



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 57 (2024)

Supporting information for article:

**Operation model of a skew-symmetric split-crystal neutron
interferometer**

Carlo P. Sasso, Giovanni Mana and Enrico Massa

Operation model of a skew-symmetric split-crystal neutron interferometer

Carlo Paolo Sasso ¹, Giovanni Mana ^{1,2}, and Enrico Massa ¹

1) INRIM – Istituto Nazionale di Ricerca Metrologica, Torino, Italy

2) UNITO – Università di Torino, Dipartimento di Fisica, Torino, Italy

3. Interferometer operation

focus coordinates, Eq. (5c)

```
Clear["Global`*"]; Remove["Global`*"];
```

```
e1 = zM1 - zF1 == -zM2 + zF2;
```

```
(* same x-axis displacement of the rays along the two paths *)
```

```
e2 = zM1 + tM1 + zF1 == zM2 + tM2 + zF2; (* same distance from the splitter *)
```

```
zF12 = Solve[{e1, e2}, {zF1, zF2}][[1]];
```

```
xF = Simplify[(zM1 - zF1) Tan[θB] /. zF12] (* x coordinate *)
```

```
xF = Simplify[(-zM2 + zF2) Tan[θB] /. zF12] (* x coordinate *)
```

```
zF = Simplify[tS + zM1 + tM1 + zF1 /. zF12] (* z coordinate *)
```

$$xF = \frac{1}{2} (tM1 - tM2 + 2 zM1 - 2 zM2) \tan[\theta B]$$

$$xF = \frac{1}{2} (tM1 - tM2 + 2 zM1 - 2 zM2) \tan[\theta B]$$

$$zF = \frac{tM1}{2} + \frac{tM2}{2} + tS + zM1 + zM2$$

rotation matrix

```
Clear["Global`*"]; Remove["Global`*"];
```

```
R = {{1, -ρ, θ}, {ρ, 1, -ψ}, {-θ, ψ, 1}};
```

```
Print["R = ", R // MatrixForm]
```

```
(* inverse of the rotation matrix, first order *)
```

```
Ri = {{1, ρ, -θ}, {-ρ, 1, ψ}, {θ, -ψ, 1}};
```

$$R = \begin{pmatrix} 1 & -\rho & \theta \\ \rho & 1 & -\psi \\ -\theta & \psi & 1 \end{pmatrix}$$

transformation $\hat{M}(z)$: restriction to V_2

```

rII = {xII, yII, zII};
(* Ko and Kh unit vectors; 0 ==> o, 1 ==> h *)
K[n_] = K {If[n == 0, -1, 1] x Sin[θB], 0, Cos[θB]};
arg = Expand[K[#].(Ri.(rII - {s, 0, 0}) - rII) & /@ {0, 1}] /.
  {Cos[θB] → Kz / K, Sin[θB] → h / (2 K)} /. xII → xII + s;
arg = Simplify[arg];
Print["⟨o| $\hat{M}$ |o⟩ = Exp[i Ko.(M-1rII - rII)] = ", Exp[I arg[[1]]] ]
Print["⟨h| $\hat{M}$ |h⟩ = Exp[i Kh.(M-1rII - rII)] = ", Exp[I arg[[2]]] ]

⟨o| $\hat{M}$ |o⟩ = Exp[i Ko.(M-1rII - rII)] = ei (1/2 h (s+zII θ-yII ρ)+Kz (xII θ-yII ψ))
⟨h| $\hat{M}$ |h⟩ = Exp[i Kh.(M-1rII - rII)] = ei (-1/2 h (s+zII θ-yII ρ)+Kz (xII θ-yII ψ))

```

transformation $\hat{M}(z)$: restriction to \mathcal{L}_2

```

rI = {xI, yI, zI};
dd = Apply[DiracDelta, Ri.(rII - {s, 0, 0}) - rI] /. xII → xII + s /.
  -zI + zII + xII θ - yII ψ → -zI + zII;
Print["⟨rII| $\hat{M}$ |rI⟩ = ", dd]

⟨rII| $\hat{M}$ |rI⟩ = DiracDelta[-zI + zII, xI - xII + zII θ - yII ρ, -yI + yII - xII ρ + zII ψ]

```

transformation $\hat{M}(z)$: direct space representation

```

M = DiagonalMatrix[Exp[I arg]] dd;
(DiagonalMatrix[Exp[I arg]] // MatrixForm) dd
DiracDelta[-zI + zII, xI - xII + zII θ - yII ρ, -yI + yII - xII ρ + zII ψ]

$$\begin{pmatrix} e^{i \left( \frac{1}{2} h (s+zII \theta-yII \rho)+Kz (xII \theta-yII \psi) \right)} & 0 \\ 0 & e^{i \left( -\frac{1}{2} h (s+zII \theta-yII \rho)+Kz (xII \theta-yII \psi) \right)} \end{pmatrix}$$


```

transformation $\hat{M}(z)$: reciprocal space representation, Eq. (6b)

(* matrix element 11 *)

```
step11 =
  FullSimplify[InverseFourierTransform[M[[1, 1]], xI, p, FourierParameters -> {0, -1}]];
step11 =
  FullSimplify[InverseFourierTransform[step11, yI, q, FourierParameters -> {0, -1}]];
step11 = FullSimplify[FourierTransform[step11, xII, p1, FourierParameters -> {0, -1}]];
step11 = FullSimplify[FourierTransform[step11, yII, q1, FourierParameters -> {0, -1}]];
step11 = step11 / 2 /. -2 p rho -> 0
```

(* matrix element 22 *)

```
step22 =
  FullSimplify[InverseFourierTransform[M[[2, 2]], xI, p, FourierParameters -> {0, -1}]];
step22 =
  FullSimplify[InverseFourierTransform[step22, yI, q, FourierParameters -> {0, -1}]];
step22 = FullSimplify[FourierTransform[step22, xII, p1, FourierParameters -> {0, -1}]];
step22 = FullSimplify[FourierTransform[step22, yII, q1, FourierParameters -> {0, -1}]];
step22 = step22 / 2 /. 2 p rho -> 0
```

$$e^{\frac{1}{2} i (h s + h z_{II} \theta - 2 p z_{II} \theta + 2 q z_{II} \psi)} \text{DiracDelta}[z_I - z_{II}] \times \\ \text{DiracDelta}[p - p_1 + K z \theta - q \rho] \times \text{DiracDelta}[-2 q + 2 q_1 + h \rho + 2 K z \psi]$$

$$e^{-\frac{1}{2} i (h s + h z_{II} \theta + 2 p z_{II} \theta - 2 q z_{II} \psi)} \text{DiracDelta}[z_I - z_{II}] \times \\ \text{DiracDelta}[p - p_1 + K z \theta - q \rho] \times \text{DiracDelta}[2 q - 2 q_1 + h \rho - 2 K z \psi]$$

$$M_{11} = \text{Simplify}\left[e^{-\frac{1}{2} i (-2 p z \theta + 2 q z \psi)} \text{step11} / . \text{DiracDelta}[z_I - z_{II}] \rightarrow 1 / . z_{II} \rightarrow z \right] /$$

$$\text{DiracDelta}[p - p_1 + K z \theta - q \rho]$$

$$M_{22} = \text{Simplify}\left[e^{-\frac{1}{2} i (-2 p z \theta + 2 q z \psi)} \text{step22} / . \text{DiracDelta}[z_I - z_{II}] \rightarrow 1 / . z_{II} \rightarrow z \right] /$$

$$\text{DiracDelta}[p - p_1 + K z \theta - q \rho]$$

Print[

" $\hat{M}(p, p_1; z) =$ ", (DiagonalMatrix[{M11, M22}] // TraditionalForm) \times

$$\text{DiracDelta}[p - p_1 + K z \theta - q \rho] \times \text{Simplify}\left[e^{-\frac{1}{2} i (-2 p z \theta + 2 q z \psi)} \right]$$

]

$$e^{\frac{1}{2} i h (s + z \theta)} \text{DiracDelta}[-2 q + 2 q_1 + h \rho + 2 K z \psi]$$

$$e^{-\frac{1}{2} i h (s + z \theta)} \text{DiracDelta}[2 q - 2 q_1 + h \rho - 2 K z \psi]$$

$$\hat{M}(p, p_1; z) = e^{i z (p \theta - q \psi)} \text{DiracDelta}[p - p_1 + K z \theta - q \rho]$$

$$\left(\begin{array}{cc} e^{\frac{1}{2} i h (s + z \theta)} \delta(-2 q + 2 q_1 + h \rho + 2 K z \psi) & 0 \\ 0 & e^{-\frac{1}{2} i h (s + z \theta)} \delta(2 q - 2 q_1 + h \rho - 2 K z \psi) \end{array} \right)$$

some tests

definitions

```
Clear["Global`*"]; Remove["Global`*"];
```

```
(* free-space propagation *)
```

```
F[p_, q_, z_] = {
  {e^{+i p z Tan[θB]}, 0},
  {0, e^{-i p z Tan[θB]}} e^{-\frac{i(\rho^2+q^2)z}{2Kz}};
```

```
(* transformation  $\hat{M}(z)$  *)
```

```
Mz1[p_, p1_, q_, q1_, z_] = {
  {e^{\frac{i h (s+\theta z)}{2}} e^{-i (p1 z \theta - q1 z \psi)} DiracDelta[p1 - p - \rho q + \theta Kz, q1 - q - \frac{h \rho}{2} - \psi Kz], 0},
  {0, e^{-\frac{i h (s+\theta z)}{2}} e^{-i (p1 z \theta - q1 z \psi)} DiracDelta[p1 - p - \rho q + \theta Kz, q1 - q + \frac{h \rho}{2} - \psi Kz]}};
```

```
(* inverse transformation  $\hat{M}^{-1}(z)$  *)
```

```
Mz2[p_, p1_, q_, q1_, z_] = Mz1[p, p1, q, q1, z] /. {s → -s, θ → -θ, ρ → -ρ, ψ → -ψ};
```

$$\hat{M}^{-1}(z) \hat{M}(z) |\psi(z)\rangle = |\psi(z)\rangle$$

```
Mz2[p, p1, q, q1, z].Mz1[p1, p2, q1, q2, z].{\tilde{\psi}_{in}[p2, q2], 0};
Integrate[%, {p2, -Infinity, +Infinity},
  Assumptions → p1 > 0 && ρ > 0 && q1 > 0 && θ > 0 && Kz > 0];
Integrate[%, {q2, -Infinity, +Infinity},
  Assumptions → p1 > 0 && ρ > 0 && q1 > 0 && θ > 0 && Kz > 0 && h > 0 && ψ > 0];
Integrate[%, {p1, -Infinity, +Infinity},
  Assumptions → ρ > 0 && θ > 0 && Kz > 0 && p > 0 && q > 0];
tmp = Integrate[%, {q1, -Infinity, +Infinity},
  Assumptions → ρ > 0 && θ > 0 && Kz > 0 && h > 0 && ψ > 0 && q > 0];
ExpandAll[tmp] /. {ρ^2 → 0, θ^2 → 0, ψ^2 → 0, ρ ψ → 0, θ ρ → 0}
{\tilde{\psi}_{in}[p, q], 0}
```

