A Novel 2D Folding Technique for Enhancing Fermi Surface Signatures in the Momentum Density

Isao Matsumoto*[1], Hiroshi Kawata[1], Nobuhiro Shiotani[2]
[1]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan
[2]Tokyo University of Fisheries, Kounan, Minato, Tokyo 108-8477, Japan

In a Compton scattering experiment one measures a directional Compton profile, $J(p_z)$, which is related to the twice integrated ground-state electron momentum density $\rho(\mathbf{p})$ by

$$J(p_z) = \iint \rho(\mathbf{p}) dp_x dp_y, \tag{1}$$

where p_z is taken along the scattering vector of the X-rays. In the independent particle approximation,

$$\rho(\mathbf{p}) = \sum_{b,\mathbf{k}}^{occ} \left| \int \psi_{b,\mathbf{k}}(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}} d\mathbf{r} \right|^2, \tag{2}$$

where $\psi_{b,\mathbf{k}}(\mathbf{r})$ is the electron wavefunction in band b and state $\mathbf{k}$. The determination of the Fermi surface (FS) geometry via the Compton spectroscopy is complicated by the presence of the double integral in Eq. (1). The standard approach to tackle these problems is to measure CP's along many different directions, and invert Eq. (1) to obtain $\rho(\mathbf{p})$ by using one of the available reconstruction methods. $\rho(\mathbf{p})$ can then be folded into the occupation number density in $\mathbf{p}$ space, $N(\mathbf{p})$, via the so-called Lock-Crisp-West (LCW) folding procedure[1]:

$$N(\mathbf{p}) \equiv \sum_{\mathbf{G}} \rho(\mathbf{p}+\mathbf{G}) = \sum_{\mathbf{G}} \sum_{b,\mathbf{k}} \delta_{\mathbf{k},\mathbf{p}+\mathbf{G}}, \tag{3}$$

where the sum over $\mathbf{G}$ runs over all reciprocal lattice vectors. The right hand side of Eq. (3) represents the occupation number density in the repeated zone scheme.

In many cases the 2D projection of the momentum density and the corresponding 2D occupation number density along a judiciously chosen direction can give most of the important features of the FS. For example the (110) projection for the *bcc* crystals works very well in sharp contrast to the *fcc* crystals in which due to overlap problems the FS image is often severely distorted. However, our analysis reveals that the problem can be solved by using a selected subset of reciprocal vectors in the folding procedure of Eq. (3).

Because we are interested specifically in projecting onto the (110) plane, it is convenient to work with new unit vectors $\hat{\mathbf{s}}$ and $\hat{\mathbf{t}}$ which lie along and perpendicular to [110]:

$$\hat{\mathbf{s}} = \frac{1}{\sqrt{2}}(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \;\; ; \;\; \hat{\mathbf{t}} = \frac{1}{\sqrt{2}}(\hat{\mathbf{x}} - \hat{\mathbf{y}}). \tag{4}$$

Then, a general lattice vector is

$$\mathbf{R} = R_s\hat{\mathbf{s}} + R_t\hat{\mathbf{t}} + R_z\hat{\mathbf{z}}, \tag{5}$$

$$\begin{aligned} R_s &= \frac{a}{2\sqrt{2}}(2u+v+w) \;\; ; \;\; R_t = \frac{a}{2\sqrt{2}}(-v+w) \;\; ; \\ R_z &= \frac{a}{2}(v+w), \end{aligned} \tag{6}$$

where u, v and w are integers, while the general reciprocal lattice vector is

$$\mathbf{G} = G_s\hat{\mathbf{s}} + G_t\hat{\mathbf{t}} + G_z\hat{\mathbf{z}}, \tag{7}$$

$$\begin{aligned} G_s &= \frac{2\pi}{a}\sqrt{2}h \;\; ; \;\; G_t = \frac{2\pi}{a}\sqrt{2}(-k+l) \;\; ; \\ G_z &= \frac{2\pi}{a}(-h+k+l), \end{aligned} \tag{8}$$

where h, k and l are integers. The two-dimensional projection of the occupation number density $N(p_t, p_z)$ can be divided into two sums involving even and odd values of h. The final result is[2]

$$N^{even}(p_t, p_z) = c \sum_{G_t^e, G_z^e}^{h:even} \sum_{b,\mathbf{k}} \delta(k_t, p_t + G_t^e)\delta(k_z, p_z + G_z^e) \tag{9}$$

and

$$N^{odd}(p_t, p_z) = c \sum_{G_t^o, G_z^o}^{h:odd} \sum_{b,\mathbf{k}} \delta(k_t, p_t + G_t^o)\delta(k_z, p_z + \frac{2\pi}{a} + G_z^o), \tag{10}$$

where the constant c collects the irrelevant prefactors and $G_t^{e(o)}$ and $G_z^{e(o)}$ are the components of $\mathbf{G}$ with even (odd) h.

The right hand side of Eq. (9) is just the projected two-dimensional $\mathbf{k}$ space occupation sampling function in the repeated zone scheme for the set of reciprocal lattice vectors with even h in Eq. (8), while the right hand side of Eq. (10) fulfills the same function for the set with odd h. Thus, the set of Fermi surface images appearing in Eq. (9), reappear in Eq. (10) but shifted by $2\pi/a$ along $\hat{\mathbf{z}}$. By carrying out the LCW folding over only one of these two sets of reciprocal lattice vectors, the Fermi surfaces corresponding to the other set are removed and thus a picture is obtained which is not complicated by superposition.

References

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*imatsu@post.kek.jp