

**Comment on “The quantum mechanics of electric conduction in crystals,” by R. J. Olsen and G. Vignale [Am. J. Phys. 78 (9), 954–960 (2010)]**

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In a recent paper, Olsen and Vignale<sup>1</sup> considered one-dimensional scattering by a potential consisting of a chain of  $N$  identical (nonoverlapping) “cells,” all separated by the same distance  $a$ . Their main goal was to study the limit  $N \rightarrow \infty$  of a potential that becomes periodic on the positive half line. This problem is not new and has been studied by many authors<sup>2–6</sup> and references cited therein.

To study the  $N \rightarrow \infty$  limit, recurrence relations were derived in Ref. 1 to allow the transmission and reflection amplitudes of the finite-periodic potential to be expressed in terms of those of its cells. Their derivation is based on the tacit assumption that it is possible to construct the transmission and reflection amplitudes by adding all the possible elementary scattering amplitudes that are associated with the different virtual paths that the particle can follow inside the potential structure, before being ultimately transmitted or reflected.

The validity of this assumption needs to be demonstrated. To do so, it is necessary to start from the Schrödinger equation and show that, if the system consists of two subsystems, the scattering matrix of the entire system factorizes, that is, its elements can be expressed in terms of those associated with the subsystems. This factorization property of the one-dimensional scattering matrix has been derived by a number of authors (see Ref. 7 and references cited therein), and it can be expressed as a convergent power series, with each term of the series describing a specific virtual path that the particle can follow when it enters the chain, before being finally transmitted or reflected (see Ref. 8, p. 2730).

We now comment on some of the statements that were made in Ref. 1. In Sec. III, the authors affirm that “Because the probability of an outcome is dependent only on the magnitude of the probability amplitude, there is no direct way to observe the phase of a particle.” This statement, as is expressed, is not entirely correct. As a counterexample, the derivative with respect to energy of the phases of the transmission and reflection coefficients is in principle directly observable, because they correspond, respectively, to the transmission and reflection time-delays.<sup>9,10</sup>

Reference 1 also states that “The total transmission coefficient includes the geometric phase gained by an electron with wave vector  $k$  as it travels through a distance  $a$  ...” This statement is incorrect, because the transmission coefficient

(or amplitude), contrary to the reflection amplitude, is not affected by the position of the potential, and consequently by the variation of the distance a particle has to travel to reach it. Rather than commenting on the reasoning presented in Appendix B of Ref. 1 in support of their assertion, we show this property explicitly. Let

$$s = \begin{pmatrix} t & r \\ l & t \end{pmatrix} \tag{1}$$

be the scattering matrix of a one-dimensional system associated with a potential  $V(x)$ , where  $t$  is the transmission amplitude, and  $l$  and  $r$  are the reflection amplitudes from the left and right, respectively, at energy  $E = \hbar^2 k^2 / 2m$  ( $m$  is the mass of the particle). A translation of the potential to the right by a distance  $a$ , that is,  $V(x) \rightarrow V(x-a)$ , is implemented by the unitary displacement operator

$$D(a) = e^{ipa/\hbar} = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}, \tag{2}$$

where  $p$  is the momentum operator. Therefore, the effect of the displacement on the  $2 \times 2$  scattering matrix is  $s \rightarrow D^\dagger(a)sD(a)$ , so that

$$\begin{aligned} s &\rightarrow \begin{pmatrix} e^{-ika} & 0 \\ 0 & e^{ika} \end{pmatrix} \begin{pmatrix} t & r \\ l & t \end{pmatrix} \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \\ &= \begin{pmatrix} t & re^{-2ika} \\ le^{2ika} & t \end{pmatrix}. \end{aligned} \tag{3}$$

Equation (3) shows that the transmission amplitude is not affected by a translation of the potential. Consequently, no additional phase factor is acquired by the transmission amplitude when the particle travels an extra distance to reach the interaction region. In contrast, an additional phase factor is gained by the reflection amplitudes as can be understood by a simple physical argument.

