Off-specular Mössbauer Reflectometry

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Abstract

Synchrotron Mössbauer Reflectometry (SMR), the grazing incidence nuclear resonant scattering of synchrotron radiation, can be applied to perform depth-selective phase analysis and to determine the isotopic and magnetic structure of thin films and multilayer. Off-specular SMR provides information from the lateral structure of multilayer. A theoretical approach of off-specular SMR is presented.

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I. INTRODUCTION

The specularly reflected radiation from layered systems does not depend on the lateral structure; it depends only on the lateral averages of material parameters.[1] For studying lateral inhomogenities, such as magnetic domains etc., off-specular reflectometry is necessary. Domain structure of AF-coupled MLs is an issue of both theoretical and technological importance. Off-specular non-polarized[2] and polarized neutron reflectometry,[3,4] soft-x-ray resonant magnetic diffuse scattering[5] and, very recently, off-specular Synchrotron Mössbauer Reflectometry (SMR) have been used to estimate the AF-domain-size distribution in magnetic MLs.[6]

The theory of the off-specular neutron reflectometry based on the Distorted Wave Born Approximation[7] (DWBA) has been published earlier.[8–10] DWBA solves the problem of diffuse (off-specular) field as perturbation around the specular field, which latter field can be easily calculated, even for general stratified media, by suitable matrix methods.[8,11–14] In case of off-specular SMR the DWBA can also be applied and similarly the solution of the specular problem is well known in the literature.[14–21] Because SMR works in the time domain, this approach is not straightforward. Our aim is the implementation of off-specular reflectometry into the data evaluation program EFFI (Environment For FItting).[22]

Starting from the general theory of Lax[1] and from the common optical formalism of polarized neutron and Mössbauer reflectometry,[14] an expression for diffuse scattering of multiple component (electromagnetic and/or quantum mechanical particle) waves on laterally inhomogeneous stratified media is obtained. As Lax has pointed out, from the point of view of specular reflection, the set of discrete atomic scattering centers can be described/replaced by homogeneous index of refraction n and solving the scattering problem is equivalent to solving the wave equation. This approach is valid only if the direction of the scattered wave is far from the direction of higher order atomic Bragg reflections. In this paper we study the grazing angle incidence limit only, for which the index of refraction approximation is valid.[17,20,21]

Our model systems are stratified media, multilayer and thin films, having lateral inhomogeneity on the mesoscopic scale, being much larger then the atomic distances. In each homogeneous part around position $\mathbf{r}$ an index of refraction $n(\mathbf{r})$ is defined. Since n for both slow neutrons and X-rays hardly differs from the 2×2 unit matrix I, the susceptibility defined by $\chi(\mathbf{r}) = 2[n(\mathbf{r})\text{-}I]$ is conveniently used (see also Ref.[14]).

II. OFF-SPECULAR SCATTERING

Using the index of refraction approximation in each homogeneous part of the system the solution of the inhomogeneous wave equvation

$$\left[\Delta + k^2 I\right] \Psi(\mathbf{r}) = -k^2 \chi(\mathbf{r}) \Psi(\mathbf{r}) \tag{2.1}$$

yields $\Psi(\mathbf{r})$, representing the two components of the electromagnetic field or the quantum mechanical spinor state of neutron at position $\mathbf{r}$, with k being the wave number in vacuum. In stratified medium we compose the susceptibility function

$$\chi(\mathbf{r}) = \sum_{l=1}^{S} \chi_l\left(\mathbf{r}_{||}\right), \tag{2.2}$$

as the sum of the susceptibility functions of the individual layers l ($l = 1..S$, the last layer S is the substrate) depending on the lateral coordinate $\mathbf{r}_{||}$ only.

