Exact theories for light, x-ray, electron, and neutron diffractions from planar media with periodic structures

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Rigorous theories in differential-equation approaches for the diffraction of all waves from planar media with general periodic structures (gratings, single-crystal slabs, etc.) are studied based upon a unified viewpoint. In order to do this without duplicating derivations of the existing theories for spinless or relativistic electrons and electromagnetic waves (light, x rays, etc.), we construct all the theories of this kind for both spinless neutrons and relativistic neutrons. Some of them are the only rigorous theories that are suitable and efficient for numerical calculations in their exact forms and at the same time provide a clear physical picture for the diffraction phenomena. We derive explicit relations between the different types of exact theories for the same wave-diffraction problem, compare the diffraction theories of the same type for different waves, and illustrate the common particulars of these theories. In addition, we present a new and most efficient form of solution for a limiting case of the diffraction systems and clarify previous misinterpretations about the limiting case.

I. INTRODUCTION

Wave diffraction from planar media with periodic structures is a common phenomenon. The waves referred to in this paper are matter waves of electrons and neutrons and electromagnetic waves (light, x rays, etc.). The slab media with periodic structures are usually gratings or ideal single crystals.

Many theories for such diffraction phenomena are proposed in the fields of spectroscopy, holography, acoustooptics, electron microscopy, and x-ray and neutron crystallography. Most of them are approximate theories[1–11] based on many simplifying assumptions such as weak coupling, a very thin or semi-infinite medium, negligible backward or forward scattering, and some "difficult-to-justify"[1] assumptions. These theories are thus applicable only in limited parameter ranges. Among the review articles and monographs,[1–11] the book by Cowley[11] introduces the crystal-diffraction theories for x rays and spinless electrons and neutrons in the unified viewpoint of an approximate integral-equation approach.

Rigorous theories based on differential-equation approaches have also been developed for the diffraction of spinless electrons[12–15] and relativistic electrons[16,17] from planar ideal crystals and for the diffraction of electromagnetic waves from gratings with one,[18–23] two,[24] and three[25,26] grating vectors. The last case includes the x-ray diffraction from ideal crystals.[25] Some of these are the only rigorous theories that are suitable and efficient for numerical calculation and at the same time provide a clear physical picture for the diffraction phenomena. A rigorous theory means here an exact solution of a wave-diffraction problem that is simulated by a given model for the diffraction system and a given equation for the wave motion.

There is also a ground of unification for all types of rigorous theories of wave diffraction from planar media with periodic structures that are based upon differential-equation approaches (Sec. II). In this paper we derive for all waves, based on this unified ground, the explicit relations between these theories through the constructions of all of these types of theories for both relativistic (Sec. III) and spinless (Sec. IV) neutrons. With such a presentation we can avoid duplicating the derivations of the aforementioned existing rigorous theories[12–26] for electromagnetic waves, spinless electrons, or relativistic electrons. General discussions and conclusions are itemized (Sec. V). In particular, a new and most efficient method to solve a limiting case of the diffraction problems is presented (Sec. III D) and, as a by-product, some previous misinterpretations about the limiting case are clarified [part (viii) in Sec. V].

II. THE COMMON MODEL AND THE METHODS OF ANALYSIS

The formulation of the theories of wave diffraction from planar media with periodic structures is usually based on the same simplifying model for the various diffraction systems. In this model, (i) the medium is planar with finite thickness d and infinite lateral extension (region II with $0 \le z \le d$ in a chosen frame) and bounded on both sides by uniform regions (region I with $-\infty < z \le 0$ and region III with $d \le z < \infty$), (ii) the interaction between the wave and the medium is terminated at the surfaces of the medium, (iii) the effect of the presence of inelastic scattering on elastic scattering may be taken into account as "absorption" by adopting complex interaction functions,[27] and (iv) the incident wave is an arbitrary stationary plane wave [coming from region I with the wave vector $\mathbf{k}_0 = k_0(\sin\theta^i, 0, \cos\theta^i)$].

The main diffraction analyses are based on integral equations,[11] differential equations,[3] and direct numerical integrations.[4] The last approach belongs to numerical analysis, in which the wave equations are directly integrated numerically through complicated algorithms to obtain numerical results. Physical insight is completely obscured. In an exact integral equation approach, the formal solution of the scattering matrix is operationally defined in terms of a perturbative series. The series cannot be summed exactly, in general, and the high-order perturbative terms are hard to calculate. This approach is not suitable for numerical calculation in its exact formulation.

In the studies of the wave diffraction from periodic structures through differential-equation approaches, mainly three types of expansion forms are used for the wave function. All are guided by the Bloch's theorem.[28] They are the Bloch-wave, coupled-wave, and semireciprocal expansions.[29] The corresponding theories are clearly established on a unified ground. It consists of the common model for all the diffraction systems of planar media with periodic structures on one hand, and the same Bloch's theorem for the basis of analyses for all the waves on the other hand. The only variations are in the wave expansion forms and the wave equations.

III. EXACT THEORIES FOR RELATIVISTIC NEUTRONS

The time-independent Dirac-type wave equation for a relativistic neutron is[30,31]

$$\{c\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m_0c^2-W+U(\mathbf{r}) -\mu\beta[\boldsymbol{\sigma}\cdot\mathbf{H}(\mathbf{r})-i\boldsymbol{\alpha}\cdot\mathbf{E}(\mathbf{r})]\}\psi(\mathbf{r})=0 \ . \quad (1)$$

Here m_0, W, and μ $(=-1.91e\hbar/2m_0c^2)$ are, respectively, the mass, the positive relativistic total energy, and the magnetic dipole moment of the neutron. c is the speed of light, $\hbar$ is Planck's constant h divided by 2π, i is the imaginary unit, and e is the magnitude of electron charge. $\mathbf{p}=-i\hbar\nabla$ is the momentum operator. β and the three components of $\boldsymbol{\alpha}$ are the Dirac spinor operators, which are 4×4 matrices in the Dirac representation:

$$\alpha_x=\begin{bmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{bmatrix},\quad \alpha_y=\begin{bmatrix}0&0&0&-i\\0&0&i&0\\0&-i&0&0\\i&0&0&0\end{bmatrix},$$
$$\alpha_z=\begin{bmatrix}0&0&1&0\\0&0&0&-1\\1&0&0&0\\0&-1&0&0\end{bmatrix},\quad \beta=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}, \quad (2)$$

The wave function ψ is then a four-component spinor. $\boldsymbol{\sigma}=-i\boldsymbol{\alpha}\times\boldsymbol{\alpha}/2$ is the spin operator.

$\mathbf{E}$ and $\mathbf{H}$ are related to the static electric potential V and magnetization $\mathbf{M}$ by $\mathbf{E}=-\nabla V$, $\mathbf{H}=\nabla\times\mathbf{A}$, and $\mathbf{A}=-\int\mathbf{M}(\mathbf{r}_1)\times\nabla(1/|\mathbf{r}-\mathbf{r}_1|)d\mathbf{r}_1$ where $d\mathbf{r}_1$ is a volume element. U is a scalar potential incorporated here to simulate the neutron-nucleus interaction by assuming zero net spin for the nucleus. Owing to the short-ranged nature of the interaction force, the Fermi point potential $U=(h^2/2\pi m_0)\sum_{i,d}b_i^{(d)}\delta(\mathbf{r}-\mathbf{R}_i^{(d)})$ may be used,[9,32] which is a sum of Dirac delta functions. Here $\mathbf{R}_i^{(d)}$ is the position vector of the dth nucleus in the ith crystalline cell, and $b_i^{(d)}$ is the bound coherent scattering length[9,10,32] of the neutron.

The functions U and V have the same periodicity of the crystal lattice. We shall consider nonmagnetic and antiferromagnetic substances only. Then the magnetization $\mathbf{M}$ is zero outside the crystal and its periods inside the crystal are the integral multiples of the periods of crystal lattice in the corresponding directions. Thus, the basic reciprocal-lattice vectors $\mathbf{b}_r$ $(r=1,2,3)$ of this periodic diffraction system as a whole are those of the periodicity of $\mathbf{M}$. In terms of them, the functions U and V as well as $\mathbf{M}$ may be Fourier analyzed. The Fourier coefficients are designated, respectively, as U_{mnt}, V_{mnt}, $\mathbf{M}_{mnt}$, $\mathbf{E}_{mnt}$, and $\mathbf{H}_{mnt}$; for example,

$$U(\mathbf{r})=\sum_{m,n,t}U_{mnt}\exp[i2\pi(m\mathbf{b}_1+n\mathbf{b}_2+t\mathbf{b}_3)\cdot\mathbf{r}] \quad (3)$$

with $m,n,t=0,\pm1,\pm2,\ldots$. The uniform regions outside the crystal are assumed here to be vacua. According to the Bloch's theorem, if the coefficients of a linear and homogeneous differential equation are truly periodic (characterized by $\mathbf{b}_r$), there are particular solutions known as the Bloch waves:

$$v_{\mathbf{K}}(\mathbf{r})=\sum_{m,n,t}v_{mnt}(\mathbf{K})\exp[i2\pi(\mathbf{K}+m\mathbf{b}_1+n\mathbf{b}_2+t\mathbf{b}_3)\cdot\mathbf{r}] , \quad (4)$$

where $v_{mnt}(\mathbf{K})$ are constants depending on the Bloch wave vector $\mathbf{K}$.

