Supplementary Information for

Cross-correlation Analysis of X-ray Photon Correlation Spectroscopy to Extract Rotational Diffusion Coefficients

Zixi Hu, Jeffrey J. Donatelli, James A. Sethian

Zixi Hu.
E-mail: zixihu@lbl.gov

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Here we provide a derivation of Eq. (8) and Eq. (11), algorithmic details of the MTECS algorithm, and other details of the numerical experiments.

Derivation of Limits

Suppose that there are \(N_p\) identical particles undergoing free Brownian motion. The position and orientation of the \(n\)-th particle at time \(t \geq 0\) are denoted by \(r_n(t)\) and \(\theta_n(t)\). Here we assume decoupling of the translational motion and the rotational motion. For dilute samples in which the hydrodynamic interaction and direct interaction between particles are absent, \(r_n\) and \(\theta_n\) can be described by mutually independent and identically distributed stochastic processes satisfying:

- \(r_n(0)\) is uniformly distributed on a large enough domain so that the characteristic function of this distribution can be viewed approximately as the indicator function of zero,

\[
\chi_0(q) = \begin{cases} 1, & \text{if } q = 0, \\ 0, & \text{if } q \neq 0, \end{cases} \tag{S1}
\]

with a initial distribution of \(\theta_n(0)\) uniform on the interval \([0, 2\pi]\).

- For any \(t > s \geq 0\),

\[
r_n(t) - r_n(s) \sim \mathcal{N}(0, 2(t-r)D_t I), \quad \theta_n(t) - \theta_n(r) \sim \mathcal{N}(0, 2(t-r)D_r), \tag{S2}
\]

where \(\mathcal{N}\) implies Gaussian variable, \(D_t\) and \(D_r\) are the translational diffusion coefficient and the rotational diffusion coefficient respectively, and \(I\) is the \(2 \times 2\) identity matrix.

- For any \(0 \leq t_1 < t_2 < \cdots < t_k\), the increments \(r_n(t_2) - r_n(t_1)\), \(\cdots\), \(r_n(t_k) - r_n(t_{k-1})\) and \(\theta_n(t_2) - \theta_n(t_1)\), \(\cdots\), \(\theta_n(t_k) - \theta_n(t_{k-1})\) are independent.

Let \(R(\theta)\) be the rotation matrix that rotates the angle \(\theta\) to angle \(0\). As in the the main text, the Cartesian coordinate in both real space and reciprocal space, \(r\) and \(q\), can also be expressed in polar coordinates as \(r = (r, \gamma)\) and \(q = (q, \phi)\), where \(r, q\) are radial coordinates, and \(\gamma, \phi\) are angular coordinates. The overall electron density distribution of the sample is

\[
\rho(r, t) = \sum_{n=1}^{N_p} \rho(R(\theta_n(t)) \cdot (r - r_n(t))). \tag{S4}
\]

The scattered field in the far-field can be modelled by the Fourier transform of \(\rho(r, t)\),

\[
E(q, t) = \int_{\mathbb{R}^2} \hat{\rho}(r, t) e^{-2\pi i q \cdot r} \, dr
\]

\[
= \sum_{n=1}^{N_p} e^{-2\pi i q \cdot r_n(t)} \int_{\mathbb{R}^2} \hat{\rho}(R(\theta_n(t)) \cdot q) e^{-2\pi i q \cdot r} \, dr
\]

\[
= \sum_{n=1}^{N_p} e^{-2\pi i q \cdot r_n(t)} \hat{\rho}(R(\theta_n(t)) \cdot q)
\]

\[
= \sum_{n=1}^{N_p} e^{-2\pi i q \cdot r_n(t)} \hat{\rho}(q, \phi - \theta_n(t)). \tag{S5}
\]

The collected images are

\[
\mathcal{J}(q, t) = |E(q, t)|^2. \tag{S6}
\]

