Coherent resonant tunneling time and velocity in finite periodic systems

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The velocity v_{res} of resonant tunneling electrons in finite periodic structures is analytically calculated in two ways. The first method is based on the fact that a transmission of unity leads to a coincidence of all still-competing tunneling time definitions. Thus, having an indisputable resonant tunneling time τ_{res}, we apply the natural definition $v_{\text{res}}=L/\tau_{\text{res}}$ to calculate the velocity. For the second method, we combine Bloch's theorem with the transfer matrix approach to decompose the wave function into two Bloch waves. The expectation value of the velocity is then calculated. Both approaches lead to the same result, showing their physical equivalence. The obtained resonant tunneling velocity v_{res} is smaller than or equal to the group velocity times the magnitude of the complex transmission amplitude of the unit cell. Only at energies at which the *unit cell* of the periodic structure has a transmission of unity does v_{res} equal the group velocity. Numerical calculations for a GaAs/AlGaAs superlattice are performed. For typical parameters, the resonant velocity is below one-third of the group velocity.

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I. INTRODUCTION

There has been an ongoing debate about the time an electron spends when it passes through a classically forbidden region (e.g., a rectangular barrier) for many decades. Despite a number of review articles[1,2] and many papers, there still exist different definitions of tunneling time. In contrast to tunneling through single barriers, periodic systems have a transmission probability of unity below the barrier potential at the individual transmission resonances, which form allowed energy bands. Stimulated by comments in Ref. 2 and recent results from the theory of finite periodic systems,[3,4] here we study the tunneling time and the velocity of electrons that *tunnel resonantly with zero reflection* through finite periodic systems (FPS). As will be shown, for the case of zero reflection, the ambiguity of the tunneling time definition vanishes. Therefore, it can be used to define a resonant tunneling velocity. Our second velocity calculation is based strictly on evaluating the expectation value of the velocity operator. We do not study the time-dependent wave function.

The paper is organized as follows. The next section gives a brief summary of the different tunneling time definitions. In Sec. III the transfer matrix approach is introduced, which is used in Sec. IV to calculate the resonant tunneling time and the corresponding velocity. In Sec. V Bloch's theorem is used together with the transfer matrix to decompose the wave function inside the (FPS) into two Bloch waves. It is shown that the velocity operator must have real expectation values at transmission resonances. The velocity expectation value is then explicitly calculated. In Sec. VI we note that both velocity approaches lead to the same result and derive an upper bound for the velocity. Further, the special case in which resonant tunneling velocity and group velocity are identical is discussed. The analytical results are applied to a semiconductor superlattice and are illustrated with a compilation of graphs in Sec. VII. Finally, we discuss the obtained results and possible extensions.

The obtained results are not restricted to a tight-binding model, but are exact as long as only coherent transport is considered.

II. TUNNELING TIMES

Most of the tunneling time studies have been performed in one of the following frameworks: (i) wave packet analysis,[1,5–8] (ii) dynamic paths including Feynman paths,[9–11] (iii) physical clocks,[12–19] (iv) flux-flux correlation functions,[20] (v) theory of weak measurements,[21] and (vi) combinations of the former.[22]

The real phase or delay time

$$\tau_{\text{phase}}(E) = \frac{\partial \arg t(E)}{\partial \omega} = \hbar \frac{\partial \arg t(E)}{\partial E}, \tag{1}$$

where $t(E)$ is the complex transmission coefficient as a function of energy, and ω is the angular frequency, arises from a stationary-phase argument for the transmitted wave packet. Many of the approaches (ii) to (vi) result at first in complex transmission tunneling times, given by one of the following expressions:

$$\tau_T^E(E) = -i\hbar \frac{\partial \ln t(E)}{\partial E} = \tau_{\text{phase}}(E) - i\hbar \frac{\partial \ln|t(E)|}{\partial E}, \tag{2}$$

$$\tau_T^V(E) = i\hbar \frac{\partial \ln t(E)}{\partial V}, \tag{3}$$

$$\tau_T^{\delta V}(E) = i\hbar \frac{\delta \ln t(E)}{\delta V(x)} = \tau_T^E(E) - i\hbar \frac{r(E) + r'(E)}{4E}, \tag{4}$$

where $\delta/\delta V(x)$ denotes the functional derivative with respect to the potential $V(x)$, and $r(E)$ and $r'(E)$ are the reflection amplitudes for particles coming from the left and right sides, respectively. The corresponding reflection times $\tau_R^X(E)$ are given by the substitution of $t(E)$ by $r(E)$ in the left equalities in Eqs. (2) and (4). In the framework of physical clocks,[12–19] the resulting times have been the real or imaginary part or the absolute value of one of the times in Eqs. (2) and (3).