A. Rigorous Bloch-wave analysis

Guided by the Bloch's theorem we may expand the wave function in each region into a linear combination of the Bloch waves (with constant coefficients):

$$\psi(\mathbf{r}')=\sum_{\varkappa}a(\varkappa)\left[\sum_{m,n,t}v_{mnt}(\varkappa)\times\exp[i(\mathbf{n}_{mnt}+\varkappa\hat{\mathbf{i}}_z)\cdot\mathbf{r}']\right] , \quad (5)$$

where

$$\mathbf{n}_{mnt}=\sin\theta^i\hat{\mathbf{i}}_x+(\varepsilon_{000}-\sin^2\theta^i)^{1/2}\hat{\mathbf{i}}_z+(m\mathbf{b}_1+n\mathbf{b}_2+t\mathbf{b}_3)/k_0 ,$$

$$\mathbf{r}'=2\pi k_0\mathbf{r} ,$$

and

$$k_0=1/\lambda=+(W^2-m_0^2c^4)^{1/2}/ch .$$

Here

$$\varepsilon_{000}=[1-\mathrm{Re}(U_{000})/(W-m_0c^2)]\times[1-\mathrm{Re}(U_{000})/(W+m_0c^2)]$$

is the permittivity for the neutron wave in a region in which the neutron-nucleus interaction energy is equal to the constant averaged value U_{000}. The symbol Re stands for taking the real part. $\hat{\mathbf{i}}_j (j=x,y,z)$ is the unit vector in the j direction. Clearly, here the Bloch wave vector is $\mathbf{K}_{\rm BW}=k_0(\sin\theta^i, 0, +(\varepsilon_{000}-\sin^2\theta^i)^{1/2}+\varkappa)$, in which only $\varkappa$ is an undetermined parameter. Here $\nu_{mnt}(\varkappa)$ is a constant spinor coefficient since the wave function ψ is a spinor function. $a(\varkappa)$ is a constant scalar coefficient. To find the allowed values of $\varkappa$ and the corresponding spinors $\nu_{mnt}(\varkappa)$, we substitute the expansion form (4) of the Bloch wave with the Bloch wave vector $\mathbf{K}=\mathbf{K}_{\rm BW}$ into Eq. (1) and obtain

$$[\boldsymbol{\alpha}\cdot(\mathbf{n}_{mnt}+\varkappa\hat{\mathbf{i}}_z)+(m_0c^2\beta-W)/chk_0]\nu_{mnt} +(1/chk_0)\sum_{u,v,w}[U_{m-u,n-v,t-w}-\mu\beta(\boldsymbol{\sigma}\cdot\mathbf{H}_{m-u,n-v,t-w}-i\boldsymbol{\alpha}\cdot\mathbf{E}_{m-u,n-v,t-w})]\nu_{uvw}=0 , \quad (6)$$

where the subscripts $u,v,w=0,\pm1,\pm2,\ldots$ are just the same as m,n,t. We may multiply the set of equations in (6) with $-\alpha_z$ and obtain an equivalent set of equations. The latter may be cast into the form of a grand matrix equation as

$$(\underline{C}-\varkappa\underline{1})\underline{\nu}=\underline{0} , \quad (7)$$

with

$$\underline{\nu}^t=(\underline{\nu}_1^t\ \underline{\nu}_2^t\ \underline{\nu}_3^t\ \underline{\nu}_4^t) , \quad (8)$$

where the superscript t stands for matrix transpose, and with

$$\underline{C}=\begin{bmatrix} i\underline{e}_z-\underline{n}_z & -\underline{n}_x+i\underline{n}_y+i\underline{e}_x+\underline{e}_y & \underline{1}/s-\underline{u}-\underline{h}_z & -\underline{h}_x+i\underline{h}_y \\ \underline{n}_x+i\underline{n}_y-i\underline{e}_x+\underline{e}_y & i\underline{e}_z-\underline{n}_z & \underline{h}_x+i\underline{h}_y & -\underline{1}/s+\underline{u}-\underline{h}_z \\ s\underline{1}-\underline{u}+\underline{h}_z & \underline{h}_x-i\underline{h}_y & -i\underline{e}_z-\underline{n}_z & -\underline{n}_x+i\underline{n}_y-i\underline{e}_x-\underline{e}_y \\ -\underline{h}_x-i\underline{h}_y & -s\underline{1}+\underline{u}+\underline{h}_z & \underline{n}_x+i\underline{n}_y+i\underline{e}_x-\underline{e}_y & -i\underline{e}_z-\underline{n}_z \end{bmatrix} . \quad (9)$$

Here $\underline{\nu}_p$ (the subscript $p,q=1,2,3,4$) is a column matrix with elements $(\underline{\nu}_p)_{mnt}=\nu_{mntp}$, while ν_{mntp} is the pth element of the spinor ν_{mnt}. The submatrix $\underline{n}_j$ is diagonal with diagonal elements n_{mntj}, which are the j components of the vectors $\mathbf{n}_{mnt}$. The elements u_{mntuvw}, $e_{jmntuvw}$, and $h_{jmntuvw}$ of the square matrices $\underline{u}$, $\underline{e}_j$, and $\underline{h}_j$ are, respectively, related to the Fourier coefficients U_{mnt}, V_{mnt}, and $\mathbf{M}_{mnt}$ of U, V, and $\mathbf{M}$ as

$$\begin{aligned} u_{mntuvw}&=(1/chk_0)U_{m-u,n-v,t-w} , \\ e_{jmntuvw}&=-i(\mu/chk_0)(n_{m-u,n-v,t-w,j}-n_{000j})V_{m-u,n-v,t-w} , \\ h_{jmntuvw}&=-(4\pi\mu/chk_0)[M_{j,m-u,n-v,t-w}-\mathbf{M}_{m-u,n-v,t-w}\cdot(\mathbf{n}_{m-u,n-v,t-w}-\mathbf{n}_{000})(n_{m-u,n-v,t-w,j}-n_{000j}) \\ &\qquad\times(\mathbf{n}_{m-u,n-v,t-w}-\mathbf{n}_{000})^{-2}] , \end{aligned} \quad (10)$$

and $s=[(W-m_0c^2)/(W+m_0c^2)]^{1/2}$. Equation (7) shows that to determine $\varkappa$ and $\underline{\nu}$ is a standard eigenvalue and eigenvector problem.

In region II, $\underline{C}=\underline{C}^{\rm II}$. The eigenvalues of $\underline{C}^{\rm II}$ and their associated eigenvectors shall be labeled as $\varkappa_{uvwq}^{\rm II}$ and $\underline{\nu}_{uvwq}^{\rm II}$, respectively. Using these and Eq. (5), we write the spinor wave function inside the crystal as

$$\psi^{\rm II}=\sum_{u,v,w,q} a_{uvwq}^{\rm II}\left[\sum_{m,n,t}\nu_{mntuvwq}^{\rm II}\exp[i(\mathbf{n}_{mnt}^{\rm II}+\varkappa_{uvwq}^{\rm II}\hat{\mathbf{i}}_z)\cdot\mathbf{r}']\right] . \quad (11)$$

Here $\nu_{mntuvwq}^{\rm II}$ is a spinor with elements $\nu_{mntpuvwq}^{\rm II}=(\underline{\nu}_{uvwq}^{\rm II})_{mntp}$, and $a_{uvwq}^{\rm II}$ is the scalar expansion coefficient associated with the (u,v,w,q)th Bloch wave.

In a vacuum region $U=V=\mathbf{M}=0$. In this case it is simpler to set $n_{mntz}=0$. The submatrices in $\underline{C}^v$ are all diagonal (here the superscript v refers to a vacuum region) and hence Eq. (7) can be decomposed into independent spinor equations

$$(C_{mnt}^v-\varkappa^v)\nu_{mnt}^v=0 , \quad (12)$$

with the spinor operator

$$C_{mnt}^v=\begin{bmatrix} 0 & -n_{mntx}+in_{mnty} & 1/s & 0 \\ n_{mnyx}+in_{mnty} & 0 & 0 & -1/s \\ s & 0 & 0 & -n_{mntx}+in_{mnty} \\ 0 & -s & n_{mntx}+in_{mnty} & 0 \end{bmatrix} . \quad (13)$$

The spinor components $\psi^{v}_{mnt}=v^{v}_{mnt}(\varkappa^{v})\exp[i(n_{mntx}x'+n_{mnty}y'+\varkappa^{v}z')]$ in a Bloch wave are already the common eigenfunctions of the Hamiltonian operator for a neutron in vacuum ($H_0=c\boldsymbol{\alpha}\cdot\mathbf{p}+m_0c^2\beta$) and the momentum operator $\mathbf{p}$, belonging to positive eigenenergy W and eigenmomentum $hk_0(n_{mntx},n_{mnty},\varkappa^{v})$. In order to study the polarization[9,33] of the neutron waves, we require each elementary wave to possess a definite helicity (which is the spin projection value along the direction of momentum in the unit of $\hbar$). This is possible because the helicity operator[33] $\boldsymbol{\sigma}\cdot\mathbf{p}/2|\mathbf{p}|$ commutes with $\mathbf{p}$ and H_0. From the requirement of $(\boldsymbol{\sigma}\cdot\mathbf{p}/2|\mathbf{p}|)\psi^{v}_{mnt}=\omega^{v}\psi^{v}_{mnt}$, we have

$$(h^{v}_{mnt}-\omega^{v})v^{v}_{mnt}=0\ , \tag{14}$$

where ω^{v} is the helicity eigenvalue and $h^{v}_{mnt}=\boldsymbol{\sigma}\cdot\mathbf{n}^{v}_{mnt}/2|\mathbf{n}^{v}_{mnt}|$ is a spinor operator. Thus, the eigenspinor v^{v}_{mnt} must satisfy both of Eqs. (12) and (14).

