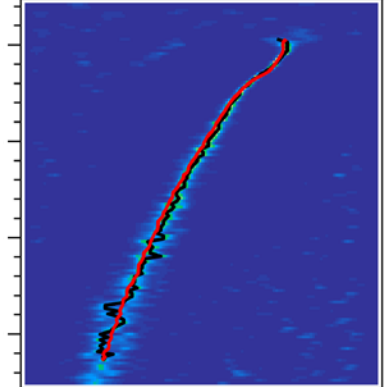
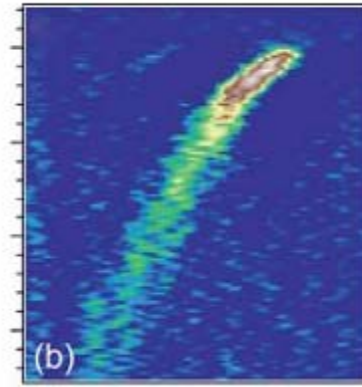
Curvature Application

Advantages:

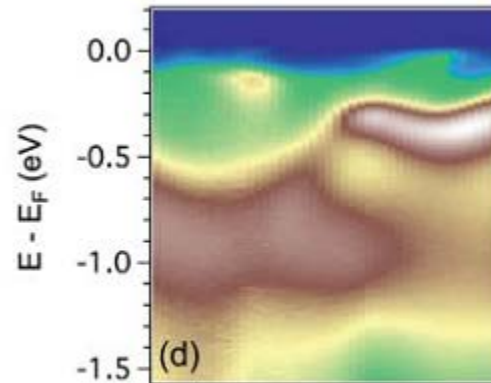
- More accurate peaks;
- Sharper bands.



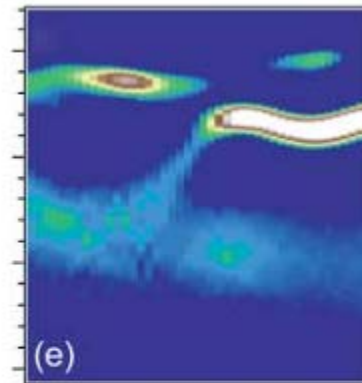
$\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$



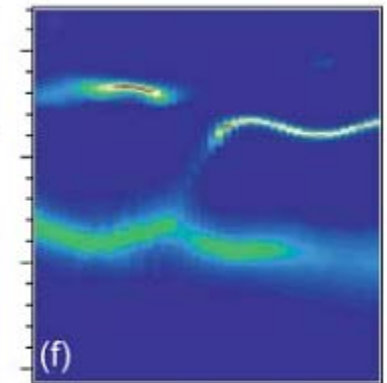
Phys. Rev. Lett. 102, 047003 (2009)