In the remainder of this section, we assume that all of the scattering vectors are non-zeros. Let \(q = (q, \phi)\) and \(q' = (q', \phi')\) in polar coordinates. We first calculate

\[
\langle \mathcal{J}(q, \phi) \mathcal{J}(q', \phi', t + \tau) \rangle = \sum_{n_1, n_2, n_3, n_4=1}^{N_p} \langle e^{-2\pi i q \cdot (r_{n_1}(\tau) - r_{n_2}(\tau))} e^{-2\pi i q' \cdot (r_{n_3}(t + \tau) - r_{n_4}(t + \tau))} \hat{\rho}(q, \phi - \theta_{n_1}(\tau)) \hat{\rho}(q', \phi' - \theta_{n_2}(\tau)) \hat{\rho}(q', \phi' - \theta_{n_3}(t + \tau)) \hat{\rho}(q, \phi - \theta_{n_4}(t + \tau)) \rangle. \tag{S7}
\]

We denote the terms in the above summation as \(S_{n_1 n_2 n_3 n_4}\). Since the motions of different particles are uncorrelated, if any of \(n_1, n_2, n_3, n_4\) is different from all the others, then \(S_{n_1 n_2 n_3 n_4}\) becomes zero (1). Therefore, the main contribution arises when \(n_1 = n_2 = n_3 = n_4, n_1 = n_2 \neq n_3 = n_4, n_1 = n_3 \neq n_2 = n_4, n_1 = n_4 \neq n_2 = n_3\).
When \( n_1 = n_2 = n_3 = n_4 \), without loss of generality, we assume that they equal to 1, then

\[
S_{1111} = \langle I(q, \phi - \theta_1 (\tau)) I(q', \phi' - \theta_1 (t + \tau)) \rangle
\]

\[
= \sum_{m, m'} \int_{m, m'}^{\infty} I_m(q) I_m(q') e^{im\phi} e^{-im\phi'} e^{-m^2 t_D} \delta_{mm'}
\]

where

\[
\delta_{mm'} = \begin{cases} 0 & \text{if } m \neq m' \\ 1 & \text{if } m = m' \end{cases}
\]

The feasibility of interchanging the order of average and summation can be ensured by the absolute convergence of the circular harmonic expansions. There are \( N_p \) such terms in the summation.

If \( n_1 = n_2 \neq n_3 = n_4 \), the terms become

\[
S_{1122} = \langle I(q, \phi - \theta_1 (\tau)) \rangle \langle I(q', \phi' - \theta_2 (t + \tau)) \rangle.
\]

Proceeding along the similar line as Eq. (S8), we have

\[
\langle I(q, \phi - \theta_1 (\tau)) \rangle = I_0(q).
\]

Hence

\[
S_{1122} = I_0(q) I_0(q').
\]

There are \( N_p (N_p - 1) \) such terms.

The terms with \( n_1 = n_4 \neq n_2 = n_3 \) can be calculated as follows:

\[
S_{1221} = \langle e^{-2\pi i (q r_1 (\tau) - q' r_1 (t + \tau))} \rangle \langle \hat{\rho}(q, \phi - \theta_1 (\tau)) \hat{\rho}(q', \phi' - \theta_1 (t + \tau)) \rangle
\]

\[
= \sum_{m = -\infty}^{\infty} e^{-im(\phi' - \phi)} \hat{\rho}_m(q) \hat{\rho}_m(q') e^{-m^2 t_D},
\]

Using the same techniques as the calculation of Eq. (S8),

\[
\langle \hat{\rho}(q, \phi - \theta_1 (\tau)) \hat{\rho}(q', \phi' - \theta_1 (t + \tau)) \rangle = \sum_{m = -\infty}^{\infty} e^{-im(\phi' - \phi)} \hat{\rho}_m(q) \hat{\rho}_m(q') e^{-m^2 t_D},
\]

and

\[
\langle e^{-2\pi i (q r_1 (\tau) - q' r_1 (t + \tau))} \rangle = \langle e^{-2\pi i (q r_1 (\tau) - q_1 (t + \tau))} \rangle \langle e^{-2\pi i (q - q') r_1 (\tau)} \rangle
\]

\[
= \chi_0(q - q') e^{-4\pi^2 q^2 t_D}.
\]

According to the above three equations,

\[
S_{1221} = \chi_0(q - q') e^{-8\pi^2 q^2 t_D} \left( \sum_{m = -\infty}^{\infty} | \hat{\rho}_m(q) |^2 e^{-m^2 t_D} \right)^2.
\]