The eigenvalue pair $(\varkappa^{v},\omega^{v})$ has four pairs of solution: $(\pm\xi_{mnt},\pm\frac{1}{2})$, where $\xi_{mnt}=+(1-n^2_{mntx}-n^2_{mnty})^{1/2}$ which takes a positive (real or imaginary) value. The four pairs of signs $(\pm,\pm)$ in the eigenvalue pairs will be used to label the associated nondegenerate eigenspinors, which are

$$\left.\begin{matrix} v^{v++}_{mnt}\\ v^{v--}_{mnt}\end{matrix}\right\}=N\begin{bmatrix}(n_{mntx}-in_{mnty})\zeta_{mnt}\\ \pm\zeta^{-1}_{mnt}\\ \pm s(n_{mntx}-in_{mnty})\zeta_{mnt}\\ s\zeta^{-1}_{mnt}\end{bmatrix}\ ,$$

$$\left.\begin{matrix} v^{v+-}_{mnt}\\ v^{v-+}_{mnt}\end{matrix}\right\}=N\begin{bmatrix}(n_{mntx}-in_{mnty})\eta_{mnt}\\ \mp\eta^{-1}_{mnt}\\ \mp s(n_{mntx}-in_{mnty})\eta_{mnt}\\ s\eta^{-1}_{mnt}\end{bmatrix}\ , \tag{15}$$

with $\zeta_{mnt}=+(1-\xi_{mnt})^{-1/2}$, $\eta_{mnt}=+(1+\xi_{mnt})^{-1/2}$, and $N=+[2(1+s^2)]^{-1/2}$.

The explicit wave function in a vacuum region is now solved analytically to be

$$\psi^{v}=\sum_{m,n,t}\sum_{p}a^{vp}_{mnt}v^{vp}_{mnt}\exp[i\mathbf{n}^{vp}_{mnt}\cdot(\mathbf{r}'-z'^{v}_0\hat{\mathbf{i}}_z)]\ , \tag{16}$$

where the superscript p in a^{vp}_{mnt} and v^{vp}_{mnt} stands now for the four sign pairs $(\pm,\pm)$, while in $\mathbf{n}^{vp}_{mnt}$ it stands only for the first signs in these pairs: $\mathbf{n}^{v\pm}_{mnt}=(n_{mntx},n_{mnty},\pm\xi_{mnt})$. z'^{v}_0 takes the value 0 in region I and the value d' $(=2\pi k_0 d)$ in region III. The eigenmomenta and wave vectors may be either real or complex since ξ_{mnt} can be real or imaginary, corresponding, respectively, to propagating waves and evanescent waves. Since the eigenspinors $v^{v\pm\pm}_{mnt}$ associated with a real ξ_{mnt} are normalized to one, their associated coefficients $a^{v\pm\pm}_{mnt}$ are the (relative) amplitudes of the corresponding (m,n,t)th-order propagating plane waves. And $|a^{v\pm\pm}_{mnt}|^2$ are the numbers of neutrons in a unit volume. Moreover, for these propagating waves, the first $\pm$ signs in the upper indices of $a^{v\pm\pm}_{mnt}$ indicate the senses of momentum projection of these (m,n,t)th-order waves along the z axis. The second $\pm$ signs label the senses of spin projection along the direction of momentum.

Before we go further, we shall show in the next subsection that the solutions of ψ^{v} and ψ^{II} just obtained by the rigorous Bloch-wave (RBW) analysis may also be obtained by the rigorous coupled-wave (RCW) analysis.

B. Rigorous coupled-wave analysis

Also guided by the Bloch's theorem, we may expand the wave function in each region as

$$\psi(\mathbf{r}')=\sum_{m,n,t}\varphi_{mnt}(z')\exp(i\mathbf{n}_{mnt}\cdot\mathbf{r}')\ . \tag{17}$$

This is a modified form of a single Bloch wave with its constant expansion coefficients of the plane-wave components being replaced by the depth-dependent coefficients $\varphi_{mnt}(z')$. Here φ_{mnt} is a spinor since ψ is. $\mathbf{n}_{mnt}$ and $\mathbf{r}'$ are defined exactly the same as in the RBW analysis (Sec. III A). Here the Bloch wave vector for the original unmodified Bloch wave is completely fixed as $\mathbf{K}_{\mathrm{CW}}=k_0(\sin\theta^i,0,+(\varepsilon_{000}-\sin^2\theta^i)^{1/2})$. Substituting the expansion form (17) into Eq. (1), we obtain a set of coupled differential equations for the variable spinor amplitudes φ_{mnt}:

$$d\varphi_{mnt}/dz'=-i\alpha_z\left\{[\boldsymbol{\alpha}\cdot\mathbf{n}_{mnt}+(m_0c^2\beta-W)/chk_0]\varphi_{mnt}+(1/chk_0)\sum_{u,v,w}[U_{m-u,n-v,t-w}-\mu\beta(\boldsymbol{\sigma}\cdot\mathbf{H}_{m-u,n-v,t-w}-i\boldsymbol{\alpha}\cdot\mathbf{E}_{m-u,n-v,t-w})]\varphi_{uvw}\right\}\ , \tag{18}$$

which may be cast into a grand matrix form as

$$d\underline{\varphi}/dz'=i\underline{C}\underline{\varphi}\ . \tag{19}$$

Here the matrix $\underline{C}$ is exactly the same as that given by Eq. (9) in the RBW analysis. $\underline{\varphi}^t=(\underline{\varphi}^t_1\ \underline{\varphi}^t_2\ \underline{\varphi}^t_3\ \underline{\varphi}^t_4)$ and the elements of the column matrix $\underline{\varphi}_p$ are φ_{mntp}, while the latter are the pth elements of the spinors φ_{mnt}.

In region II, $\underline{C}=\underline{C}^{\mathrm{II}}$. Equation (19) is a linear and homogeneous matrix differential equation of first order with the constant matrix coefficient $\underline{C}^{\mathrm{II}}$. According to matrix theory, its solution has the following two equivalent forms:

$$\underline{\varphi}^{\mathrm{II}}(z')=\exp(i\underline{C}^{\mathrm{II}}z')\underline{\varphi}^{\mathrm{II}}(0)=\underline{T}^{\mathrm{II}}\exp(i\underline{\varkappa}^{\mathrm{II}}z')\underline{a}^{\mathrm{II}}\ . \tag{20}$$

Here $\underline{\varkappa}^{\mathrm{II}}$ is a diagonal matrix with the eigenvalues $\varkappa^{\mathrm{II}}_{uvwq}$ of $\underline{C}^{\mathrm{II}}$ as its diagonal elements. $\underline{T}^{\mathrm{II}}$ is a square matrix which consists of a row of the column eigenvectors $\underline{v}^{\mathrm{II}}_{uvwq}$ belonging, respectively, to eigenvalues $\varkappa^{\mathrm{II}}_{uvwq}$, and these column matrices are arranged in $\underline{T}^{\mathrm{II}}$ in the same sequence as $\varkappa^{\mathrm{II}}_{uvwq}$ are arranged in $\underline{\varkappa}^{\mathrm{II}}$. That is, the elements are $T^{\mathrm{II}}_{mntpuvwq}=(\underline{v}^{\mathrm{II}}_{uvwq})_{mntp}$. $\underline{a}^{\mathrm{II}}$ is an arbitrary constant column matrix. From the solution of $\underline{\varphi}^{\mathrm{II}}$ given by Eq. (20), we obtain the solution of the spinor $\varphi^{\mathrm{II}}_{mnt}$ as

$$\varphi^{\mathrm{II}}_{mnt}(z')=\sum_{u,v,w} T^{\mathrm{II}}_{mntuvw}\exp(i\varkappa^{\mathrm{II}}_{uvw}z')a^{\mathrm{II}}_{uvw} \,. \tag{21}$$

Here T^{II}_{mntuvw} and $\varkappa^{\mathrm{II}}_{uvw}$ are, respectively, the spinor operators with elements $(T^{\mathrm{II}}_{mntuvw})_{pq}=T^{\mathrm{II}}_{mntpuvwq}$ and $(\varkappa^{\mathrm{II}}_{uvw})_{pq}=\varkappa^{\mathrm{II}}_{uvwq}\delta_{pq}$, where δ_{pq} is a Kronecker delta. a^{II}_{uvw} is clearly an arbitrary constant spinor. Substituting Eq. (21) back into Eq. (17), we obtain the general solution of the wave function inside the crystal as

$$\psi^{\mathrm{II}}=\sum_{m,n,t}\sum_{u,v,w} T^{\mathrm{II}}_{mntuvw}\exp[i(\mathbf{n}^{\mathrm{II}}_{mnt}+\varkappa^{\mathrm{II}}_{uvw}\hat{\mathbf{i}}_z)\cdot\mathbf{r}']a^{\mathrm{II}}_{uvw} \,. \tag{22}$$

This solution is in fact exactly the same as that obtained in Eq. (11) by the RBW analysis.

In a vacuum region, it is again more convenient to set $n_{mntz}=0$ as we did before in the Bloch-wave analysis. In this case, $\underline{u}=\underline{e}_j=\underline{h}_j=0$. Then, Eq. (19) may be decomposed into independent spinor equations

$$d\varphi^{v}_{mnt}/dz'=iC^{v}_{mnt}\varphi^{v}_{mnt} \,. \tag{23}$$

Here C^{v}_{mnt} is also exactly the same as that given by Eq. (13). The general solution of Eq. (23) is in the form $\varphi^{v}_{mnt}(z')=\exp(iC^{v}_{mnt}z')\varphi^{v}_{mnt}(0)$. Furthermore, we also require this spinor to be expanded into helicity eigenstates as we did in the RBW analysis. Then, it has the form

$$\varphi^{v}_{mnt}(z')=T^{v}_{mnt}\exp[i\varkappa^{v}_{mnt}(z'-z'^{v}_0)]a^{v}_{mnt} \,, \tag{24}$$

with $T^{v}_{mnt}=(v^{v++}_{mnt}\ v^{v+-}_{mnt}\ v^{v-+}_{mnt}\ v^{v--}_{mnt})$, where the spinors $v^{v\pm\pm}_{mnt}$ are exactly those given by Eq. (15). $\varkappa^{v}_{mnt}$ is a diagonal spinor operator with diagonal elements ξ_{mnt}, ξ_{mnt}, $-\xi_{mnt}$, and $-\xi_{mnt}$ arranged in this very sequence. $(a^{v}_{mnt})^t=(a^{v++}_{mnt}\ a^{v+-}_{mnt}\ a^{v-+}_{mnt}\ a^{v--}_{mnt})$ is an arbitrary spinor with constant elements. Substituting the solution (24) back into Eq. (17), we obtain the wave function in a vacuum region as

$$\psi^{v}=\sum_{m,n,t}T^{v}_{mnt}\exp[i\mathbf{n}^{v}_{mnt}\cdot(\mathbf{r}'-z'^{v}_0\hat{\mathbf{i}}_z)]a^{v}_{mnt} \,, \tag{25}$$

where $\mathbf{n}^{v}_{mnt}=(n_{mntx},n_{mnty},\varkappa^{v}_{mnt})$ is rather a spinor operator. This solution is also exactly the same as that given by Eq. (16) in the RBW analysis.