As mentioned, the energy derivative of the phase  $\alpha_t = \arg t$  of the transmission amplitude gives the transmission time-delay

$$\tau_t = \hbar \frac{d\alpha_t}{dE} = \frac{1}{v} \frac{d\alpha_t}{dk}, \tag{4}$$

where  $v = \hbar k / m$  is the incoming velocity. Therefore, if displacing the potential a distance  $a$  to the right causes the

transmission phase  $\alpha_t$ , to acquire an energy-dependent term  $ka$ , then, according to Eq. (4), the transmission time-delay is increased by  $a/v$ . This increase would be in contradiction to the definition of the time-delay, which is a relative quantity obtained by comparing an interaction time with a free reference time. When the interacting particle is transmitted, it necessarily travels the same distance as the free reference particle, independent of the position of the potential, which therefore cannot affect the transmission time-delay. Consequently, there cannot be any additional energy-dependent phase factor in the transmission amplitude.

In contrast, the situation is different for the reflection time-delays from the left and the right, which are respectively given by

$$\tau_l = \frac{1}{v} \frac{d\alpha_l}{dk}, \quad \tau_r = \frac{1}{v} \frac{d\alpha_r}{dk}, \quad (5)$$

where  $\alpha_l = \arg l$  and  $\alpha_r = \arg r$ . Unlike a free reference particle, the total distance traveled by a reflected particle is affected by the position of the potential. If the particle comes from the left, and the potential is displaced by a distance  $a$  to the right, the particle has to travel (back and forth) an extra distance  $2a$ , giving an additional free flight contribution of  $2a/v$  to the reflection time-delay from the left. After integration, this contribution yields the extra  $2ka$  positive term in the phase of the reflection amplitude from the left, in agreement with Eq. (3). Similarly, the situation for the reflection time-delay from the right is reduced by  $2a/v$ , giving a negative additional term  $-2ka$  in the phase of the reflection amplitude from the right, also in agreement with Eq. (3).

In Ref. 1, Sec. III, the authors derive recurrence formulas for the transmission and reflection amplitudes for a chain of equally spaced potential cells. The interpretation of their Eqs. (9) and (10) is partially invalidated by the transformation properties of the transmission and reflection amplitudes. There is another reason why these expressions are not correct. Although the authors are aware that the reflection amplitudes from the left and the right differ for nonsymmetric potentials (see their Sec. IV), they apparently overlooked this fact in their derivation. Even if we assume that the unit cell is symmetric (that is, parity invariant), as soon as we add to it a second cell to the right, the symmetry of the two-potential system is lost. Therefore, in the derivation of the recurrence formulas for the transmission and reflection amplitudes, it is necessary to take into account the distinction between reflection amplitudes from the left and the right.

We introduce the following notation (which differs from the notation in Ref. 1). We denote by  $s_N$  the scattering matrix associated with the  $N$ th single-cell, a distance  $(N-1)a$  from the first cell, which is described by the scattering matrix  $s_1 \equiv s$ . We denote by  $s^{(N)}$  the scattering matrix associated with the finite-periodic chain of  $N$  equally spaced cells, with  $s^{(1)} = s_1 = s$ . If we use the same notation for the elements of the scattering matrices and assume that the cells are iteratively added to the right of the chain, we have for the transmission amplitude

$$t^{(N+1)} = t^{(N)} [1 + l_{N+1} r^{(N)} + \dots] t_{N+1}, \quad (6)$$

$$= \frac{t^{(N)} t_{N+1}}{1 - l_{N+1} r^{(N)}} = \frac{t^{(N)} t}{1 - l r^{(N)} e^{2ikNa}}, \quad (7)$$

where the last equality follows from Eq. (3). Similarly, for the reflection amplitude from the left, we have the recurrence relation

$$l^{(N+1)} = l^{(N)} + t^{(N)} l_{N+1} [1 + r^{(N)} l_{N+1} + \dots] t^{(N)}, \quad (8)$$

$$= l^{(N)} + \frac{(t^{(N)})^2 l_{N+1}}{1 - l_{N+1} r^{(N)}} = l^{(N)} + \frac{(t^{(N)})^2 l e^{2ikNa}}{1 - l r^{(N)} e^{2ikNa}}. \quad (9)$$

Equations (7) and (9), which take into account the transformation property (3) and the necessary distinction between the left and the right reflection amplitudes, are the corrected versions of Eqs. (9) and (10) of Ref. 1.