$$\hat{M}^{-1}(z) \hat{F}(z) M(0) |\psi(0)\rangle = F(z) |\psi(0)\rangle$$

```
Mz2[p, p1, q, q1, z].F[p1, q1, z].Mz1[p1, p2, q1, q2, 0].{\tilde{\psi}_{in}[p2, q2], 0};
Integrate[%, {p2, -Infinity, +Infinity},
  Assumptions → p1 > 0 && ρ > 0 && q1 > 0 && θ > 0 && Kz > 0];
Integrate[%, {q2, -Infinity, +Infinity},
  Assumptions → p1 > 0 && ρ > 0 && q1 > 0 && θ > 0 && Kz > 0 && h > 0 && ψ > 0];
Integrate[%, {p1, -Infinity, +Infinity},
  Assumptions → ρ > 0 && θ > 0 && Kz > 0 && p > 0 && q > 0];
tmp = Integrate[%, {q1, -Infinity, +Infinity},
  Assumptions → ρ > 0 && θ > 0 && Kz > 0 && h > 0 && ψ > 0 && q > 0];
ExpandAll[tmp /. {ρ^2 → 0}] /.
  {ρ^2 → 0, θ^2 → 0, ψ^2 → 0, ρ ψ → 0, θ ρ → 0, h → 2 Kz Tan[θB], p q → 0}
{e^{-\frac{i p^2 z}{2 Kz} - \frac{i q^2 z}{2 Kz} + i p z Tan[θB]} \tilde{\psi}_{in}[p, q], 0}
```

$$\hat{M}(z)|\psi(0)\rangle = |\psi(z)\rangle$$

```
Mz1[p, p2, q, q2, z].{ψ̃_in[p2, q2, z], θ};
Integrate[%, {p2, -Infinity, +Infinity},
  Assumptions → p > 0 && ρ > 0 && q > 0 && θ > 0 && Kz > 0];
Integrate[%, {q2, -Infinity, +Infinity},
  Assumptions → p > 0 && ρ > 0 && q > 0 && θ > 0 && Kz > 0 && h > 0 && ψ > 0];
% /. {ρ → θ, θ² → θ, ψ² → θ, ρ ψ → θ, θ ρ → θ, h → 2 Kz Tan[θB], p q → θ, s → θ} // MatrixForm
( e^(1/2 i (2 z (-p θ + q ψ) + 2 Kz z θ Tan[θB])) ψ̃_in[p - Kz θ, q + Kz ψ, z] )
  θ
```

4. Input wave: partially coherent source

direct-space representation of the density matrix, Eq. (9a-b)

```
Clear["Global`*"]; Remove["Global`*"]
φ[x_] = e^(-((x-x0)²)/l0² + i φ0 + i p0 x);
(* j(x1, x2) = ∫_k ⟨x1|φ(k)⟩⟨φ(k)|x2⟩dk, Cohen-Tannoudji pag. 305, Eq. (28) *)
step1 = φ[x1] (φ[x2] /. i → -i);
step2 =
  1 / (sqrt(2) π σp) Integrate[step1 e^(-p²/(2 σp²)), {p0, -Infinity, +Infinity}, Assumptions → σp > 0];
(* we assume w0 >> l0 *)
step3 = sqrt(2/π) sqrt(1/l0² + 1/w0²) Integrate[step2 e^(-2 x0²/w0²),
  {x0, -Infinity, +Infinity}, Assumptions → w0 > 0 && l0 > 0] /. l0² + w0² → w0²;
Collect[step3[[2]], {x1² + x2², (x1 - x2)²}, Together] /. (-1 - l0² σp²) / l0² → -1 / l0
(* l0 definition *)
Print["j[x1,x2] = ", Exp[%]] (* Eq. (10b) *)
j[x1,x2] = e^(-x1²+x2²/w0² - (x1-x2)²/2 l0)
```

without assuming w0 >> l0 (redefinitions of w0 and l0)

```

step2 =
  
$$\frac{1}{\sqrt{2\pi}\sigma} \text{Integrate}\left[\text{step1 } e^{-\frac{p\theta^2}{2\sigma^2}}, \{p\theta, -\text{Infinity}, +\text{Infinity}\}, \text{Assumptions} \rightarrow \sigma > 0\right];$$

step3 = 
$$\sqrt{\frac{2}{\pi}} \sqrt{\frac{1}{l\theta^2} + \frac{1}{w\theta^2}}$$

  Integrate[step2 e- $\frac{2x\theta^2}{w\theta^2}$ , {xθ, -Infinity, +Infinity}, Assumptions → wθ > 0 && lθ > 0];
(* wθ redefinition and lθ definition *)
Collect[step3[[2]], {x12 + x22, (x1 - x2)2}, Together] /.
  {-lθ2 - wθ2 → -wθ2,  $\frac{-w\theta^2 - l\theta^4 \sigma^2 - l\theta^2 w\theta^2 \sigma^2}{l\theta^2 (l\theta^2 + w\theta^2)} \rightarrow 1 / l\theta$ };
step3 = Exp[%];
Print["j[x1,x2] = ", step3]
(* perfectly coherent state *)
Print["j[x1,x2] = ", Limit[step3, lθ → Infinity]]
j[x1,x2] = e- $\frac{x1^2+x2^2}{w\theta^2} + \frac{(x1-x2)^2}{2l\theta}$ 
j[x1,x2] = e- $\frac{x1^2+x2^2}{w\theta^2}$ 

```

reciprocal-space representation of the density matrix, Eq. (9c-d)

```

Clear["Global`*"]; Remove["Global`*"]
j[x1_, x2_] = e- $\frac{x1^2+x2^2}{w\theta^2} - \frac{(x1-x2)^2}{2l\theta^2}$ ;
step1 =  $\sqrt{2\pi} \sqrt{\frac{2}{w\theta^2} + \frac{1}{l\theta^2}}$ 
  InverseFourierTransform[j[x1, x2], {x2}, {p2}, FourierParameters → {1, -1}];
step2 =  $\frac{\sqrt{\frac{1}{w\theta^2} + \frac{1}{w\theta^2 + 2l\theta^2}}}{\sqrt{\pi}}$ 
  FullSimplify[FourierTransform[step1, {x1}, {p1}, FourierParameters → {1, -1}]];
% /. wθ2 + lθ2 → wθ2; (* lθ << wθ *)
j~[p1, p2] = FullSimplify[%] (* Eq. (9d) *)
Print["j~[p1,p2] =", Limit[step2, lθ → Infinity]] (* Eq. (9e) *)
j~[p1, p2] = e- $\frac{1}{8} (p1-p2)^2 w\theta^2 - \frac{1}{4} (p1^2+p2^2) l\theta^2$ 
j~[p1, p2] = e- $\frac{1}{4} (p1^2+p2^2) w\theta^2$ 

```

5. Exit waves: coherent source

definitions

Clear["Global`*"]; Remove["Global`*"];

U0[p_, q_, z_] = {
 {T[p, z], R[p, z]},
 {R[p, z], T[-p, z]}} e^{- $\frac{i(p^2+q^2)z}{2Kz}$} ; (* Eq. (4a) *)

F[p_, q_, z_] = {
 {e^{+i p z Tan[θB]}, θ},
 {θ, e^{-i p z Tan[θB]}}} e^{- $\frac{i(p^2+q^2)z}{2Kz}$} ; (* Eq. (3c) *)

(* transformation (6b) *)

Mz1[p_, p1_, q_, q1_, z_] = {
 {e ^{$\frac{i h (s+\theta z)}{2}$} DiracDelta[p1 - p - ρ q + θ Kz, q1 - q - $\frac{h \rho}{2}$ - ψ Kz], θ},
 {θ, e ^{$\frac{i h (s+\theta z)}{2}$} DiracDelta[p1 - p - ρ q + θ Kz, q1 - q + $\frac{h \rho}{2}$ - ψ Kz]}}
 } e^{-i (p z θ - q z ψ)}; (* Eq. (6b) *)

(* inverse of the transformation (6b) *)

Mz2[p_, p1_, q_, q1_, z_] = Mz1[p, p1, q, q1, z] /. {s → -s, θ → -θ, ρ → -ρ, ψ → -ψ};

Po = {{1, θ}, {θ, θ}};

Ph = {{θ, θ}, {θ, 1}};

arm1 = F[p, q, zD].Mz2[p, p1, q, q1, Δz + tA].U0[p1, q1, tA].Mz1[p1, p2, q1, q2, Δz].
 F[p2, q2, zA1].Ph.U0[p2, q2, tM1].F[p2, q2, zM1].
 Po.U0[p2, q2, tS].F[p2, q2, zS].{ψ_{in}[p2, q2], θ}; (* Eq. (7b) *)

arm2 = F[p, q, zD].Mz2[p, p1, q, q1, Δz + tA].U0[p1, q1, tA].
 F[p1, q1, zA2].Po.U0[p1, q1, tM2].Mz1[p1, p2, q1, q2, Δz - tM2 - zA2].
 F[p2, q2, zM2].Ph.U0[p2, q2, tS].F[p2, q2, zS].{ψ_{in}[p2, q2], θ}; (* Eq. (7c) *)

(* the factor of 4 is form δ[p1-p-ρq+θKz,q1-q-hρ/2] =

2δ[2q-2q1+hρ,-p+p1+Kzθ-qρ] *)

arm1o = arm1[[1]] / 4

arm1h = arm1[[2]] / 4

arm2o = arm2[[1]] / 4

arm2h = arm2[[2]] / 4

e ^{$\frac{i(p^2+q^2)tA}{2Kz} - \frac{i(p^2+q^2)tM1}{2Kz} - \frac{i(p^2+q^2)tS}{2Kz} - \frac{i(p^2+q^2)zA1}{2Kz} - \frac{i(p^2+q^2)zD}{2Kz} - \frac{i(p^2+q^2)zM1}{2Kz} - \frac{i(p^2+q^2)zS}{2Kz} - \frac{1}{2} i h (s+\Delta z \theta) + \frac{1}{2} i h (-s - (tA+\Delta z) \theta) - i (p1 \Delta z \theta -$}
 DiracDelta[-p + p1 - Kz θ + q ρ, -2 q + 2 q1 + h ρ + 2 Kz ψ] ×
 DiracDelta[-p1 + p2 + Kz θ - q1 ρ, -2 q1 + 2 q2 + h ρ - 2 Kz ψ] ×
 R[p1, tA] × R[p2, tM1] × T[p2, tS] ψ_{in}[p2, q2]