If the homogeneous parts of the system are large compared to the wavelength, we may assume that the exact solution $\Psi(\mathbf{r})$ is close to the solution $\Psi_{\text{coh}}(\mathbf{r})$ of the coherent (specular) field equation[1]

$$\left[\Delta + k^2 I\right] \Psi_{\text{coh}}(\mathbf{r}) = -k^2 \sum \overline{\chi}_l \Psi_{\text{coh}}(\mathbf{r}), \tag{2.3}$$

which is obtained from Eq. (2.1) by replacing the susceptibilities $\chi_l\left(\mathbf{r}_{||}\right)$ by the average susceptibility $\overline{\chi}_l = \left\langle \chi_l\left(\mathbf{r}_{||}\right)\right\rangle$ of each layer l. In order to arrive at a perturbation equation, the sum $-k^2 \sum \overline{\chi} \Psi(\mathbf{r})$ is added and subtracted at the right hand side of Eq. (2.1)

$$\left[\Delta + k^2 I\right] \Psi(\mathbf{r}) = -k^2 \sum \overline{\chi}_l \Psi(\mathbf{r}) - k^2 \sum \left(\chi_l\left(\mathbf{r}_{||}\right) - \overline{\chi}_l\right) \Psi(\mathbf{r}). \tag{2.4}$$

For homogeneous layers $\chi_l\left(\mathbf{r}_{||}\right) = \overline{\chi_l}$ the second sum vanishes on the right, so that Eq. (2.4) is equivalent to Eq. (2.3), the basic equation of the specular reflectometry.[10,14,20,22]

We look for the general solutions

$$\Psi\left(\mathbf{r}\right) = \Psi_{\mathrm{coh}}\left(\mathbf{r}\right) + \Psi_{\mathrm{off}}\left(\mathbf{r}\right) \tag{2.5}$$

of Eq. (2.4) as the sum of the coherent field $\Psi_{\mathrm{coh}}\left(\mathbf{r}\right)$, which vanishes out of the specular direction, and the off-specular field $\Psi_{\mathrm{off}}\left(\mathbf{r}\right)$. Substituting Eq. (2.4) into Eq. (2.3) gives

$$\left[\Delta + k^2 I\right]\Psi_{\mathrm{off}}\left(\mathbf{r}\right) = -k^2 \sum \left(\chi_l\left(\mathbf{r}_{||}\right) - \overline{\chi_l}\right)\Psi_{\mathrm{coh}}\left(\mathbf{r}\right) - k^2 \sum \chi_l\left(\mathbf{r}_{||}\right)\Psi_{\mathrm{off}}\left(\mathbf{r}\right). \tag{2.6}$$

By the optical method[14] the coherent field $\Psi_{\mathrm{coh}}\left(\mathbf{r}\right)$, the solution of Eq. (2.3), is obtained

$$\Psi_{\mathrm{coh}}\left(\mathbf{r}\right) = T\left(\mathbf{r}_{\perp}\right)\Psi^{\mathrm{in}}\exp\left(i\mathbf{k}_{||}\cdot\mathbf{r}_{||}\right) \tag{2.7}$$

(see Appendix), where $\mathbf{r}_{\perp}$ and $\mathbf{r}_{||}$ are the perpendicular and lateral components of $\mathbf{r}$, respectively and Ψ^{in} the amplitude of the incident plane wave

$$T\left(\mathbf{r}_{\perp}\right) = L^{[21]}\left(\mathbf{r}_{\perp}\right)\left(I - R_{\mathrm{sp}}\right) + L^{[22]}\left(\mathbf{r}_{\perp}\right)\left(I + R_{\mathrm{sp}}\right) \tag{2.8}$$

is the transmission factor of the coherent field between the top surface $\mathbf{r}_{\perp} = 0$ and an arbitrary depth $\mathbf{r}_{\perp}$. R_{sp} is the 2×2 specular reflectivity matrix of the system[14], $L^{[21]}\left(\mathbf{r}_{\perp}\right)$ and $L^{[22]}\left(\mathbf{r}_{\perp}\right)$ are the 2×2 submatrices of the 4×4 characteristic matrix L at depth $\mathbf{r}_{\perp}$.[14,20]

Eq. (2.6) can be solved up to arbitrary accuracy applying higher order Born approximations. As our first approximation the second term of the right hand side is neglected, so the solution can be given by using the Green function technique,

$$\Psi_{\mathrm{off}}\left(\mathbf{r}\right) = \frac{k^2}{4\pi}\sum_l \int \frac{\exp\left(ikR\right)}{R}\left(\chi_l\left(\mathbf{r}'_{||}\right) - \overline{\chi_l}\right)\Psi_{\mathrm{coh}}\left(\mathbf{r}'\right)\mathbf{d}^3\mathbf{r}', \tag{2.9}$$

where $R = \left|\mathbf{r} - \mathbf{r}'\right|$. The approximation requires $\left\|\Psi_{\mathrm{coh}}\left(\mathbf{r}\right)\right\| \gg \left\|\Psi_{\mathrm{off}}\left(\mathbf{r}\right)\right\|$, which condition is expected to be valid for magnetic domains in multilayer, where large enough homogeneous domains are observed,[6,9] so that the exact solution $\Psi\left(\mathbf{r}\right)$ is close to the coherent field $\Psi_{\mathrm{coh}}\left(\mathbf{r}\right)$ according to the above condition.

