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PEROVSKITES Solid-state X-ray detector

QUANTUM CASCADE LASERS Sub-hertz linewidth

TWO-DIMENSIONAL MATERIALS Population inversion

Kramers-Kronig revisited



Spatial Kramers-Kronig relations and the reflection of waves

S. A. R. Horsley^{1*}, M. Artoni^{2,3} and G. C. La Rocca⁴

When a planar dielectric medium has a permittivity profile that is an analytic function in the upper or lower half of the complex position plane x = x' + ix'' then the real and imaginary parts of its permittivity are related by the spatial Kramers-Kronig relations. We find that such a medium will not reflect radiation incident from one side, whatever the angle of incidence. Using the spatial Kramers-Kronig relations, one can derive a real part of a permittivity profile from some given imaginary part (or vice versa) such that the reflection is guaranteed to be zero. This result is valid for both scalar and vector wave theories and may have relevance for designing materials that efficiently absorb radiation or for the creation of a new type of anti-reflection surface.

A wave propagating through an inhomogeneous medium is usually partially reflected, which is often undesirable from a practical point of view. Although the reflection from a sharp interface can be suppressed by applying an anti-reflection coating¹, less is understood about what is required in order for a generic inhomogeneous medium not to reflect any radiation. There are some well-known examples of non-reflecting material profiles, such as the hyperbolic secant profile described by Landau and Lifshitz2, which has been discussed by Lekner³ (see ref. 4 for an experimental realization). More recently, the design technique of transformation optics^{5,6} has made significant strides forward, giving us a strategy for finding inhomogeneous, anisotropic materials (transformation media) that reflect no radiation, whatever the incident field^{5,7,8}. In the same vein, perfectly matched layers⁹ are a family of anisotropic lossy media that are often used in computer simulations to mimic an infinitely extended system and are closely connected to transformation media, absorbing a wave without producing any reflection¹⁰⁻¹². The last few years have seen increasing interest in the property of parity-time (PT) symmetry in optics^{13–15}, partly because media with this property can suppress reflection 16,17. For complex permittivities this requires regions of gain $(\text{Im}[\epsilon(x)] < 0)$ as well as loss $(\text{Im}[\epsilon(x)] > 0)$ and has been connected to the use of complex coordinates in transformation optics¹⁸. Realizing any of these non-reflecting materials is challenging, but suitably structured metamaterials¹⁹ are promising, because a wide range of material parameters can be achieved through the use of specially designed sub-wavelength elements. In particular, recent work on 'dispersion engineering'²⁰ has seen simultaneous control of the real and imaginary parts of the permittivity and permeability, which is necessary to realize PT-symmetric media, as well as the materials proposed in this work.

Here, we find a new and very general relation between the real and imaginary parts of a (locally isotropic) planar permittivity profile $\epsilon(x)$ that guarantees zero reflection. The result makes use of the properties of $\epsilon(x)$ at complex values of the spatial coordinate x = x' + ix'' to predict what happens to the wave when x is real. In short, when the permittivity profile $\epsilon(x' + ix'')$ is an analytic function

(that is, without poles or branch cuts) in the upper or lower half of the complex position plane—and therefore obeys the Kramers-Kronig relations in space—the reflection from respectively the left or right of the profile vanishes, whatever the angle of incidence. We note at the outset that this condition is only sufficient and not necessary for zero reflection. As a corollary of our finding, if the real part of such a non-reflecting permittivity profile is symmetric about some point in space, then the corresponding imaginary part always turns out to be antisymmetric about this point, thus exhibiting PT-symmetry. We stress, however, that the spatial Kramers-Kronig relations do not require any definite symmetry under inversion of space or reversal of time, so they lead to an enormous class of reflectionless metamaterials. Furthermore, while requiring appropriate dispersion engineering in space, the requisite materials are locally isotropic, non-magnetic and do not rely in general on the presence of gain or negatively refracting media. This makes our findings quite distinct from those based on PT-symmetry, which always need gain or make use of transformation optics (for example, ref. 18), which nearly always require anisotropic magnetic materials.