For later purposes, we give the recurrence relation for the reflection amplitude from the right. In this case, we have

$$r^{(N+1)} = r_{N+1} + t_{N+1} r^{(N)} [1 + l_{N+1} r^{(N)} + \dots] t_{N+1}, \quad (10)$$

$$= r_{N+1} + \frac{t_{N+1}^2 r^{(N)}}{1 - l_{N+1} r^{(N)}} \\ = r e^{2ik(N+1)a} + \frac{t^2 r^{(N)}}{1 - l r^{(N)} e^{2ikNa}}. \quad (11)$$

It is also possible to derive a recurrence relation for the reflection amplitude from the right which is similar to Eq. (9) and is expressed in terms of the transmission amplitude  $t^{(N)}$ . We start from a  $N$ -cell chain that is displaced to the right a distance  $a$  and add an additional cell to the left to obtain the  $(N+1)$ -cell structure. By taking into consideration the effects of the  $a$ -displacement on the phases of the reflection amplitudes, we find

$$r^{(N+1)} = r^{(N)} e^{-2ika} + t^{(N)} r [1 + l^{(N)} e^{2ika} r + \dots] t^{(N)}, \quad (12)$$

$$= r^{(N)} e^{-2ika} + \frac{(t^{(N)})^2 r}{1 - l^{(N)} r e^{2ika}}. \quad (13)$$

We now reproduce the argument in Ref. 1 and determine the conditions for which the transmission amplitude  $t^{(N)}$  goes to zero as  $N \rightarrow \infty$ . From Eq. (9), it is clear that if we assume  $t^{(N)} \rightarrow 0$  as  $N \rightarrow \infty$  for a given  $k$ , we have that  $l^{(N+1)} = l^{(N)} + o(1)$  in the same limit. Thus, the reflection amplitude from the left approaches a constant as the number of cells increases. By conservation of probability this constant has to be a pure phase factor, that is,  $l^{(\infty)} = e^{i\alpha_l^{(\infty)}}$ . Olsen and Vignale<sup>1</sup> use this property to deduce that the phase of the transmission amplitude  $t^{(N)}$  approaches a constant as  $N \rightarrow \infty$ . To do so, they exploit that for a parity invariant potential the relative phase difference between  $l^{(N)}$  and  $t^{(N)}$  is  $\pi/2$ ,

$$\alpha_l^{(N)} - \alpha_t^{(N)} = \pi/2 \pmod{\pi}. \quad (14)$$

As we have emphasized, the potential is not parity invariant, and therefore it is not possible to use Eq. (14) to infer that  $\alpha_t^{(N)}$  also approaches a constant value, as  $\alpha_l^{(N)}$  does. There is no way to infer such a result, as  $\alpha_t^{(N)}$  does not converge to a constant value as  $N \rightarrow \infty$ .

To understand this latter result, we observe that from the unitarity of the scattering matrix a general relation between the phases of the transmission and reflection amplitudes can be derived, which is also valid for nonsymmetric potentials,

$$\frac{1}{2}(\alpha_t^{(N)} + \alpha_r^{(N)}) - \alpha_i^{(N)} = \pi/2 \text{ mod } \pi. \quad (15)$$