$$\begin{aligned}
& e^{-\frac{i(p_1^2+q_1^2)tA}{2Kz} - \frac{i(p_2^2+q_2^2)tM_1}{2Kz} - \frac{i(p_2^2+q_2^2)tS}{2Kz} - \frac{i(p_2^2+q_2^2)zA_1}{2Kz} - \frac{i(p^2+q^2)zD}{2Kz} - \frac{i(p_2^2+q_2^2)zM_1}{2Kz} - \frac{i(p_2^2+q_2^2)zS}{2Kz} - \frac{1}{2}i h (s+\Delta z \theta) - \frac{1}{2}i h (-s-(tA+\Delta z)\theta) - i(p_1 \Delta z \theta -} \\
& \text{DiracDelta}[-p+p_1-Kz\theta+q\rho, 2q-2q_1+h\rho-2Kz\psi] \times \\
& \text{DiracDelta}[-p_1+p_2+Kz\theta-q_1\rho, -2q_1+2q_2+h\rho-2Kz\psi] \times \\
& R[p_2, tM_1] \times T[-p_1, tA] \times T[p_2, tS] \tilde{\psi}_{in}[p_2, q_2] \\
& e^{-\frac{i(p_1^2+q_1^2)tA}{2Kz} - \frac{i(p_1^2+q_1^2)tM_2}{2Kz} - \frac{i(p_2^2+q_2^2)tS}{2Kz} - \frac{i(p_1^2+q_1^2)zA_2}{2Kz} - \frac{i(p^2+q^2)zD}{2Kz} - \frac{i(p_2^2+q_2^2)zM_2}{2Kz} - \frac{i(p_2^2+q_2^2)zS}{2Kz} + \frac{1}{2}i h (-s-(tA+\Delta z)\theta) - \frac{1}{2}i h (s+(-tM_2-zA_2+\Delta z)\theta)} \\
& \text{DiracDelta}[-p+p_1-Kz\theta+q\rho, -2q+2q_1+h\rho+2Kz\psi] \times \\
& \text{DiracDelta}[-p_1+p_2+Kz\theta-q_1\rho, -2q_1+2q_2+h\rho-2Kz\psi] \times \\
& R[p_1, tM_2] \times R[p_2, tS] \times T[p_1, tA] \tilde{\psi}_{in}[p_2, q_2] \\
& e^{-\frac{i(p_1^2+q_1^2)tA}{2Kz} - \frac{i(p_1^2+q_1^2)tM_2}{2Kz} - \frac{i(p_2^2+q_2^2)tS}{2Kz} - \frac{i(p_1^2+q_1^2)zA_2}{2Kz} - \frac{i(p^2+q^2)zD}{2Kz} - \frac{i(p_2^2+q_2^2)zM_2}{2Kz} - \frac{i(p_2^2+q_2^2)zS}{2Kz} - \frac{1}{2}i h (-s-(tA+\Delta z)\theta) - \frac{1}{2}i h (s+(-tM_2-zA_2+\Delta z)\theta)} \\
& \text{DiracDelta}[-p+p_1-Kz\theta+q\rho, 2q-2q_1+h\rho-2Kz\psi] \times \\
& \text{DiracDelta}[-p_1+p_2+Kz\theta-q_1\rho, -2q_1+2q_2+h\rho-2Kz\psi] \times \\
& R[p_1, tA] \times R[p_1, tM_2] \times R[p_2, tS] \tilde{\psi}_{in}[p_2, q_2]
\end{aligned}$$

final states, Eq. (11a-d)

```

{-2 q + 2 q1 + h ρ + 2 Kz ψ == 0, -p + p1 - Kz θ + q ρ == 0,
-2 q1 + 2 q2 + h ρ - 2 Kz ψ == 0, -p1 + p2 + Kz θ - q1 ρ == 0};
Expand[Solve[%, {p1, q1, p2, q2}] /. {ρ^2 → 0, ρ ψ → 0}] [[1]]
arm1o /. %; (* this is equivalent to the integrations over p2 and p1 *)
ExpandAll[%] /. {ρ^2 → 0, θ^2 → 0, θ ρ → 0, p θ → 0, p ρ → 0, ψ^2 → 0, ψ ρ → 0} /.
DiracDelta[0, 0]^2 → 1 / 2;
(* omission of the phase terms shared by ψ̃o1 and ψ̃o2 *)
tmp = ExpandAll[
% e^{-i p (zS+zD) Tan[θB]} e^{i h s} e^{-\frac{i h q tA ρ}{2 Kz}} e^{\frac{1}{2} i h θ tA} e^{i h Δz θ} e^{i p (zA1-zM1) Tan[θB]} e^{\frac{-i h q (tM1+tS+zA1+zM1+zS) ρ}{Kz}}];
Collect[Part[%, 1, 2], {p, q}, Simplify] /. {tA + tM1 + tS + zA1 + zD + zM1 + zS → zD}
ψ̃o1 == ReplacePart[tmp, 1 → e^{Collect[%, zD, Simplify]}] (* Eq. (11.a) *)
{p1 → p + Kz θ - q ρ, q1 → q - \frac{h ρ}{2} - Kz ψ, p2 → p, q2 → q - h ρ}
-\frac{i p^2 zD}{2 Kz} - \frac{i q^2 zD}{2 Kz}
ψ̃o1 == e^{-\frac{i (p^2+q^2) zD}{2 Kz}} R[p, tM1] × R[p + Kz θ - q ρ, tA] × T[p, tS] ψ̃in[p, q - h ρ]

```

```

{-2 q + 2 q1 + h ρ + 2 Kz ψ == 0, -p + p1 - Kz θ + q ρ == 0,
 -2 q1 + 2 q2 + h ρ - 2 Kz ψ == 0, -p1 + p2 + Kz θ - q1 ρ == 0};
Expand[Solve[%, {p1, q1, p2, q2}] /. {ρ^2 → 0, ρ ψ → 0}][[1]]
arm2o /. %; (* this is equivalent to the integrations over p2 and p1 *)
ExpandAll[%] /. {ρ^2 → 0, θ^2 → 0, θ ρ → 0, p θ → 0, p ρ → 0, ψ^2 → 0, ψ ρ → 0} /.
DiracDelta[0, 0]^2 → 1 / 2;
(* omission of the shared phase terms, ψ̃o1 and ψ̃o2 *)
tmp = ExpandAll[
% e^{-i p (zS+zD) Tan[θB]} e^{i h s} e^{\frac{1}{2} i h θ tA} e^{-\frac{i h q tA ρ}{2 Kz}} e^{i h Δz θ} e^{i p (zA1-zM1) Tan[θB]} e^{\frac{-i h q (tM1+tS+zA1+zM1+zS) ρ}{Kz}}];
Collect[Part[%, 1, 2], {p, q}, Simplify] /. {tA + tM2 + tS + zA2 + zD + zM2 + zS → zD,
(zA1 + zA2 - zM1 - zM2) Tan[θB] → Δx, Tan[θB] → h / (2 Kz)};
Collect[%, {p, q, ρ}, Simplify] /.
{ (tM2 + 2 zA2) θ → 2 s0, -\frac{i h (2 tM1 - tM2 + 2 (zA1 + zM1 - zM2)) ρ}{2 Kz} → -i Δy }
ψ̃o2 == ReplacePart[tmp, 1 → e^{Collect[%, zD, Simplify]}] (* Eq. (11.b) *)
{p1 → p + Kz θ - q ρ, q1 → q - \frac{h ρ}{2} - Kz ψ, p2 → p - Kz ρ ψ, q2 → q - h ρ}
i h s0 - \frac{i p^2 zD}{2 Kz} - \frac{i q^2 zD}{2 Kz} + i p Δx - i q Δy
ψ̃o2 ==
e^{-\frac{i (p^2+q^2) zD}{2 Kz} + i (h s0+p Δx-q Δy)} R[p, tS] × R[p + Kz θ - q ρ, tM2] × T[p + Kz θ - q ρ, tA] ψ̃in[p, q - h ρ]

{2 q - 2 q1 + h ρ - 2 Kz ψ == 0, -p + p1 - Kz θ + q ρ == 0,
 -2 q1 + 2 q2 + h ρ - 2 Kz ψ == 0, -p1 + p2 + Kz θ - q1 ρ == 0};
Expand[Solve[%, {p1, q1, p2, q2}] /. {ρ^2 → 0, ρ ψ → 0}][[1]]
arm1h /. %; (* integrations over p2 and p1 *)
ExpandAll[%] /. {ρ^2 → 0, θ^2 → 0, θ ρ → 0, p θ → 0, p ρ → 0, ψ^2 → 0, ψ ρ → 0} /.
DiracDelta[0, 0]^2 → 1 / 2;
(* omission of the shared phase terms, ψ̃h1 and ψ̃h2 *)
tmp = ExpandAll[
% e^{-i p (zS-zD) Tan[θB]} e^{-\frac{1}{2} i h θ tA} e^{\frac{i h q tA ρ}{2 Kz}} e^{i p (zA1-zM1) Tan[θB]}];
Collect[Part[%, 1, 2], {p, q}, Simplify] /. {tA + tM1 + tS + zA1 + zD + zM1 + zS → zD}
ψ̃h1 == ReplacePart[tmp, 1 → e^{Collect[%, zD, Simplify]}] (* Eq. (11.c) *)
{p1 → p + Kz θ - q ρ, q1 → q + \frac{h ρ}{2} - Kz ψ, p2 → p - Kz ρ ψ, q2 → q}
-\frac{i p^2 zD}{2 Kz} - \frac{i q^2 zD}{2 Kz}
ψ̃h1 == e^{-\frac{i (p^2+q^2) zD}{2 Kz}} R[p, tM1] × T[p, tS] × T[-p - Kz θ + q ρ, tA] ψ̃in[p, q]

```

```

{2 q - 2 q1 + h ρ - 2 Kz ψ == 0, -p + p1 - Kz θ + q ρ == 0,
 -2 q1 + 2 q2 + h ρ - 2 Kz ψ == 0, -p1 + p2 + Kz θ - q1 ρ == 0};
Expand[Solve[%, {p1, q1, p2, q2}] /. {ρ^2 → 0, ρ ψ → 0}][[1]]
arm2h /. %; (* integrations over p2 and p1 *)
ExpandAll[%] /. {ρ^2 → 0, θ^2 → 0, θ ρ → 0, p θ → 0, p ρ → 0, ψ^2 → 0, ψ ρ → 0} /.
DiracDelta[0, 0]^2 → 1 / 2;
(* omission of the shared phase terms, ψ̃h1 and ψ̃h2 *)
tmp = ExpandAll[% e-i p (zS-zD) Tan[θB] e- $\frac{1}{2}$  i h θ tA e $\frac{i h q tA ρ}{2 Kz}$  ei p (zA1-zM1) Tan[θB]];
Simplify[#] & /@ Collect[Part[%, 1, 2], {p, q, θ, ρ}] /.
{tA + tM2 + tS + zA2 + zD + zM2 + zS → zD,
 (zA1 + zA2 - zM1 - zM2) Tan[θB] → Δx, Tan[θB] → h / (2 Kz)};
Collect[%, {p, q}, Simplify] /. {(tM2 + 2 zA2) θ → 2 sθ, - $\frac{i h q (tM2 + 2 zA2) ρ}{2 Kz}$  → -i q Δy}
ψ̃h2 == ReplacePart[tmp, 1 → eCollect[%, zD, Simplify]] (* Eq. (11.d) *)
{p1 → p + Kz θ - q ρ, q1 → q +  $\frac{h ρ}{2}$  - Kz ψ, p2 → p - Kz ρ ψ, q2 → q}
i h sθ -  $\frac{i p^2 zD}{2 Kz}$  -  $\frac{i q^2 zD}{2 Kz}$  + i p Δx - i q Δy
ψ̃h2 == e $-\frac{i(p^2+q^2)zD}{2Kz} + i(h s\theta + p \Delta x - q \Delta y)$  R[p, tS] × R[p + Kz θ - q ρ, tA] × R[p + Kz θ - q ρ, tM2] ψ̃in[p, q]