Consider a monochromatic electromagnetic wave of frequency ω propagating in the x-y plane within a medium with an inhomogeneous permittivity e(x) that tends to a constant positive value e_b as $x \to \pm \infty$. A schematic of this situation is shown in Fig. 1a. The two polarizations are transverse electric (TE, electric field along z) and transverse magnetic (TM, magnetic field along z). For TE polarization we can write the electric field as

$$E_z(x, y) = e_z(x)e^{ik_y y} \tag{1}$$

where k_y determines the angle of incidence and the *x*-dependent amplitude e_z obeys the one-dimensional Helmholtz equation:

$$\frac{d^2 e_z}{dx^2} + [K^2 + k_0^2 \alpha(x)]e_z = 0$$
 (2)

In equation (2), $K = \pm (\epsilon_b k_0^2 - k_y^2)^{1/2}$ and the permittivity has the assumed form of the positive background contribution ϵ_b plus a spatially varying part

$$\epsilon(x) = \epsilon_{\rm b} + \alpha(x) \tag{3}$$

with $k_0 = \omega/c$. The spatially varying part of the permittivity $\alpha(x)$ vanishes at large distances from the origin, where the field is composed of plane waves $\exp(\pm iKx)$. Now suppose that a right-going wave comes from infinity $x = -\infty$ and onto the inhomogeneous permittivity profile. The effect is to produce a scattered field e_s , and we can write the total field as

$$e_{z}(x) = E_0 e^{iKx} + e_{s}(x) \tag{4}$$

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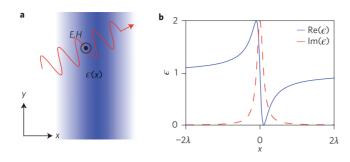


Figure 1 | Wave propagation through inhomogeneous media. a, A wave propagating in the x-y plane in an inhomogeneous medium with permittivity $\varepsilon(x)$ (indicated by blue shading). The TE polarization has an electric field pointing only along z and the TM polarization has a magnetic field pointing only along z. When the real (blue) and imaginary (red) parts of the permittivity are related to one another by the Kramers-Kronig relations (as in **b**) then the reflection vanishes for all angles of incidence. **b**, Permittivity profile $\varepsilon(x)$ given by equation (11) for parameters A = 2.0 and $\xi = 0.1\lambda$ with $\lambda = 2\pi/k_0$.

where K > 0. Inserting equation (4) into equation (2), we find the inhomogeneous differential equation that governs the scattered field:

$$\left[\frac{d^2}{dx^2} + K^2 + k_0^2 \alpha(x)\right] e_s(x) = -k_0^2 \alpha(x) E_0 e^{iKx}$$
 (5)

One well-known way to solve equation (5) is to expand e_s as a series, $e_s = \sum_n e_s^{(n)}$, where the *n*th term is proportional to the *n*th power of α . The first term in this series—known as the Born approximation in scattering calculations—can be found immediately and is

$$e_{\rm s}^{(1)}(x) = -E_0 k_0^2 \int \frac{{\rm d}k}{2\pi} G(k) \tilde{\alpha}(k-K) {\rm e}^{{\rm i}kx}$$
 (6)

where $\tilde{\alpha}$ is the spatial Fourier transform of $\alpha(x)$ and G(k) is the retarded Green function (η is an infinitesimal positive number)

$$G(k) = \frac{1}{(K + in)^2 - k^2}$$
 (7)

Notice that if $\tilde{\alpha}(k < 0) = 0$, then the Born approximation to the scattered field (equation (6)) is made up of only right-going waves, whatever the value of K (that is, whatever the angle of incidence). This means that to first order in $\alpha(x)$ there is no back-scattering from such a permittivity profile. As a first order result this is not all that remarkable, but by examining all the other terms in the series expression for e_s we can see that there is actually no backscattering to any order. To prove this, consider the nth term in the scattering series:

$$e_{s}^{(n)}(x) = -k_{0}^{2} \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} G(k) \tilde{\alpha}(k-k') \tilde{e}_{s}^{(n-1)}(k') e^{ikx}$$
 (8)

This term is also made up of only right-going waves if (1) the Fourier components of the scattered electric field $\tilde{e}^{(n-1)}$ are zero for left-going waves $\tilde{e}^{(n-1)}(k<0)=0$ and (2) the Fourier components of the permittivity profile are also zero for left-going waves $\tilde{\alpha}(k<0)=0$. We have already established that $e_s^{(1)}$ is made up of entirely right-going waves when $\tilde{\alpha}(k<0)=0$, so every successive term also contains only right-going waves. There is thus zero back-scattering to every order when $\tilde{\alpha}(k<0)=0$. One way to understand this result is to think that when a wave scatters multiple times from an object, for each scattering event there is a momentum change Δk that occurs with an amplitude proportional to $\tilde{\alpha}(\Delta k)$.