By hypothesis, we know that  $\alpha_i^{(N)} = \alpha_i^{(\infty)} + o(1)$ . Thus, according to Eq. (15), to determine the behavior of  $\alpha_i^{(N)}$  for large  $N$ , we need only to determine the behavior of  $\alpha_r^{(N)}$ . Using Eq. (13), we find that as  $N \rightarrow \infty$ ,

$$r^{(N+1)} = r^{(N)} e^{-2ika} + o(1), \quad (16)$$

which means that, in this limit,

$$\alpha_r^{(N+1)} = \alpha_r^{(N)} - 2ka + o(1), \quad (17)$$

and the reflection amplitude from the right possesses the asymptotic form

$$\alpha_r^{(N)} = \alpha - 2Nka + o(1), \quad (18)$$

where  $\alpha$  is a  $N$ -independent (but energy-dependent) constant. It follows from Eq. (15) that the asymptotic behavior of the transmission phase is

$$\alpha_t^{(N)} = \beta - Nka + o(1), \quad (19)$$

where  $\beta$  is a constant. Thus, we find that  $\alpha_t^{(N)}$  diverges as  $N \rightarrow \infty$ .

According to Eq. (19), the transmission time-delay for a  $N$ -cell periodic potential and for a particle with incoming energy  $E = \hbar^2 k^2 / 2m = v^2 / 2m$ , such that  $t^{(N)} \rightarrow 0$  as  $N \rightarrow \infty$ , has the limiting behavior

$$\tau_t^{(N)} = \frac{1}{v} \frac{d\alpha_t^{(N)}}{dk} = \frac{1}{v} \frac{d\alpha}{dk} - \frac{Na}{v} + o(1), \quad (20)$$

$$= -\frac{Na}{v} [1 + o(1)]. \quad (21)$$

Equation (21) is an expression of the Hartman effect.<sup>11,12</sup> If we define the time  $T_t^{(N)}$  spent by the transmitted particle inside the interaction region as the sum of the transmission time-delay  $\tau_t^{(N)}$  and the time  $Na/v$ , it takes for a free particle of velocity  $v$  to travel the distance  $Na$ ,<sup>13</sup>

$$T_t^{(N)} = \frac{Na}{v} + \tau_t^{(N)}, \quad (22)$$

then, by substituting Eq. (21) into Eq. (22), we find that  $T_t^{(N)} \rightarrow 0$ , as  $N \rightarrow \infty$ . Thus, for sufficiently long chains, when the transmission probability approaches zero, the effective group velocity of the transmitted particle inside the potential becomes arbitrarily large, allowing for traversal group velocities larger than the speed of light in vacuum.<sup>14</sup>

We will now explain how to use the argument in Ref. 1 to derive the condition for the total reflection in the limit  $N \rightarrow \infty$ . We multiply Eq. (7) by  $e^{ika}$  and write

$$\frac{t^{(N+1)} e^{ika}}{t^{(N)}} = \frac{t e^{ika}}{1 - l r^{(N)} e^{2ikNa}}. \quad (23)$$

From Eq. (19), the left-hand side of Eq. (23) approaches a real value as  $N \rightarrow \infty$ . Therefore, in this limit, the imaginary part of the right-hand side of Eq. (23) must go to zero. By using Eq. (18), we obtain the condition

$$\text{Im} \frac{|t|}{e^{-i(\alpha_t + ka)} - |l| e^{i\theta}} = 0, \quad (24)$$

where we have defined  $\theta = \alpha + \alpha_l - \alpha_t - ka$ . Because the numerator is real, Eq. (24) is satisfied if the imaginary part of the denominator is 0, giving

$$\frac{\sin(\alpha_t + ka)}{|l|} = \sin \theta. \quad (25)$$

Equation (25) implies that

$$\frac{|\sin(\alpha_t + ka)|}{|l|} = |\sin \theta| \leq 1. \quad (26)$$

If we use  $|l|^2 = 1 - |t|^2$ , and  $\sin^2 x = 1 - \cos^2 x$ , we obtain the condition for total reflection in the limit of a potential that becomes periodic on the positive half line,

$$\frac{\cos(\alpha_t + ka)}{|t|} \geq 1. \quad (27)$$

This condition is compatible with the one found in Refs. 2, 4, and 6, where the Cayley–Hamilton theorem and Chebyshev polynomials of the second kind were used to solve the recurrence relations and express the transmission probability  $|t^{(N)}|^2$  in terms of only the transmission amplitude of the (first) single-cell,