On the other hand, it was shown that the simultaneous process of (a) the determination whether a particle is transmitted and (b) if so, how long it took to traverse the barrier, corresponds to two noncommuting observables.[23] There was also some direct evidence that the imaginary part of the tunneling time results from the back action on the particle due to the measurement process.[21]

In contrast, the time an electron spends under the barrier, either finally reflected by or transmitted through the barrier, is consistently given by the dwell time,[24] also called sojourn time, which is defined as the ratio of the number of particles within the barrier (extending from a to b) to the incident flux:[13]

$$\tau_D(E) = \frac{1}{v_{\text{in}}}\int_a^b |\Psi|^2 dx. \tag{5}$$

A Hermitian sojourn time operator exists,[25] which shows that this time is measurable.

Again, there has been no general agreement whether a relation of the following form must hold:

$$\tau_D(E) = |t(E)|^2\tau_T(E) + |r(E)|^2\tau_R(E). \tag{6}$$

Based on the argument that reflection and transmission are mutually exclusive events, which exhaust all possibilities in the sense of Feynman, this relation served as a point of focus in an early review.[1] The complex tunneling times $\tau_{T,R}^{\delta V}$ fulfill Eq. (6).[9] Nevertheless, the arguments for Eq. (6) have also been criticized, arguing that the approach used goes beyond Feynman's original interpretation.[2]

A. Tunneling times in the case of the transmission equal to unity

Given that $|t|=1$, for a certain energy, it was shown that phase time and dwell time are identical, not only for the single barrier (at energies higher than the potential energy of the barrier),[13] but also for arbitrary structures.[1,7] The tunneling times τ_T^E, τ_T^V, and $\tau_T^{\delta V}$, [Eqs. (2) and (4)], also simplify to the phase time τ_{phase}, [Eq. (1)], for $|t|=1$ in any arbitrary structure. Thus, we have

$$|t(E')| = 1 \Rightarrow \tau_{\text{phase}}(E') = \tau_D(E') = \tau_T^E(E') = \tau_T^V(E') = \tau_T^{\delta V}(E'). \tag{7}$$

In accordance with the real character of the phase time, the aforementioned problem of noncommuting observables vanishes in the case $|t(E')|=1$, since all particles tunnel finally through the structure; there is neither reflection nor interference between reflected and transmitted particles.

Due to Eq. (7) we can choose any time definition [Eqs. (1)–(5)] to calculate the tunneling time at resonance. We will use the phase delay time [Eq. (1)], and make use of the results obtained in Refs. 4 and 26.

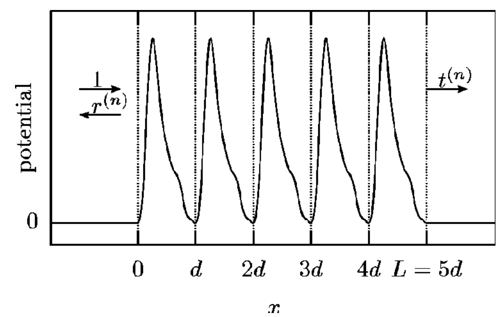

FIG. 1. Periodic potential (drawn for five periods) embedded between two infinite half-spaces. Arrows denote the wave function (plane waves).

B. Group velocity

At first view, a similiar approach to the phase time is the concept of the group velocity

$$v_g = \frac{\partial\omega}{\partial k}, \tag{8}$$

which is the velocity of the envelope of a propagating wave packet in a medium. Here ω is the angular frequency and k is the wave number. The function $\omega(k)$ is normally referred to as dispersion. The solutions of the Schrödinger equation for a periodic potential also yield a (band) dispersion relation between the Bloch wave number q and the angular frequency ω. Using $E=\hbar\omega$, the group velocity then reads

$$v_g = \left(\hbar\frac{\partial q}{\partial E}\right)^{-1}. \tag{9}$$

In Ref. 2, the following relation between the tunneling time and the group velocity was given (for the tight-binding limit), neglecting terms due to the matching of the wave functions at the ends of the system:

$$v_g \cong L/|\tau_T^E|. \tag{10}$$

Here L is the length of the periodic system. Recent numerical calculations for FPS embedded in regions of constant potential showed that the equality in Eq. (10), *does not hold* in general.[27] At first glance, it might seem paradoxical that the group velocity and the phase delay time, which are both based on a wave packet approach, lead to conflicting results.