In the same manner, for \( n_1 = n_3 \neq n_2 = n_4 \),

\[
S_{1212} = \chi_0(q + q') e^{-8\pi^2 q^2 t_D} \left( \sum_{m = -\infty}^{\infty} (-1)^m | \hat{\rho}_m(q) |^2 e^{-m^2 t_D} \right)^2.
\]

Combination of Eq. (S8), Eq. (S12), Eq. (S16) and Eq. (S17) gives

\[
\langle \mathcal{J}(q, \phi, \tau) \mathcal{J}(q', \phi', t + \tau) \rangle = N_p \sum_{m = -\infty}^{\infty} e^{-im(\phi' - \phi)} I_m(q) I_m(q') e^{-m^2 t_D}
\]

\[
+ N_p (N_p - 1) I_0(q) I_0(q') + N_p (N_p - 1) \chi_0(q - q') e^{-8\pi^2 q^2 t_D} \left( \sum_{m = -\infty}^{\infty} | \hat{\rho}_m(q) |^2 e^{-m^2 t_D} \right)^2
\]

\[
+ N_p (N_p - 1) \chi_0(q + q') e^{-8\pi^2 q^2 t_D} \left( \sum_{m = -\infty}^{\infty} (-1)^m | \hat{\rho}_m(q) |^2 e^{-m^2 t_D} \right)^2.
\]
Likewise,

\[ \langle \mathcal{J}(q, \phi, \tau) \rangle = N_p I_0(q). \]  

[S19]

Taking \( q = q' \) and \( \phi = \phi' \), i.e. \( q = q' \), in Eq. (S18) and combining with Eq. (S19), when \( N_p \) is large enough,

\[
g_2(q, \phi, t) = \frac{\langle \mathcal{J}(q, \phi, \tau) \mathcal{J}(q, \phi, \tau + t) \rangle}{\langle \mathcal{J}(q, \phi, \tau) \rangle^2} = \frac{1}{N_p} \sum_{m=-\infty}^{\infty} \frac{|I_m(q)|^2 e^{-m^2 tD_r}}{|I_0(q)|^2} + \frac{N_p - 1}{N_p} + \frac{N_p - 1}{N_p} \frac{\sum_{m=-\infty}^{\infty} |\hat{\rho}_m(q)|^2 e^{-m^2 tD_r}}{I_0(q)^2} \approx 1 + e^{-8\pi^2 q^2 tD_r} \left( \frac{\sum_{m=-\infty}^{\infty} |\hat{\rho}_m(q)|^2 e^{-m^2 tD_r}}{\sum_{\ell=-\infty}^{\infty} |\hat{\rho}_\ell(q)|^2} \right)^2.
\]

[S20]

The derivation of Eq. (8) in main text is completed.

Let \( \phi' = \phi + \Delta \phi \) where \( \Delta \phi \neq 0 \) and \( \tau \), which implies \( q \neq q' \) and \( q = -q' \). Then Eq. (S18) reads,

\[
\langle \mathcal{J}(q, \phi, \tau) \mathcal{J}(q', \phi + \Delta \phi, t + \tau) \rangle = N_p \sum_{m=-\infty}^{\infty} e^{i m \Delta \phi} \frac{|I_m(q')| |I_m(q)| e^{-m^2 tD_r}}{I_0(q')} + N_p (N_p - 1) I_0(q) I_0(q').
\]

[S21]

Combining with Eq. (S19), the Eq. (11) in the main text followings immediately by omitting \( N_p \) and setting \( I_m = 0 \) for odd \( m \), which is due to the Friedel’s symmetry. When \( \Delta \phi = 0 \) or \( \tau = 0 \) and \( q = q' \), the third or fourth term in the right hand side of Eq. (S18) remains in Eq. (S21). In such cases, the right hand side of Eq. (11) in the main text contains a term with the factor \( N_p(N_p - 1) \) rather than merely a term with the factor \( N_p \), leading to the peaks depicted by Fig. 4 in the main text.

