Epilogue

Recall $M(\mathbb{R}^d)$ (all complex Radon measures on $\mathbb{R}^d$) $= C^c(\mathbb{R}^d)^* \ni \varphi$

($\int \varphi(x)\,\mu(dx) \in \mathbb{C}$)

For $\mu \in M(\mathbb{R}^d)$, $f_1, \cdots, f_n \in C^c(\mathbb{R}^d)$, $\varepsilon > 0$, we set

$U(\mu, f_1, \cdots, f_n, \varepsilon) = \{\nu \in M(\mathbb{R}^d) \mid |\mu(f_j) - \nu(f_j)| < \varepsilon \ \forall j = 1, \cdots, n\}$

$\{U(\mu, f_1, \cdots, f_n, \varepsilon) \mid f_1, \cdots, f_n \in C^c(\mathbb{R}^d), \varepsilon > 0\}$ is a ngd. base for μ in $M(\mathbb{R}^d)$, and we call the corresponding topology the weak* topology.

(or the vague topology)

Recall that for $\mu \in M(\mathbb{R}^d)$ for $R > 0$ we set

$\gamma_\mu^R = \frac{1}{\mathrm{vol}(B_R)} \mu|_{B_R} * \tilde{\mu}|_{B_R}$ (in [GB]) or $\gamma_\mu^R = \frac{1}{L^d} \mu|_{C_L} * \tilde{\mu}|_{C_L}$ (in Hof)

Lemma

If $\mu \in M(\mathbb{R}^d)$ is translation bounded, then

then γ_μ^R is translation bounded

and $\{\gamma_\mu^R\}_{R>0}$ is precompact in $M(\mathbb{R}^d)$ for the weak* topology

(closure in w*-topology)

$\hookrightarrow K := \overline{\{\gamma_\mu^R\}}_{R>0}$ is compact

Corollory

Since $\{\gamma_\mu^R\}$ is a net in K, which is compact,

it has at least one convergent subnet.

We call the limit of this convergent subnet an autocorrelation for μ.

"Every accumulation point of $\{\gamma_\mu^R\}_{R>0}$ in vague topology is called an autocorrelation for μ. If $\lim_{R\to 0} \gamma_\mu^R$ exists, in the vague topology, we call it the natual autocorrelation measure.

<u>Conclusion on diffraction</u>

From the lecture of B. Gelloz and from pages 66 and 67 of his slides, we have

$$\text{Amplitude of scattering} \quad F(k) = \int_{\text{solid}} \rho(r)\, e^{-ik\cdot r}\, dr \qquad (*)$$

$$= \hat{\rho}(k)$$

with ρ the distribution of mater (electrons).

The intensity I is then given by $I = |F|^2 = |\hat{\rho}|^2$.

Now $(*)$ is meaningful only if "solid" is small, but the relation $\rho(r+R) = \rho(r)$ implies that the solid is in the entire space. Seems like a contradiction

However, for ρ in L^1 the following diagram is commutative

$$\begin{tikzcd} \rho \arrow[r, "*"] \arrow[d, "\mathcal{F}"'] & \rho * \tilde{\rho} \arrow[d, "\mathcal{F}"] \\ \hat{\rho} \arrow[r, "|\cdot|^2"'] & |\hat{\rho}|^2 \end{tikzcd}$$

[Hof, B6]

Gelloz

We have used the second arrow to give a meaning to diffraction. Indeed, following [B6], we considered

For any $\rho \in \mathcal{M}(\mathbb{R}^d)$ translation bounded

$$\rho|_{B_R} * \tilde{\rho}|_{B_R}$$ is well defined, translation bounded

and the net

$$\mathbb{R} \ni R \longmapsto \frac{1}{\mathrm{Vol}(B_R)} \rho|_{B_R} * \tilde{\rho}|_{B_R} \equiv \gamma_\rho^R$$

a net in the w^* compact set $K := \overline{\{ \gamma_\rho^R \}}^{w^*\text{-top.}}$.

Thus it has a least one converging subnet, and this limit is called the auto-correlation γ_ρ

Then $I = |\hat{\gamma}_\rho|^2$ with the Fourier transform always well defined on $\mathcal{M}(\mathbb{R}^d)$, also in a suitable sense.

Note that the autocorrelation might not be unique, but the theory allows it.