NE1A1/2002G188

Equivalence of LCW-folding and Schuelke's method

Nobuhiro SHIOTANI*
KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

Introduction

Fermiology by high-resolution Compton scattering has been developed to such that it can now provide the long sought experimental evidence for Fermi surface geometry related phenomena in disordered alloys, metals and compounds in high temperature phases.

To map out the Fermi surface from high resolution Compton profiles, we have to take three steps: 1) we measure Compton profiles along n (n=15~30) different crystalline directions, 2) we reconstruct three-dimensional momentum density using one of established methods, 3) we convert momentum density to occupation number density using the so-called LCW-folding [1], and we look for edges of the Fermi surface in the reduced zone (the first Brillouin zone). There is another path, 2') we reconstruct the so-called B-function [2], 3') we calculate the occupation number density using Schuelke's method [3, 4], and we look for edges of Fermi surface in the reduced zone. Although Schuelke's method is known to be analogous to the LCW-folding, to the best of the author's knowledge, equivalence of the two methods has not explicitly been documented.

Equivalence of the two methods

The following is one way to show the equivalence of the two methods.

The so-called B-function is defined as a Fourier transform of momentum density ρ(**p**),

$$\mathrm{B}(\mathbf{r}) = \int \rho(\mathbf{p}) \exp(-\mathrm{i}\,\mathbf{p}\cdot\mathbf{r})\, \mathrm{d}\mathbf{p}\,, \qquad (1)$$

and inversely,

$$\rho(\boldsymbol{p}) = (2\pi)^{-3} \int B(\boldsymbol{r}) \exp(i\,\boldsymbol{p}\cdot\boldsymbol{r})\, d\boldsymbol{r}\,. \qquad (1')$$

The LCW-folding is written as,

$$\sum_{\boldsymbol{G}_i} \rho(\boldsymbol{p}+\boldsymbol{G}_i) = C \sum_{\boldsymbol{G}_i} \sum_{b,\boldsymbol{k}}^{occ} \delta_{\boldsymbol{k},\,\boldsymbol{p}+\boldsymbol{G}_i}\,, \qquad (2)$$

where $\boldsymbol{G}_i$ represents the reciprocal lattice vectors, and the constant C collects the irrelevant prefactors. The right hand side is the occupation number density $N(\mathbf{k})$ in the repeated zone scheme which is explicitly expressed by the summation over $\boldsymbol{G}_i$. Schuelke's method is expressed as,

$$C \sum_{\boldsymbol{R}_i} B(\boldsymbol{R}_i) \exp(i\,\boldsymbol{k}\cdot\boldsymbol{R}_i) = N(\boldsymbol{k})\,, \qquad (3)$$

where $\boldsymbol{R}_i$ represents the lattice translation vectors.

We rewrite the left hand side of Eq. (2) using Eq. (1'),

$$\sum_{\mathbf{G}_i} \rho(\mathbf{p}+\mathbf{G}_i) = C \sum_{\mathbf{G}_i} \int d\mathbf{r}\, B(\mathbf{r}) \times \exp(i(\mathbf{p}+\mathbf{G}_i)\cdot\mathbf{r}).$$

We divide the integration over the whole space into the sum of integrations over the unit cells,

$$\int d\boldsymbol{r} \Rightarrow \sum_{\boldsymbol{R}_i} \int_{cell} d\boldsymbol{r}'\,.$$

Then

$$\sum_{\mathbf{G}_i} \rho(\mathbf{p}+\mathbf{G}_i)$$

$$= C \sum_{\boldsymbol{G}_i} \sum_{\boldsymbol{R}_i} \int_{cell} d\boldsymbol{r}'\, B(\boldsymbol{R}_i+\boldsymbol{r}') \times \exp(i\,(\boldsymbol{p}+\boldsymbol{G}_i)\cdot(\boldsymbol{R}_i+\boldsymbol{r}'))$$

$$= C \sum_{\mathbf{R}_i} \int_{cell} d\mathbf{r}'\, B(\mathbf{R}_i+\mathbf{r}') \times \exp(i\,\mathbf{p}\cdot(\mathbf{R}_i+\mathbf{r}')) \cdot \sum_{\mathbf{G}_i} \exp(i\,\mathbf{G}_i\cdot(\mathbf{R}_i+\mathbf{r}'))$$

Using the following identities,

$\exp(i\boldsymbol{G}_i\cdot\boldsymbol{R}_i)=1$, and $\sum_{\boldsymbol{G}_i} \exp(i\boldsymbol{G}_i\cdot\boldsymbol{r}') = C'\,\delta_{\boldsymbol{r}',0}$

we get

$$= C \sum_{\boldsymbol{R}_i} \int_{cell} d\boldsymbol{r}'\, B(\boldsymbol{R}_i+\boldsymbol{r}') \exp(i\,\boldsymbol{p}\cdot(\boldsymbol{R}_i+\boldsymbol{r}'))\,\delta_{\boldsymbol{r}',0}$$

$$= C \sum_{\boldsymbol{R}_i} B(\boldsymbol{R}_i) \exp(i\,\boldsymbol{p}\cdot\boldsymbol{R}_i)\,.$$

Finally, we equate the above to the right hand side of Eq. (2),

$$\sum_{\mathbf{G}_i} \rho(\mathbf{p}+\mathbf{G}_i) = C \sum_{\mathbf{R}_i} B(\mathbf{R}_i) \exp(i\,\mathbf{p}\cdot\mathbf{R}_i)$$

$$= C \sum_{\mathbf{G}_i} \sum_{b,\mathbf{k}}^{occ} \delta_{\mathbf{k},\,\mathbf{p}+\mathbf{G}_i}\,.$$

Since $\boldsymbol{p}$ is always reduced to $\boldsymbol{k}$ by the δ-function in the right hand, we replace $\boldsymbol{p}$ in the left hand side by $\boldsymbol{k}$ and we have explicitly retrieved Schuelke's method, Eq. (3).

References

[1] D. G. Lock, V. H. C. Crisp, and R. N. West, J. Phys. F3 (1973) 561.
[2] P. Pattison, W. Weyrich, and B. G. Williams, Solid State Commun. 21 (1977) 967.
[3] W. Schuelke, phys. stat. sol. (b) 80 (1977) K67.
[4] W. Schuelke, G. Stutz, F. Wohlert, and A. Kaprolat, Phys. Rev. B 54 (1996) 14381.

*Shiotani@post.kek.jp