mPD, mPCLP and mDCLP surfaces) have been determined.

For IPMS in the regular class the explicit calculation of surface coordinates, *via* numerical integration of the Weierstrass representation, is readily performed. As each of the s branches of the Weierstrass function only differs by a constant factor $\exp(i\psi_p)$, the traversal of the Riemann surface induced in such a calculation is easily traced. Numerical generation of the *Flächenstück* is extremely useful in visualizing the lower-symmetry examples in which the plane lines of curvature and/or linear asymptotes do not define a boundary circuit. Even in higher-symmetry cases the computation is worthwhile since the interpenetrating labyrinth networks partitioned by the IPMS are not always immediately apparent.

The technique we have used also leads naturally to nonclassical minimal surfaces that are orientationally ordered but lack translational symmetry. Whether these surfaces are physically relevant remains to be seen. However, the recent interest in quasicrystalline structures and orientational order warrants there inclusion here. We have looked for surfaces whose point-group symmetries are those of the icosahedron, since these are allowed symmetries on the sphere, however, no such minimal surface exists within the regular class. (Note that such an icosahedral surface does exist as an irregular surface, of higher genus.) However, special positions on one of these new noncrystallographic surfaces, the pentagonal CLP surface, exhibits the same point-group symmetry as that of the so-called T-phases in rapidly quenched alloys (Bendersky, 1985). This symmetry has also been observed in a lyotropic liquid crystal (Fontell, 1991).

Having concluded our study of the regular class of IPMS, the question of possible extension of the construction algorithm to all IPMS arises. The recognition of this special class is a somewhat arbitrary one, introduced for the sake of simplicity of the Riemann-surface structure of the Weierstrass function, thus facilitating an exhaustive listing of all such possible surfaces. This listing serves a dual purpose - firstly, in unifying all previously discovered IPMS (*e.g.* D, P and CLP surfaces) within a systematic parametrization scheme that permits generalization to reduced-symmetry families and isolating new IPMS such as the VAL surface illustrated in Fig. 17(*b*) and (*c*) and, secondly, in the converse statement that there exists no other IPMS in this class. However, the limitations of this class are clear, both from the existence of 'irregular' IPMS, such as the Neovius [or C(P)] surface, and from the existence of 'regular' IPMS, such as the I-WP surface, which pass into the irregular class on crystallographic distortion. The construction framework of topological, geometrical and Riemann surface features established here permits a natural generalization of the above to the irregular class. This is addressed in a forthcoming study (Fogden, 1992).

References

BENDERSKY, L. (1985). *Phys. Rev. Lett.* **55**, 1461.

FISCHER, W. & KOCH, E. (1989). *Acta Cryst.* A**45**, 726-732.

FOGDEN, A. (1991). PhD thesis, Australian National Univ., Canberra, Australia.

FOGDEN, A. (1992). Submitted to *Acta Cryst.* A.

FOGDEN, A. & HYDE, S. T. (1992). *Acta Cryst.* A**48**, 442-451.

FONTELL, K. (1991). Private communication.

LIDIN, S. (1988). *J. Phys. (Paris)*, **49**, 421-427.

LIDIN, S. & HYDE, S. T. (1987). *J. Phys. (Paris)*, **48**, 1585-1590.

LIDIN, S., HYDE, S. T. & NINHAM, B. W. (1990). *J. Phys. (Paris)*, **51**, 801-813.

LIDIN, S. & LARSSON, S. (1990). *J. Chem. Soc. Faraday Trans.* **86**, 769-775.

SCHOEN, A. H. (1970). *Infinite Periodic Minimal Surfaces Without Self-Intersection. NASA Tech. Note* No. D-5541.

SCHWARZ, H. A. (1890). *Gesammelte Mathematische Abhandlungen.* Berlin: Springer.

Acta Cryst. (1992). A**48**, 591-595

Reciprocity in Electron Diffraction

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Abstract

The symmetry of reciprocity is reviewed in the context of relativistic quantum mechanics with the specific aim of relating to C, P and T invariances. From this investigation global time reversal is found to be a sufficient condition for reciprocity to hold in scattering from a vector potential. The present proof is free from assumptions of small-angle scattering and from restrictions on z-dependent terms in the scattering equation, and by avoiding S-matrix theory is thought to be accessible to undergraduate teaching.