Far from the scattering system the Fraunhofer approximation

$$\frac{\exp(ikR)}{R} \approx \frac{\exp(ikr)}{r} \exp\left(-i\mathbf{k}' \cdot \mathbf{r}'\right) \tag{2.10}$$

is applied and the final result reads ,

$$\Psi_{\text{off}}(\mathbf{r}) = \sqrt{\frac{\pi}{2}} \frac{k^2}{r} \exp(ikr) \sum_l S_l\left(\mathbf{K}_{||}\right) T_l\left(\mathbf{k}'_\perp\right) \Psi^{\text{in}}, \tag{2.11}$$

where

$$T_l\left(\mathbf{k}'_\perp\right) = \frac{1}{\sqrt{2\pi}} \int\limits_{Z_l} \exp\left(-i\mathbf{k}'_\perp \mathbf{r}_\perp\right) T\left(\mathbf{r}_\perp\right) \mathbf{dr}_\perp \tag{2.12}$$

is the Fourier integral over the one dimensional interval Z_l of layer l;

$$S_l\left(\mathbf{K}_{||}\right) = \frac{1}{2\pi} \int \exp\left(-i\mathbf{K}_{||}\mathbf{r}_{||}\right) \left(\chi_l\left(\mathbf{r}_{||}\right) - \overline{\chi_l}\right) \mathbf{d}^2\mathbf{r}_{||} \tag{2.13}$$

is the two dimensional Fourier transform of $\left(\chi_l\left(\mathbf{r}_{||}\right) - \overline{\chi}\right)$ and $\mathbf{K}_{||}$ is the lateral component of the momentum transfer vector $\mathbf{K} = \mathbf{k}' - \mathbf{k}$.

The off-specularly scattered intensity $I_{\text{off}} = (\Psi_{\text{off}}, \Psi_{\text{off}})$reads

$$I_{\text{off}} = \frac{\pi k^4}{2r^2} \sum_{ll'} \left(\Psi^{\text{in}}, T_l^+\left(\mathbf{k}'_\perp\right) S_l^+\left(\mathbf{K}_{||}\right) S_{l'}\left(\mathbf{K}_{||}\right) T_{l'}\left(\mathbf{k}'_\perp\right) \cdot \Psi^{\text{in}}\right), \tag{2.14}$$

which for arbitrary incident polarization is written as

$$I_{\text{off}} = \frac{\pi k^4}{2r^2} \sum_{ll'} \mathbf{Tr}\left[T_l^+\left(\mathbf{k}'_\perp\right) S_l^+\left(\mathbf{K}_{||}\right) S_{l'}\left(\mathbf{K}_{||}\right) T_{l'}\left(\mathbf{k}'_\perp\right) \cdot \rho\right], \tag{2.15}$$

where ρ is the polarization density matrix of the incident radiation.[23] From the convolution theorem follows that the Fourier transform $C_{ll'}\left(\mathbf{R}_{||}\right)$ of

$$C_{ll'}\left(\mathbf{K}_{||}\right) = \frac{1}{2\pi} S_l^+\left(\mathbf{K}_{||}\right) S_{l'}\left(\mathbf{K}_{||}\right), \tag{2.16}$$

is the cross correlation function of the susceptibilities between layers l and l'

$$C_{ll'}\left(\mathbf{R}_{||}\right) = \frac{1}{A} \int \left(\chi_l\left(\mathbf{R}_{||} + \mathbf{r}_{||}\right) - \overline{\chi}_l\right)^+ \left(\chi_{l'}\left(\mathbf{r}_{||}\right) - \overline{\chi}_{l'}\right) \mathbf{d}^2\mathbf{r}_{||} \tag{2.17}$$

A is the area of the surface ($A \to \infty$). The final result then becomes

$$I_{\text{off}} = \frac{\pi k^4}{2r^2} \sum_{ll'} \mathbf{Tr}\left[T_l^+\left(\mathbf{k}'_\perp\right) C_{ll'}\left(\mathbf{K}_{||}\right) T_{l'}\left(\mathbf{k}'_\perp\right) \cdot \rho\right], \tag{2.18}$$

which expression is very convenient in case of randomly distributed lateral inhomogenities.