Our analytical calculations will on one hand, show that Eq. (10) taken from Ref. 2 gives indeed a wrong estimation when the unit cell transmission amplitude is small and will, on the other hand, resolve the mentioned paradox.

III. FINITE PERIODIC SYSTEMS

Our one-dimensional model system consists of an n-fold periodic structure, extending from $x=0$ to $x=L=nd$ (d is the length of the unit cell), embedded between two semi-infinite half-spaces with zero potential (Fig. 1).

Assuming a plane wave, $\exp(ikx)$, traveling from the left towards the FPS, the wave function is given by

$$\Psi(x)=\begin{cases}\exp(ikx)+r^{(n)}\exp(-ikx), & x\leqslant 0\\ \Psi^{(n)}_{\mathrm{FPS}}(x), & 0\leqslant x\leqslant L=nd\\ t^{(n)}\exp[ik(x-L)], & x\geqslant L\end{cases} \tag{11}$$

where $k=\sqrt{2mE}/\hbar$ is the electron wave vector in the semi-infinite half-spaces, and $r^{(n)}$ and $t^{(n)}$ are the complex reflection and transmission coefficients of the n-fold periodic structure, respectively.

We start by briefly reviewing some important properties of one-dimensional FPS.[3,4] The wave functions at the left and right interfaces of a certain region, Ψ_L and Ψ_R, respectively, are related by the transfer matrix $\mathbf{M}$ through[28]

$$\begin{pmatrix}A_L^+\\ A_L^-\end{pmatrix}=\mathbf{M}\begin{pmatrix}A_R^+\\ A_R^-\end{pmatrix},$$

where

$$\Psi_{L,R}=(1\quad 1)\begin{pmatrix}A_{L,R}^+\\ A_{L,R}^-\end{pmatrix}=A_{L,R}^+ + A_{L,R}^-.$$

Neglecting spin, the time reversal invariance and the conservation of the probability density current lead to the structure[29] of the transfer matrix $\mathbf{M}$

$$\mathbf{M}=\begin{pmatrix}a & b\\ b^* & a^*\end{pmatrix}, \tag{12}$$

where additionally $\det\mathbf{M}=1$ holds (x^* denotes the complex conjugate of x). In terms of the transmission and reflection coefficients t and r, the transfer matrix can be written as[30]

$$\mathbf{M}=\begin{pmatrix}1/t & r^*/t^*\\ r/t & 1/t^*\end{pmatrix}. \tag{13}$$

Since by construction the transfer matrix of a sequence of layers is the product of the transfer matrices of each layer, the transfer matrix of a potential consisting of n periods is the nth power of the transfer matrix of one period:

$$\mathbf{M}^n=\begin{pmatrix}a^{(n)} & b^{(n)}\\ b^{(n)*} & a^{(n)*}\end{pmatrix}. \tag{14}$$

For $n\geqslant 2$, $a^{(n)}$ and $b^{(n)}$ can be expanded to[31]

$$a^{(n)}=aU_{n-1}(\mathrm{Re}\{a\})-U_{n-2}(\mathrm{Re}\{a\}), \tag{15}$$

$$b^{(n)}=bU_{n-1}(\mathrm{Re}\{a\}), \tag{16}$$

where $U_n(x)$ denote the Chebyshev polynomials of the second kind. The transmission $T^{(n)}$ of any (field-free) n-fold periodic structure is given by[3,4,30,32,33]

$$T^{(n)}=|a^{(n)}|^{-2}=[1+|b|^2U^2_{n-1}(\mathrm{Re}\{a\})]^{-1}. \tag{17}$$

Resonances with $T^{(n)}=1$ occur if and only if $b^{(n)}=bU_{n-1}(\mathrm{Re}\{a\})=0$. This leads to the following independent conditions of transmission resonances[3,34]

$$T^{(n)}=1\Leftrightarrow \mathrm{Re}\{a\}=\cos(j\pi/n)\vee|a|=1, \tag{18}$$

where $j\in\{1,\ldots,n-1\}$. For the case $\mathrm{Re}\{a\}=\cos(j\pi/n)$, the corresponding Bloch wave vectors q_j^{res} are given by the condition $\mathrm{Re}\{a\}=\cos qd$:

$$q_j^{\mathrm{res}}=\pm\frac{j\pi}{nd},\ j=1,\ldots,n-1. \tag{19}$$

Inserting $\mathrm{Re}\{a\}=\cos(j\pi/n)$ into Eq. (15), we obtain at these resonances:

$$a^{(n)}(q_j^{\mathrm{res}})=t^{(n)}(q_j^{\mathrm{res}})=(-1)^j. \tag{20}$$

Additional transmission resonances with $T^{(n)}=1$ occur if $|a|=|t|^{-1}=1$; i.e., when the transmission probability of the unit cell equals unity.

IV. VELOCITY FROM TUNNELING TIME

Recently, the phase time for a system with n periods, $\tau^{(n)}_{\mathrm{phase}}$, has been calculated with the help of Eqs. (1), (13), and (15):[4,26]

$$\tau^{(n)}_{\mathrm{phase}}=\hbar T^{(n)}\left[\left(n-\frac{\mathrm{Re}\{a\}}{2}U_{2n-1}(\mathrm{Re}\{a\})\right)\times\frac{\mathrm{Im}\{a\}}{1-\mathrm{Re}^2\{a\}}\frac{\partial\,\mathrm{Re}\{a\}}{\partial E}-\frac{1}{2}U_{2n-1}(\mathrm{Re}\{a\})\frac{\partial\,\mathrm{Im}\{a\}}{\partial E}\right], \tag{21}$$

where $T^{(n)}$ is the transmission probability of the periodic structure given by Eq. (17). Here we are only interested in the phase time at resonance energies of the transmission. For energies at which $T^{(n)}=1$, the phase time is equal to the tunneling time as we discussed in Sec. I. In both cases of Eq. (18), Eq. (21) can be reduced to the in-resonance phase time[4] or resonant tunneling time:

$$\tau^{(n)}_{\mathrm{res}}=\hbar n\frac{\mathrm{Im}\{a\}}{1-\mathrm{Re}^2\{a\}}\frac{\partial\,\mathrm{Re}\{a\}}{\partial E}. \tag{22}$$

Clearly, $\tau^{(n)}_{\mathrm{res}}$ is proportional to the number of periods n. Using the natural definition

$$v_{\mathrm{res}}=L/\tau^{(n)}_{\mathrm{res}}, \tag{23}$$

we get the following resonant tunneling velocity:

$$v_{\mathrm{res}}=\hbar^{-1}d\frac{1-\mathrm{Re}^2\{a\}}{-\mathrm{Im}\{a\}}\left(-\frac{\partial\,\mathrm{Re}\{a\}}{\partial E}\right)^{-1}, \tag{24}$$

which does not depend on the number of periods n. For the sake of completeness, we give the result in terms of the transmission amplitude $t=1/a$ of the unit cell:

$$v_{\mathrm{res}}=\hbar^{-1}d\frac{|t|^4-\mathrm{Re}^2\{t\}}{\mathrm{Im}\{t\}}\left(-\frac{\partial\,\mathrm{Re}\{t\}}{\partial E}\right)^{-1}. \tag{25}$$

Now it is interesting to compare this tunneling velocity v_{res} to the group velocity v_g. From the dispersion relation $\mathrm{Re}\{a\}=\cos(qd)$, we obtain

$$v_g = \left(\hbar \frac{\partial q}{\partial E}\right)^{-1} = \hbar^{-1} d\sqrt{1-\mathrm{Re}^2\{a\}}\left(-\frac{\partial\,\mathrm{Re}\{a\}}{\partial E}\right)^{-1}. \quad (26)$$

Using Eqs. (24)–(26), the resonant tunneling velocity and the group velocity are related by

$$v_{\mathrm{res}} = \frac{\sqrt{1-\mathrm{Re}^2\{a\}}}{-\mathrm{Im}\{a\}} v_g = \frac{\sqrt{|t|^4-\mathrm{Re}^2\{t\}}}{\mathrm{Im}\{t\}} v_g. \quad (27)$$

Note that the equations for the resonant tunneling time and the resonant velocity are only meaningful if they are evaluated at energies at which the FPS has a transmission probability of unity.

V. EXPECTATION VALUE OF VELOCITY OPERATOR

In the following, we calculate the expectation value of the velocity operator applied to the exact wave function inside the FPS.