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1. Introduction

The theorem of reciprocity has found everyday application in electron diffraction. Initially, through the work of von Laue (1935) and Cowley (1969), and later Moodie (1972) and Buxton, Eades, Steeds & Rackham (1976), this theorem has become a basic element in electron diffraction analysis and analysis of z symmetries in electron-microscope contrast. However, little progress has been made in relating these symmetries directly to those of relativistic quantum mechanics. Standard derivations of the reciprocity relation using time-reversal (TR) symmetry and the S-matrix formalism (see, for example, Merzbacher, 1961) are dependent upon the invariance of a Hermitian Hamiltonian under TR. This leaves something to be desired in terms of the specifics of the time-stationary N-beam solution; see, for example, Portier & Gratias (1982).

On the other hand, Pogany & Turner (1968) gave a proof that relied only on the symmetry of a Green's function involved in the solution of the non-relativistic Schrödinger equation following an earlier proof by Bilhorn, Foldy, Thaler & Tobocam (1964). In this present note we aim to extend their method to the Klein–Gordon equation and to the presence of a vector potential. This latter consideration is interesting because of the experimental observation by Tonomura, Matsuda & Endo (1986) of the breakdown of reciprocity for a magnetic specimen (the actual purpose of these authors was to exploit this breakdown in separating electrostatic and magnetic phase changes, but in so doing their results gave an experimental verification).

Elastic scattering is assumed in the present paper, which deals exclusively with the scattering of a charged particle by an electromagnetic field. However, derivations for electromagnetic radiation and a dielectric field, and for a charged particle undergoing specific inelastic processes, will be considered in the near future.

2. Derivation

Models

Electron diffraction can be modelled by an electron plane wave scattering off some object in which the four-potential $A^\alpha = (\varphi, \mathbf{A})$ is nonzero within the volume Ω occupied by the scatter. The source of particles (an electron gun) is denoted by the point P and the detector (a plate) by the point Q.

For small accelerating potentials, the electrons are nonrelativistic and may be treated with the Schrödinger equation but, for large accelerating potentials, the Dirac equation should be used. Since the effect of the electron spin is usually negligible in both cases, the Klein–Gordon equation may be used in the relativistic case.

Reciprocity

If $\Psi_P(\mathbf{r})$ denotes the scattered wave function at $\mathbf{r}$ with the source at P, then this notation can be used to define the notion of reciprocity:

$$|\Psi_Q(\mathbf{r}_P)| = |\Psi_P(\mathbf{r}_Q)|. \tag{1}$$

What this amounts to is an interchange of source and detector or, in the particular case of elastic scattering, a rotation of 180° of the scatterer about the direction defined by the direction of the change-in-momentum vector $\Delta\mathbf{p} = \mathbf{p}_f - \mathbf{p}_i$, where $\mathbf{p}_i$ and $\mathbf{p}_f$ are the incident and scattered electron momenta respectively (see Fig. 1). Although the following discussion is confined to spherical waves, these directions are still well defined when the source–scatterer and detector–scatterer distances are large compared with the dimensions of the scatterer.

We seek to find under which conditions (*i.e.* the constraints on the potentials φ, $\mathbf{A}$) an experiment can be said to be subject to the reciprocity condition (1). This amounts to finding the constraints on φ and $\mathbf{A}$ that guarantee an identical beam intensity at the point Q on the plate when the scatterer is rotated as described above. The relationship of this symmetry to other fundamental quantum-mechanical symmetries (C, P and T) will be discussed.

Motivation from classical results

The relativistic but classical (*i.e.* non-quantum-mechanical) path of the electron can be computed uniquely from the Lagrangian

$$L_c(\mathbf{u}, \mathbf{A}, \varphi, e) = -\mu c^2(1 - u^2/c^2)^{1/2} + (e/c)\mathbf{u}\cdot\mathbf{A} - e\varphi,$$

where the potentials are in general non-parity-invariant (*i.e.* unsymmetric). Table 1 shows the effect of the fundamental transformations C, P and T on the potentials A^α, the charge e and the velocity (momentum) $\mathbf{u}(\mathbf{p})$. This assumes a global transformation – as if the experimenter were able to change the fields inside the sample as well as the direction of the electron beam.