$$|t^{(N)}|^2 = \frac{1}{1 + U_{N-1}^2(z) \frac{1 - |t|^2}{|t|^2}}. \quad (28)$$

$U_N(z)$  is the  $N$ th Chebyshev polynomial of the second kind and  $z = \cos(\alpha_t + ka) / |t|$ . By inspection of Eq. (28), it is clear that  $t^{(N)} \rightarrow 0$  as  $N \rightarrow \infty$ , if and only if  $U_N(z) \rightarrow \infty$  in the same limit. By using the trigonometric identity

$$U_N(\cos \gamma) = \frac{\sin[(N+1)\gamma]}{\sin \gamma} \quad (29)$$

and the properties of the hyperbolic functions, we can easily deduce that  $|U_N(\cos \gamma)| \rightarrow \infty$  as  $N \rightarrow \infty$  if  $|\cos \gamma| > 1$ , yielding the total reflection condition  $|z| = \cos(\alpha_t + ka) / |t| > 1$ , with a strict inequality, which is the one usually mentioned in the literature [see, for instance, Eq. (22) of Ref. 2]. However, for  $z = \pm 1$  we have  $U_N(1) = N+1$ , and  $U_N(-1) = (N+1)(-1)^N$ . Therefore, it is also true that  $|U_N(\pm 1)| = O(N+1)$  as  $N \rightarrow \infty$ , so that Eq. (28) also gives Eq. (27).

In Sec. III of Ref. 1, the authors affirm that ‘‘There are also some conditions where the transmission coefficient of an infinite chain is nonzero ....’’ Strictly speaking, this statement is incorrect. Although Eq. (27) correctly describes the energies for which the transmission amplitude converges to zero in the limit  $N \rightarrow \infty$ , it is not possible to conclude that for

energies breaking this condition, that is,  $\cos(\alpha_r + ka)/|t| < 1$ , the transmission probability would converge to a finite value as  $N \rightarrow \infty$ . The limit of the transmission amplitude does not exist for these energies, as it is clear from the fact that it oscillates. If instead of a monoenergetic incoming wave, we consider a wave packet with a small range of energies, then, using the Riemann–Lebesgue lemma and a power expansion, we can show that the transmission probability converges in this case to a finite average value.<sup>5</sup>

In conclusion, we have used the notion of time-delay to explain the meaning of the transformation properties of the transmission and reflection amplitudes as a result of a displacement of the potential. We then reconsidered the derivation in Ref. 1 to obtain the condition for total reflection in the limit of an infinite number of cells composing the periodic potential. We also obtained an expression for Hartman’s effect, showing that the group velocity of the transmitted particle inside the chain can become arbitrary large as  $N \rightarrow \infty$ .

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<sup>1</sup>R. J. Olsen and G. Vignale, “The quantum mechanics of electric conduction in crystals,” *Am. J. Phys.* **78** (9), 954–960 (2010).

<sup>2</sup>D. J. Griffiths and N. F. Taussig, “Scattering from a locally periodic potential,” *Am. J. Phys.* **60** (10), 883–888 (1992).

<sup>3</sup>S. J. Blundell, “The Dirac comb and the Kronig–Penney model: Comment on ‘Scattering from a locally periodic potential,’ by D. J. Griffiths and N. F. Taussig [*Am. J. Phys.* 60, 883–888 (1992)],” *Am. J. Phys.* **61** (12),

1147–1148 (1993).

<sup>4</sup>D. W. L. Sprung, H. Wu, and J. Martorell, “Scattering by a finite periodic potential,” *Am. J. Phys.* **61** (12), 1118–1124 (1993).

<sup>5</sup>R. G. Newton, “Comment on ‘Scattering by a finite periodic potential,’ by Sprung, Wu, and Martorell [*Am. J. Phys.* 61, 1118–1124 (1993)],” *Am. J. Phys.* **62** (11), 1042–1043 (1994).