A. Decomposition of Ψ into two Bloch waves

In 1929, Bloch calculated the eigenfunctions of the Schrödinger equation for crystal lattices.[35] He modeled the lattice by a periodic potential that spans the whole space. Using group theory together with periodic (Born–von Kármán) boundary conditions, he proved that the base solutions of the Schrödinger equation for a lattice potential [i.e., $V(\mathbf{x}) = V(\mathbf{x}+\mathbf{R}_i)$, where $\mathbf{R}_i$ is any lattice vector], are of the form

$$\Psi^B_{\mathbf{q}}(\mathbf{x}) = u_{\mathbf{q}}(\mathbf{x})\exp(i\mathbf{q}\cdot\mathbf{x}). \quad (28)$$

Here $\mathbf{q}$ is in modern terms a reciprocal lattice vector and

$$u_{\mathbf{q}}(\mathbf{x}) = u_{\mathbf{q}}(\mathbf{x}+\mathbf{R}_i) \quad (29)$$

is a lattice periodic function. This fact is well known as Bloch's theorem. Actually, in the mathematical literature, the same theorem for linear differential equations with periodic coefficients was proved by Floquet[36] much earlier. Since Bloch derived the theorem originally for an infinite domain, this infinite domain is sometimes considered as necessary.

Therefore, we will start by briefly showing that Bloch's theorem gives also the exact wave functions in finite systems.

Mathematically spoken, for the case of the infinite periodic potential $V:\mathbb{R}^3 \to \mathbb{R}$ considered by Bloch, the domain of the Schrödinger differential equation and its solutions $\Psi^B_{\mathbf{q}}$ is $D=\mathbb{R}^3$. If we reduce the domain of the periodic potential (and thus of the Schrödinger equation) to any finite subdomain $\tilde{D} \subset \mathbb{R}^3$ and choose an arbitrary potential in the domain $\mathbb{R}^3 \setminus \tilde{D}$, the base solutions of the differential equation inside $\tilde{D}$ are not changed. The physical consequence is that despite the loss of the global translation invariance of the Hamiltonian in a finite system, the wave functions are still *exactly* given by superpositions of Bloch waves [Eq. (28)].

If we neglect spin, the time inversion symmetry of the Hamiltonian leads to Kramers degeneracy; i.e., $E(\mathbf{q}) = E(-\mathbf{q})$.

Therefore, the two linear independent solutions of Schrödinger's equation for the one-dimensional periodic potential in a finite domain are given by Ψ^B_q and $(\Psi^B_q)^*(x) = \Psi^B_{-q}(x)$. Having clarified this, we use the following wave function in any one-dimensional n-fold periodic system inside an allowed band:

$$\Psi^{(n)}_{\mathrm{FPS}}(x) = \alpha^{(n)}_q u_q(x)\exp(iqx) + \alpha^{(n)}_{-q} u^*_q(x)\exp(-iqx), \quad 0 \leq x \leq nd, \quad (30)$$

$$u_q(x+d) = u_q(x), \quad u^*_q(x) = u_{-q}(x).$$

See also Ref. 37 (Chap. 8, Sec. 1.1, Sec. 1.2) for another rigorous justification. The dimensionless coefficients $\alpha^{(n)}_q$ and $\alpha^{(n)}_{-q}$ are determined by inital value conditions; i.e., by $\Psi(0)$ and $\Psi'(0)$. In the following, we choose the $u_q(x)$ to be normalized:

$$\int_0^d dx\, u^*_q(x) u_q(x) = d/(2\pi). \quad (31)$$

B. The velocity operator has real expectation values at transmission resonances

Any physical state is represented by a wave function that is an element of the Hilbert space of the square integrable functions $\mathcal{H} = L^2(\mathbb{R}^3)$. The Hermiticity of the velocity (and the momentum) operator comes from the fact that the normalization $\langle\Psi|\Psi\rangle = 1$ leads to $\Psi(\mathbf{x}) = 0$ as $|\mathbf{x}| \to \infty$.

The states we consider [Eq. (11)] are scattering states that do not belong to $L^2(\mathbb{R}^3)$. Therefore, we cannot expect that the velocity operator applied to any finite subdomain is Hermitian. Nevertheless, we show that the expectation values of the velocity operator inside the periodic structure are real for resonant tunneling states.