Momentum
 $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$



Momentum



Momentum

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

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

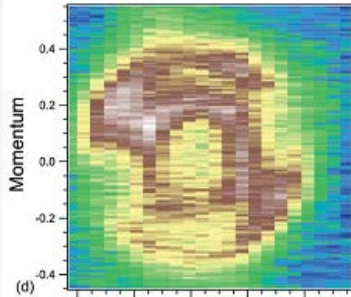
- Using the second order terms

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

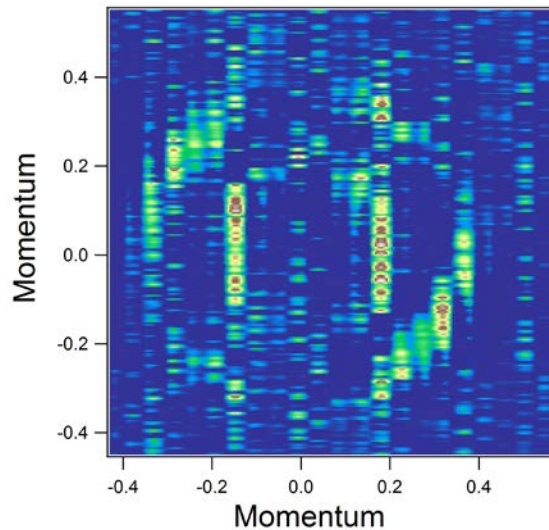
- We got

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

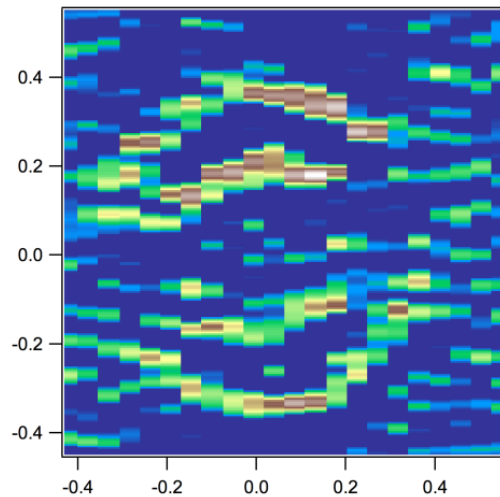
Application



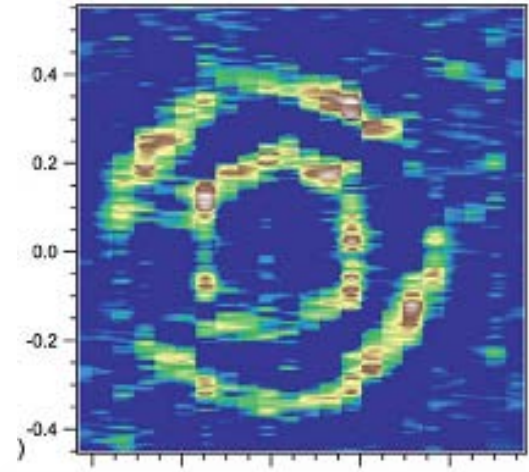
Raw data



Horizontal
second derivative



Vertical
second derivative



2D
second derivative

2D curvature

- Mean curvature in 2D

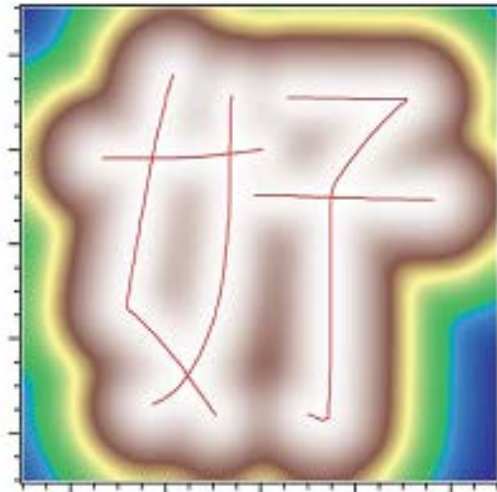
$$C(x, y) = \frac{[1 + (\frac{\partial f}{\partial x})^2] \frac{\partial^2 f}{\partial y^2} - 2 \frac{\partial f}{\partial x} \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial x \partial y} + [1 + (\frac{\partial f}{\partial y})^2] \frac{\partial^2 f}{\partial x^2}}{[1 + (\frac{\partial f}{\partial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

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

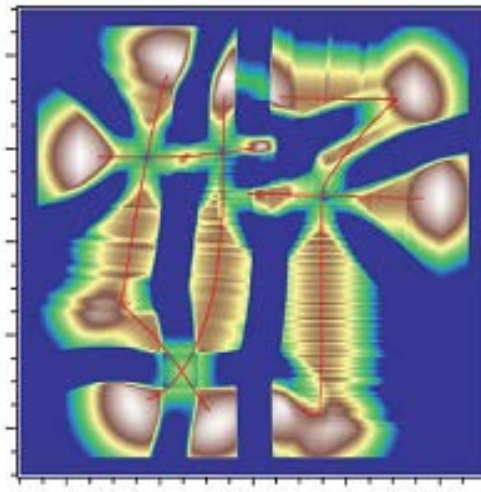
$$C(x, y) \sim \frac{\left[1 + C_x \left(\frac{\partial f}{\partial x}\right)^2\right] C_y \frac{\partial^2 f}{\partial y^2} - 2 C_x C_y \frac{\partial f}{\partial x} \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial x \partial y} + \left[1 + C_y \left(\frac{\partial f}{\partial y}\right)^2\right]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