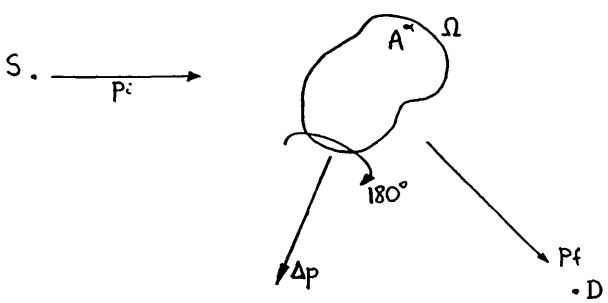

Fig. 1. Schematic diagram showing the equivalence of a 180° rotation of the scatterer about $\Delta\mathbf{p}$ to the reciprocity symmetry.

Table 1. *Global C, P and T transformations*

Transformation	$\mathbf{A}'(\mathbf{r}')$	$\varphi'(\mathbf{r}')$	$\mathbf{u}', \mathbf{p}'$	e'	L_c'
C	$-\mathbf{A}(\mathbf{r})$	$-\varphi(\mathbf{r})$	$\mathbf{u}, \mathbf{p}$	$-e$	L_c
P	$\mathbf{A}(-\mathbf{r})$	$\varphi(-\mathbf{r})$	$-\mathbf{u}, -\mathbf{p}$	e	?
T	$-\mathbf{A}(\mathbf{r})$	$\varphi(\mathbf{r})$	$-\mathbf{u}, -\mathbf{p}$	e	L_c
CT	$\mathbf{A}(\mathbf{r})$	$-\varphi(\mathbf{r})$	$-\mathbf{u}, -\mathbf{p}$	$-e$	L_c

Table 2. *Restricted C, P and T transformations*

Transformation	$\mathbf{A}'(\mathbf{r}')$	$\varphi'(\mathbf{r}')$	$\mathbf{u}', \mathbf{p}'$	e'	L_c'
C	$\mathbf{A}(\mathbf{r})$	$\varphi(\mathbf{r})$	$\mathbf{u}, \mathbf{p}$	$-e$	?
P	$\mathbf{A}(\mathbf{r})$	$\varphi(\mathbf{r})$	$-\mathbf{u}, -\mathbf{p}$	e	?
T	$\mathbf{A}(\mathbf{r})$	$\varphi(\mathbf{r})$	$-\mathbf{u}, -\mathbf{p}$	e	?
CT	$\mathbf{A}(\mathbf{r})$	$\varphi(\mathbf{r})$	$-\mathbf{u}, -\mathbf{p}$	$-e$	?

The entries in Table 1 imply that the electron path is classically reversible (and therefore reciprocal) under any combination of C or T global transformations. This is also clear by inspection of the Lorentz force

$$\mathbf{F} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) = e(-\nabla\varphi + \mathbf{v} \times \nabla \times \mathbf{A}),$$

where conservation of the force $\mathbf{F}$ under reversal of the velocity $\mathbf{v}$ requires conservation of the sign of $e\varphi$ and a flip in the sign of $e\mathbf{A}$. More realistically, however, the experimenter will only be able to change the direction and charge of the particles being fired at the specimen and not the internal fields: see Table 2. Thus the Lagrangian is noninvariant and the experimenter cannot expect to see a reciprocal system. In the special case of a negligible magnetic field (which turns out to be relevant to a very wide class of materials), the system is reciprocal under 'restricted' time reversal, which corresponds to the 180° rotation described above. The condition for this is

$$\beta = \frac{u}{c} \ll \frac{\varphi}{A} \sim \frac{\text{electric field}}{\text{magnetic field}}.$$