```

6. Exit waves: partially coherent source

definitions

```

Clear["Global`*"]; Remove["Global`*"];

(* crystal diffraction, Laue *)
U0[p_, q_, z_] = {
  T[p, z], R[p, z]},
  {R[p, z], T[-p, z]} } e-i (p2+q2) z / (2 Kz); (* Eq. (4a) *)

(* free-space propagation *)
F[p_, q_, z_] = {
  e+i p z Tan[θB], θ},
  {θ, e-i p z Tan[θB]} } e-i (p2+q2) z / (2 Kz); (* Eq. (3c) *)

(* transformation (6b) *)
Mz1[p_, p1_, q_, q1_, z_] = {
  ei h (s+θ z) / 2 DiracDelta[p1 - p - ρ q + θ Kz, q1 - q - h ρ / 2 - ψ Kz], θ},
  {θ, e-i h (s+θ z) / 2 DiracDelta[p1 - p - ρ q + θ Kz, q1 - q + h ρ / 2 - ψ Kz]} }
  e-i (p z θ - q z ψ); (* Eq. (6b) *)

(* inverse of the transformation (6b) *)
Mz2[p_, p1_, q_, q1_, z_] = Mz1[p, p1, q, q1, z] /. {s → -s, θ → -θ, ρ → -ρ, ψ → -ψ};

(* o and h projectors *)
Po = {{1, θ}, {θ, θ}};
Ph = {{θ, θ}, {θ, 1}};

(* ⟨p,q|X1 Po|p1,q1⟩, to be integrated over p2 and q2, see Eq. (19) *)
arm1 = F[p, q, zDA].Mz2[p, p2, q, q2, Δz + tA].U0[p2, q2, tA].Mz1[p2, p1, q2, q1, Δz].
  F[p1, q1, zA1].Ph.U0[p1, q1, tM1].F[p1, q1, zM1].Po.U0[p1, q1, tS].F[p1, q1, zS].Po;

(* ⟨p,q|X2 Po|p1,q1⟩, to be integrated over p2 and q2, see Eq. (19) *)
arm2 = F[p, q, zDA].Mz2[p, p2, q, q2, Δz + tA].U0[p2, q2, tA].
  F[p2, q2, zA2].Po.U0[p2, q2, tM2].Mz1[p2, p1, q2, q1, Δz - tM2 - zA2].
  F[p1, q1, zM2].Ph.U0[p1, q1, tS].F[p1, q1, zS].Po;

(* the factor of 4 is form δ[p1-p-ρ q+θ Kz,q1-q-hρ/2] =
  2δ[2 q-2 q1+h ρ,-p+p1+Kz θ-q ρ] *)
X1Poo = arm1[[1, 1]] / 4
X1Poh = arm1[[2, 1]] / 4
X2Poo = arm2[[1, 1]] / 4
X2Poh = arm2[[2, 1]] / 4

e-i (p22+q22) tA / (2 Kz) - i (p12+q12) tM1 / (2 Kz) - i (p12+q12) tS / (2 Kz) - i (p12+q12) zA1 / (2 Kz) - i (p22+q22) zDA / (2 Kz) - i (p12+q12) zM1 / (2 Kz) - i (p12+q12) zS / (2 Kz) - 1/2 i h (s+Δz θ) + 1/2 i h (-s-(tA+Δz) θ) - i (p2 Δz θ -
  DiracDelta[-p + p2 - Kz θ + q ρ, -2 q + 2 q2 + h ρ + 2 Kz ψ] ×
  DiracDelta[p1 - p2 + Kz θ - q2 ρ, 2 q1 - 2 q2 + h ρ - 2 Kz ψ] × R[p1, tM1] × R[p2, tA] × T[p1, tS]

```

$$\begin{aligned}
& e^{-\frac{i(p_2^2+q_2^2)t_A}{2Kz} - \frac{i(p_1^2+q_1^2)t_{M1}}{2Kz} - \frac{i(p_1^2+q_1^2)t_S}{2Kz} - \frac{i(p_1^2+q_1^2)z_{A1}}{2Kz} - \frac{i(p^2+q^2)z_{DA}}{2Kz} - \frac{i(p_1^2+q_1^2)z_{M1}}{2Kz} - \frac{i(p_1^2+q_1^2)z_S}{2Kz} - \frac{1}{2}i h (s+\Delta z \theta) - \frac{1}{2}i h (-s-(t_A+\Delta z) \theta) - i(p_2 \Delta z \theta)} \\
& \text{DiracDelta}[-p+p_2-Kz\theta+q\rho, 2q-2q_2+h\rho-2Kz\psi] \times \\
& \text{DiracDelta}[p_1-p_2+Kz\theta-q_2\rho, 2q_1-2q_2+h\rho-2Kz\psi] \times R[p_1, t_{M1}] \times T[p_1, t_S] \times T[-p_2, t_A] \\
& e^{-\frac{i(p_2^2+q_2^2)t_A}{2Kz} - \frac{i(p_2^2+q_2^2)t_{M2}}{2Kz} - \frac{i(p_1^2+q_1^2)t_S}{2Kz} - \frac{i(p_2^2+q_2^2)z_{A2}}{2Kz} - \frac{i(p^2+q^2)z_{DA}}{2Kz} - \frac{i(p_1^2+q_1^2)z_{M2}}{2Kz} - \frac{i(p_1^2+q_1^2)z_S}{2Kz} - \frac{1}{2}i h (-s-(t_A+\Delta z) \theta) - \frac{1}{2}i h (s+(-t_{M2}-z_{A2}+\Delta z) \theta)} \\
& \text{DiracDelta}[-p+p_2-Kz\theta+q\rho, -2q+2q_2+h\rho+2Kz\psi] \times \\
& \text{DiracDelta}[p_1-p_2+Kz\theta-q_2\rho, 2q_1-2q_2+h\rho-2Kz\psi] \times R[p_1, t_S] \times R[p_2, t_{M2}] \times T[p_2, t_A] \\
& e^{-\frac{i(p_2^2+q_2^2)t_A}{2Kz} - \frac{i(p_2^2+q_2^2)t_{M2}}{2Kz} - \frac{i(p_1^2+q_1^2)t_S}{2Kz} - \frac{i(p_2^2+q_2^2)z_{A2}}{2Kz} - \frac{i(p^2+q^2)z_{DA}}{2Kz} - \frac{i(p_1^2+q_1^2)z_{M2}}{2Kz} - \frac{i(p_1^2+q_1^2)z_S}{2Kz} - \frac{1}{2}i h (-s-(t_A+\Delta z) \theta) - \frac{1}{2}i h (s+(-t_{M2}-z_{A2}+\Delta z) \theta)} \\
& \text{DiracDelta}[-p+p_2-Kz\theta+q\rho, 2q-2q_2+h\rho-2Kz\psi] \times \\
& \text{DiracDelta}[p_1-p_2+Kz\theta-q_2\rho, 2q_1-2q_2+h\rho-2Kz\psi] \times R[p_1, t_S] \times R[p_2, t_A] \times R[p_2, t_{M2}]
\end{aligned}$$

Appendix C

calculation of $(XPO)_i^{nn}[p, q, p_1, q_1]$ in Eq. (19)

the integration over p_2 is because of the transformation (6b)

the phase terms shared by $(XPO)_1^{nn}$ and $(XPO)_2^{nn}$ are omitted

```

{-2 q + 2 q2 + h ρ + 2 Kz ψ == 0, -p + p2 - Kz θ + q ρ == 0,
 2 q1 - 2 q2 + h ρ - 2 Kz ψ == 0, p1 - p2 + Kz θ - q2 ρ == 0};
rule = Expand[Solve[%, {p2, q2, p1, q1}] /. {ρ^2 -> 0, ρ ψ -> 0}] [[1]]
X1Poo /. (* integrations over p2 *);
ExpandAll[% / 2] /. {ρ^2 -> 0, θ^2 -> 0, ψ^2 -> 0, θ ρ -> 0, ρ ψ -> 0, p ρ -> 0, p θ -> 0} /.
DiracDelta[0, 0]^2 -> DiracDelta[p1 - (p1 /. rule), q1 - (q1 /. rule)];
(* omission of the shared phase terms, Xoo1 and Xoo2 *)
tmp = ExpandAll[
  % e^{-i p (zS+zDA) Tan[θB]} e^{i h s} e^{-\frac{i h q t_A \rho}{2 Kz}} e^{\frac{1}{2} i h \theta t_A} e^{i h \Delta z \theta} e^{i p (zA1-zM1) Tan[θB]} e^{\frac{-i h q (tM1+tS+zA1+zM1+zS) \rho}{Kz}}];
Collect[Part[%, 1, 2], {p, q}, Simplify] /. {tA + tM1 + tS + zA1 + zDA + zM1 + zS -> zD}
Xoo1 = ReplacePart[tmp, 1 -> e^{Collect[%, zD, Simplify]}];
Print["Xoo1 = ", Xoo1]

{p2 -> p + Kz θ - q ρ, q2 -> q - \frac{h \rho}{2} - Kz ψ, p1 -> p, q1 -> q - h ρ}

-\frac{i p^2 zD}{2 Kz} - \frac{i q^2 zD}{2 Kz}
Xoo1 = e^{-\frac{i(p^2+q^2)zD}{2Kz}} DiracDelta[-p+p1, -q+q1+h\rho] \times R[p, t_{M1}] \times R[p+Kz\theta-q\rho, t_A] \times T[p, t_S]

```

```

{-p + p2 - Kz θ + q ρ == 0, -2 q + 2 q2 + h ρ + 2 Kz ψ == 0,
 p1 - p2 + Kz θ - q2 ρ == 0, 2 q1 - 2 q2 + h ρ - 2 Kz ψ == 0};
rule = Expand[Solve[%, {p2, q2, p1, q1}] /. {ρ^2 → 0, ρ ψ → 0}] [[1]]
X2Poo /. %; (* integrations over p2 *);
ExpandAll[% / 2] /. {ρ^2 → 0, θ^2 → 0, ψ^2 → 0, θ ρ → 0, ρ ψ → 0, p ρ → 0, p θ → 0} /.
 DiracDelta[0, 0]^2 → DiracDelta[p1 - (p1 /. rule), q1 - (q1 /. rule)];
(* omission of the shared phase terms, X001 and X002 *)
tmp = ExpandAll[
 % e^{-i p (zS+zDA) Tan[θB]} e^{i h s} e^{-\frac{i h q tA ρ}{2 Kz}} e^{\frac{1}{2} i h θ tA} e^{i h Δz θ} e^{i p (zA1-zM1) Tan[θB]} e^{\frac{-i h q (tM1+tS+zA1+zM1+zS) ρ}{Kz}}];
Collect[Part[%, 1, 2], {p, q}, Simplify] /. {tA + tM2 + tS + zA2 + zDA + zM2 + zS → zD,
 (zA1 + zA2 - zM1 - zM2) Tan[θB] → Δx, Tan[θB] → h / (2 Kz)};
Collect[%, {p, q, ρ}, Simplify] /.
 { (tM2 + 2 zA2) θ → 2 s0, -\frac{i h (2 tM1 - tM2 + 2 (zA1 + zM1 - zM2)) ρ}{2 Kz} → -i Δy}
X002 = ReplacePart[tmp, 1 → e^{Collect[%, zD, Simplify]}];
Print["X002 = ", X002]

{p2 → p + Kz θ - q ρ, q2 → q - \frac{h ρ}{2} - Kz ψ, p1 → p, q1 → q - h ρ}

i h s0 - \frac{i p^2 zD}{2 Kz} - \frac{i q^2 zD}{2 Kz} + i p Δx - i q Δy

X002 = e^{-\frac{i (p^2+q^2) zD}{2 Kz} + i (h s0+p Δx-q Δy)} DiracDelta[-p + p1, -q + q1 + h ρ] ×
 R[p, tS] × R[p + Kz θ - q ρ, tM2] × T[p + Kz θ - q ρ, tA]

{-p + p2 - Kz θ + q ρ == 0, 2 q - 2 q2 + h ρ - 2 Kz ψ == 0,
 p1 - p2 + Kz θ - q2 ρ == 0, 2 q1 - 2 q2 + h ρ - 2 Kz ψ == 0};
rule = Expand[Solve[%, {p2, q2, p1, q1}] /. {ρ^2 → 0, ρ ψ → 0}] [[1]]
X1Poh /. %; (* integrations over p2 *);
ExpandAll[% / 2] /. {ρ^2 → 0, θ^2 → 0, ψ^2 → 0, θ ρ → 0, ρ ψ → 0, p ρ → 0, p θ → 0} /.
 DiracDelta[0, 0]^2 → DiracDelta[p1 - (p1 /. rule), q1 - (q1 /. rule)];
(* omission of the shared phase terms, Xh1 and Xh2 *)
tmp = ExpandAll[
 % e^{-i p (zS-zDA) Tan[θB]} e^{-\frac{1}{2} i h θ tA} e^{\frac{i h q tA ρ}{2 Kz}} e^{i p (zA1-zM1) Tan[θB]}];
Collect[Part[%, 1, 2], {p, q}, Simplify] /. {tA + tM1 + tS + zA1 + zDA + zM1 + zS → zD}
Xh1 = ReplacePart[tmp, 1 → e^{Collect[%, zD, Simplify]}];
Print["Xh1 = ", Xh1]

{p2 → p + Kz θ - q ρ, q2 → q + \frac{h ρ}{2} - Kz ψ, p1 → p, q1 → q}

\frac{i p^2 zD}{2 Kz} - \frac{i q^2 zD}{2 Kz}

Xh1 = e^{-\frac{i (p^2+q^2) zD}{2 Kz}} DiracDelta[-p + p1, -q + q1] × R[p, tM1] × T[p, tS] × T[-p - Kz θ + q ρ, tA]