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

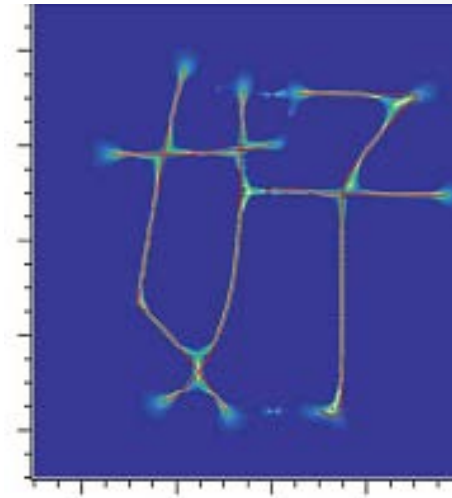
2D Curvature Application



Raw data



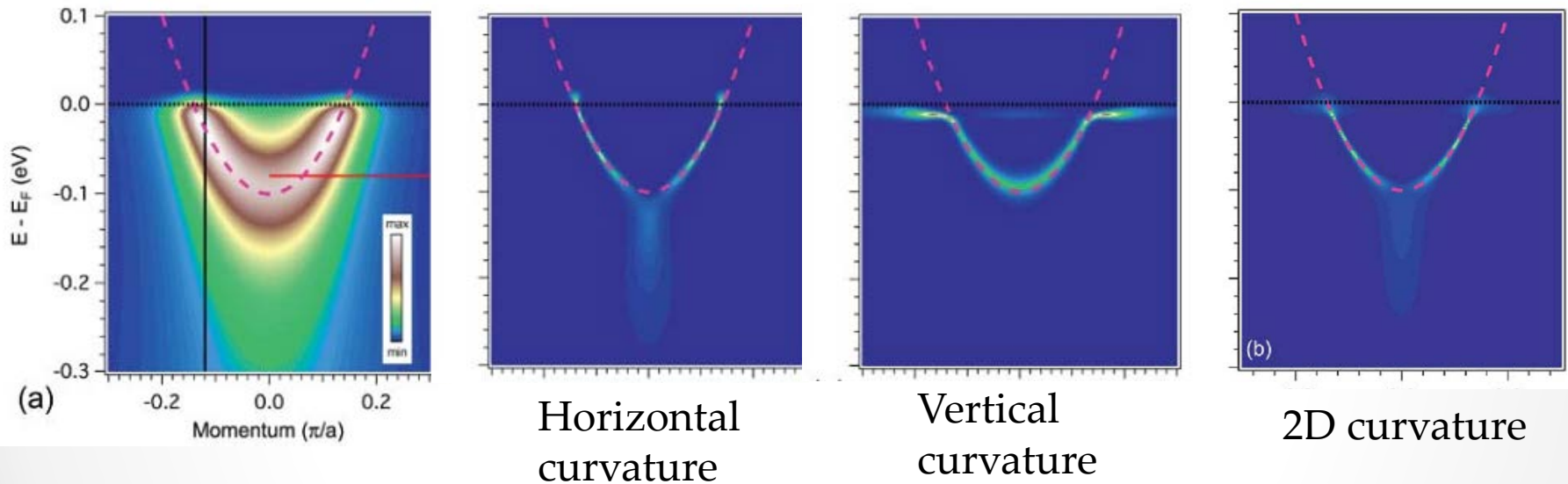
2D second derivative



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.

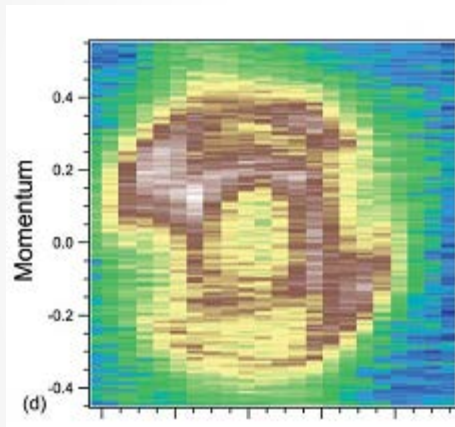
2D Curvature Application



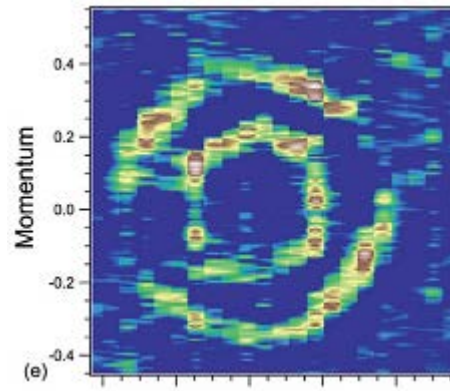
- 2D curvature method tracks the original band dispersion with higher accuracy over the whole range of energy.