<sup>6</sup>D. J. Griffiths and C. A. Steinke, “Waves in locally periodic media,” *Am. J. Phys.* **69** (2), 137–157 (2001).

<sup>7</sup>M. Sassoli de Bianchi, “Comment on ‘Generalized composition law from  $2 \times 2$  matrices,’ by R. Giust, J.-M. Vigoureux, and J. Lages [*Am. J. Phys.* 77, 1068–1073 (2009)],” *Am. J. Phys.* **78** (6), 645–646 (2010).

<sup>8</sup>M. Sassoli de Bianchi, “Levinson’s theorem, zero-energy resonances, and time delay in one-dimensional scattering systems,” *J. Math. Phys.* **35** (6), 2719–2733 (1994).

<sup>9</sup>E. H. Hauge and J. A. Stovneng, “Tunneling times: A critical review,” *Rev. Mod. Phys.* **61** (4), 917–936 (1989).

<sup>10</sup>M. Sassoli de Bianchi, “Conditional time-delay in scattering theory,” *Helv. Phys. Acta* **66**, 361–377 (1993).

<sup>11</sup>T. E. Hartman, “Tunneling of a wave packet,” *J. Appl. Phys.* **33**, 3427–3433 (1962).

<sup>12</sup>M. Sassoli de Bianchi, “A simple semiclassical derivation of Hartman’s effect,” *Eur. J. Phys.* **21**, L21–L23 (2000).

<sup>13</sup>Unlike transmission and reflection time-delays, the notions of transmission and reflection travel times do not have a unique definition in quantum mechanics, because they correspond to the joint measurement of two incompatible observables. See Refs. 9 and 10 and references therein.

<sup>14</sup>This superluminal phenomenon does not mean that information can be conveyed faster than light. See, for instance, the experiment with single photons in Ref. 15 and references cited therein.

<sup>15</sup>A. M. Steinberg and R. Y. Chiao, “Subfemtosecond determination of transmission delay times for a dielectric mirror (photonic band gap) as a function of the angle of incidence,” *Phys. Rev. A* **51**, 3525–3528 (1995).

## Reply to “Comment on ‘The quantum mechanics of electric conduction in crystals,’ ” by Massimiliano Sassoli de Bianchi [*Am. J. Phys.* **79** (5), 549–551 (2010)]

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We thank Sassoli de Bianchi for his comment,<sup>1</sup> which provides the opportunity to clarify the nature of the formalism that we introduced in Appendix B of our paper.<sup>2</sup> We will show that there is no difference between the derivation in our paper and that of Ref. 1 if the results are compared in the same coordinate system. In addition, we will show that using our formalism, the problem may be solved more elegantly without the necessity of considering the subtle points involved in Sassoli de Bianchi’s derivation.

In the standard formalism, the transmission (reflection) coefficient gives the phase of the transmitted (reflected) part of the wave at any position on the opposite (same) side of the potential from the incident wave, relative to a wave with identical wavevector  $\vec{k}$ , which has not encountered the potential. This situation is shown in Fig. 1(a) for a potential of width  $a$  centered at  $c$ . This wave that has not encountered the potential does not exist; it is merely used as a convenient reference in the standard treatment. A more meaningful alternative is to give the phase of the transmitted (reflected) part of the wave relative to the incident wave, which can be done

by setting the phase of the incident wave  $A = e^{-ik(c-a/2)}$ , such that the incident wave is equal to one just to the left of the potential, making the transmitted part of the wave equal to  $te^{ik(x-c+a/2)}$ . However, this transformation is clumsy because the position of the center of the potential is now part of the transmitted wave.