A permittivity profile that has only positive Fourier components therefore cannot convert a right-going wave to a left-going one. It might appear that this argument relies on a smallness condition for $\alpha(x)$, but in Supplementary Section A we give an alternative argument that does not rely on a series expansion of the electric field, and in Supplementary Section B we derive two exact solutions for propagation in such profiles that confirm the effect. Supplementary Section C contains a numerical investigation to show that an order-of-magnitude increase in $\alpha(x)$ does not disturb the non-reflecting behaviour.

In light of these properties, such non-reflecting permittivity profiles can generally be written as

$$\epsilon(x) = \epsilon_{\rm b} + \int_{0}^{\infty} \frac{\mathrm{d}k}{2\pi} \tilde{\alpha}(k) \mathrm{e}^{\mathrm{i}kx} \tag{9}$$

which is necessarily a complex function of position. The spatial distribution of the reactive and dissipative parts of such a material response together completely suppress reflection. To make use of this finding, we note that equation (9) is the same in form as the relationship between the susceptibility in the frequency and time domains, which embodies the causality principle²¹, and one need only make the replacements $k \to t$ and $x \to \omega$ in equation (9) to recover this well-known formula. As a consequence^{22,23}, the non-reflecting permittivity profile $\alpha(x)$ is an analytic function in the upper half complex position plane and satisfies the Kramers–Kronig relations in space:

$$\operatorname{Re}[\alpha(x)] = \frac{1}{\pi} \operatorname{P} \int_{-\infty}^{\infty} \frac{\operatorname{Im}[\alpha(s)]}{s - x} ds$$
 (10)

where P indicates the principal part of the integral. Therefore, if we were given some $\text{Im}[\alpha(s)]$, say as a (square integrable) function of position, a corresponding real part can be constructed from equation (10) such that the reflection from the complex susceptibility profile is zero. We note that if the imaginary part of $\alpha(x)$ is symmetric about x = 0, then the real part calculated from equation (10) will be antisymmetric and vice versa. Accordingly, the Kramers-Kronig relations generate a whole family of permittivity profiles that exhibit PT-symmetry $(\alpha(-x) = \alpha^*(x))$. Similarly, we also have a whole family of non-reflecting profiles where $\alpha(x)$ exhibits PT-antisymmetry ($\alpha(-x) = -\alpha^*(x)$), a property that has already been associated with zero back-scattering in optics²⁴, just as is the case for PT-symmetry²⁵. In fact, even purely lossy periodic media can be engineered²⁶ such that their Bragg reflection from one side vanishes when the real and imaginary parts of their susceptibility are spatially out of phase, which is a characteristic property of Hilbert transform pairs. However, our findings are more general than these known results, as they are also compatible with nonreflecting profiles exhibiting no definite PT-symmetry at all.

As an initial illustration of this finding, we consider the simplest example: a permittivity profile with a single pole in the lower half position plane

$$\epsilon(x) = \epsilon_{\rm b} + A \frac{\mathrm{i} - x/\xi}{1 + (x/\xi)^2} \tag{11}$$

where ξ sets the spatial scale of the profile and A the amplitude. Equation (11) is plotted in Fig. 1 and takes a form that would be very familiar if the x-axis represented frequency rather than space. The non-reflecting behaviour is demonstrated in Fig. 2, which shows the absolute value of the electric field for a point source (a line source in two dimensions) placed either side of x=0 and compares the behaviour of the full profile (equation (11)) versus its real and imaginary parts separately.

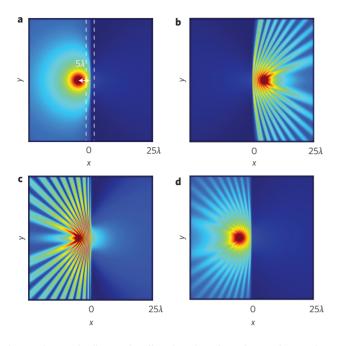


Figure 2 | Test of reflection for all angles of incidence by simulating a line source (pointing out of the page) placed within the inhomogeneous permittivity profile shown in Fig. 1b. Simulations were performed using COMSOL Multiphysics. **a,b**, Absolute values of the electric field of a line source placed at positions $x = -5\lambda$ (**a**) and $x = +5\lambda$ (**b**) in the permittivity profile. The region between the vertical dashed lines in **a** indicates the region plotted in Fig. 1b. **c,d**, As in **a,b**, with identical parameters, but taking only the real (**c**) and imaginary (**d**) parts of the permittivity. The absence of any oscillations in **a** shows that the reflection is completely suppressed for incidence from the left, for all incident angles.