Reciprocity theorems in quantum mechanics

Nonrelativistic case. The proof of reciprocity for the nonrelativistic case follows closely that of Bilhorn *et al.* (1964), but we incorporate the magnetic field to obtain greater generality. Natural units ($\hbar = c = 1$) are used throughout. We assume the scatterer and electron system can be described by a Hamiltonian of form

$$H = (1/2\mu)(\mathbf{p} - e\mathbf{A})^2 + e\varphi(\mathbf{r}),$$

where no spin interactions have been incorporated. We claim that the equation

$$(H - i\partial_t)\Psi_P(\mathbf{r}, t) = \delta(\mathbf{r} - \mathbf{r}_P)\exp(-iEt),$$

which can be written in the separated form (providing the potentials are time-independent)

$$(H - E)\Psi_P(\mathbf{r}, t) = \delta(\mathbf{r} - \mathbf{r}_P),$$

$$\Psi_P(\mathbf{r}, t) = \Psi_P(\mathbf{r})\exp(-iEt),$$

corresponds to a source at point P (an electron gun) of electrons of energy E that are in stationary states. This is justified by the fact that the 'incident' wave function on the volume Ω will have the asymptotic form

$$\Psi_P(\mathbf{r}, t) \sim |\mathbf{r} - \mathbf{r}_P|^{-1} \exp\{i[\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_P) - Et]\}, \quad (2)$$

which looks exactly like the plane wave assumed in conventional scattering theory when $|\mathbf{r} - \mathbf{r}_P|$ is large compared to the dimensions of the scatterer (*i.e.* $|\mathbf{r} - \mathbf{r}_P|$ will be virtually constant over the range of the interaction). This is manifestly true in, say, an electron microscope, where $|\mathbf{r} - \mathbf{r}_P|$ will be the gun-specimen distance.

A point source at A of electrons of energy E will then be described by the equation

$$[(1/2\mu)(-i\nabla - e\mathbf{A})^2 + e\varphi(\mathbf{r}) - E]\Psi_A(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_A) \quad (3)$$

and an identical point source at B will be described by

$$[(1/2\mu)(-i\nabla - e\mathbf{A})^2 + e\varphi(\mathbf{r}) - E]\Psi_B(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_B). \quad (4)$$

If we integrate the result of multiplying equation (3) by $\Psi_B(\mathbf{r})$ and subtracting equation (4) multiplied by $\Psi_A(\mathbf{r})$ over all space, we obtain

$$\begin{aligned}\Psi_B(\mathbf{r}_A) - \Psi_A(\mathbf{r}_B) &= (1/2\mu)\int[(\Psi_A\nabla^2\Psi_B - \Psi_B\nabla^2\Psi_A) \\ &\quad + 2ie\mathbf{A} \cdot (\Psi_A\nabla\Psi_B - \Psi_B\nabla\Psi_A)]\,\mathrm{d}^3r.\end{aligned}$$

The first term in the integral can be written

$$\int \nabla \cdot (\Psi_A\nabla\Psi_B - \Psi_B\nabla\Psi_A)\mathrm{d}^3r = \int_{\partial S} (\Psi_A\nabla\Psi_B - \Psi_B\nabla\Psi_A) \cdot \mathrm{d}\mathbf{S}.$$

But since the Ψs satisfy homogeneous boundary conditions of the form

$$\alpha\Psi + \beta\,\partial\Psi/\partial n = 0$$

at the bounding surface ∂S at infinity (Bilhorn *et al.*, 1964), this contribution to the integral vanishes and the final result is

$$\Psi_B(\mathbf{r}_A) - \Psi_A(\mathbf{r}_B) = (ie/\mu)\int \mathbf{A} \cdot (\Psi_A\nabla\Psi_B - \Psi_B\nabla\Psi_A)\,\mathrm{d}^3r \neq 0 \quad (5)$$

in general.

Now one possible description of a zero magnetic field is $\mathbf{A} = \mathbf{0}$, in which case it is obvious that the integral in (5) vanishes and the system is reciprocal, *i.e.* $\Psi_B(\mathbf{r}_A) = \Psi_A(\mathbf{r}_B)$. The immediate question is then whether this is a gauge-invariant result, *i.e.* can $\Psi_B(\mathbf{r}_A)$ and $\Psi_A(\mathbf{r}_B)$ be made to differ by more than a phase factor by the action of gauge transformations.