We can simplify the situation considerably by having different coordinate systems:  $x' = x - c + a/2$  to the left and  $x'' = x - c - a/2$  to the right of the potential. This situation is depicted in Fig. 1(b). The transmitted part of the wave is equal to  $te^{ika}e^{ikx''} = \tilde{t}e^{ikx''}$ , where  $\tilde{t} = te^{ika}$  is the total transmission coefficient, as defined in Appendix B of Ref. 2. Likewise, the reflected part of the wave is equal to  $re^{ika}e^{ikx''} = \tilde{r}e^{ikx''}$ , where  $\tilde{r} = re^{ika}$  is the total reflection coefficient. These coefficients give the phase of the waves that have encountered the potential relative to the incident wave before it encounters the potential.

In the standard formalism for an electron incident from the left, the transmission coefficient is valid only to the right of

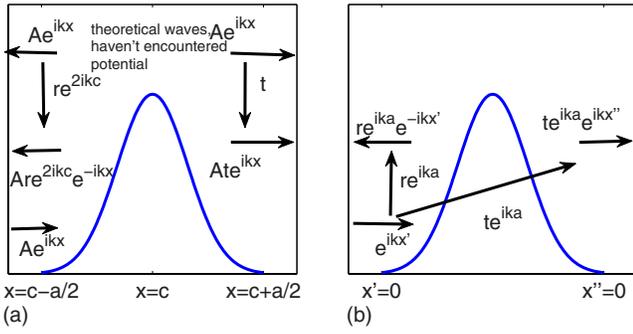


Fig. 1. An electron is incident from the right on a single potential. (a) The transmission (reflection) coefficient gives the phase between the transmitted (reflected) wave and a wave that has not encountered the potential. (b) The total transmission (reflection) coefficient gives the phase between the transmitted (reflected) wave and the incident wave just as it hits the potential.

the potential and the reflection coefficient is valid only to the left of the potential. Therefore, it is necessary to keep track of where a given position is relative to the potential. Our formalism encodes the same information in a different way, with the  $x'$  coordinate system used to the left of the potential and the  $x''$  coordinate system used to the right of the potential. This method has two pedagogical advantages.

- (1) The total coefficients include the geometric phase due to the spatial extent of the potential. Therefore, the change in the phase of a plane wave as a function of position does not need to be explained separately; the total effect of the potential can simply be used.
- (2) Although the reflection coefficients change as the potential is shifted, the total reflection coefficients do not. Therefore, the displacement operator does not need to be introduced. As a result, the scattering matrix does not need to be introduced, and different reflection coefficients for a wave incident from the right or the left do not need to be used unless the effects of disorder are discussed.

We will now show how the equations derived in Ref. 1 are recovered with our approach. In Ref. 2, we defined the total transmission and reflection coefficients by beginning with a parity invariant potential of width  $a$  in the coordinate system  $x$  centered at  $x=0$ . In the new coordinate system,  $x'=x+a/2$  gives the position relative to the left edge of the barrier and  $x''=x-a/2$  gives the position relative to the right edge of the barrier. In this new coordinate system,  $x'=0$  is at the left edge of the potential and  $x''=0$  is at the right edge of the potential. Therefore,  $e^{ikx'}=e^{-ikx''}=e^{ikx}=1$ , meaning that there is no geometric phase in these new coordinates; rather, it has been incorporated into the total transmission and reflection amplitudes. As we add cells to the periodic potential, we will similarly define new coordinate systems  $x'''$  and so forth, with a different coordinate system after each potential block. After we have created the composite potential using our method, we may transform back to the original coordinate system  $x$ . First, we perform the inverse transformation using the notation of Ref. 1 in which  $t^{(N)}$  is defined as the transmission coefficient of the composite potential composed of  $N$  individual potentials in the  $x$  coordinate system,

$$t^{(N)} = \tilde{t}_N e^{-ikNa}, \quad (1)$$

$$r^{(N)} = l^{(N)} = \tilde{r}_N e^{-ikNa}. \quad (2)$$

By definition, this transformation makes the composite potential parity invariant in the  $x$  coordinate system; thus, the composite potential is shifted from the composite potential derived in Ref. 1. As mentioned in Ref. 1, the transmission coefficient is invariant to shifts in the position of the potential. Therefore, we see that although the total transmission coefficient goes to a constant  $\beta$ , the phase of the transmission coefficient goes to  $\alpha_t^N = \beta - Nka$ , resolving one of the issues raised in Ref. 1 with our derivation.<sup>2</sup> Also because the composite potential is parity invariant, the reflection coefficient for a wave incident from the right  $r$  is the same as for a wave incident from the left  $l$ , which resolves another concern raised in Ref. 1.