We note that, as is well known, the Helmholtz equation (2) is equivalent to a Schrödinger equation in which $-\alpha(x)$ plays the role of a potential profile. Thus, the spatial Kramers–Kronig relations generate a large family of complex non-reflecting potential profiles. Needless to say, as the relation given by equation (9) is a sufficient, but not necessary condition, real non-reflecting profiles also exist that are perfectly transparent (for example, as mentioned earlier the potential $V(x) = U_0 \mathrm{sech}^2(x/a)$ is known to be non-reflecting for quantum particles when U_0 takes specific values^{2,3}).

The above analysis was carried out for TE polarization, but how is TM polarized radiation affected by the permittivity profile (equation (3))? This polarization obeys a different wave equation,

$$\nabla \cdot \left[\epsilon^{-1}(x) \nabla H_z \right] + k_0^2 H_z = 0 \tag{12}$$

Writing $\epsilon^{-1}(x) = \epsilon_{\rm b}^{-1} + \beta(x)$ and $H_z = h_z(x)e^{{\rm i}k_y y}$, equation (12) becomes

$$\frac{\mathrm{d}^2 h_z(x)}{\mathrm{d}x^2} + K^2 h_z(x) = -\epsilon_b \left[\frac{\mathrm{d}}{\mathrm{d}x} \left(\beta(x) \frac{\mathrm{d}h_z(x)}{\mathrm{d}x} \right) - k_y^2 \beta(x) h_z(x) \right]$$
(13)

Comparing this with equation (2), we can show that the equivalent of equation (8) is given by

$$h_{s}^{(n)}(x) = \epsilon_{b} \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} G(k) \tilde{\beta}(k-k') (k_{y}^{2} + kk') \tilde{h}_{s}^{(n-1)}(k') e^{ikx}$$
 (14)

Therefore, if $\tilde{\beta}(k < 0) = 0$, then reflection of the TM polarization is also suppressed. However, it is not necessarily the case that both $\tilde{\alpha}(k < 0) = 0$ and $\tilde{\beta}(k < 0) = 0$. For both equations to hold we need

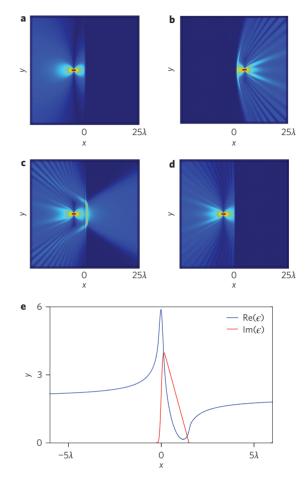


Figure 3 | In cases where the permittivity has neither poles nor zeros in the upper half position plane, the reflection also vanishes for TM polarization. **a**, Field of a dipole source aligned along the y axis (so that the field is TM polarized) and placed at $x = -5\lambda$ in the permittivity profile in **e**. **b**, A dipole radiating in the same profile but at $x = +5\lambda$. **c**.**d**, Reflection from just the real (**c**) and imaginary (**d**) parts of the profile. **e**, Permittivity profile, the imaginary part of which is given by equation (15), with $\epsilon_b = 2$, $L = 1.5\lambda$, $\xi = 0.1\lambda$ and h = 4.5. The real part of the profile was calculated numerically using equation (10).

both $\epsilon(x) - \epsilon_{\rm b}$ and $\epsilon^{-1}(x) - \epsilon_{\rm b}^{-1}$ to be analytic functions in the upper half complex position plane. In particular, if $\epsilon(x)$ satisfies the spatial Kramers–Kronig relations, it will be free of zeros in the upper half plane when ${\rm Im}[\epsilon(x)] > 0$ along the real axis²⁷. Therefore lossy media obeying the Kramers–Kronig relations in space will not reflect radiation of either polarization for any angle of incidence. Meanwhile, for profiles exhibiting gain (or more precisely zeros in the upper half position plane), reflection will be suppressed for only one of the two polarizations.