The calculation is restricted to the one-dimensional region between $x=0$ and $x=L$ inside the FPS. The expectation value of the velocity of any state $|\Psi\rangle$ is given by $\langle\hat{v}\rangle = \langle\Psi|\hat{v}|\Psi\rangle / \langle\Psi|\Psi\rangle$. In our case the numerator can be denoted as $\langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{v}\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle$, where $\hat{P}_{\mathrm{FPS}}$ is the projection operator onto the space region of the FPS:

$$\hat{P}_{\mathrm{FPS}} = \int_0^L dx |x\rangle\langle x|. \quad (32)$$

Partial integration (assuming a constant effective electron mass m) leads to

$$\langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{v}\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle = \left(\frac{-ih}{m}\right)|\Psi^{(n)}_{\mathrm{FPS}}|^2\big|_0^L + \langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{v}\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle^*. \quad (33)$$

Equation (11) yields immediately that $\Psi^{(n)}_{\mathrm{FPS}}(0) = 1 + r^{(n)}$, $\Psi^{(n)}_{\mathrm{FPS}}(L) = t^{(n)}$. Thus, when $|t^{(n)}| = 1 \Leftrightarrow r^{(n)} = 0$ holds, we have $\Psi^{(n)}_{\mathrm{FPS}}(0) = 1$ and $|\Psi^{(n)}_{\mathrm{FPS}}(L)| = 1$, and the term $|\Psi^{(n)}_{\mathrm{FPS}}(L)|^2 - |\Psi^{(n)}_{\mathrm{FPS}}(0)|^2$ vanishes. Therefore, we obtain

$$|t^{(n)}| = 1 \Rightarrow \langle \Psi_{\mathrm{FPS}}^{(n)} | \hat{v} \hat{P}_{\mathrm{FPS}} | \Psi_{\mathrm{FPS}}^{(n)} \rangle = \langle \Psi_{\mathrm{FPS}}^{(n)} | \hat{v} \hat{P}_{\mathrm{FPS}} | \Psi_{\mathrm{FPS}}^{(n)} \rangle^*, \tag{34}$$

i.e., the velocity has a real value at resonances with $|t^{(n)}|=1$.

In this derivation, we did not use the periodicity of the potential nor that of the base solutions; thus, it holds for arbitrary potentials if $|t|=1$ (strictly speaking, it holds if and only if $|1+r|=|t|$).

Note that in the calculation of eigenstates bounded by infinite barriers on both sides, a different relation, i.e., $\Psi_{\mathrm{FPS}}^{(n)}(0)=\Psi_{\mathrm{FPS}}^{(n)}(L)=0$, holds, which leads to a velocity expectation value of zero.

C. Expectation value of the velocity at resonance

The expectation value of the velocity in the n-periodic system at resonance is given by

$$\langle \hat{v}_{\mathrm{FPS}}^{(n)} \rangle = \frac{\langle \Psi_{\mathrm{FPS}}^{(n)} | \hat{v} \hat{P}_{\mathrm{FPS}} | \Psi_{\mathrm{FPS}}^{(n)} \rangle}{\langle \Psi_{\mathrm{FPS}}^{(n)} | \hat{P}_{\mathrm{FPS}} | \Psi_{\mathrm{FPS}}^{(n)} \rangle}. \tag{35}$$

With the help of Eqs. (30) and (31), the numerator is given by

$$\langle \Psi_{\mathrm{FPS}}^{(n)} | \hat{v} \hat{P}_{\mathrm{FPS}} | \Psi_{\mathrm{FPS}}^{(n)} \rangle = \frac{L}{2\pi} (|\alpha_q^{(n)}|^2 - |\alpha_{-q}^{(n)}|^2) v_g(q). \tag{36}$$

The denominator of Eq. (35) is given by

$$\langle \Psi_{\mathrm{FPS}}^{(n)} | \hat{P}_{\mathrm{FPS}} | \Psi_{\mathrm{FPS}}^{(n)} \rangle = \frac{L}{2\pi} (|\alpha_q^{(n)}|^2 + |\alpha_{-q}^{(n)}|^2). \tag{37}$$

A detailed derivation of both equations is given in Appendixes A and B, respectively. From Eqs. (35)–(37) we obtain the velocity expectation value at resonance:

$$\langle \hat{v}_{\mathrm{FPS}}^{(n)} \rangle = \frac{|\alpha_q^{(n)}|^2 - |\alpha_{-q}^{(n)}|^2}{|\alpha_q^{(n)}|^2 + |\alpha_{-q}^{(n)}|^2} v_g = \frac{1 - |\alpha_{-q}^{(n)}/\alpha_q^{(n)}|^2}{1 + |\alpha_{-q}^{(n)}/\alpha_q^{(n)}|^2} v_g. \tag{38}$$

An interpretation of this formula will be given in the next section.