To answer this question it is necessary to recall that Green's functions $\Psi_A(\mathbf{r})$ and $\Psi_B(\mathbf{r})$ are not gauge invariant and, under the usual gauge transformations

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\chi(\mathbf{r})$$
$$\varphi \to \varphi' = \varphi - \partial\chi(\mathbf{r})/\partial t = \varphi$$
$$\Psi(\mathbf{r}) \to \Psi'(\mathbf{r}) = \Psi(\mathbf{r}) \exp[ie\chi(\mathbf{r})]$$
$$(\chi \in \mathbf{R} \text{ necessarily}),$$

the new wave function $\Psi_A'(\mathbf{r})$ satisfies the equation

$$(H' - E)\Psi_A'(\mathbf{r}) = \exp[ie\chi(\mathbf{r}_A)]\delta(\mathbf{r} - \mathbf{r}_A), \quad (6)$$

which amounts simply to a phase shift in the source. Such a phase shift is in principle not measurable, which suggests that the reciprocity result above is gauge invariant. By repeating the above derivation starting from (6) we obtain the result

$$\begin{aligned}
&\Psi_B(\mathbf{r}_A)\exp[ie\chi(\mathbf{r}_A)] - \Psi_A(\mathbf{r}_B)\exp[ie\chi(\mathbf{r}_B)] \\
&= (1/2\mu)\int[(\Psi_A'\nabla^2\Psi_B' - \Psi_B'\nabla^2\Psi_A') \\
&\quad + 2ie\mathbf{A}'\cdot(\Psi_A'\nabla\Psi_B' - \Psi_B'\nabla\Psi_A')]\,d^3r \\
&= (ie/\mu)\int(\mathbf{A} + \nabla\chi) \\
&\quad \times(\Psi_A\nabla\Psi_B - \Psi_B\nabla\Psi_A)\exp(2ie\chi)\,d^3r, \quad (7)
\end{aligned}$$

where the first part of the integral vanishes by the argument used above.

If we put $\mathbf{A} = \nabla\xi$ in (5) to take into account all possible expressions of the magnetic potential corresponding to zero magnetic field, then clearly a choice of gauge transformation $\chi = -\xi$ renders the integral in (7) trivially zero, so we may write

$$\Psi_B(\mathbf{r}_A)\exp[-ie\xi(\mathbf{r}_A)] = \Psi_A(\mathbf{r}_B)\exp[-ie\xi(\mathbf{r}_B)]$$

and therefore

$$|\Psi_B(\mathbf{r}_A)| = |\Psi_A(\mathbf{r}_B)|,$$

which is the desired reciprocity result. This indicates that reciprocity holds at least in the nonrelativistic case in the absence of magnetic fields.

Relativistic case. The proof for the Klein-Gordon and Dirac equations follows along similar lines; under the same assumptions of time-independent potentials and stationary-wave functions of energy E, the Klein-Gordon equation for a source at point A is

$$[(E - e\varphi)^2 - (-i\nabla - e\mathbf{A})^2 - \mu^2]\Psi_A(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_A). \quad (8)$$

Writing the same equation for a source at point B and cross-multiplying and integrating as before, we obtain

$$\begin{aligned}
&\Psi_B(\mathbf{r}_A) - \Psi_A(\mathbf{r}_B) \\
&= [(\Psi_B\nabla^2\Psi_A - \Psi_A\nabla^2\Psi_B) \\
&\quad + 2ie\mathbf{A}\cdot(\Psi_A\nabla\Psi_B - \Psi_B\nabla\Psi_A)]\,d^3r. \quad (9)
\end{aligned}$$

The first part of the integral vanishes by the same arguments advanced previously and so we have the result

$$\begin{aligned}
&\Psi_B(\mathbf{r}_A) - \Psi_A(\mathbf{r}_B) \\
&\quad = 2ie\int\mathbf{A}\cdot(\Psi_A\nabla\Psi_B - \Psi_B\nabla\Psi_A)\,d^3r \neq 0 \quad (10)
\end{aligned}$$

in general.