C. Exact RBW-RCW theory

By applying RBW and RCW analyses, we have obtained in the last two subsections exactly the same general wave solution in each region. Apparently, here the RBW theory and the RCW theory are not only equivalent as they ought to be. They are actually the same theory. Under our choice of the Bloch wave vectors in the Bloch-wave and coupled-wave expansions (namely, $\mathbf{K}_{\mathrm{BW}}=\mathbf{K}_{\mathrm{CW}}+k_0\varkappa\hat{\mathbf{i}}_z$), the close relationship between the RBW and RCW analyses are transparent in each step. For instance, by comparing the expansion forms (5) and (17), we can see the correspondence

$$\varphi_{mnt}(z')=\sum_{\varkappa}a(\varkappa)v_{mnt}(\varkappa)\exp(i\varkappa z') \tag{26}$$

between the factors in the two kinds of expansion forms. This equality simply means that the depth-dependent amplitude $\varphi_{mnt}(z')$ in the RCW analysis is further expanded as such in the RBW analysis. If we substitute the expansion form (26) into Eqs. (18) and (19) in the RCW analysis, we immediately obtain their corresponding equations (6) and (7) in the RBW analysis, respectively.

The boundary conditions $\psi^{\mathrm{I}}(x,y,0)=\psi^{\mathrm{II}}(x,y,0)$, and $\psi^{\mathrm{II}}(x,y,d)=\psi^{\mathrm{III}}(x,y,d)$ imply

$$\begin{aligned}\sum_p a^{\mathrm{I}p}_{mnt}v^{vp}_{mnt}&=\sum_{u,v,w,q}a^{\mathrm{II}}_{uvwq}v^{\mathrm{II}}_{mntuvwq}\,,\\ \sum_p a^{\mathrm{III}p}_{mnt}v^{vp}_{mnt}&=\sum_{u,v,w,q}a^{\mathrm{II}}_{uvwq}v^{\mathrm{II}}_{mntuvwq}\\ &\quad\times\exp[i(n^{\mathrm{II}}_{mntz}+\varkappa^{\mathrm{II}}_{uvwq})d']\end{aligned} \tag{27a}$$

when Eqs. (16) and (11) are used; or equivalently

$$\begin{aligned}T^{v}_{mnt}a^{\mathrm{I}}_{mnt}&=\sum_{u,v,w}T^{\mathrm{II}}_{mntuvw}a^{\mathrm{II}}_{uvw}\,,\\ T^{v}_{mnt}a^{\mathrm{III}}_{mnt}&=\sum_{u,v,w}T^{\mathrm{II}}_{mntuvw}\\ &\quad\times\exp[i(n^{\mathrm{II}}_{mntz}+\varkappa^{\mathrm{II}}_{uvw}d')]a^{\mathrm{II}}_{uvw}\end{aligned} \tag{27b}$$

when Eqs. (22) and (25) are used. Either Eqs. (27a) or (27b) may be cast into the same grand matrix forms as

$$\begin{aligned}&\underline{T}^{v}\underline{a}^{\mathrm{I}}=\underline{T}^{\mathrm{II}}\underline{a}^{\mathrm{II}}\,,\\ &\underline{T}^{v}\underline{a}^{\mathrm{III}}=\underline{X}(i\underline{n}^{\mathrm{II}}_z d')\underline{T}^{\mathrm{II}}\exp(i\underline{\varkappa}^{\mathrm{II}}d')\underline{a}^{\mathrm{II}}\,,\end{aligned} \tag{27c}$$

where

$$\underline{a}^{v}=\begin{bmatrix}\underline{a}^{v+}\\ \underline{a}^{v-}\end{bmatrix},\quad \underline{a}^{v+}=\begin{bmatrix}\underline{a}^{v++}\\ \underline{a}^{v+-}\end{bmatrix},\quad \underline{a}^{v-}=\begin{bmatrix}\underline{a}^{v-+}\\ \underline{a}^{v--}\end{bmatrix}, \tag{28}$$

with the superscript v in $\underline{a}^{v\pm\pm}$ standing for I or III. The elements of $\underline{a}^{v\pm\pm}$ are $a^{v\pm\pm}_{mnt}$, $\underline{X}(i\underline{n}^{\mathrm{II}}_z d')=[\exp(i\underline{n}^{\mathrm{II}}_z d')\delta_{pq}]$, and

$$\underline{T}^{v}=N\begin{bmatrix}(\underline{n}_x-i\underline{n}_y)\underline{\xi} & (\underline{n}_x-i\underline{n}_y)\underline{\eta} & (\underline{n}_x-i\underline{n}_y)\underline{\eta} & (\underline{n}_x-i\underline{n}_y)\underline{\xi}\\ \underline{\xi}^{-1} & -\underline{\eta}^{-1} & \underline{\eta}^{-1} & -\underline{\xi}^{-1}\\ s(\underline{n}_x-i\underline{n}_y)\underline{\xi} & -s(\underline{n}_x-in_y)\underline{\eta} & s(\underline{n}_x-i\underline{n}_y)\underline{\eta} & -s(\underline{n}_x-i\underline{n}_y)\underline{\xi}\\ s\underline{\xi}^{-1} & s\underline{\eta}^{-1} & s\underline{\eta}^{-1} & s\underline{\xi}^{-1}\end{bmatrix}. \tag{29}$$

Eliminating $\underline{a}^{\mathrm{II}}$ from Eqs. (27c), we have

$$\underline{a}^{\mathrm{I}}=\underline{M}\,\underline{a}^{\mathrm{III}} \tag{30}$$

with

$$\underline{M}=(\underline{T}^{v})^{-1}\underline{T}^{\mathrm{II}}\exp(-i\underline{\varkappa}^{\mathrm{II}}d')(\underline{T}^{\mathrm{II}})^{-1}\underline{X}(-i\underline{n}_z^{\mathrm{II}}d')\underline{T}^{v}\ . \tag{31}$$

The given "initial conditions" are that the incident neutron wave is a single stationary plane wave coming form region I and it belongs to the positive relativistic total energy W and the wave vector $\mathbf{k}_0=k_0\mathbf{n}_{000}^{v+}$. Thus we have $\underline{a}^{\mathrm{III}-+}=\underline{a}^{\mathrm{III}--}=\underline{0}$, $\underline{a}^{\mathrm{I}++}=b^{+}(0\ \cdots\ 0\ 1\ 0\ \cdots\ 0)^t$ and $\underline{a}^{\mathrm{I}+-}=b^{-}(0\ \cdots\ 0\ 1\ 0\ \cdots\ 0)^t$, when the (0,0,0)th elements $a_{000}^{v\pm\pm}$ are arranged in the middle of the corresponding column matrices $\underline{a}^{v\pm\pm}$. These and Eq. (30) determine the diffraction amplitudes $a_{mnt}^{\mathrm{I}-+}$, $a_{mnt}^{\mathrm{I}--}$, $a_{mnt}^{\mathrm{III}++}$, and $a_{mnt}^{\mathrm{III}+-}$.[17,25] And we have $\psi_{inc}=(b^{+}v_{000}^{v++}+b^{-}v_{000}^{v+-})\exp(i\mathbf{n}_{000}^{v+}\cdot\mathbf{r}')$. Clearly, $|b^{\pm}|^2$ are the numbers of incident neutrons per unit volume with the eigenmomentum $h\mathbf{k}_0$ and, respectively, the helicity eigenvalues $\pm\frac{1}{2}$. The explicit expression of the wave solution is then

$$\begin{aligned}\psi^{\mathrm{I}}&=(b^{+}v_{000}^{v++}+b^{-}v_{000}^{v+-})\exp(i2\pi\mathbf{k}_0\cdot\mathbf{r})+\sum_{m,n,t}(a_{mnt}^{\mathrm{I}-+}v_{mnt}^{v-+}+a_{mnt}^{\mathrm{I}--}v_{mnt}^{v--})\exp(i2\pi\mathbf{k}_{mnt}^{R}\cdot\mathbf{r})\ ,\\ \psi^{\mathrm{II}}&=\sum_{m,n,t}\sum_{u,v,w,q}a_{uvwq}^{\mathrm{II}}v_{mntuvwq}^{\mathrm{II}}\exp(i2\pi\mathbf{k}_{mntuvwq}^{\mathrm{II}}\cdot\mathbf{r})\ ,\\ \psi^{\mathrm{III}}&=\sum_{m,n,t}(a_{mnt}^{\mathrm{III}++}v_{mnt}^{v++}+a_{mnt}^{\mathrm{III}+-}v_{mnt}^{v+-})\exp[i2\pi\mathbf{k}_{mnt}^{T}\cdot(\mathbf{r}-d\hat{\mathbf{i}}_z)]\end{aligned} \tag{32}$$

with

$$\mathbf{k}_{mntuvwq}^{\mathrm{II}}=k_0\sin\theta^i\hat{\mathbf{i}}_x+k_0[(\varepsilon_{000}^{\mathrm{II}}-\sin^2\theta^i)^{1/2}+\varkappa_{uvwq}^{\mathrm{II}}]\hat{\mathbf{i}}_z+m\mathbf{b}_1+n\mathbf{b}_2+t\mathbf{b}_3\ ,$$

$$\mathbf{k}_{mnt}^{R}=k_0\mathbf{n}_{mnt}^{v-},\quad\text{and }\mathbf{k}_{mnt}^{T}=k_0\mathbf{n}_{mnt}^{v+}\ .$$