III. OFF-SPECULAR SMR

The result of Eq. (2.18) is valid for neutron and x-ray reflectometry working in the energy domain. However, in case of SMR we detect the time response after the synchrotron pulse,[24] which is

$$\Psi_{\text{off}}\left(\mathbf{r},t\right)=\frac{1}{\hbar\sqrt{2\pi}}\int\limits_{-\infty}^{\infty}\Psi_{\text{off}}\left(\mathbf{r},E\right)\exp\left(-iEt/\hbar\right)\mathbf{d}E, \tag{3.1}$$

the Fourier transform of the off-specular field. As both the susceptibilities $\left(\chi_l\left(\mathbf{r}'_{||},E\right)-\overline{\chi_l}\left(E\right)\right)$and the coherent field $\Psi_{\text{coh}}\left(\mathbf{r}',E\right)$ strongly depend on the energy[24] E and according to the definitions of Eqs. (2.8), (2.12) and (2.13), the energy dependence also regards to $S_l\left(\mathbf{K}_{||},E\right)$ and $T_l\left(\mathbf{k}'_{\perp},E\right)$, Eq. (2.18) can not been applied.

In order to work out Eq. (3.1) we define a geometric distribution function $\Omega_l^{\mu}\left(\mathbf{r}_{||}\right)$ of each homogeneous region $\mu=1,..,M$ in layer l. $\Omega_l^{\mu}\left(\mathbf{r}_{||}\right)$ describes the homogeneous area with an energy dependent susceptibility $\chi_l^{\mu}\left(E\right)$. Over the region of $\chi_l^{\mu}\left(E\right)$ the distribution function $\Omega_l^{\mu}\left(\mathbf{r}_{||}\right)=1$ otherwise $\Omega_l^{\mu}\left(\mathbf{r}_{||}\right)=0$, so that the total inhomogeneous susceptibility is the sum

$$\chi\left(\mathbf{r},E\right)=\sum_{\mu=1}^{M}\sum_{l=1}^{S}\Omega_l^{\mu}\left(\mathbf{r}_{||}\right)\chi_l^{\mu}\left(E\right), \tag{3.2}$$

where the space and energy dependent parts of $\chi\left(\mathbf{r},E\right)$ have been separated. The average susceptibility inside layer l reads

$$\overline{\chi_l}\left(E\right)=\frac{1}{A}\sum_{\mu=1}^{M}A_l^{\mu}\chi_l^{\mu}\left(E\right), \tag{3.3}$$

where $A_l^{\mu}=\int\Omega_l^{\mu}\left(\mathbf{r}_{||}\right)\mathbf{d}^2\mathbf{r}_{||}$ is the total area of the homogeneous part μ inside layer l. Starting from Eqs. (2.13), (3.2) and (3.3)

$$S_l\left(\mathbf{K}_{||},E\right)=\sum_{\mu=1}^{M}G_l^{\mu}\left(\mathbf{K}_{||}\right)\overline{\chi}_l^{\mu}\left(E\right), \tag{3.4}$$

with

$$G_l^{\mu}\left(\mathbf{K}_{||}\right)=\frac{1}{2\pi}\int\exp\left(-i\mathbf{K}_{||}\mathbf{r}_{||}\right)\left(\Omega_l^{\mu}\left(\mathbf{r}_{||}\right)-\frac{1}{A}A_l^{\mu}\right)\mathbf{d}^2\mathbf{r}_{||}, \tag{3.5}$$

we finally get the energy dependent off-specular field

$$\Psi_{\text{off}}\left(\mathbf{r},E\right)=\sqrt{\frac{\pi}{2}}\frac{k^2}{r}\exp\left(ikr\right)\sum_{l,\mu}G_l^{\mu}\left(\mathbf{K}_{\|}\right)\chi_l^{\mu}\left(E\right)T_l\left(\mathbf{k}'_{\perp},E\right)\Psi^{\text{in}} \tag{3.6}$$

and the off-specular intensity

$$I_{\text{off}}\left(E\right)=\frac{k^4}{4r^2}\sum_{ll'\mu\mu'}C_{l'l}^{\mu'\mu}\left(\mathbf{K}_{\|}\right)\mathbf{Tr}\left[\left(\Gamma_{l'}^{\mu'}\right)^{+}\left(\mathbf{k}'_{\perp},E\right)\Gamma_l^{\mu}\left(\mathbf{k}'_{\perp},E\right)\cdot\rho\right]. \tag{3.7}$$