```

```

{-p + p2 - Kz θ + q ρ == 0, 2 q - 2 q2 + h ρ - 2 Kz ψ == 0,
 p1 - p2 + Kz θ - q2 ρ == 0, 2 q1 - 2 q2 + h ρ - 2 Kz ψ == 0};
rule = Expand[Solve[%, {p2, q2, p1, q1}] /. {ρ^2 → 0, ρ ψ → 0}][[1]]
X2Poh /. % (* integrations over p2 *);
ExpandAll[% / 2] /. {ρ^2 → 0, θ^2 → 0, ψ^2 → 0, θ ρ → 0, ρ ψ → 0, p ρ → 0, p θ → 0} /.
 DiracDelta[0, 0]^2 → DiracDelta[p1 - (p1 /. rule), q1 - (q1 /. rule)];
(* omission of the shared phase terms, Xhñ1 and Xhñ2 *)
tmp = ExpandAll[% e^{-i p (zS-zDA) Tan[θB]} e^{-\frac{1}{2} i h θ tA} e^{\frac{i h q tA ρ}{2 Kz}} e^{i p (zA1-zM1) Tan[θB]}];
Simplify[#] & @Collect[Part[%, 1, 2], {p, q, θ, ρ}] /.
 {tA + tM2 + tS + zA2 + zDA + zM2 + zS → zD,
 (zA1 + zA2 - zM1 - zM2) Tan[θB] → Δx, Tan[θB] → h / (2 Kz)};
Collect[%, {p, q}, Simplify] /. {(tM2 + 2 zA2) θ → 2 sθ, -\frac{i h q (tM2 + 2 zA2) ρ}{2 Kz} → -i q Δy}
Xhñ2 = ReplacePart[tmp, 1 → e^{Collect[%, zD, Simplify]}];
Print["Xhñ2 = ", Xhñ2]

{p2 → p + Kz θ - q ρ, q2 → q + \frac{h ρ}{2} - Kz ψ, p1 → p, q1 → q}

i h sθ - \frac{i p^2 zD}{2 Kz} - \frac{i q^2 zD}{2 Kz} + i p Δx - i q Δy

Xhñ2 = e^{-\frac{i (p^2+q^2) zD}{2 Kz} + i (h sθ+p Δx-q Δy)} DiracDelta[-p + p1, -q + q1] ×
 R[p, tS] × R[p + Kz θ - q ρ, tA] × R[p + Kz θ - q ρ, tM2]

```

Appendix C

calculation of $(XPo)_i^{*nn}[p, q, p2, q2]$ in Eq. (19)

```

Xōō1* = Xōō1 /. Exp[x_] → Exp[-x] /. {p1 → p2, q1 → q2} /.
 {R[x_, y_] → R*[x, y], T[x_, y_] → T*[x, y]}
Xōō2* = Xōō2 /. Exp[x_] → Exp[-x] /. {p1 → p2, q1 → q2} /.
 {R[x_, y_] → R*[x, y], T[x_, y_] → T*[x, y]}
Xhñ1* = Xhñ1 /. Exp[x_] → Exp[-x] /. {p1 → p2, q1 → q2} /.
 {R[x_, y_] → R*[x, y], T[x_, y_] → T*[x, y]}
Xhñ2* = Xhñ2 /. Exp[x_] → Exp[-x] /. {p1 → p2, q1 → q2} /.
 {R[x_, y_] → R*[x, y], T[x_, y_] → T*[x, y]}

e^{\frac{i (p^2+q^2) zD}{2 Kz}} DiracDelta[-p + p2, -q + q2 + h ρ] R*[p, tM1] R*[p + Kz θ - q ρ, tA] T*[p, tS]

e^{\frac{i (p^2+q^2) zD}{2 Kz} - i (h sθ+p Δx-q Δy)} DiracDelta[-p + p2, -q + q2 + h ρ]
 R*[p, tS] R*[p + Kz θ - q ρ, tM2] T*[p + Kz θ - q ρ, tA]

e^{\frac{i (p^2+q^2) zD}{2 Kz}} DiracDelta[-p + p2, -q + q2] R*[p, tM1] T*[p, tS] T*[-p - Kz θ + q ρ, tA]

e^{\frac{i (p^2+q^2) zD}{2 Kz} - i (h sθ+p Δx-q Δy)} DiracDelta[-p + p2, -q + q2]
 R*[p, tS] R*[p + Kz θ - q ρ, tA] R*[p + Kz θ - q ρ, tM2]

```

Appendix C

calculation of $j_o^{ij}[pa, qa, pb, qb]$

$(X\tilde{o}o1 /. \{p \rightarrow pa, q \rightarrow qa\}) (X\tilde{o}o1^* /. \{p \rightarrow pb, q \rightarrow qb\}) jin[p1, q1, p2, q2];$
`tmp = Integrate[%, {p1, -Infinity, +Infinity}, {q1, -Infinity, +Infinity},`
`{p2, -Infinity, +Infinity}, {q2, -Infinity, +Infinity}, Assumptions $\rightarrow pa \in \mathbb{R}$];`
`Collect[tmp[[1, 2]], zD, Simplify]`
 $j\tilde{o}11 = \text{ReplacePart}[tmp, \{1, 2\} \rightarrow \%] (* \text{Eq. (C.1b)} *)$

$$-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz}$$

$$j\tilde{o}11 = e^{-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz}} jin[pa, qa - h \rho, pb, qb - h \rho] \times R[pa, tM1] \times$$

$$R[pa + Kz \theta - qa \rho, tA] \times T[pa, tS] R^*[pb, tM1] R^*[pb + Kz \theta - qb \rho, tA] T^*[pb, tS]$$

$(X\tilde{o}o2 /. \{p \rightarrow pa, q \rightarrow qa\}) (X\tilde{o}o2^* /. \{p \rightarrow pb, q \rightarrow qb\}) jin[p1, q1, p2, q2];$
`tmp = Integrate[%, {p1, -Infinity, +Infinity}, {q1, -Infinity, +Infinity},`
`{p2, -Infinity, +Infinity}, {q2, -Infinity, +Infinity}, Assumptions $\rightarrow pa \in \mathbb{R}$];`
`Collect[tmp[[1, 2]], {Δx, zD}, Simplify]`
 $j\tilde{o}22 = \text{ReplacePart}[tmp, \{1, 2\} \rightarrow \%] (* \text{Eq. (C.1c)} *)$

$$-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz} + i (pa - pb) \Delta x - i (qa - qb) \Delta y$$

$$j\tilde{o}22 = e^{-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz} + i (pa - pb) \Delta x - i (qa - qb) \Delta y}$$

$$jin[pa, qa - h \rho, pb, qb - h \rho] \times R[pa, tS] \times R[pa + Kz \theta - qa \rho, tM2] \times$$

$$T[pa + Kz \theta - qa \rho, tA] R^*[pb, tS] R^*[pb + Kz \theta - qb \rho, tM2] T^*[pb + Kz \theta - qb \rho, tA]$$

$(X\tilde{o}o1 /. \{p \rightarrow pa, q \rightarrow qa\}) (X\tilde{o}o2^* /. \{p \rightarrow pb, q \rightarrow qb\}) jin[p1, q1, p2, q2];$
`tmp = Integrate[%, {p1, -Infinity, +Infinity}, {q1, -Infinity, +Infinity},`
`{p2, -Infinity, +Infinity}, {q2, -Infinity, +Infinity}, Assumptions $\rightarrow pa \in \mathbb{R}$];`
`Collect[tmp[[1, 2]], zD, Simplify]`
 $j\tilde{o}12 = \text{ReplacePart}[tmp, \{1, 2\} \rightarrow \%] (* \text{Eq. (C.1d)} *)$

$$-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz} - i (h s\theta + pb \Delta x - qb \Delta y)$$

$$j\tilde{o}12 = e^{-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz} - i (h s\theta + pb \Delta x - qb \Delta y)} jin[pa, qa - h \rho, pb, qb - h \rho] \times R[pa, tM1] \times$$

$$R[pa + Kz \theta - qa \rho, tA] \times T[pa, tS] R^*[pb, tS] R^*[pb + Kz \theta - qb \rho, tM2] T^*[pb + Kz \theta - qb \rho, tA]$$

$(X\tilde{o}o2 /. \{p \rightarrow pa, q \rightarrow qa\}) (X\tilde{o}o1^* /. \{p \rightarrow pb, q \rightarrow qb\}) jin[p1, q1, p2, q2];$
`tmp = Integrate[%, {p1, -Infinity, +Infinity}, {q1, -Infinity, +Infinity},`
`{p2, -Infinity, +Infinity}, {q2, -Infinity, +Infinity}, Assumptions $\rightarrow pa \in \mathbb{R}$];`
`Collect[tmp[[1, 2]], zD, Simplify]`
 $j\tilde{o}21 = \text{ReplacePart}[tmp, \{1, 2\} \rightarrow \%] (* \text{Eq. (C.1e)} *)$

$$\frac{i (-pa^2 + pb^2 - qa^2 + qb^2) zD}{2 Kz} + i (h s\theta + pa \Delta x - qa \Delta y)$$

$$j\tilde{o}21 = e^{\frac{i (-pa^2 + pb^2 - qa^2 + qb^2) zD}{2 Kz} + i (h s\theta + pa \Delta x - qa \Delta y)} jin[pa, qa - h \rho, pb, qb - h \rho] \times R[pa, tS] \times$$

$$R[pa + Kz \theta - qa \rho, tM2] \times T[pa + Kz \theta - qa \rho, tA] R^*[pb, tM1] R^*[pb + Kz \theta - qb \rho, tA] T^*[pb, tS]$$

Appendix C

calculation of $j_h^{ij}[pa, qa, pb, qb]$

$(X\tilde{h}1 /. \{p \rightarrow pa, q \rightarrow qa\}) (X\tilde{h}1^* /. \{p \rightarrow pb, q \rightarrow qb\}) \text{jin}[p1, q1, p2, q2];$
 $\text{tmp} = \text{Integrate}[\%, \{p1, -\text{Infinity}, +\text{Infinity}\}, \{q1, -\text{Infinity}, +\text{Infinity}\},$
 $\{p2, -\text{Infinity}, +\text{Infinity}\}, \{q2, -\text{Infinity}, +\text{Infinity}\}, \text{Assumptions} \rightarrow pa \in \mathbb{R}];$
 $\text{Collect}[\text{tmp}[[1, 2]], zD, \text{Simplify}]$