D. Determination of Bloch coefficients

Next we have to determine the ratio $|\alpha_{-q}^{(n)}/\alpha_q^{(n)}|$. For the calculation of the expectation value, it would be sufficient to consider only the wave function at resonance; nevertheless, we will derive a more general result that is valid for any q value.

We rewrite the ansatz for the wave function (30) in a reduced form

$$\Psi_{\mathrm{FPS}}^{(n)}(x) = \tilde{u}_q(x)\exp(iqx) + \tilde{\alpha}_{-q}^{(n)} \tilde{u}_q^*(x)\exp(-iqx), \tag{39a}$$

$$\tilde{u}_q(x) = \alpha_q^{(n)} u_q(x), \tag{39b}$$

$$\tilde{\alpha}_{-q}^{(n)} = \alpha_{-q}^{(n)}/(\alpha_q^{(n)})^*. \tag{39c}$$

By formally replacing q with $-q$ and taking the complex conjugate in Eq. (39c),

$$\tilde{\alpha}_{-q}^{(n)} = 1/(\tilde{\alpha}_q^{(n)})^* \tag{39d}$$

is obtained.

As stated above, the remaining coefficient $\tilde{\alpha}_{-q}^{(n)}$ is determined by the initial values $\Psi(0)$ and $\Psi'(0)$, obtained from the continuity of the wave function and the probability current density across the boundary at $x=0$. To simplify the algebra, we make use of the fact that these continuity conditions are inherently incorporated in the transfer matrix approach. Therefore, to determine $\tilde{\alpha}_{-q}^{(n)}$, we use the continuity of the wave function at $x=0$ and two different representations of $\Psi_{\mathrm{FPS}}^{(n)}$ at $x=d$. This way, the derivative of the wave function is not needed in an explicit form.[38] The continuity of the wave function (11) at $x=0$ leads to

$$1 + r^{(n)} = \tilde{u}_q(0) + \tilde{\alpha}_{-q}^{(n)} \tilde{u}_q^*(0). \tag{40}$$

With Eq. (39a), the periodicity of the $\tilde{u}_q(x)$ gives the wave function at $x=d$:

$$\Psi_{\mathrm{FPS}}^{(n)}(d) = \tilde{u}_q(0)\exp(iqd) + \tilde{\alpha}_{-q}^{(n)} \tilde{u}_q^*(0)\exp(-iqd). \tag{41}$$

On the other hand, $\Psi_{\mathrm{FPS}}^{(n)}(d)$ can be obtained through the transfer matrix (12) of the unit cell:

$$\Psi_{\mathrm{FPS}}^{(n)}(d) = (1\ \ 1)\mathbf{M}^{-1}\begin{pmatrix} 1 \\ r^{(n)} \end{pmatrix} = a^* - b^* + r^{(n)}(a-b). \tag{42}$$

Again, we note that the continuity of the probability current density is fully incorporated in this treatment in the reflection coefficient $r^{(n)}$. Equations (40) and (41), together with (42), form two nonlinear equations in $\tilde{u}_q(0)$ and $\tilde{\alpha}_{-q}^{(n)}$. The solution for $\tilde{\alpha}_{-q}^{(n)}$ is given by

$$\tilde{\alpha}_{-q}^{(n)} = \frac{a^* - b^* - \xi + r^{(n)}(a-b-\xi)}{a - b - \xi + r^{(n)*}(a^* - b^* - \xi)}, \tag{43}$$

where $\xi=\exp(iqd)$ is introduced. From Eqs. (13)–(16), we obtain

$$r^{(n)} = \frac{b^{(n)*}}{a^{(n)}} = \frac{b^* U_{n-1}(\mathrm{Re}\{a\})}{aU_{n-1}(\mathrm{Re}\{a\}) - U_{n-2}(\mathrm{Re}\{a\})}. \tag{44}$$

