4) Diffraction and the autocorrelation

Consider an assvembly of N identical structurelers atoms at positions $x_1, x_2, \cdots, x_N$. One can model the system by the delta measure:

$$\varrho = \sum_{j=1}^{N} \delta_{x_j} \text{ (bounded)}$$

If this assembly is irradiated by a tradiation of wavelength λ from the direction Q_0, then the intasity of radiation scattered elastically into Q is given by

$$I(q) = \left| \sum_{j=1}^{N} e^{-2\pi i (q, x_j)} \right|^2, \text{ with } q = \frac{Q - Q_0}{\lambda}$$

I is called "distribution of scattering power" or "diffraction intensity".

Recall

1) $\hat{\delta}_a(\cdot) = e^{-2\pi i (a, \cdot)}$
2) $\hat{\tilde{\varrho}} = \overline{\hat{\varrho}}$
3) $\cancel{\hat{\mu} * \nu}$ $\widehat{\mu * \nu} = \hat{\mu}\hat{\nu}$

One observes: $I(q) = |\hat{\varrho}|^2 = \hat{\varrho}\,\overline{\hat{\varrho}} = \hat{\varrho}\,\hat{\tilde{\varrho}} = \widehat{\varrho * \tilde{\varrho}}$

$\varrho * \tilde{\varrho}$ is known as "Pattesson function" (actually a measure)

One can prove that

$$\int I(q)[\phi * \tilde{\phi}](q)\,dq \geqslant \int N[\phi * \tilde{\phi}](q)\,dq \quad \forall \phi \in \mathcal{K}$$

$$\because \quad I(q) = \left(\sum_{j=1}^{N} e^{-2\pi i (q, x_j)} \right) \left(\sum_{l=1}^{N} e^{\cancel{2\pi i} 2\pi i (q, x_l)} \right) = N + \sum_{j \neq l} e^{2\pi i (q, x_0 - x_j)}$$

$$\Rightarrow \int I(q)[\phi * \tilde{\phi}](q)\,dq = N \int [\phi * \tilde{\phi}](q)\,dq + \sum_{j \neq l} \int e^{2\pi i (q, x_0 - x_j)} [\phi * \tilde{\phi}](q)\,dq$$

$$\geqslant N \int [\phi * \tilde{\phi}](q)\,dq + 0 \qquad \square$$

$I\cancel{q}(q)$ won't converge as $N \to \infty$.

Instead, one has to consider $\frac{I}{N}$, scattering power per atom

One has that if the infinite system has a unique autocorrelation γ, then $\frac{I}{N} \xrightarrow{N \to \infty} \frac{\hat{\gamma}}{\gamma(\{0\})}$ $\quad \gamma(\{0\})$ is called "particle density"

One has $\hat{\gamma} = \hat{\gamma}_{pp} + \hat{\gamma}_{ac} + \hat{\gamma}_{sc}$

$\hat{\gamma}_{pp}$: sign of order. Note that point mass at 0 is always present.

$\hat{\gamma}_{ac}$: sign of disorder

$\hat{\gamma}_{sc}$: sign of order between quasisperiodic and randomness

Remark: I/N is continuous (a.c. measure)

· Discrete and s.c. parts only appear in the limit of definite system

Ex: For a crystal, of which lattice is $\mathbb{Z}^d$: $\Gamma = \mathbb{Z}^d$, $|\hat{\Gamma}| = 1$, $\Gamma^* = \mathbb{Z}^d$

Let ϱ be a decorator of unit cell by N atoms

(i.e. all coordinate x_j between $0 \sim 1$).

Then the crystal is modeled by

$$\mu = \varrho * \sum_{n \in \mathbb{Z}^d} \delta_n$$

$$\Rightarrow \gamma_\mu = \lim_{L \to \infty} \frac{1}{L^d} (\mu_{C_L} * \tilde{\mu}_{C_L}) = \lim_{L \to \infty} \frac{1}{L^d} ((\varrho * \sum_{n \in \mathbb{Z}^d} \delta_n) * (\tilde{\varrho} * \sum_{n \in \mathbb{Z}^d} \tilde{\delta}_n))$$

$$= \lim_{L \to \infty} \frac{1}{L^d} [(\overset{\text{rho}}{\varrho} * \tilde{\varrho}) * (\sum_{n \in \mathbb{Z}^d} \delta_n * \sum_{n \in \mathbb{Z}^d} \tilde{\delta}_n)]$$

$$\underline{\underline{\text{L.D.C}}} \ (\varrho * \tilde{\varrho}) * \left(\lim_{L \to \infty} \frac{1}{L^d} \sum_{n \in \mathbb{Z}^d} \delta_{n_{C_L}} * \sum_{n \in \mathbb{Z}^d} \delta_{n_{C_L}} \right)$$

$$\underline{\underline{\text{S.H.'s presentation}}} \ (\varrho * \tilde{\varrho}) * \sum_{n \in \mathbb{Z}^d} \delta_n$$

$$\hat{\gamma}_\mu = \widehat{(\varrho * \tilde{\varrho})} \sum_{n \in \mathbb{Z}^d} \hat{\delta}_n$$

From Poisson simnation formula

$$\widehat{\delta_{\Gamma^*}} = |\hat{\Gamma}| \, \delta_\Gamma = 1 \cdot \sum_{n \in \mathbb{Z}^d} \delta_n$$

$$= |\hat{\varrho}|^2 \sum_{n \in \mathbb{Z}^d} \delta_n$$

□