$\text{jh}\tilde{1}1 = \text{ReplacePart}[\text{tmp}, \{1, 2\} \rightarrow \%] (* \text{Eq. (C.1f)} *)$

$$-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz}$$

$$\text{jh}\tilde{1}1 = e^{-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz}} \text{jin}[pa, qa, pb, qb] \times R[pa, tM1] \times T[pa, tS] \times$$

$$T[-pa - Kz \theta + qa \rho, tA] R^*[pb, tM1] T^*[pb, tS] T^*[-pb - Kz \theta + qb \rho, tA]$$

$(X\tilde{h}2 /. \{p \rightarrow pa, q \rightarrow qa\}) (X\tilde{h}2^* /. \{p \rightarrow pb, q \rightarrow qb\}) \text{jin}[p1, q1, p2, q2];$
 $\text{tmp} = \text{Integrate}[\%, \{p1, -\text{Infinity}, +\text{Infinity}\}, \{q1, -\text{Infinity}, +\text{Infinity}\},$
 $\{p2, -\text{Infinity}, +\text{Infinity}\}, \{q2, -\text{Infinity}, +\text{Infinity}\}, \text{Assumptions} \rightarrow pa \in \mathbb{R}];$
 $\text{Collect}[\text{tmp}[[1, 2]], \{\Delta x, zD\}, \text{Simplify}]$

$\text{jh}\tilde{2}2 = \text{ReplacePart}[\text{tmp}, \{1, 2\} \rightarrow \%] (* \text{Eq. (C.1g)} *)$

$$-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz} + i (pa - pb) \Delta x + i (-qa + qb) \Delta y$$

$\text{jh}\tilde{2}2 =$

$$e^{-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz} + i (pa - pb) \Delta x + i (-qa + qb) \Delta y} \text{jin}[pa, qa, pb, qb] \times R[pa, tS] \times R[pa + Kz \theta - qa \rho, tA] \times$$

$$R[pa + Kz \theta - qa \rho, tM2] R^*[pb, tS] R^*[pb + Kz \theta - qb \rho, tA] R^*[pb + Kz \theta - qb \rho, tM2]$$

$(X\tilde{h}1 /. \{p \rightarrow pa, q \rightarrow qa\}) (X\tilde{h}2^* /. \{p \rightarrow pb, q \rightarrow qb\}) \text{jin}[p1, q1, p2, q2];$
 $\text{tmp} = \text{Integrate}[\%, \{p1, -\text{Infinity}, +\text{Infinity}\}, \{q1, -\text{Infinity}, +\text{Infinity}\},$
 $\{p2, -\text{Infinity}, +\text{Infinity}\}, \{q2, -\text{Infinity}, +\text{Infinity}\}, \text{Assumptions} \rightarrow pa \in \mathbb{R}];$
 $\text{Collect}[\text{tmp}[[1, 2]], zD, \text{Simplify}]$

$\text{jh}\tilde{1}2 = \text{ReplacePart}[\text{tmp}, \{1, 2\} \rightarrow \%] (* \text{Eq. (C.1h)} *)$

$$-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz} - i (hs \theta + pb \Delta x - qb \Delta y)$$

$$\text{jh}\tilde{1}2 = e^{-\frac{i (pa^2 - pb^2 + qa^2 - qb^2) zD}{2 Kz} - i (hs \theta + pb \Delta x - qb \Delta y)} \text{jin}[pa, qa, pb, qb] \times R[pa, tM1] \times T[pa, tS] \times$$

$$T[-pa - Kz \theta + qa \rho, tA] R^*[pb, tS] R^*[pb + Kz \theta - qb \rho, tA] R^*[pb + Kz \theta - qb \rho, tM2]$$

$(X\tilde{h}2 /. \{p \rightarrow pa, q \rightarrow qa\}) (X\tilde{h}1^* /. \{p \rightarrow pb, q \rightarrow qb\}) \text{jin}[p1, q1, p2, q2];$
 $\text{tmp} = \text{Integrate}[\%, \{p1, -\text{Infinity}, +\text{Infinity}\}, \{q1, -\text{Infinity}, +\text{Infinity}\},$
 $\{p2, -\text{Infinity}, +\text{Infinity}\}, \{q2, -\text{Infinity}, +\text{Infinity}\}, \text{Assumptions} \rightarrow pa \in \mathbb{R}];$
 $\text{Collect}[\text{tmp}[[1, 2]], zD, \text{Simplify}];$

$\text{jh}\tilde{2}1 = \text{ReplacePart}[\text{tmp}, \{1, 2\} \rightarrow \%] (* \text{Eq. (C.1i)} *)$

$$\text{jh}\tilde{2}1 = e^{\frac{i (-pa^2 + pb^2 - qa^2 + qb^2) zD}{2 Kz} + i (hs \theta + pa \Delta x - qa \Delta y)} \text{jin}[pa, qa, pb, qb] \times R[pa, tS] \times R[pa + Kz \theta - qa \rho, tA] \times$$

$$R[pa + Kz \theta - qa \rho, tM2] R^*[pb, tM1] T^*[pb, tS] T^*[-pb - Kz \theta + qb \rho, tA]$$

Appendix C

calculation of j_{00}^{ii} and j_{00}^{ij} , case $p_a = p_b$ and $q_a = q_b$

```

Xõo1 Xõo1* jin[p1, q1, p2, q2];
Jõ11 = Integrate[%, {p1, -Infinity, +Infinity},
  {q1, -Infinity, +Infinity}, {p2, -Infinity, +Infinity},
  {q2, -Infinity, +Infinity}, Assumptions -> p ∈ ℝ] (* Eq. (C.2a) *)

Xõo2 Xõo2* jin[p1, q1, p2, q2];
Jõ22 = Integrate[%, {p1, -Infinity, +Infinity},
  {q1, -Infinity, +Infinity}, {p2, -Infinity, +Infinity},
  {q2, -Infinity, +Infinity}, Assumptions -> p ∈ ℝ] (* Eq. (C.2b) *)

Xõo1 Xõo2* jin[p1, q1, p2, q2];
Jõ12 = Integrate[%, {p1, -Infinity, +Infinity},
  {q1, -Infinity, +Infinity}, {p2, -Infinity, +Infinity},
  {q2, -Infinity, +Infinity}, Assumptions -> p ∈ ℝ] (* Eq. (C.2c) *)

Xõo2 Xõo1* jin[p1, q1, p2, q2];
Jõ21 = Integrate[%, {p1, -Infinity, +Infinity},
  {q1, -Infinity, +Infinity}, {p2, -Infinity, +Infinity},
  {q2, -Infinity, +Infinity}, Assumptions -> p ∈ ℝ] (* Eq. (C.2d) *)

Jõ11 = jin[p, q - h ρ, p, q - h ρ] × R[p, tM1] ×
  R[p + Kz θ - q ρ, tA] × T[p, tS] R*[p, tM1] R*[p + Kz θ - q ρ, tA] T*[p, tS]

Jõ22 = jin[p, q - h ρ, p, q - h ρ] × R[p, tS] × R[p + Kz θ - q ρ, tM2] ×
  T[p + Kz θ - q ρ, tA] R*[p, tS] R*[p + Kz θ - q ρ, tM2] T*[p + Kz θ - q ρ, tA]

Jõ12 = e-i (h s θ + p Δx - q Δy) jin[p, q - h ρ, p, q - h ρ] × R[p, tM1] ×
  R[p + Kz θ - q ρ, tA] × T[p, tS] R*[p, tS] R*[p + Kz θ - q ρ, tM2] T*[p + Kz θ - q ρ, tA]

Jõ21 = ei (h s θ + p Δx - q Δy) jin[p, q - h ρ, p, q - h ρ] × R[p, tS] ×
  R[p + Kz θ - q ρ, tM2] × T[p + Kz θ - q ρ, tA] R*[p, tM1] R*[p + Kz θ - q ρ, tA] T*[p, tS]

```

Appendix C

calculation of j_{hh}^{ii} and j_{hh}^{jj} , case $p_a = p_b$ and $q_a = q_b$

```

Xhñ1 Xhñ1* jin[p1, q1, p2, q2];
Jhñ1 = Integrate[%, {p1, -Infinity, +Infinity},
  {q1, -Infinity, +Infinity}, {p2, -Infinity, +Infinity},
  {q2, -Infinity, +Infinity}, Assumptions -> p ∈ ℝ] (* Eq. (C.2e) *)

Xhñ2 Xhñ2* jin[p1, q1, p2, q2];
Jhñ2 = Integrate[%, {p1, -Infinity, +Infinity},
  {q1, -Infinity, +Infinity}, {p2, -Infinity, +Infinity},
  {q2, -Infinity, +Infinity}, Assumptions -> p ∈ ℝ] (* Eq. (C.2f) *)

Xhñ1 Xhñ2* jin[p1, q1, p2, q2];
Jhñ12 = Integrate[%, {p1, -Infinity, +Infinity},
  {q1, -Infinity, +Infinity}, {p2, -Infinity, +Infinity},
  {q2, -Infinity, +Infinity}, Assumptions -> p ∈ ℝ] (* Eq. (C.2g) *)

Xhñ2 Xhñ1* jin[p1, q1, p2, q2];
Jhñ21 = Integrate[%, {p1, -Infinity, +Infinity},
  {q1, -Infinity, +Infinity}, {p2, -Infinity, +Infinity},
  {q2, -Infinity, +Infinity}, Assumptions -> p ∈ ℝ] (* Eq. (C.2h) *)

Jhñ1 = jin[p, q, p, q] × R[p, tM1] × T[p, tS] ×
  T[-p - Kz θ + q ρ, tA] R*[p, tM1] T*[p, tS] T*[-p - Kz θ + q ρ, tA]

Jhñ2 = jin[p, q, p, q] × R[p, tS] × R[p + Kz θ - q ρ, tA] ×
  R[p + Kz θ - q ρ, tM2] R*[p, tS] R*[p + Kz θ - q ρ, tA] R*[p + Kz θ - q ρ, tM2]

Jhñ12 = e-i (h s θ + p Δx - q Δy) jin[p, q, p, q] × R[p, tM1] × T[p, tS] ×
  T[-p - Kz θ + q ρ, tA] R*[p, tS] R*[p + Kz θ - q ρ, tA] R*[p + Kz θ - q ρ, tM2]

Jhñ21 = ei (h s θ + p Δx - q Δy) jin[p, q, p, q] × R[p, tS] × R[p + Kz θ - q ρ, tA] ×
  R[p + Kz θ - q ρ, tM2] R*[p, tM1] T*[p, tS] T*[-p - Kz θ + q ρ, tA]