**Details of MTECS**

**Angular Average Subtraction.** Here we discuss the evaluation of the cross-correlation data, which is the left-hand side of Eq. (11). The first term can be computed by Eq. (10). The second term, \( \langle \mathcal{J}(q, \phi, \tau) \rangle \cdot \langle \mathcal{J}(q', \phi, \tau) \rangle \), can be assessed as the product of the angular-temporal averages of the images,

\[
\langle \mathcal{J}(q, \phi, \tau) \rangle \cdot \langle \mathcal{J}(q', \phi, \tau) \rangle = \left( \frac{1}{2\pi N_{\text{sp}}} \sum_{k=0}^{N_{\text{sp}}-1} \int_0^{2\pi} \mathcal{J}(q, \phi, k \Delta t) d\phi \right) \left( \frac{1}{2\pi N_{\text{sp}}} \sum_{k=0}^{N_{\text{sp}}-1} \int_0^{2\pi} \mathcal{J}(q', \phi, k \Delta t) d\phi \right).
\]

[S22]

To ameliorate the bias resulted from such estimation of angular average, a further operation can be conducted. We first calculate the full singular value decomposition of \( E \),

\[
E = U_C \Lambda_C V_C^*.
\]

[S23]

\[
U_C = [U_{C1}, U_{C2}],
\]

where \( U_{C1} \) consists of the first \( 2M \) columns of \( U_C \), and the remaining \( N_{\phi} - 2M \) columns form \( U_{C2} \). For each \( l, l', k \), we seek out the real number \( \alpha_{ll'k} \) to make \( C_{ll',k} - \alpha_{ll'k} \mathbf{1} \) as close to the column space of \( E \) as possible,

\[
\alpha_{ll'k} = \arg\min_{\alpha \in \mathbb{R}} \|U_{C2}^* (C_{ll',k} - \alpha \mathbf{1})\|^2
\]

[S24]

\[
= \Re \left( (U_{C2}^*)^* (U_{C2}^* C_{ll',k}) \right) \frac{\|U_{C2}^* \mathbf{1}\|^2}{\|U_{C2}^* \mathbf{1}\|^2},
\]

where \( \mathbf{1} \) is the all-ones vector and \( \Re (\cdot) \) takes the real part of a complex number, and then we perform

\[
C_{ll',k} := C_{ll',k} - \alpha_{ll'k} \mathbf{1}.
\]

[S25]

**Parameter Selection and Solver to Correlation Noise Projector.** In this subsection, we follow the approach outlined in (2). The parameter \( \sigma_{ll'k} \) can be chosen by how well the mathematical model describes the cross-correlation data \( C \). Specifically, we select

\[
\sigma_{ll'k}^2 = \frac{\|U_{C2}^* C_{ll',k}\|^2}{N_{\phi} - 2M},
\]

[S26]

which in fact is an estimation of the inconsistency between the cross-correlation data \( C_{ll',k} \) and Eq. (12, 14).

To choose \( \tau_k \), we first let \( B_{:k} = \mathbf{0} \). The \( q/l' \) factor in the objective function of optimization Eq. (17) is resulted from the \( q \) factor in the orthogonality of the basis function Eq. (S35) (See Eq. (S37)). By vectorizing and rescaling the tensors, the Tikhonov regularization Eq. (17) can be written in conventional constrained linear regression,

\[
\min_{\Delta \mathcal{T}} \|\Delta \mathcal{T}\|^2 \text{ s.t. } \|\mathcal{T} - \bar{E} \cdot \Delta \mathcal{T}\|^2 \leq \tau_k,
\]

[S27]
where $\overline{C} \in \mathbb{R}^{N_x^2N_y}$ and $\overline{E} \in \mathbb{C}^{N_x^2N_y \times 2N_x^2M}$. A large $\tau_k$ tends to oversmooth the solution $\Delta \overline{B}$, while a small one may cause overfitting and thus make the regularization fail to filter out the noises. A good heuristic is

$$
\tau_k = \left(1 + \frac{2}{N_y - 2M - 2}\right) \left(1 - \frac{2M(\|\overline{C}\|^2 - 1)}{N_y(\|\overline{C}\|^2 - 1) + 2M}\right).
$$

[S28]

where the first term is based on Chi-square distribution statistics and the second one is based on the estimated magnitude of errors.