The matrices for area μ, l

$$\Gamma_l^{\mu}\left(\mathbf{k}'_{\perp},E\right)=\chi_l^{\mu}\left(E\right)T_l\left(\mathbf{k}'_{\perp},E\right), \tag{3.8}$$

are the products of the homogeneous solution $T_l\left(\mathbf{k}'_{\perp},E\right)$ and the susceptibility $\chi_l^{\mu}\left(E\right)$ of that area.

$$C_{l'l}^{\mu'\mu}\left(\mathbf{K}_{\|}\right)=\frac{1}{2\pi}G_l^{\mu'}\left(\mathbf{K}_{\|}\right)^{*}G_l^{\mu}\left(\mathbf{K}_{\|}\right) \tag{3.9}$$

is the geometrical correlation function between layers l and l', homogeneous parts μ and μ'. In Eq. (3.7) the geometrical correlation function is separated from the energy dependent functions, and can therefore be applied for time domain and energy domain measurements, as well. Now the Fourier transformation can be worked out. With Eq. (3.1) the time dependent intensity becomes

$$I_{\text{off}}\left(t\right)=\frac{k^4}{4r^2}\sum_{ll'\mu\mu'}C_{l'l}^{\mu'\mu}\left(\mathbf{K}_{\|}\right)\mathbf{Tr}\left[\left(\Gamma_{l'}^{\mu'}\right)^{+}\left(\mathbf{k}'_{\perp},t\right)\Gamma_l^{\mu}\left(\mathbf{k}'_{\perp},t\right)\cdot\rho\right], \tag{3.10}$$

where

$$\Gamma_l^{\mu}\left(\mathbf{k}'_{\perp},t\right)=\frac{1}{\hbar\sqrt{2\pi}}\int_{-\infty}^{\infty}\Gamma_l^{\mu}\left(\mathbf{k}'_{\perp},E\right)\exp\left(-iEt/\hbar\right)\mathbf{d}E \tag{3.11}$$

IV. TIME INTEGRATED OFF-SPECULAR SMR

One possibility for off-specular reflectometry is the geometry called 'ω-scan', where we set the value of 2θ (we fix the height of the detector) and vary the sample orientation ω (leaving the constraint of specular reflection $\omega=\theta$). In the special case of ω- scan the lateral components of the momentum transfer vector $\mathbf{K}_{\|}$ and the perpendicular component of the wave vector of the out coming wave $\mathbf{k}'_{\perp}$can be expressed by the grazing angle θ and by ω

$$\mathbf{K}_{\|} = 2k \sin\theta \sin(\theta - \omega) \tag{4.1}$$

$$\mathbf{k}'_{\perp} = k \sin\omega. \tag{4.2}$$

The time-integrated intensity is $I(\omega, \theta) = \int_{t^1}^{t^2} I_{\text{off}}(t)\, \mathbf{d}t$, where t_1 and t_2 define the time window of the measurements after the synchrotron bunch. Applying Eqs. (3.10) and (3.11) the final form reads

$$I(\omega, \theta) = \frac{N\tau}{t_{\text{Bunch}}} \frac{k^4}{4\hbar r^2} \sum_{n=-\infty}^{\infty} S_n \int_{-\infty}^{\infty} \mathbf{d}E \sum_{ll'\mu\mu'} C_{l'l}^{\mu'\mu}\left(\mathbf{K}_{\|}\right) \mathbf{Tr}\left[\left(\Gamma_{l'}^{\mu'}\right)^{+}(\mathbf{k}'_{\perp}, E + n\hbar\Omega)\, \Gamma_l^{\mu}(\mathbf{k}'_{\perp}, E)\, \rho\right], \tag{4.3}$$

where N is the number of photons in the incident synchrotron bunch, τ is the duration of the synchrotron bunch ($\tau \approx 50$ ps at ESRF), t_{Bunch} is the time interval between the synchrotron bunches, $\Omega = \frac{2\pi}{t_{\text{Bunch}}}$ and S_n are the discrete Fourier components of the periodical time window function $S(t) = \sum_{n=-\infty}^{\infty} S_n \exp(in\Omega t)$of the experiment defined by $S(t) = 1$ for $t_1 < t < t_2$, otherwise $S(t) = 0$ after each synchrotron bunch.