```

6.1 moiré fringes

fringe period

```

Clear["Global`*"]; Remove["Global`*"]
jñ[q1_, q2_] = e- $\frac{i}{8} (q1-q2)^2 w\theta^2 - \frac{i}{4} (q1^2+q2^2) l\theta^2$ ; (* Eq. (22) *)
Jhñ11[q1_, q2_] = e- $\frac{i (q1^2-q2^2) zD}{2 Kz}$  jñ[q1, q2]; (* Eq. (21.a) *)
Jhñ22[q1_, q2_] = e- $\frac{i (q1^2-q2^2) zD}{2 Kz} - i (q1-q2) \Delta y$  jñ[q1, q2]; (* Eq. (21.b) *)
Jhñ12[q1_, q2_] = e- $\frac{i (q1^2-q2^2) zD}{2 Kz} + i q2 \Delta y$  jñ[q1, q2]; (* Eq. (21.c) *)
(* inverse Fourier transforms; jo1[y], jo2[y],
and jo12[y] have the same normalising constant *)
Simplify[PowerExpand[InverseFourierTransform[Jhñ11[q1, q2],
    {q1, q2}, {y, x}, FourierParameters → {1, -1}] /. x → -y]];
Jhh11 = Simplify[Part[%, 1] /. l $\theta^2$  + w $\theta^2$  → w $\theta^2$  /. Kz2 l $\theta^2$  w $\theta^2$  + 4 zD2 → wD2 Kz2 l $\theta^2$ 
    (* by using (B2.a) *) /. h → 2 Kz Tan[ $\theta$ B]] (* Eq. (23.a) *)
Simplify[PowerExpand[InverseFourierTransform[Jhñ22[q1, q2],
    {q1, q2}, {y, x}, FourierParameters → {1, -1}] /. x → -y]];
Jhh22 = Simplify[Part[%, 1] /. l $\theta^2$  + w $\theta^2$  → w $\theta^2$  /. Kz2 l $\theta^2$  w $\theta^2$  + 4 zD2 → wD2 Kz2 l $\theta^2$ 
    (* by using (B2.a) *) /. h → 2 Kz Tan[ $\theta$ B]] (* Eq. (23.b) *)
Jhh12 = Simplify[PowerExpand[InverseFourierTransform[Jhñ12[q1, q2],
    {q1, q2}, {y, x}, FourierParameters → {1, -1}] /. x → -y]];
(* Jhh12 exponent *)
exponent = Jhh12[[1, 2]] /. 2 Kz2 l $\theta^2$  (l $\theta^2$  + w $\theta^2$ ) + 8 zD2 → 2 wD2 Kz2 l $\theta^2$ ;
(* by setting l $\theta^4$  =  $\theta$  and using (B2.a) *)
(* Jhh12 exponent: real part *)
real =
    FullSimplify[ComplexExpand[Re[exponent]] /. h → 2 Kz Tan[ $\theta$ B] /. - $\frac{w\theta^2 \Delta y^2}{2 l\theta^2 wD^2}$  → - $\frac{\Delta y^2}{2 lD^2}$ ];
(* by using (B2.a) and the  $\theta$ s and  $\theta$ c definitons *)
(* Jhh12 exponent: imaginary part *)
imaginary = ComplexExpand[Im[exponent]];
imaginary = % /.  $\Delta y^2$  →  $\theta$  /. zD →  $\frac{Kz^2 l\theta^2 wD^2}{4 rD}$ 
    (* by using (B2.c) *) /.  $\Delta y$  → 2 (zA2 + tM2 / 2)  $\rho$  Tan[ $\theta$ B] /. Tan[ $\theta$ B] →  $\frac{h}{2 Kz}$ ;
Print["Jhh12 = ", Exp[real + I imaginary] (* Eq. (23.c) *)]

$$\Delta\rho = \frac{2\pi y}{\text{imaginary}} /. h \rightarrow 2\pi / d$$
 (* Eq. (26) *)

$$Jhh11 = e^{-\frac{2y^2}{w\theta^2}}$$


$$Jhh22 = e^{-\frac{2(y-\Delta y)^2}{w\theta^2}}$$

    
```

$$J_{hh12} = e^{-\frac{\Delta y^2}{2 \omega D^2} - \frac{2 y^2 - 2 y \Delta y + \Delta y^2}{\omega D^2} + \frac{i h y \left(\frac{t M_2}{2} + z A_2 \right) \rho}{r D}}$$

$$\Delta \rho = \frac{d r D}{\left(\frac{t M_2}{2} + z A_2 \right) \rho}$$

fringe visibility

```
Clear["Global`*"]; Remove["Global`*"]
```

```
Jhh11 = e^{-\frac{2 y^2}{\omega D^2}} (* Eq. (23a) *); Jhh22 = e^{-\frac{2 (y-\Delta y)^2}{\omega D^2}} (* Eq. (23b) *);
```

```
Jhh12 = e^{-\frac{\Delta y^2}{2 \omega D^2} - \frac{2 y^2 - 2 y \Delta y + \Delta y^2}{\omega D^2} + \frac{i h y \left( \frac{t M_2}{2} + z A_2 \right) \rho}{r D}} (* Eq. (23c) *);
```

```
Print["\Gamma = ", FullSimplify[\frac{2 ComplexExpand[Abs[Jhh12]]}{Jhh11 + Jhh22}]] (* Eq. (26) *)
```

$$\Gamma = e^{-\frac{\Delta y^2}{2 \omega D^2}} \operatorname{Sech}\left[\frac{(2 y - \Delta y) \Delta y}{\omega D^2}\right]$$

7. results

7.2 Rocking curves symmetries

```
Clear["Global`*"]; Remove["Global`*"];
```

$$R[\eta_, \xi_] = \frac{i \operatorname{Sin}\left[\xi \sqrt{1 + \eta^2}\right]}{\sqrt{1 + \eta^2}};$$

```
T[\eta_, \xi_] = Cos[\xi Sqrt[\eta^2 + 1]] + \eta R[\eta, \xi];
(* zero absorption case: |T(\eta, \xi)|^2 = 1 - |R(\eta, \xi)|^2 *)
```

```
R2[\eta_, \xi_] = ComplexExpand[Abs[R[\eta, \xi]]]^2;
```

```
T2[\eta_, \xi_] = ComplexExpand[Abs[T[\eta, \xi]]]^2;
```

```
test = Simplify[R2[\eta, \xi] + T2[\eta, \xi]]
```

```
test == 1
```

The rocking curve symmetry $J_n^{(i)}(-\theta) = J_n^{(i)}(\theta)$ is a consequence of the symmetry $\eta \rightarrow -\eta$ of the integrand in (29), provided $\rho = 0$ and the symmetry $\tilde{J}_{in}(p, q, p, q) = \tilde{J}_{in}(-p, q, -p, q)$.

We set $\eta_1 = \Delta_e (K_z \theta) \tan(\Theta_B) / \pi$.

```
(* change of the integration variables,  $\eta = y - \eta_1/2$  and  $\eta = -y + \eta_1/2$  *)
test = {
  Simplify[RRT[y -  $\eta_1/2$ ,  $\eta_1$ ] - RRT[-y +  $\eta_1/2$ , - $\eta_1$ ]],
  Simplify[TRR[y -  $\eta_1/2$ ,  $\eta_1$ ] - TRR[-y +  $\eta_1/2$ , - $\eta_1$ ]],
  Simplify[RRR[y -  $\eta_1/2$ ,  $\eta_1$ ] - RRR[-y +  $\eta_1/2$ , - $\eta_1$ ]],
  Simplify[TRT[y -  $\eta_1/2$ ,  $\eta_1$ ] - TRT[-y +  $\eta_1/2$ , - $\eta_1$ ]]
}
test = {0, 0, 0, 0}
```

The identity of the rocking curves TRR and RRT, $J_o^{(1)}(\theta) = J_o^{(2)}(\theta)$, is a consequence of the identity of the integrands in (29) after suitable changes of the integration variable, provided $\rho = 0$ and the symmetry $\tilde{j}_{in}(p, q, p, q) = \tilde{j}_{in}(-p, q, -p, q)$. We set $\eta_1 = \Delta_e(K_z \theta) \tan(\Theta_B)/\pi$.

```
(* T2 = 1 - R2 *)
RRT[ $\eta_1$ _,  $\eta_1$ _] = R2[ $\eta$ ,  $\xi S$ ]  $\times$  R2[ $\eta + \eta_1$ ,  $\xi M$ ] (1 - R2[ $\eta + \eta_1$ ,  $\xi S$ ]); (* Jo22 *)
TRR[ $\eta_1$ _,  $\eta_1$ _] = (1 - R2[ $\eta$ ,  $\xi S$ ]) R2[ $\eta$ ,  $\xi M$ ]  $\times$  R2[ $\eta + \eta_1$ ,  $\xi S$ ]; (* Jo11 *)
RRR[ $\eta_1$ _,  $\eta_1$ _] = R[ $\eta$ ,  $\xi S$ ]  $\times$  R2[ $\eta + \eta_1$ ,  $\xi M$ ]  $\times$  R2[ $\eta + \eta_1$ ,  $\xi S$ ]; (* Jh22 *)
TRT[ $\eta_1$ _,  $\eta_1$ _] = (1 - R2[ $\eta$ ,  $\xi S$ ]) R2[ $\eta$ ,  $\xi M$ ] (1 - R2[- $\eta - \eta_1$ ,  $\xi S$ ]); (* Jh11 *)

(* change of the integration variables,  $\eta = y - \eta_1/2$  and  $\eta = y + \eta_1/2$  *)
test = RRT[y -  $\eta_1/2$ ,  $\eta_1$ ] - TRR[y +  $\eta_1/2$ , - $\eta_1$ ]
test = 0
```

7.3 fringe visibility

```
Clear["Global`*"]; Remove["Global`*"]
(* for the sake of algebraic simplicity, calculations are made for the h state *)
 $\tilde{j}_{in}[q_1_, q_2_] = e^{-\frac{1}{8}(q_1 - q_2)^2 w_0^2 - \frac{1}{4}(q_1^2 + q_2^2) l_0^2}$ ; (* Eq. (22) *)
 $\tilde{J}_{h11}[q_] = \tilde{j}_{in}[q, q]$ ; (* Eq. (C.2e) *)
 $\tilde{J}_{h22}[q_] = \tilde{j}_{in}[q, q]$ ; (* Eq. (C.2f) *)
 $\tilde{J}_{h12}[q_] = e^{\pm q \Delta y} \tilde{j}_{in}[q, q]$ ; (* Eq. (C.2g) *)

Integrate[ $\tilde{J}_{h11}[q]$ , {q, -Infinity, +Infinity}, Assumptions  $\rightarrow w_0 > 0 \ \&\& \ l_0 > 0$ ];
(* Eq. 20.b *)
 $J_h = \% + \text{Integrate}[\tilde{J}_{h22}[q], \{q, -Infinity, +Infinity\}, \text{Assumptions} \rightarrow w_0 > 0 \ \&\& \ l_0 > 0]$ ;
(* Eq. 20.b *)
Print["Jh = ", Jh]
 $\Xi_h = \text{Integrate}[\tilde{J}_{h12}[q], \{q, -Infinity, +Infinity\}, \text{Assumptions} \rightarrow w_0 > 0 \ \&\& \ l_0 > 0 \ \&\& \ \Delta y \in \text{Reals}]$ ; (* Eq. 20.c *)
Print[" $\Xi_h$  = ",  $\Xi_h$ ]
Print[" $\Gamma$  = ", PowerExpand[ $\frac{2 \text{ComplexExpand}[\text{Abs}[\Xi_h]]}{J_h}$ ]] (* Eq. 29 *)
```

$$J_h = \frac{2 \sqrt{2} \pi}{l_0}$$

$$\Xi_h = \frac{e^{-\frac{\Delta y^2}{2 l_0^2}} \sqrt{2} \pi}{l_0}$$

$$\Gamma = e^{-\frac{\Delta y^2}{2 l_0^2}}$$

Appendix B - free-space propagation

propagation of the single particle wave function (Gaussian model)

```
Clear["Global`*"]; Remove["Global`*"];
(* Gaussian wave packet; reciprocal-space representation;
p and l0 are measured orthogonally to the optical axis z *)

$$\tilde{\psi}_{in}[p_] = e^{-\frac{p^2 l_0^2}{4}};$$

(* free-space propagator; z is measured along the propagation axis;
pm = +1 if propagation is along Ko;
pm = -1 if propagation is along Kh;
pm = 0 if p → q and x → y *)

$$F[p_, z_] = e^{-\frac{i p^2 z}{2 k z}} e^{i p m p z \text{Tan}[\theta B]};$$

(* free-space propagation *)
InverseFourierTransform[F[p, z]  $\tilde{\psi}_{in}[p]$ , p, x, FourierParameters → {0, -1}];
Print[" $\tilde{\psi}_{in}[X; Z] \propto$  ", Part[%, 2]]
```

$$\tilde{\psi}_{in}[X; Z] \propto e^{-\frac{Kz (x + pm z \text{Tan}[\theta B])^2}{Kz l_0^2 + 2 i z}}$$

$$\tilde{\psi}_{in}[X; Z] \propto e^{-\frac{(x + pm z \text{Tan}[\theta B])^2}{l_z^2} + \frac{i Kz (x + pm z \text{Tan}[\theta B])^2}{2 r z}}$$

lz : beam radius

```
Simplify[ComplexExpand[Re[- $\frac{Kz (x + pm z \text{Tan}[\theta B])^2}{Kz l_0^2 + 2 i z}$ ]]];
```

$$l_z^2 = \text{Expand}\left[\text{Expand}\left[-\frac{(x + pm z \text{Tan}[\theta B])^2}{\%}\right] /. \frac{4}{Kz^2 l_0^2} \rightarrow \text{Tan}[\theta s]^2\right]$$