2D Curvature Application

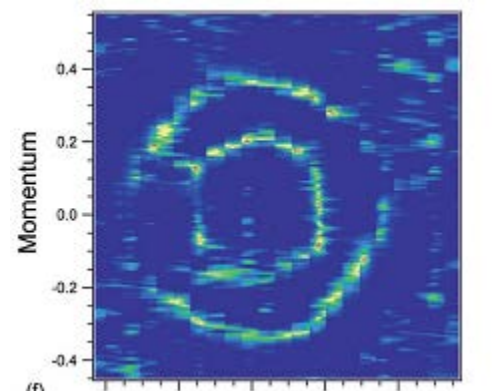
- Fermi surface contour of $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$



Raw data



2D second derivative



2D curvature

Conclusions

- 1D curvature

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

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

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

zhangpeng@lbl.gov

Igor Macro online

The screenshot shows a web browser window with the address bar containing ex7.iphy.ac.cn. The website header features the logo "EX7" with a globe icon and the text "Photoelectron Spectroscopy Research Group, IOP Beijing National Laboratory for Condensed Matter Physics". A navigation menu on the left includes links for HOME, RESEARCH, PUBLICATIONS, FACILITIES, PEOPLE, COLLABORATION, EVENTS, OPPORTUNITIES, and LINKS. The "PUBLICATIONS" section is expanded, showing a list of papers. The "List" link is highlighted with a red circle. The first paper in the list is (104) T. Qian, X.-P. Wang, W.-C. Ji, P. Zhang, P. Richard, G. Xu, X. Dai, Z. Fang, J.-G. Guo, X.-L. Chen, and H. Ding, "Absence of a Holelike Fermi Surface for the Iron-Based $K0.8Fe1.7Se2$ Superconductor Revealed by Angle-Resolved Photoemission Spectroscopy", *Physical Review Letters* 106, 187001 (2011) [download PDF]. Other papers listed include (103) H. Ding, K. Nakayama, P. Richard, S. Souma, T. Sato, T. Takahashi, M. Neupane, Y.-M. Xu, Z.-H. Pan, A.V. Federov, Z. Wang, X. Dai, Z. Fang, G.F. Chen, J.L. Luo, and N.L. Wang, "Electronic structure of optimally doped pnictide $Ba_{0.6}K_{0.4}Fe_2As_2$: a comprehensive angle-resolved photoemission spectroscopy investigation", *Journal of Physics: Condensed Matter* 23, 135701 (2011) [download PDF]; (102) M. Neupane, P. Richard, Y.-M. Xu, K. Nakayama, T. Sato, T. Takahashi, A. V. Federov, G. Xu, X. Dai, Z. Fang, Z. Wang, G.-F. Chen, N.-L. Wang, H.-H. Wen, and H. Ding, "Electron-hole asymmetry in the superconductivity of doped $BaFe_2As_2$ seen via the rigid chemical-potential shift in photoemission", *Physical Review B* 83, 094522 (2011) [download PDF]; (101) T. Qian, N. Xu, Y.-B. Shi, K. Nakayama, P. Richard, T. Kawahara, T. Sato, T. Takahashi, M. Neupane, Y.-M. Xu, X.-P. Wang, G. Xu, X. Dai, Z. Fang, P. Cheng, H.-H. Wen, and H. Ding, "Quasinested Fe orbitals versus Mott-insulating V orbitals in superconducting $Sr_2VFeAsO_3$ as seen from angle-resolved photoemission", *Physical Review B* 83, 140513 (2011) [download PDF]; (100) P. Zhang, P. Richard, T. Qian, Y.-M. Xu, X. Dai, and H. Ding, "A precise method for visualizing dispersive features in image plots", *Review of Scientific Instruments* 82, 043712 (2011) [download PDF] [Igor curvature macro and its instruction]; (99) X.-P. Wang, T. Qian, P. Richard, P. Zhang, J. Dong, H.-D. Wang, C.-H. Dong, M.-H. Fang and H. Ding, "Strong nodeless pairing on separate electron Fermi surface sheets in $(Ti, K)Fe_{1.78}Se_2$ probed by ARPES", *Europhysics Letters* 93, 57001 (2011) [download PDF]; (98) Y.-M. Xu, Y.-B. Huang, X.-Y. Cui, R. Elia, R. Milan, M. Shi, G.-F. Chen, P. Zheng, N.-L. Wang, P.-C. Dai, J.-P. Hu, Z. Wang, and H. Ding, "Observation of a ubiquitous three-dimensional superconducting gap function in optimally doped $Ba_{0.6}K_{0.4}Fe_2As_2$ ", *Nature Physics* 7, 198 (2011) [download PDF]; (97) K. Nakayama, T. Sato, P. Richard, Y.-M. Xu, T. Kawahara, K. Umezawa, T. Qian, M. Neupane, G. F. Chen, H. Ding, and T. Takahashi, "Universality of superconducting gaps in overdoped