We now need to shift our potential  $(N-1)a/2$  to the right to match Sassoli de Bianchi's derivation,<sup>1</sup> whose composite potential is made of  $N+1$  individual potentials and begins at  $x=-a/2$  (the beginning of the first potential, which is taken to be parity invariant). If we use the displacement operator, the transformations that link his notation to ours are found to be

$$t^{(N)} = \tilde{t}_N e^{-ikNa}, \quad (3)$$

$$r^{(N)} = \tilde{r}_N e^{-ik(2N-1)a}, \quad (4)$$

$$l^{(N)} = \tilde{r}_N e^{-ika}. \quad (5)$$

Using these transformations, we convert his Eq. (7) for the transmission coefficient to our notation and find

$$\tilde{t}_{N+1} e^{-ik(N+1)a} = \frac{\tilde{t}_N e^{-ikNa} \tilde{t}_N e^{-ika}}{1 - \tilde{r}_N e^{-ika} \tilde{r}_N e^{-ik(2N-1)a} e^{2ikNa}}, \quad (6)$$

$$\tilde{t}_{N+1} = \frac{\tilde{t}_N \tilde{t}_N}{1 - \tilde{r}_N \tilde{r}_N}. \quad (7)$$

Equation (7), which was found by starting with the derivation of Ref. 1 and applying the definition of the total transmission coefficient and the displacement operator, is identical to Eq. (9) of Ref. 2. Similar transformations can be done to obtain Eq. (10) of Ref. 2. We conclude that the only difference between our derivations is that of notation.

Sassoli de Bianchi objected to our statement that "Because the probability of an outcome is dependent only on the magnitude of the probability amplitude, there is no direct way to observe the phase of a particle," saying that "To give a counter example, the derivative with respect to energy of the phases of the transmission and reflection amplitudes are in principle directly observable, as they correspond, respectively, to the transmission and reflection time delays." Our statement refers to the phase of the particle itself, which is not observable, rather than the phase of the transmission and reflection amplitudes. Even with interference, all that is observable is the relative difference in phase of the particle that has traveled different paths, not the absolute phase of the particle itself.

Sassoli de Bianchi cited our statement “There are also some conditions where the transmission coefficient of an infinite chain is nonzero,” saying “one is not allowed to conclude that for energies breaking that condition... the transmission probability would converge to a finite value.” We did not intend to imply that the transmission coefficient converges to a finite value, merely that it is nonzero (though oscillating). These oscillations are demonstrated in Fig. 3 of Ref. 2, where the transmission probability inside the band is shown to oscillate about a nonzero value.

In conclusion, our original paper<sup>2</sup> showed that the phase of the total transmission coefficient converges to a finite value at the edge of the band. As shown in Eq. (2), this behavior means that the phase of the transmission coefficient is di-

rectly proportional to  $Na$ , which is the width of the potential. This property may be used, as shown in Ref. 1, to demonstrate the Hartman effect. The total transmission and reflection coefficients were introduced as a pedagogical tool so that conduction bands in a one-dimensional system may be introduced to undergraduate students without introducing the concepts of the scattering matrix and displacement operator or considering the coordinate system at all.

<sup>1</sup>M. Sassoli de Bianchi, “Comment on ‘The quantum mechanics of electric conduction in crystals,’ by R. J. Olsen and G. Vignale [Am. J. Phys. 78 (9), 954–960 (2010)],” Am. J. Phys. 79 (5), 549–551 (2010).

<sup>2</sup>R. J. Olsen and G. Vignale, “The quantum mechanics of electric conduction in crystals,” Am. J. Phys. 78 (9), 954–960 (2010).