(* Eq. (B.1a), Tan[θs] definition *)

$$l_z^2 = l_0^2 + z^2 \text{Tan}[\theta s]^2$$

$$\tilde{\psi}_{in}[X; Z] \propto e^{-\frac{(x + pm z \text{Tan}[\theta B])^2}{l_z^2} + \frac{i Kz (x + pm z \text{Tan}[\theta B])^2}{2 r z}}$$

rz : wavefront radius of curvature

```

Simplify[ComplexExpand[Im[- $\frac{Kz (x + pm z \text{Tan}[\theta B])^2}{Kz l\theta^2 + 2 i z}$ ]]];
Expand[ $\frac{Kz (x + pm z \text{Tan}[\theta B])^2}{2 \times \%}$ ] /.  $\frac{Kz^2 l\theta^4}{4} \rightarrow \frac{l\theta^2}{\text{Tan}[\theta s]^2}$ 
(* Eq. (B.1b), Tan[θs] definition *);
Print["rz = ", %]
Simplify[ComplexExpand[Im[- $\frac{Kz (x + pm z \text{Tan}[\theta B])^2}{Kz l\theta^2 + 2 i z}$ ]]];
Together[ $\frac{Kz (x + pm z \text{Tan}[\theta B])^2}{2 \times \%}$ ] /.  $Kz^2 l\theta^4 + 4 z^2 \rightarrow Kz^2 l\theta^2 lz^2$ 
(* by the Tan[θs] and lz definitions *);
Print["rz = ", %]
rz = z +  $\frac{l\theta^2 \text{Cot}[\theta s]^2}{z}$ 
rz =  $\frac{Kz^2 l\theta^2 lz^2}{4 z}$ 
    
```

propagation of the density matrix (Gauss Schell-model)

```

Clear["Global`*"]; Remove["Global`*"]
jin[q1_, q2_] = e- $\frac{1}{8} (q1-q2)^2 w\theta^2 - \frac{1}{4} (q1^2+q2^2) l\theta^2$ ;
F[q_, z_] = e- $\frac{i q^2 z}{2 Kz}$ ;
(* propagation *)
jz[q1_, q2_] = F[q1, z] jin[q1, q2] (Conjugate[F[q2, z]] /. Conjugate[a_] -> a);
(* transformation back to the direct space *)
Part[InverseFourierTransform[jz[q1, q2],
    {q1, q2}, {y1, x}, FourierParameters -> {1, -1}] /. x -> -y2, 1];
jz[y1_, y2_] = % /. lθ2 + wθ2 -> wθ2; (* lθ << wθ *)
Print["jz[y1,y2] = ", jz[y1, y2]]
jz[y1,y2] = e- $\frac{Kz (Kz w\theta^2 (y1-y2)^2 + 2 Kz l\theta^2 (y1^2+y2^2) + 4 i (-y1^2+y2^2) z)}{2 Kz^2 l\theta^2 w\theta^2 + 8 z^2}$ 
    
```

beam radius and correlation length


```

Simplify[ComplexExpand[Re[Part[jz[y1, y2], 2]]]];
tmp = Collect[%, (y1 - y2)^2, Simplify];
Print["exponent: real part = ", %]
-Simplify[ $\frac{1}{\text{Coefficient}[tmp, y1^2 + y2^2]}$ ] /.  $\frac{4}{Kz^2 l\theta^2} \rightarrow \text{Tan}[\theta s]^2$ 
(* Eq. (B.1c),  $\theta s$  definition *);
Print["wz2 = ", %] (* Eq. (B.2a) *)
-Simplify[1 / (2 Coefficient[tmp, (y1 - y2)^2])] /.  $\frac{4}{Kz^2 w\theta^2} \rightarrow \text{Tan}[\theta c]^2$ 
(* Eq. (B.2d),  $\theta c$  definition *);
Print["lz2 = ", %] (* Eq. (B.2b) *)

```

$$\text{exponent: real part} = -\frac{Kz^2 l\theta^2 (y1^2 + y2^2)}{Kz^2 l\theta^2 w\theta^2 + 4 z^2} - \frac{Kz^2 w\theta^2 (y1 - y2)^2}{2 Kz^2 l\theta^2 w\theta^2 + 8 z^2}$$

$$w_z^2 = w\theta^2 + z^2 \text{Tan}[\theta s]^2$$

$$l_z^2 = l\theta^2 + z^2 \text{Tan}[\theta c]^2$$

curvature radius

```

tmp = Simplify[ComplexExpand[Im[Part[jz[y1, y2], 2]]]];
Print["imaginary part = ", %]
Expand[ $\frac{Kz (y1^2 - y2^2)}{2 tmp}$ ] /.  $\frac{Kz^2 w\theta^2}{4} \rightarrow \frac{1}{\text{Tan}[\theta c]^2}$  (*  $\theta c$  definition, Eq. (B.2d) *);
Print["rz = ", %] (* Eq. (B.2c) *)
Together[ $\frac{Kz (y1^2 - y2^2)}{2 tmp}$ ] /.  $Kz^2 l\theta^2 w\theta^2 + 4 z^2 \rightarrow Kz^2 l\theta^2 w_z^2$ 
(* by the Tan[ $\theta s$ ] and lz definitions *);
Print["rz = ", %] (* Eq. (B.2c) *)

```

$$\text{imaginary part} = \frac{2 Kz (y1^2 - y2^2) z}{Kz^2 l\theta^2 w\theta^2 + 4 z^2}$$

$$r_z = z + \frac{l\theta^2 \text{Cot}[\theta c]^2}{z}$$

$$r_z = \frac{Kz^2 l\theta^2 w_z^2}{4 z}$$

Appendix D - shear interferometry

interference of parallel Gaussian beams

```

Clear["Global`*"]; Remove["Global`*"];

$$\phi_1 = e^{-\frac{y^2}{1z^2} + \frac{i Kz y^2}{2 rz}}$$


$$\phi_2 = e^{-\frac{(y-\Delta y)^2}{1z^2} + \frac{i Kz (y-\Delta y)^2}{2 rz}}$$


$$\phi_1 \text{ FullSimplify[ComplexExpand[Conjugate[\phi_2]]]}$$


$$\Xi = \text{Integrate}[\%, \{y, -\text{Infinity}, +\text{Infinity}\},$$


$$\text{Assumptions} \rightarrow lz > 0 \&\& rz > 0 \&\& \Delta y > 0 \&\& Kz > 0];$$

Print[" $\Xi =$ ",  $\Xi$ ]

$$J_1 = \text{Integrate}\left[e^{-\frac{2y^2}{1z^2}}, \{y, -\text{Infinity}, +\text{Infinity}\}, \text{Assumptions} \rightarrow lz > 0\right];$$

Print["J1 = ", J1]

$$J_2 = \text{Integrate}\left[e^{-\frac{2(y-\Delta y)^2}{1z^2}}, \{y, -\text{Infinity}, +\text{Infinity}\}, \text{Assumptions} \rightarrow lz > 0 \&\& x0 > 0\right];$$

Print["J2 = ", J2]

$$\Gamma = \frac{2 \Xi}{J_1 + J_2} \text{ (* visibility *)}; \text{Print["}\Gamma = ", \Gamma]$$

(* by using (B1-a), (B1-b), and (B1-c) *)
Simplify[\Gamma[[2]] /. {lz \to Sqrt[1\theta^2 + z^2 Tan[\theta s]^2],

$$rz \to z + \frac{1\theta^2 \text{Cot}[\theta s]^2}{z}, \text{Tan}[\theta s] \to \frac{2}{Kz 1\theta}, \text{Cot}[\theta s] \to \frac{Kz 1\theta}{2}}];$$

Print["\Gamma = ", Exp[\%]]

$$e^{-\frac{y^2}{1z^2} + \frac{i Kz y^2}{2 rz} - \frac{i (Kz 1z^2 - 2 i rz) (y-\Delta y)^2}{2 1z^2 rz}}$$


$$\Xi = e^{-\frac{(Kz^2 1z^4 + 4 rz^2) \Delta y^2}{8 1z^2 rz^2}} 1z \sqrt{\frac{\pi}{2}}$$


$$J_1 = 1z \sqrt{\frac{\pi}{2}}$$


$$J_2 = 1z \sqrt{\frac{\pi}{2}}$$


$$\Gamma = e^{-\frac{(Kz^2 1z^4 + 4 rz^2) \Delta y^2}{8 1z^2 rz^2}}$$


$$\Gamma = e^{-\frac{\Delta y^2}{2 1\theta^2}}$$


```

interference of intersecting Gaussian beams

```
Clear["Global`*"]; Remove["Global`*"];
```

$$\phi_1 = e^{-\frac{y^2}{1z^2} + \frac{iKz y^2}{2rz}};$$

$$\phi_2 = e^{-\frac{y^2}{1z^2} + \frac{iKz y^2}{2rz} + iKz \rho \theta y};$$

```
\Xi = Integrate[\phi1 FullSimplify[ComplexExpand[Conjugate[\phi2]]],  
  {y, -Infinity, +Infinity}, Assumptions -> lz > 0 && rz > 0 && Kz > 0 && \rho\theta > 0];
```

```
Print["\Xi = ", \Xi]
```

```
J1 = Integrate[e^{-\frac{2y^2}{1z^2}}, {y, -Infinity, +Infinity}, Assumptions -> lz > 0];
```

```
Print["J2 = J1 = ", J1]
```

```
J2 = J1;
```

```
\Gamma = 2 \Xi / (J1 + J2) (* visibility *);
```

```
Print["\Gamma = ", \Gamma]
```

$$\Xi = e^{-\frac{1}{8} Kz^2 1z^2 \rho \theta^2} 1z \sqrt{\frac{\pi}{2}}$$

$$J2 = J1 = 1z \sqrt{\frac{\pi}{2}}$$

$$\Gamma = e^{-\frac{1}{8} Kz^2 1z^2 \rho \theta^2}$$