As an example to demonstrate the general applicability of equation (10) in eliminating the reflection of both polarizations, we take a more complicated permittivity profile with an imaginary part given by

$$\operatorname{Im}[\epsilon(x)] = \frac{h(L-x)}{4L} \left[1 + \operatorname{erf}\left(\frac{x}{\xi}\right) \right] \left[1 + \operatorname{erf}\left(\frac{(L-x)}{\xi}\right) \right] \tag{15}$$

which represents a smoothed triangle function, where 'erf' is an error function, h is the height, L the length, and ξ characterizes the smoothness of the corners. Numerically calculating the integral (10), we obtain the real part of the permittivity that, when added to 'i' times equation (15), is necessary to reduce the reflection to zero.

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The full function is shown in Fig. 3e and, unlike equation (11), has no definite parity symmetry. Figure 3a–d shows that a combination of the real and imaginary parts of the resulting profile suppresses the reflection of TM polarized waves incident from the left (we have also verified that this profile is non-reflecting for TE waves).

A general result in the theory of reflection is that when waves are incident onto a generic planar interface, at angles close to grazing $(k_y \sim k_0)$ the reflectivity usually approaches unity (see, for example, ref. 28). The above findings at first sight appear to contradict this result. However, strictly speaking, the profiles we have calculated are of infinite extent, so there is no 'interface' to speak of, as can be seen from the long tails evident in the real parts of $\epsilon(x)$ shown in Figs 1 and 3. We could, however, confine these infinite profiles to a finite region of space by truncating these tails, multiplying the profile by an envelope function U(x):

$$\alpha'(x) = \alpha(x)U(x)$$

$$\to \tilde{\alpha}'(k) = \int_0^\infty \frac{\mathrm{d}k'}{2\pi} \tilde{U}(k'-k)\tilde{\alpha}(k')$$

where U(x)=0 at some distance from the centre of the profile. The price of prematurely truncating the long tails is that $\alpha'(k<0)\neq 0$. However, if $\tilde{U}(\Delta k)$ is sharply peaked around $\Delta k=0$, $\tilde{\alpha}'$ will only be non-zero for negative k of a small magnitude. For example, if we use $U(x)=\exp(-(x/a)^2)$, then $\tilde{U}(\Delta k)=(a/2\sqrt{\pi})\exp(-a^2(\Delta k)^2/4)$, which rapidly goes to zero beyond around $\Delta k=-2/a$. The consequence of this is that waves close to grazing will now be reflected by the profile, but the angle at which this is significant approaches $\pi/2$ as a is made ever larger. A numerical investigation of this effect can be found in the Supplementary Information.

The non-reflecting properties of specific classes of potential profiles have long been studied²⁹, but more recently the analogous behaviour of PT-symmetric complex susceptibility profiles have been considered in optics. However, to the best of our knowledge, the simple and much more general relation discussed here between the one-sided absence of reflection and the analytic extension of the spatially dependent susceptibility to one half of the complex position plane has not been pointed out before. We have shown how the corresponding Kramers-Kronig relations in space can be used to generate a very large family of non-reflecting profiles. If the profile is also free of zeros in the upper or lower half complex position plane (the half plane being determined by whether reflection vanishes from the left or the right), then the profile is also nonreflecting for both polarizations. In practice, the catch is that the profiles have very long tails that must be truncated, and where one chooses to perform the truncation determines the range of angles that are not reflected. Nevertheless, the advantage of this method is that it does not require magnetic or anisotropic media and only requires control over the real and imaginary parts of an isotropic permittivity (without necessarily requiring gain or taking negative values). The method is also in principle applicable to any wave equation, including the Schrödinger equation. The Kramers-Kronig relations in the frequency domain are a cornerstone of optics, but it is hoped that the spatial Kramers-Kronig relations will provide at least some guidance and insight in the development of metamaterials based on judiciously chosen susceptibility profiles.

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Author contributions

S.A.R.H. devised the theory, performed the simulations and wrote the manuscript. M.A. and G.C.L.R. worked on the theory and co-wrote the manuscript.

Additional information

Supplementary information is available in the online version of the paper. Reprints and permissions information is available online at www.nature.com/reprints. Correspondence and requests for materials should be addressed to S.A.R.H.

Competing financial interests

The authors declare no competing financial interests.