The optimization Eq. (S27) is equivalent to Tikhonov regularization with Morozov’s discrepancy principle (3), which can be solved by finding

$$
\Delta \overline{B}(\lambda) = (\overline{E}^* \overline{E} + \lambda I)^{-1} \overline{E}^* \overline{C}
$$

[S29]
satisfying

$$
\|\overline{C} - \overline{E} \Delta \overline{B}(\lambda)\|^2 = \tau_k.
$$

[S30]

In (4), it is shown that the left hand side of Eq. (S30) is a monotonic function of $\lambda$, which in our implementation Eq. (S30) was solved by the Newton–Raphson method coupled with the bisection method when the bound constraints are broken.

**Derivation of Band-limiting Projector and Choice of $N_m$.** First, we present derivation of the basis function $v_{mn}(q)$. The density-density autocorrelation function is defined as

$$
A(r) = \int_{\mathbb{R}^2} \rho(r + r')\rho(r')dr'.
$$

[S31]

whose circular harmonic coefficient $A_m(r)$ is supported on $[0, L]$, so can be represented in Fourier-Bessel series

$$
A_m(r) = \sum_{n} a_{mn} \sqrt{2} J_{m}(\frac{u_{mn}r}{L}) = \sum_{n} a_{mn} \sqrt{2} J_{m+1}(\frac{u_{mn}r}{L})\frac{J_{m}(2\pi qr)}{u_{mn} - (2\pi qr)^2}.
$$

[S32]

Since the Fourier transform of $A(r)$ is $I(q)$ (5), the circular harmonic coefficient $I_m$ can be obtained by the Hankel transform of $A_m$,

$$
I_m(q) = 2\pi(-1)^m \int_0^L A_m(r)J_m(2\pi qr)dr.
$$

[S33]

Combining Eq. (S32) and Eq. (S33) gives

$$
I_m(q) = \sum_{n=1}^{\infty} a_{mn} \frac{2\sqrt{2}\pi(-1)^m}{LJ_{m+1}(u_{mn})} \int_0^L J_m(\frac{u_{mn}r}{L})J_m(2\pi qr)dr
$$

[S34]

$$
= \sum_{n=1}^{\infty} \frac{2\sqrt{2}\pi(-1)^m L u_{mn} J_m(2\pi qL)}{u_{mn}^2 - (2\pi qL)^2}.
$$

Then let

$$
v_{mn}(q) = \begin{cases} 
\sqrt{2}\pi(-1)^m LJ_{m+1}(u_{mn}) & \text{if } q = \frac{u_{mn}}{2\pi L} \\
2\sqrt{2}\pi(-1)^m L u_{mn} J_m(2\pi qL) & \text{otherwise}
\end{cases}
$$

[S35]

The size $N_m$ of the truncation, which is the number of columns of $V_m$, should be chosen as the maximal $n$ such that

$$
\frac{u_{mn}}{2\pi L} \leq \alpha q_{max}.
$$

[S36]

We used $\alpha = 8$. The basis functions $v_{mn}$ are orthogonal to each other in the sense that

$$
\int_0^\infty v_{mn}(q)v_{m'n'}(q)q dq = \delta_{nn'}.
$$

[S37]

Therefore, prior to computation of the pseudoinverse $V_m^\dagger$, we weight $V_m$ by multiplying the $n$-th row by $\sqrt{q_n d_n}$ with $d_n = \frac{u_{n+1} - u_n}{2}$. This weighted $V_m$ is denoted by $\overline{V}_m$. We calculate the singular value decomposition of $\overline{V}_m$,

$$
\overline{V}_m = U_B \Lambda_B V_B^*,
$$

[S38]

and then the pseudoinverse of $\overline{V}_m$ as

$$
\overline{V}_m^\dagger = V_B \Lambda_B^{inv} U_B^*.
$$

[S39]

where $\Lambda_B^{inv}$ is a diagonal matrix with diagonal entries

$$
(\Lambda_B^{inv})_{nn} = \begin{cases} 
\frac{1}{(\Lambda_B)_{nn}} & \text{if } (\Lambda_B)_{nn} \geq \beta(\Lambda_B)_{11} \\
0 & \text{if } (\Lambda_B)_{nn} < \beta(\Lambda_B)_{11}
\end{cases}
$$

[S40]