Under the standard gauge transformations above, the transformed wave function satisfies

$$\begin{aligned}
&[(E - e\varphi')^2 - (i\nabla - eA')^2 - \mu^2]\Psi_A(\mathbf{r})' \\
&\quad = \exp[ie\chi(\mathbf{r}_A)]\delta(\mathbf{r} - \mathbf{r}_A) \quad (11)
\end{aligned}$$

and a repetition of the derivation shows that the difference integral is

$$\begin{aligned}
&\Psi_B(\mathbf{r}_A)\exp[ie\chi(\mathbf{r}_A)] - \Psi_A(\mathbf{r}_B)\exp[ie\chi(\mathbf{r}_B)] \\
&= \int[(\Psi_A'\nabla^2\Psi_B' - \Psi_B'\nabla^2\Psi_A') \\
&\quad + 2ie\mathbf{A}'\cdot(\Psi_A'\nabla\Psi_B' - \Psi_B'\nabla\Psi_A')]\,d^3r \\
&= 2ie\int(\mathbf{A} + \nabla\chi)\cdot(\Psi_A'\nabla\Psi_B' - \Psi_B'\nabla\Psi_A')\,d^3r. \quad (12)
\end{aligned}$$

The gauge invariance of the zero-magnetic-field reciprocity displayed by (10) is readily proved by choosing $\mathbf{A} = \nabla\xi$ and a gauge transform $\chi = -\xi$ such that the integral in (12) vanishes and thus

$$|\Psi_B(\mathbf{r}_A)| = |\Psi_A(\mathbf{r}_B)|. \quad (13)$$

The proof for the Dirac equation follows immediately upon recollection of the fact that each of the components of the Dirac four-spinor ψ (in the usual representation) satisfies the Klein-Gordon equation, and the homogeneous boundary conditions may be written

$$\lambda\psi + \rho\frac{\partial\psi}{\partial n} = 0 \Leftrightarrow \lambda_{ii}\psi_i + \rho_{ii}\frac{\partial\psi_i}{\partial n} = 0,$$

where λ and ρ are some 4×4 diagonal matrices whose elements will not be independent because of the normalization of ψ. But this implies that each component ψ_i of the spinor satisfies the reciprocity relation (13), and since the Dirac probability density is

$$P(\mathbf{r}) = \psi(\mathbf{r})^\dagger\psi(\mathbf{r}) = \sum_{i=1}^{4}|\psi_i(\mathbf{r})|^2,$$

clearly the probability density is also reciprocal;

$$P_B(\mathbf{r}_A) = P_A(\mathbf{r}_B).$$

Reciprocity under global T or CT transformations

This section gives the proofs for the Klein-Gordon case (and thus by implication the Dirac and Schrödinger cases) when the change of the source location to point B is also accompanied by a global transformation T or CT on all the fields and charges. Note that these transformations are generally not experimentally realizable except in certain trivial cases (*e.g.* $\mathbf{B} = \mathbf{0}$).

From Table 1 it is clear that the product $e\mathbf{A}$ reverses sign under global T or CT transformations, and the product $e\varphi$ remains constant, so (8) with the source shifted to point B and $e\mathbf{A} \rightarrow -e\mathbf{A}$ becomes

$$[(E-e\varphi)^2-(-i\nabla+e\mathbf{A})^2-\mu^2]\Psi_B(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}_B). \quad (14)$$

Note that this is not a formal time-reversal operation involving a complex conjugation; (14) is simply the answer to the question 'what equation describes the evolution of a particle $\psi_B(\mathbf{r})$ of energy E, charge $\pm e$, with a source at point B and the field $e\mathbf{A}$ reversed in direction whilst the electrostatic interaction is unchanged?' Since time reversal interchanges the processes of emission and absorption, this effect is incorporated by interchanging the spatial locations of the source and detector. Repeating the usual derivation using (8) and (14) then yields

$$\psi_B(\mathbf{r}_A)-\psi_A(\mathbf{r}_B) = -2ie\int \nabla\cdot(\mathbf{A}\Psi_A\Psi_B)\,\mathrm{d}^3r. \quad (15)$$