D. The limiting case and a new approach

There is a limiting case for the diffraction systems. It is the case that a basic reciprocal-lattice (or grating) vector, say $\mathbf{b}_3$, is exactly perpendicular to the medium surfaces (i.e., $\mathbf{b}_3=b_3\hat{\mathbf{i}}_z$). In such a limit, the x and y components of $\mathbf{n}_{mnt}$ will become independent of the subscript t. Thus, in the vacuum regions, the wave vectors and hence all the t-dependent quantities in the wave function given by Eq. (16) become t independent. Hence, instead of Eq. (16) or Eq. (25), we have

$$\psi^{v}=\sum_{m,n}\sum_{p}a_{mn}^{vp}v_{mn}^{vp}\exp[i\mathbf{n}_{mn}^{vp}\cdot(\mathbf{r}'-z_0'^{v}\hat{\mathbf{i}}_z)]\ , \tag{33}$$

in which the wave vectors are $\mathbf{k}_{mn}^{T}=k_0\mathbf{n}_{mn}^{v+}=k_0(n_{mnx},n_{mny},\xi_{mn})$ and $\mathbf{k}_{mn}^{R}=k_0\mathbf{n}_{mn}^{v-}=k_0(n_{mnx},n_{mny},-\xi_{mn})$ with $\xi_{mn}=+(1-n_{mnx}^2-n_{mny}^2)^{1/2}$. The eigenspinor v_{mn}^{vp} have the same from as Eq. (15) with the subscript t suppressed. While inside the crystal, the wave vectors have t dependence only in their z components:

$$\mathbf{k}_{mntuvwq}^{\mathrm{II}}=k_0\sin\theta^i\hat{\mathbf{i}}_x+[k_0(\varepsilon_{000}^{\mathrm{II}}-\sin^2\theta^i)^{1/2}+k_0\varkappa_{uvwq}^{\mathrm{II}}+tb_3]\hat{\mathbf{i}}_z+m\mathbf{b}_1+n\mathbf{b}_2\ .$$

There are two methods to solve for the amplitudes $a_{mn}^{\mathrm{I}-\pm}$ and $a_{mn}^{\mathrm{III}+\pm}$ of the (m,n)th-order diffraction waves. We shall introduce them in the RBW analysis only.

The first method is to use still the expansion form (11) for the wave function in the crystal. Applying the boundary conditions to wave functions in Eqs. (11) and (33), we obtain

$$\begin{aligned}\sum_p a_{mn}^{\mathrm{I}p}v_{mn}^{\mathrm{I}p}&=\sum_t\sum_{u,v,w,q}a_{uvwq}^{\mathrm{II}}v_{mntuvwq}^{\mathrm{II}}\ ,\\ \sum_p a_{mn}^{\mathrm{III}p}v_{mn}^{vp}&=\sum_t\sum_{u,v,w,q}a_{uvwq}^{\mathrm{II}}v_{mntuvwq}^{\mathrm{II}}\times\exp[i(n_{mntz}^{\mathrm{II}}+\varkappa_{uvwq}^{\mathrm{II}})d']\ .\end{aligned} \tag{34}$$

Now we use Eq. (27a) with $v_{mnt}^{vp}=v_{mn}^{vp}$ *to define* the auxiliary quantities $a_{mnt}^{\mathrm{I}p}$ and $a_{mnt}^{\mathrm{III}p}$. These are then related by Eq. (30), as we have shown. By comparing Eqs. (27a) and (34), we see that the unknowns $a_{mn}^{\mathrm{I}p}$ and $a_{mn}^{\mathrm{III}p}$ may be calculated from the simple summations:

$$a_{mn}^{\mathrm{I}p}=\sum_t a_{mnt}^{\mathrm{I}p},\quad a_{mn}^{\mathrm{III}p}=\sum_t a_{mnt}^{\mathrm{III}p}\ . \tag{35}$$

Thus, the RBW-RCW theory for the general case is still applicable to the limiting case with the help of Eqs. (35). Physically, this result means that when the direction of $\mathbf{b}_3$ approaches in the limit to that of the crystal's normal, the diffraction waves with different order number t but with the same order numbers m and n, the same sense of propagation, and the same helicity collapse into a single (m,n)th-order wave. Consequently, their amplitudes must be summed coherently as given by Eqs. (35). This is the same as the corresponding approach in the RCW theories in Refs. 15, 17, and 25.

The second method that we shall introduce is a new approach. In Eq. (11), the wave function inside the crystal is expanded by *all* the Bloch waves for the particular periodic system. Now we shall expand it instead by subset of the Bloch waves:

$$\psi^{\rm II}=\sum_{u,v,q} a^{\rm II}_{uvq}\left[\sum_{m,n,t} v^{\rm II}_{mntuvwq} \times \exp[i(\mathbf{n}^{\rm II}_{mnt}+\varkappa^{\rm II}_{uvwq}\hat{\mathbf{i}}_z)\cdot\mathbf{r}']\right] . \quad (36)$$

This may be obtained from Eq. (11) by deleting the summation on the subscript w. Here w takes an arbitrarily fixed value for each given triple of u, v, and q.

When the boundary conditions are applied to the reduced expansion form of $\psi^{\rm II}$ in Eq. (36) and the waves $\psi^{\rm I}$ and $\psi^{\rm III}$ given by Eq. (33), the result may be also be cast into a grand matrix from like Eq. (30), namely $\underline{a}^{\rm I}=\underline{M}\,\underline{a}^{\rm III}$; but the contents in each matrix are different. Here,

$$\underline{M}=(\underline{T}^{v})^{-1}\left[\sum_t \underline{T}^{\rm II}_T\right]\exp(i\underline{\varkappa}^{\rm II}d') \times\left[\sum_t \underline{X}(i\underline{n}^{\rm II}_{tz}d')\underline{T}^{\rm II}_t\right]^{-1}\underline{T}^{v} . \quad (37)$$

The column matrices $\underline{a}^{\rm I}$ and $\underline{a}^{\rm III}$ and the square matrix $\underline{T}^{v}$ have the same form as defined, respectively, in Eqs. (28) and (29). But in them the column submatrices $\underline{a}^{v\pm\pm}$ and the diagonal submatrices $\underline{n}_x$, $\underline{n}_y$, $\underline{\zeta}$, and η have instead, the elements $a^{v\pm\pm}_{mn}$ and the diagonal elements $n_{mnx}=\sin\theta^i+(mb_{1x}+nb_{2x})/k_0$, $n_{mny}=(mb_{1y}+nb_{2y})/k_0$, $\zeta_{mn}=+(1-\xi_{mn})^{-1/2}$, and $\eta_{mn}=+(1+\xi_{mn})^{-1/2}$, respectively. The diagonal elements of the diagonal matrices $\underline{n}^{\rm II}_{tz}$ and $\underline{\varkappa}^{\rm II}$ are $n^{\rm II}_{mntz}$ and $\varkappa^{\rm II}_{uvwq}$ (with an arbitrarily fixed w for each given triple of u, v, and q). And $\underline{T}^{\rm II}_t$ is a square matrix with elements $(\underline{T}^{\rm II}_t)_{mnpuvq}=(\underline{v}^{\rm II}_{uvwq})_{mntp}$ (with w fixed exactly the same as in $\varkappa^{\rm II}_{uvwq}$).

The explicit expression of the wave function in this limiting case is then

$$\psi^{\rm I}=(b^{+}v^{v++}_{00}+b^{-}v^{v+-}_{00})\exp(i2\pi\mathbf{k}_0\cdot\mathbf{r}) + \sum_{m,n}(a^{I-+}_{mn}v^{v-+}_{mn}+a^{\rm I--}_{mn}v^{v--}_{mn}) \times\exp(i2\pi\mathbf{k}^{R}_{mn}\cdot\mathbf{r}) ,$$

$$\psi^{\rm II}=\sum_{u,v,q}\sum_{m,n,t} a^{\rm II}_{uvq}v^{\rm II}_{mntuvwq} \times\exp(i2\pi\mathbf{k}^{\rm II}_{mntuvwq}\cdot\mathbf{r}) , \quad (38)$$

$$\psi^{\rm III}=\sum_{m,n}(a^{\rm III++}_{mn}v^{v++}_{mn}+a^{\rm III+-}_{mn}v^{v+-}_{mn}) \times\exp[i2\pi\mathbf{k}^{T}_{mn}\cdot(\mathbf{r}-d\hat{\mathbf{i}}_z)] .$$

In both of the approaches to the limiting case, the same standard eigenvalue and eigenvector problem is involved. The advantage of the first approach is that no separate considerations for the limiting case is necessary. The main computation scheme, and hence the main computer program, for the general case is still applicable. But since here the number of the equations involved is greater than that of the variables to be solved, this approach is inefficient. In the second approach, only about two-thirds of the eigenvalues and their associated eigenvectors need to be calculated and the dimension of the diffraction-amplitude matrices to be handled is also reduced by one third. This is the most efficient method.