V. CONCLUSION

Off-specular SMR is sensitive to the lateral structure of the hyperfine fields, so it can be used for studying magnetic domains in multilayer. Because of the underlying common optical approach the same theory can be applied for SMR, x-ray reflectometry, spin polarized neutron reflectometry[14] and x-ray resonance exchange scattering[25,26] for both specular and off-specular reflection. Using perturbation theory (DWBA), the off-specularly reflected intensity of SMR has been expressed by the geometrical correlation functions of the lateral structure and by the specular field profile in the layers. A newer version of the data evaluation computer program **EFFI** (**E**nvironment **F**or **FI**tting), based on this calculus, will be freely soon available.[22,27]

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APPENDIX: GENERAL SOLUTION OF THE COHERENT FIELD EQUATION

The solution of Eq. (2.3) was given in Refs.[14,20,22], where instead of the second order differential equation regarding to $\Psi_{\mathrm{coh}}(\mathbf{r})$, after defining the derivative field $\Phi(\mathbf{r}_\perp) = (ik\sin\Theta)^{-1}\Psi'(\mathbf{r}_\perp)$, a system of first order differential equations was used.[14] The solution was given in terms of the 4×4 characteristic matrix L of the system.[14,20,22]

$$\begin{pmatrix}\Phi(\mathbf{r}_\perp)\\ \Psi(\mathbf{r}_\perp)\end{pmatrix} = L(\mathbf{r}_\perp)\begin{pmatrix}\Phi(0)\\ \Psi(0)\end{pmatrix}, \tag{A1}$$

which equation has the physical meaning that there is linear connection between the fields in depth $\mathbf{r}_\perp = 0$ and in arbitrary depth $\mathbf{r}_\perp$ the characteristic matrix L being the matrix coefficient. Taking into account the boundary conditions, the field at the top surfaces of the system ($\mathbf{r}_\perp = 0$) is

$$\Psi(0) = \Psi^{\mathrm{in}} + R_{\mathrm{sp}}\Psi^{\mathrm{in}}, \tag{A2}$$

the sum of the incident Ψ^{in} and the reflected $R_{\mathrm{sp}}\Psi^{\mathrm{in}}$ waves so Eq. (A1) reads

$$\begin{pmatrix}\Phi(\mathbf{r}_\perp)\\ \Psi(\mathbf{r}_\perp)\end{pmatrix} = L(\mathbf{r}_\perp)\begin{pmatrix}\Psi^{\mathrm{in}} - R_{\mathrm{sp}}\Psi^{\mathrm{in}}\\ \Psi^{\mathrm{in}} + R_{\mathrm{sp}}\Psi^{\mathrm{in}}\end{pmatrix}, \tag{A3}$$

where the concept of impedance tensors was used,[28] taking into account that the fields at $\mathbf{r}_\perp = 0$ are in vacuum (see Eqs. (21) and (22) of Ref.[14]). Expressing the second component from Eq. (A3), the field at arbitrary depth $\mathbf{r}_\perp$ reads

$$\Psi(\mathbf{r}_\perp) = \left\lfloor L^{[21]}(\mathbf{r}_\perp)(I - R_{\mathrm{sp}}) + L^{[22]}(\mathbf{r}_\perp)(I + R_{\mathrm{sp}})\right\rfloor \Psi^{\mathrm{in}}, \tag{A4}$$

and using the notation $T\left(\mathbf{r}_{\perp}\right)=L^{[21]}\left(\mathbf{r}_{\perp}\right)\left(I-R_{\mathrm{sp}}\right)+L^{[22]}\left(\mathbf{r}_{\perp}\right)\left(I+R_{\mathrm{sp}}\right)$the solution of the three dimensional homogeneous wave equation is

$$\Psi_{\mathrm{coh}}\left(\mathbf{r}\right)=T\left(\mathbf{r}_{\perp}\right)\Psi^{\mathrm{in}}\exp\left(i\mathbf{k}_{\|}\cdot\mathbf{r}_{\|}\right). \tag{A5}$$

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