We selected $\beta = 0.1$ in our implementation. The pseudoinverse $V_m^\dagger$ is attained by dividing the $n$-th column of $\overline{V}_m^\dagger$ by $\sqrt{q_n d_n}$.
Solution to Rank-one Tensor Decomposition. This subpart can be solved by a modified alternating least square algorithm (6) that iterates between the subproblem of the optimization with respect to $A_m$ and $R_m$. In particular, initializing $R_m$ to be all zeros except $R_{0m} = 1$, the $A_m$-subproblem is equivalent to

$$\min_{A_m \in \mathbb{C}^{N_m}} \left\| \frac{1}{\| w_{td} \circ R_m \|^2} \sum_{k=0}^{K-1} (w_{td})^2 R_{km} G_{.,k} - A_m A_m^* \right\|_F$$

where $\circ$ is the element-wise multiplication. The solution to the above minimization is $A_m = \lambda_0 v_0$ where $\lambda_0$ is the largest positive eigenvalue and $v_0$ is the corresponding eigenvector of the matrix

$$\frac{1}{\| w_{td} \circ R_m \|^2} \sum_{k=0}^{K-1} (w_{td})^2 R_{km} G_{.,k}.$$ 

The $R_m$-subproblem can be solved element-wisely, for each $k > 0$

$$\min_{0 \leq R_{km} \leq 1} \left\| G_{.,k} - R_{km} A_m A_m^* \right\|_F.$$ 

The solution to the above minimization is

$$R_{km} = P_{[0,1]} \left( \frac{3R(A_m^* A_m) G_{.,k}}{\| A_m \|^4} \right),$$

where $P_{[0,1]}$ projects any real number to $[0,1]$,

$$P_{[0,1]}(x) = \begin{cases} 0 & \text{if } x < 0, \\ x & \text{if } 0 \leq x \leq 1, \\ 1 & \text{if } x > 1. \end{cases}$$

In the first iteration of MTECS, $w_{td}$ was set to be all zeros except the first entry, and in the following iterations, $w_{td}$ was selected based on the current estimation of $D_r$,

$$(w_{td})_k = e^{-4m^2 k^2 H^2 (p)}.$$ 

Details of Numerical Experiments

In the numerical experiments, the electron density $\rho$ at $r = (r_1, r_2)$ in Cartesian coordinate system is, up to a scaling constant,

$$\rho(r) = \begin{cases} \sqrt{W^2 - 4r_2^2} & \text{if } 2|r_1| \leq T \text{ and } 2|r_2| \leq W, \\ 2\sqrt{H^2 - (r_1 - (H + T/2))^2 - r_2^2} & \text{if } (r_1 - (H + T/2))^2 + r_2^2 \leq H^2, \\ 2\sqrt{H^2 - (r_1 + (H + T/2))^2 - r_2^2} & \text{if } (r_1 + (H + T/2))^2 + r_2^2 \leq H^2, \\ 0 & \text{otherwise}, \end{cases}$$

where $H = W = \frac{4}{2047}$, and $T = \frac{8}{2047}$. And the intensity function $I$ is

$$I(q, \phi) = \frac{TW J_1(\pi W q \sin \phi) \sin(T q \cos \phi)}{2T q^2 \sin \phi \cos \phi} + \frac{2H^{3/2} J_{3/2}(2\pi H q) \cos(2\pi(T/2 + H)q \cos \phi)}{q^{3/2}}.$$ 

See Fig. S1a for illustration of $I$. The Fig. S1b shows part of a synthesized images.

According to Eq. (12) and Eq. (13), $B$ is actually the circular harmonic coefficients of the cross-correlation data $C$. Theoretically,

$$B_{i',m'} = I_{2m}(q_{i'}) \overline{I_{2m}(q')}.$$ 

In Fig. S2, we show the $B'(p)$ output by the last iteration of the algorithm, denoted by $B_{\text{filtered}}$, against the measure $q$. This figure also demonstrates the capability of the MTECS algorithm to filter the cross-correlation data.
Fig. S1. (a) The intensity function $I$. (b) Part of an example of the simulated samples.
Fig. S2. The $\log(g^{\text{filtered}}_{i|m=0})$ (in orange) and $\log |I_{2m}(q_i)|^2$ (in blue) versus measured $q_i$. 
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