Furthermore, the minimal number of different Bloch waves used inside the crystal in the second approach must be equal (or one-to-one corresponding) to the number of waves in either of the vacuum regions. But the choice of this subset is entirely arbitrary. Inside the crystal, the nonuniqueness of the amplitudes of the Bloch waves in the first approach and the arbitrarines of the choice of the subset of the Bloch waves in the second approach are expected to come from the same origin. Indeed, looking at a single Bloch wave in this limiting case,

$$v^{\rm II}_{uvwq}=\exp(i\varkappa^{\rm II}_{uvwq}z') \times\sum_{m,n,t} v^{\rm II}_{mntuvwq}\exp[i(n_{mnx}x'+n_{mny}y' +n^{\rm II}_{mntz}z')] , \quad (39)$$

we see that it can in fact phase match a plane wave of any order in a vacuum region on the interface. The Bloch waves are thus all equivalent in this limited sense. This is the reason why any arbitrary subset of them may expand the wave function inside the crystal as long as the number of the different Bloch waves in the subset is equal to (or greater than) the number of plane waves in either of the vacuum regions.

E. Rigorous semireciprocal theory

In addition to the Bloch-wave and coupled-wave expansions, there is still another expansion form that is also guided by the Bloch's theorem. it may be obtained by absorbing the z-dependent phase factors in the coupled-wave expansion form (17) into the z-dependent spinor amplitudes. Namely,

$$\psi(\mathbf{r}')=\sum_{m,n,t}\Phi_{mnt}(z')\exp[i(n_{mntx}x'+n_{mnty}y')] . \quad (40)$$

This is called semireciprocal approach because only part of the spatial-coodinate (namely, x and y) dependence is Fourier analyzed.

Substituting Eq. (40) into Eq. (1) and casting the resulting equation in a matrix form, we obtain

$$d\underline{\Phi}/dz'=i\underline{D}(z')\underline{\Phi} , \quad (41)$$

where $\underline{\Phi}^t=(\underline{\Phi}^t_1\ \underline{\Phi}^t_2\ \underline{\Phi}^t_3\ \underline{\Phi}^t_4)$ and the elements of the column matrix $\underline{\Phi}_p (p=1, 2, 3, \text{ or } 4)$ are Φ_{mntp} which are the pth elements of the spinors Φ_{mnt}. But here we shall have no need to write down the coefficient matrix $\underline{D}(z')$ explicitly, except for pointing out that it is z dependent for the region inside the crystal. In the vacuum regions, we have $\underline{D}^{v}=\underline{C}^{v}$ and $\underline{\Phi}^{v}=\underline{\varphi}^{v}$, where $\underline{C}^{v}$ and $\underline{\varphi}^{v}$ are defined in Sec. III B and $\underline{\varphi}^{v}$ has already been solved there. Inside the crystal, we may formally write down the solution of Eq. (41) as[13]

$$\underline{\Phi}^{\rm II}(z')=\exp\left[T\int_0^{z'} i\underline{D}^{\rm II}(z')dz'\right]\underline{\Phi}^{\rm II}(0) , \quad (42)$$

where T is the Dyson ordered-product operator. This is rather an integral-equation approach to the diffraction problem, since the exponential matrix-operator function in Eq. (42) is only defined operationally by a perturbative series. Consequently, the rigorous semireciprocal (RSR) theory is not suitable for numerical calculation in its exact form.[13]

IV. EXACT THEORIES FOR SPINLESS NEUTRONS

The time-independent wave equation for a spinless neutron is the Scrhödinger equation for a scalar wave function $\psi(\mathbf{r})$ belonging to a nonrelativistic total energy E:

$$\{\nabla^2+(2m_0/\hbar^2)[E-U(\mathbf{r})]\}\psi(\mathbf{r})=0 \; . \tag{43}$$

Only RBW and RCW theories shall be constructed for spinless neutrons since an RSR theory is not suitable for numerical calculation[13] just as we have seen in the relativistic case. We shall see below that the RBW and RCW theories for spinless neutrons are not identical as are those for relativistic neutrons. Furthermore, the derivations of the former theories and their relation are less straightforward. The reason is that while the differential wave equation for a relativistic spin-$\frac{1}{2}$ particle (the Dirac-type equation) is of first order, its nonrelativistic spinless limit (the Schrödinger equation) is of second order. Moreover, this difference gives rise to more complicated boundary conditions for the spinless case.

A. Rigorous Bloch-wave theory

Substituting the expansion form (4) for a scalar Bloch wave $v_{\mathbf{K}}(\mathbf{r})$ with the Bloch wave vector $\mathbf{K}=\mathbf{K}_{\mathrm{BW}}$ (defined in Sec. III A) into Eq. (43) and rearranging the resulting coupled equations of the scalar coefficients v_{mnt} into a grand matrix form, we have

$$[\underline{\hat{\varepsilon}}-\underline{n}_x^2-\underline{n}_y^2-(\underline{n}_z+\varkappa\underline{1})^2]\underline{v}=0 \; . \tag{44}$$

Here $\underline{n}_j$ stands for the same quantity defined in Sec. III A. The elements of the column matrix $\underline{v}$ and square matrix $\underline{\hat{\varepsilon}}$ are, respectively, v_{mnt} and $\hat{\varepsilon}_{mntuvw}=\hat{\varepsilon}_{m-u,n-v,t-w}$, while $\hat{\varepsilon}_{mnt}=\delta_{m0}\delta_{n0}\delta_{t0}-U_{mnt}/E$ is the Fourier coefficient of the complex permittivity $1-U(\mathbf{r})/E$ for the nonrelativistic spinless neutron wave. In particular, the averaged real permittivity $\varepsilon_{000}=\mathrm{Re}(\hat{\varepsilon}_{000})=1-\mathrm{Re}(U_{000})/E$ is involved in the definition of $\mathbf{K}_{\mathrm{BW}}$ for this nonrelativistic case. We note that since no magnetic interaction may be considered, here the $\mathbf{b}_r$'s stand for the basic reciprocal-lattice vectors of the true lattice structure of the medium.

The allowed values of $\varkappa$ in this spinless neutron case are to be solved from the determinantal equation

$$\det[\underline{\hat{\varepsilon}}-\underline{n}_x^2-\underline{n}_y^2-(\underline{n}_z+\varkappa\underline{1})^2]=0 \; , \tag{45a}$$

which is equivalent[12] to the usual form of secular equation

$$\det(\underline{C}-\varkappa\underline{1})=0 \tag{45b}$$

with

$$\underline{C}=\begin{bmatrix} -\underline{n}_z & \underline{1} \\ \underline{\hat{\varepsilon}}-\underline{n}_x^2-\underline{n}_y^2 & -\underline{n}_z \end{bmatrix} . \tag{46}$$

Equation (45b) is a standard eigenvalue equation for matrix $\underline{C}$. Apparently, Eq. (44) is a generalized eigenvalue and eigenvector equation. Since this equation is quadratic in its eigenvalue $\varkappa$, the correspondence between the eigenvalues $\varkappa$ and the eigenvectors $\underline{v}$ is two to one.

In region II, $U=U^{\mathrm{II}}$ and $\underline{C}=\underline{C}^{\mathrm{II}}$. The eigenvalue pairs and their associated eigenvectors shall be labeled as $\varkappa_{uvw}^{\mathrm{II}q}$ and $\underline{v}_{uvw}^{\mathrm{II}}$ (here the superscript q or p stands for the sign symbol + or −). The former may be calculated by Eq. (45b). This is an eigenvalue problem in the standard form. By using its results, the latter are calculated by Eq. (44). This is an eigenvector problem also in its standard form. The general solution is then

$$\psi^{\mathrm{II}}=\sum_{u,v,w,q} a_{uvw}^{\mathrm{II}q}\left[\sum_{m,n,t} v_{mntuvw}^{\mathrm{II}}\exp[i(\mathbf{n}_{mnt}^{\mathrm{II}}+\varkappa_{uvw}^{\mathrm{II}q}\hat{\mathbf{i}}_z)\cdot\mathbf{r}']\right] , \tag{47}$$

where $v_{mntuvw}^{\mathrm{II}}=(\underline{v}_{uvw}^{\mathrm{II}})_{mnt}$. In a vacuum region, $U=0$ and $\underline{\hat{\varepsilon}}=\underline{1}$. Here we may also set $n_{mntz}=0$. Hence, Eq. (44) may be decomposed into the scalar equations $[1-n_{mntx}^2-n_{mnty}^2-(\varkappa^v)^2]v_{mnt}^v=0$. Thus, the eigenvalues are $\varkappa_{mnt}^{v\pm}=\pm\xi_{mnt}$. The general solution is then

$$\psi^v(\mathbf{r}')=\sum_{m,n,t,p} a_{mnt}^{vp}\exp[i\mathbf{n}_{mnt}^{vp}\cdot(\mathbf{r}'-z_0'^{v}\hat{\mathbf{i}}_z)] \; . \tag{48}$$

Here ξ_{mnt}, $\mathbf{n}_{mnt}^{v\pm}$, and $z_0'^{v}$ are also defined exactly the same as in Sec. III A