Any realistic potential can be written as

$$\mathbf{A} = \mathbf{A}_{\text{phys}} + \nabla\xi,$$

where $\mathbf{A}_{\text{phys}}$ is a physical potential of form

$$\mathbf{A}_{\text{phys}}(\mathbf{r}) \sim \int [\mathbf{j}(\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|]\,\mathrm{d}^3r$$

and ξ is any arbitrary gauge variable. $\mathbf{j}(\mathbf{r}')$ is nonzero only in the region Ω, so $\mathbf{A}_{\text{phys}}(\mathbf{r}) \sim r^{-1}$ at large distances, as do the wave functions $\Psi_A(\mathbf{r})$ and $\psi_B(\mathbf{r})$ as a consequence of having a point source. Hence the integral

$$\int \nabla\cdot(\mathbf{A}_{\text{phys}}\psi_A\psi_B)\,\mathrm{d}^3r = \int_{\partial S} \mathbf{A}_{\text{phys}}\psi_B\psi_A\cdot\mathrm{d}\mathbf{S} \sim \lim_{R_s\rightarrow\infty}(4\pi R_s^2/R_s^3) = 0.$$

Under the usual gauge transform {with $\psi_B(\mathbf{r})' = \psi_B(\mathbf{r})\exp[\pm ie\chi(\mathbf{r})]$ depending of course on whether charge conjugation has been employed}, (15) becomes

$$\psi_B(\mathbf{r}_A)\exp[ie\chi(\mathbf{r}_A)]-\psi_A(\mathbf{r}_B)\exp[\pm ie\chi(\mathbf{r}_B)] = -2ie\int\nabla\cdot[(\mathbf{A}+\nabla_\chi)\psi'_A\psi'_B]\,\mathrm{d}^3r$$

and if we choose $\chi = -\xi$, then the right-hand side behaves exactly like the integral in (16), which is identically zero, so once again we have $|\psi_B(\mathbf{r}_A)| = |\psi_A(\mathbf{r}_B)|$ as a gauge-independent result.

3. Results and discussion

The main conclusion reached from the above derivation is that global time reversal (GTR) lies behind the symmetry we call reciprocity in electron diffraction. These investigations have also highlighted the main conceptual difficulty that has prevented a ready acceptance of this fact in the past, that is, that working within the formalism of stationary states as required for the calculation of coherently scattered electron intensities precludes the use of 'initial' and 'final' states needed in TR proofs. The problem here, like that formulated in the Aharanov–Bohm effect, arises from particle-wave duality: the N-beam diffraction is envisaged (and computed as in multislice methods) as a monochromatic and classical wave equation. Finally, however, the interpretation requires a source and detector for each diffraction channel involving electrons as particles.

A not unexpected consequence of the requirement of GTR is that reciprocity will not hold for a magnetic specimen, since reversal of the internal currents and hence magnetic field are part of that requirement.

Finally, the present proof is not dependent on assumption of 'small-angle' scattering and so is equally applicable to LEED (low-energy electron diffraction). For this reason it should replace earlier use of the small-angle approximation, which initially appeared to provide a simple picture of reciprocity as a z-reversal symmetry. However, when it was later found (Portier & Gratias, 1982) that this picture was valid only for the exact Bragg condition, the simplification became counter-productive, even as a teaching aid.

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References

BILHORN, D. E., FOLDY, L. L., THALER, R. M. & TOBOCAM, W. (1964). *J. Math. Phys. (NY)*, **5**, 435-441.
BUXTON, B. F., EADES, J. A., STEEDS, J. W. & RACKHAM, G. M. (1976). *Philos. Trans. R. Soc. Ser. A*, **281**, 171-194.
COWLEY, J. M. (1969). *Appl. Phys. Lett.* **15**, 58.
LAUE, M. VON (1935). *Ann. Phys. (Leipzig)*, **23**, 705.
MERZBACHER, E. (1961). *Quantum Mechanics*, p. 506. New York: John Wiley.
MOODIE, A. F. (1972). *Z. Naturforsch. Teil A*, **27**, 437-440.
POGANY, A. P. & TURNER, P. S. (1968). *Acta Cryst.* A**24**, 103-109.
PORTIER, R. & GRATIAS, D. (1982). In *Electron Microscopy and Analysis* 1981, edited by M. J. GORINGE, pp. 275-278. Bristol: Institute of Physics.
TONOMURA, A., MATSUDA, T. & ENDO, J. (1986). *Phys. Rev. B*, **34**, 3397-3402.