The boundary conditions for the scalar wave function governed by the (second-order) Schrödinger equation are $\psi^{\mathrm{I}}(x,y,0)=\psi^{\mathrm{II}}(x,y,0)$, $(\partial\psi^{\mathrm{I}}/\partial z)_{z=0}=(\partial\psi^{\mathrm{II}}/\partial z)_{z=0}$, $\psi^{\mathrm{III}}(x,y,d)=\psi^{\mathrm{II}}(x,y,d)$, and $(\partial\psi^{\mathrm{III}}/\partial z)_{z=d}=(\partial\psi^{\mathrm{II}}/\partial z)_{z=d}$. Applying these to the solutions of ψ^{I} and ψ^{III} given in Eq. (48) and ψ^{II} in Eq. (47), we have

$$\begin{aligned}
&\sum_p a_{mnt}^{\mathrm{I}p}=\sum_{u,v,w,q} v_{mntuvw}^{\mathrm{II}}a_{uvw}^{\mathrm{II}q} \; , \\
&\sum_p n_{mntz}^{vp}a_{mnt}^{\mathrm{I}p}=\sum_{u,v,w,q}(n_{mntz}^{\mathrm{II}}+\varkappa_{uvw}^{\mathrm{II}q})v_{mntuvw}^{\mathrm{II}}a_{uvw}^{\mathrm{II}q} \; , \\
&\sum_p a_{mnt}^{\mathrm{III}p}=\sum_{u,v,w,q} v_{mntuvw}^{\mathrm{II}}\exp[i(n_{mntz}^{\mathrm{II}}+\varkappa_{uvw}^{\mathrm{II}q})d']a_{uvw}^{\mathrm{II}q} \; , \\
&\sum_p n_{mntz}^{vp}a_{mnt}^{\mathrm{III}p}=\sum_{u,v,w,q}(n_{mntz}^{\mathrm{II}}+\varkappa_{uvw}^{\mathrm{II}q})v_{mntuvw}^{\mathrm{II}}\exp[i(n_{mntz}^{\mathrm{II}}+\varkappa_{uvw}^{\mathrm{II}q})d']a_{uvw}^{\mathrm{II}q} \; .
\end{aligned} \tag{49}$$

The first (last) two equations may be combined into one boundary condition at $z=0$ ($z=d$) in a matrix form. Namely,

$$\underline{T}^v\underline{a}^{\rm I}=\underline{T}^{\rm II}\underline{a}^{\rm II} ,$$
$$\underline{T}^v\underline{a}^{\rm III}=\underline{X}(i\underline{n}_z^{\rm II}d')\underline{T}^{\rm II}\exp(i\underline{\varkappa}^{\rm II}d')\underline{a}^{\rm II} , \tag{50}$$

with

$$\underline{T}^v=\begin{bmatrix}\underline{1} & \underline{1}\\ \underline{\xi} & -\underline{\xi}\end{bmatrix},\quad \underline{a}^v=\begin{bmatrix}\underline{a}^{v+}\\ \underline{a}^{v-}\end{bmatrix} . \tag{51}$$

Here $\underline{\varkappa}^{\rm II}$ is a block matrix with two diagonal submatrices $\underline{\varkappa}^{\rm II+}$ and $\underline{\varkappa}^{\rm II-}$ on its diagonal in this very sequence. The elements of $\underline{a}^{v\pm}$ and the diagonal elements of $\underline{\varkappa}^{\rm II\pm}$ are $a_{mnt}^{v\pm}$ and $\varkappa_{mnt}^{\rm II\pm}$, respectively. $\underline{X}(i\underline{n}_z^{\rm II}d')$ is a block matrix with two identical submatrices $\exp(i\underline{n}_z^{\rm II}d')$ on its diagonal, while $\underline{n}_z^{\rm II}$ is defined just the same as in Sec. III. And,

$$\underline{T}^{\rm II}=\begin{bmatrix}\underline{1} & \underline{1}\\ \underline{n}_z^{\rm II} & \underline{n}_z^{\rm II}\end{bmatrix}\begin{bmatrix}\underline{\Upsilon}^{\rm II} & \underline{0}\\ \underline{0} & \underline{\Upsilon}^{\rm II}\end{bmatrix}+\begin{bmatrix}\underline{\Upsilon}^{\rm II} & \underline{0}\\ \underline{0} & \underline{\Upsilon}^{\rm II}\end{bmatrix}\begin{bmatrix}\underline{0} & \underline{0}\\ \underline{\varkappa}^{\rm II+} & \underline{\varkappa}^{\rm II-}\end{bmatrix} . \tag{52}$$

Here $\underline{\Upsilon}^{\rm II}$ is the square matrix consisting in a row of the column eigenvectors $\underline{v}_{uvw}^{\rm II}$, in the same sequence as $\varkappa_{uvw}^{{\rm II}q}$ are arranged in $\underline{\varkappa}^{{\rm II}q}$. That is, its elements are $(\underline{\Upsilon}^{\rm II})_{mntuvw}=(\underline{v}_{uvw}^{\rm II})_{mnt}$.

Eliminating $\underline{a}^{\rm II}$ from Eqs. (50), we obtain

$$\underline{a}^{\rm I}=\underline{M}\,\underline{a}^{\rm III} , \tag{53}$$

with

$$\underline{M}=(\underline{T}^v)^{-1}\underline{T}^{\rm II}\exp(-i\underline{\varkappa}^{\rm II}d')\times(\underline{T}^{\rm II})^{-1}\underline{X}(-i\underline{n}_z^{\rm II}d')\underline{T}^v . \tag{54}$$

These have exactly the same forms as Eqs. (30) and (31) for the relativistic case, but the contents in each matrix factor in this nonrelativistic case are different. In particular, the dimension of the matrix factors here is less by a factor of 2.

B. Rigorous coupled-wave theory

Substituting the coupled-wave expansion form (17) for a scalar wave function ψ into Eq. (43), we obtain

$$d^2\varphi_{mnt}/dz'^2+i2n_{mntz}d\varphi_{mnt}/dz' -\mathbf{n}_{mnt}^2\varphi_{mnt}+\sum_{u,v,w}\hat{\varepsilon}_{m-u,n-v,t-w}\varphi_{uvw}=0 , \tag{55}$$

where φ_{mnt} is a scalar function. All the other symbols have been defined previously. Use the so-called "state variable"[34] conjugate to φ_{mnt}, which is set to be[15]

$$\chi_{mnt}=-id\varphi_{mnt}/dz'+n_{mntz}\varphi_{mnt} . \tag{56}$$

Then, the whole set of equations in (55) and (56) may be converted into a set of first-order equations for the conjugate pairs of variables φ_{mnt} and χ_{mnt}. The latter set may be then combined into a grand matrix form as[15]

$$d\underline{f}/dz'=i\underline{C}\,\underline{f} \tag{57}$$

with $\underline{f}^t=(\underline{\varphi}^t\underline{\chi}^t)$, where $\underline{\varphi}$ and $\underline{\chi}$ are column matrices with elements φ_{mnt} and χ_{mnt}, respectively. Here the matrix $\underline{C}$ is exactly the same $\underline{C}$ matrix given in Eq. (46).

In region II, the solution of Eq. (57) is

$$\underline{f}^{\rm II}(z')=\underline{T}^{\rm II}\exp(i\underline{\varkappa}^{\rm II}z')\underline{a}^{\rm II} , \tag{58}$$

where $\underline{T}^{\rm II}$ is a square matrix consisting in a row of the column eigenvectors $\underline{\mu}_{uvw}^{{\rm II}q}$ of $\underline{C}^{\rm II}$, belonging, respectively, to the latter's eigenvalues $\varkappa_{uvw}^{{\rm II}q}$. These eigenvectors are arranged in $\underline{T}^{\rm II}$ in the same sequence as the eigenvalues $\underline{\varkappa}_{uvw}^{{\rm II}q}$ are arranged in the diagonal matrix $\underline{\varkappa}^{\rm II}$. We will show that the $\underline{T}^{\rm II}$ defined here is exactly equal to the $\underline{T}^{\rm II}$ defined in Sec. IV A.

Since in a vacuum region the submatrices in $\underline{C}^v$ are diagonal, Eq. (57) can be decomposed into

$$d\underline{f}_{mnt}^v/dz'=i\underline{C}_{mnt}^v\underline{f}_{mnt}^v \tag{59}$$

with $\underline{f}_{mnt}^v=(\varphi_{mnt}^v\,\chi_{mnt}^v)^t$ and

$$\underline{C}_{mnt}^v=\begin{bmatrix}0 & 1\\ 1-n_{mntx}^2-n_{mnty}^2 & 0\end{bmatrix} , \tag{60}$$

where we have set $n_{mntz}=0$ as before. The eigenvalues of $\underline{C}_{mnt}^v$ and their associated eigenvectors are $\pm\xi_{mnt}$ and $\underline{\mu}_{mnt}^{v\pm}=(1\ \pm\xi_{mnt})^t$, respectively. Hence

$$\underline{f}_{mnt}^v(z')=\underline{T}_{mnt}^v\exp[i\underline{\varkappa}_{mnt}^v(z'-z_0'^v)]\underline{a}_{mnt}^v , \tag{61}$$

where $\underline{\varkappa}_{mnt}^v$ is a 2×2 diagonal matrix with diagonal elements ξ_{mnt} and $-\xi_{mnt}$, arranged in this very sequence. $\underline{T}_{mnt}^v=(\underline{\mu}_{mnt}^{v+}\ \underline{\mu}_{mnt}^{v-})$ and $\underline{a}_{mnt}^v=(a_{mnt}^{v+}\ a_{mnt}^{v-})^t$. The solutions $\underline{f}_{mnt}^v$ in Eq. (61) may be combined into the solution of $\underline{f}^v$ as

$$\underline{f}^v(z')=\underline{T}^v\exp[i\underline{\varkappa}^v(z'-z_0'^v)]\underline{a}^v , \tag{62}$$

with $\underline{T}^v$ and $\underline{a}^v$ defined the same as in Sec. IV A. Here $\underline{\varkappa}^v$ is a block matrix with two diagonal submatices $\underline{\varkappa}^{v+}$ and $\underline{\varkappa}^{v-}$ on its diagonal in this sequence, while the elements of $\underline{\varkappa}^{v\pm}$ are $\varkappa_{mnt}^{v\pm}=\pm\xi_{mnt}$.

From the definitions of φ_{mnt} and χ_{mnt} given by Eqs. (17) and (56), we can see that the continuity of wave function and its partial derivative across a boundary imply the continuity of the matrix function $\underline{X}(i\underline{n}_zz')\underline{f}(z')$, where the function $\underline{X}$ has been defined previously. Thus, the boudary conditions are $\underline{f}^{\rm I}(0)=\underline{f}^{\rm II}(0)$ and $\underline{f}^{\rm III}(d')=\underline{X}(i\underline{n}_z^{\rm II}d')\underline{f}^{\rm II}(d')$. The simplicity of this form of boundary conditions for the matrix amplitude $\underline{f}$ is the reason why we define the state variable χ_{mnt} in the form of Eq. (56). Substituting the solution of $\underline{f}$ in each region as given by Eqs. (58) and (62) into these boundary conditions and eliminating the common factor $\underline{a}^{\text{II}}$, we obtain the same relation between $\underline{a}^{\text{I}}$ and $\underline{a}^{\text{III}}$ as given by Eqs. (53) and (54).

Now we start to show that the $\underline{T}^{\text{II}}$ defined here is the same as the $\underline{T}^{\text{II}}$ defined in Eq. (52). In another word, the matrix $\underline{T}^{\text{II}}$ that consists in a row of eigenvectors of $\underline{C}^{\text{II}}$ and the matrix $\underline{\Upsilon}^{\text{II}}$ that consists in a row of eigenvectors of Eq. (44) for region II are related by Eq. (52). From the definitions of $\underline{f}$ and χ_{mnt} we have

$$\underline{f}=\begin{bmatrix}\underline{\varphi}\\ -id\underline{\varphi}/dz'+\underline{n}_z\underline{\varphi}\end{bmatrix} . \tag{63}$$

The correspondence between the Bloch-wave expansion and the coupled-wave expansion, Eq. (26), may be rewritten more explicitly for region II as

$$\varphi^{\text{II}}_{mnt}(z')=\sum_{u,v,w,q} a^{\text{II}q}_{uvw} v^{\text{II}}_{mntuvw}\exp(i\varkappa^{\text{II}q}_{uvw}z') \tag{64a}$$

or

$$\underline{\varphi}^{\text{II}}(z')=\underline{\Upsilon}^{\text{II}}\sum_{q=1}^{2}\exp(i\underline{\varkappa}^{\text{II}q}z')\underline{a}^{\text{II}q} . \tag{64b}$$

Substituting Eqs. (64b) and (58) into Eq. (63) and then setting $z=0$, we obtain

$$\underline{T}^{\text{II}}\underline{a}^{\text{II}}=\begin{bmatrix}\underline{\Upsilon}^{\text{II}}\sum_q \underline{a}^{\text{II}q}\\ \underline{\Upsilon}^{\text{II}}\sum_q \underline{\varkappa}^{\text{II}q}\underline{a}^{\text{II}q}+\underline{n}_z^{\text{II}}\underline{\Upsilon}^{\text{II}}\sum_q \underline{a}^{\text{II}q}\end{bmatrix} . \tag{65}$$

This implies Eq. (52). Q.E.D. Thus, the RBW and RCW theories for spinless neutrons are equivalent as they ought to be. And here we have derived the explicit relation between them, Eq. (52).

The given incident wave in this spinless case is $\psi_{\text{inc}}=b\exp(i2\pi\mathbf{k}_0\cdot\mathbf{r})$, which implies the "initial conditions:" $\underline{a}^{\text{III}-}=\underline{0}$ and $\underline{a}^{\text{I}+}=b(0\ \cdots\ 0\ 1\ 0\ \cdots\ 0)^t$. These and Eq. (53) determine the diffraction amplitudes $a^{\text{I}-}_{mnt}$ and $a^{\text{III}+}_{mnt}$. The wave solution is

$$\psi^{\text{I}}=b\exp(i2\pi\mathbf{k}_0\cdot\mathbf{r})+\sum_{m,n,t}a^{\text{I}-}_{mnt}\exp(i2\pi\mathbf{k}^R_{mnt}\cdot\mathbf{r}) ,$$

$$\psi^{\text{II}}=\sum_{u,v,w,q}\sum_{m,n,t}a^{\text{II}q}_{uvw}v^{\text{II}}_{mntuvw}\exp(i2\pi\mathbf{k}^{\text{II}q}_{mntuvw}\cdot\mathbf{r}) , \tag{66}$$

$$\psi^{\text{III}}=\sum_{m,n,t}a^{\text{III}+}_{mnt}\exp[i2\pi\mathbf{k}^T_{mnt}\cdot(\mathbf{r}-d\hat{\mathbf{i}}_z)] ,$$

where

$$\mathbf{k}^{\text{II}q}_{mntuvw}=k_0\sin\theta^i\hat{\mathbf{i}}_x+k_0[(\varepsilon^{\text{II}}_{000}-\sin^2\theta^i)^{1/2}+\varkappa^{\text{II}q}_{uvw}]\hat{\mathbf{i}}_z +m\mathbf{b}_1+n\mathbf{b}_2+t\mathbf{b}_3 ,$$

and $\mathbf{k}^T_{mnt}$ and $\mathbf{k}^R_{mnt}$ are defined in Sec. III C.

V. DISCUSSIONS AND CONCLUSIONS

(i) We have formulated here the rigorous Bloch-wave and coupled-wave theories for both spinless neutrons and relativistic neutrons, basing upon the unified ground of (a) a common model for the wave diffractions from planar media with periodic structures and (b) the same Bloch theorem for the basis of wave expansions. The wave equations are characterized by the particle's spin values and the particle-medium interactions. The rigorous theories that are based on the common model and the same wave equation but different expansion forms are equivalent, of course.[3] We have pointed out that the RBW and RCW theories are the only rigorous diffraction theories that are convenient for numerical calculation in their exact forms and at the same time provide a clear physical insight to the diffraction phenomena. These conclusions are obviously true also for other waves such as electromagnetic waves and relativistic and spinless electrons since for them the equations of motion are also linear and homogeneous (cf. Refs. 15, 17, and 25).

(ii) The amplitudes of spinless and relativistic neutron diffraction waves in the RBW and RCW theories are formally solved in explicit matrix forms, which display a simple numerical calculation shceme and hence can be implemented on digital computers in a straightforward manner. No approximations have to be made except for the necessary finite truncation in series calculations. Precision of arbitrary levels may be achieved in principle, as long as the model based on which the theories are constructed remains applicable. All of these are also evidently true for all other waves (cf. Refs. 15, 17, and 19–25).

(iii) We have shown that the RBW and RCW analyses yield the same theory for the relativistic neutrons owing to the fact that a Dirac-type wave equation is of first order in spatial derivatives. The conclusion is also apparently true for relativistic electrons and electromagnetic waves since the Dirac equation of electron and the Maxwell equations are also first-order differential equations. Moreover, the RBW-RCW theory for relativistic neutrons has exactly the same form as the relativistic electron diffraction theory which is derived in RCW analysis in Ref. 17, except for the contents of the characteristic coefficient matrix $\underline{C}$ which contains the particular wave-medium interaction information of the given diffraction system. This is because both electron and neutron have the same spin value, $\frac{1}{2}$. The rigorous diffraction theory of electromagnetic waves (spin 1) derived via RCW analysis in Ref. 25 also has a very similar form.

(iv) The RBW and RCW theories are different (though equivalent) for the spinless neutrons. We have derived their explicit relation [Eq. (52)]. Clearly, the same relation should also exist for spinless electrons and TE and TM -polarized electromagnetic waves since they are all governed by second-order scalar differential equations of the same form. Besides, the RCW theory for spinless neutrons is of exactly the same form as that for spinless electrons given in Ref. 15, except that the electon-medium interaction $-eV$ is replaced by the neutron-medium interaction U,[35] while the RBW theory of spinless neutrons should have similar connection with Colella's[12] RBW theory for spinless electrons.

(v) In a nonrelativistic theory for neutrons or electrons, the Schrödinger equation is adopted as the equation of motion. The spin (i.e., polarization) and magnetic effects are then entirely neglected. These effects could be approximately accounted for by adopting, instead, the Pauli equation for a spin-$\frac{1}{2}$ nonrelativistic particle. But the corresponding RBW and RCW theories would have the same complexity and equally large dimension in the eigenvalue problems as a fully relativistic RBW-RCW theory.

(vi) For wave diffraction problems, the important topics of scattering matrix, transmittance and reflectance, conservation laws, polarization, Bragg's law, the convergence rate in numerical calculation, and the relation to the problems of guided wave in periodic structures have all been discussed in details for spinless and relativistic electrons in Refs. 15 and 17, respectively. The results are totally applicable to the spinless and relativistic neutrons, as apparent from our foregoing comparisons.

(vii) We have presented here two methods to solve the problem of relativistic neutron diffraction from planar crystals in the limiting case. Clearly, they are also applicable to the diffraction of all waves from slab media with periodic structures that are characterized either by one, two, or three grating vectors or by three reciprocal-lattice vectors when one vector is perpendicular to the slab surfaces. The second method is a new and most efficient approach to treat such a limiting case

(viii) Moon[36] has argued that in the limiting case (a) the RBW approach of Colella[12] has an insufficiency in the number of boundary conditions to fix all the unknown amplitudes, (b) this approach is inefficient in the use of computer time in numerical calculation, and (c) there exist subsets of equivalent eigenvalues to produce identical Bloch waves. But Colella[37] maintains that in his treatment[12] the number of boundary conditions is exactly matched to the number of unknowns in any case. From our derivation in the first approach for the limiting case, which is essentially the same as the Colella's,[12] we can see that the matching conditions on the boundaries are explicitly displayed in matrix forms and there is no insufficiency. But as we have pointed out, it is truly an inefficient method. From our discussions on the new approach, however, we see that the degeneracy in the limiting case is not caused by what is asserted by Moon.[36]

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