Inserting into Eq. (43), we obtain after some algebra,

$$\tilde{\alpha}_{-q}^{(n)} = \frac{a^* - b^* - \xi}{a - b - \xi} \frac{a^{(n)*}}{a^{(n)}} = \frac{a^* - b^* - \xi}{a - b - \xi} \frac{t^{(n)}}{t^{(n)*}}. \tag{45}$$

Consistent with Eq. (39d), $\tilde{\alpha}_{-q}^{(n)}=1/(\tilde{\alpha}_q^{(n)})^*$ is fulfilled. In Appendix C, Eq. (45) is used to calculate $\tilde{u}_q(x)$ and $\Psi_{\mathrm{FPS}}^{(n)}(x)$. Further, we prove in Appendix D 1 the interesting identity

$$\langle \Psi_{\mathrm{FPS}}^{(n)} | \hat{v} \hat{P}_{\mathrm{FPS}} | \Psi_{\mathrm{FPS}}^{(n)} \rangle = j_{\mathrm{in}} L, \tag{46}$$

where j_{in} is the incident probability current. Equation (46) is used for the calculation of $\alpha_{-q}^{(n)}$ and $\alpha_q^{(n)}$ in Appendix D 3.

As a consequence of Eq. (45), the absolute value of $\tilde{\alpha}_{-q}^{(n)}$ does not depend on n:

$$|\tilde{\alpha}_{-q}^{(n)}| = \left| \frac{a^* - b^* - \xi}{a - b - \xi} \right|. \tag{47}$$

This shows that the ratio of the amplitude of the left- and right-going Bloch wave does not depend on the number of periods and is a property of the unit cell only.

Using $\mathrm{Re}\{a\}=\cos(qd)$, $|a|^2-|b|^2=1$, and $\xi=\exp(iqd)$, the absolute value squared of $\tilde{\alpha}_{-q}^{(n)}$ inside a band can be simplified to

$$|\tilde{\alpha}_{-q}^{(n)}|^2 = \frac{\mathrm{Im}\{a\} + \sqrt{1-\mathrm{Re}^2\{a\}}}{\mathrm{Im}\{a\} - \sqrt{1-\mathrm{Re}^2\{a\}}}. \tag{48}$$

Taking $|\tilde{\alpha}_{-q}^{(n)}|=|\alpha_{-q}^{(n)}/\alpha_{q}^{(n)}|$ into consideration, inserting Eq. (48) into Eq. (38) gives

$$\langle \hat{v}_{\mathrm{FPS}}^{(n)} \rangle = \frac{1-|\tilde{\alpha}_{-q}^{(n)}|^2}{1+|\tilde{\alpha}_{-q}^{(n)}|^2} v_g = \frac{\sqrt{1-\mathrm{Re}^2\{a\}}}{-\mathrm{Im}\{a\}} v_g. \tag{49}$$

However, this result is not true for the off-resonant case when the first equality does not hold. Nevertheless, the behavior of $\langle \hat{v}_{\mathrm{FPS}}^{(n)} \rangle$ as a continuous function of E or q is of interest, since any rational multiple of π/d can be obtained as q_{res}, by choosing proper values for j and n [see Eq. (19)].

For the sake of completeness, in the resonant case, in which q_{res} is given by Eq. (19), and $t^{(n)}=\pm 1$ holds, Eq. (45) can be simplified to

$$\tilde{\alpha}_{-q_{\mathrm{res}}}^{(n)} = \frac{a^* - b^* - \xi}{a - b - \xi}. \tag{50}$$

In the second resonant case, in which $|t|=|a|^{-1}=1$, either the numerator or the denominator of the right-hand side of Eq. (48) vanishes; i.e.,

$$|t| = 1 \Rightarrow \alpha_{-q}^{(n)} = 0 \vee \alpha_{q}^{(n)} = 0. \tag{51}$$

VI. IDENTITY OF TUNNELING TIME APPROACH AND VELOCITY EXPECTATION VALUE APPROACH

Comparing Eqs. (27) and (49), we get the important identity

$$\langle \hat{v}_{\mathrm{FPS}}^{(n)} \rangle = v_{\mathrm{res}}. \tag{52}$$

Consequently, the tunneling time approach and the velocity expectation value approach are physically equivalent at resonance. We use the term v_{res} as the electron velocity in resonant tunneling through a FPS in the following. From the first identity in Eq. (49), it follows that the electron velocity is bounded above by the group velocity v_g:

$$v_{\mathrm{res}} \leqslant |v_g|. \tag{53}$$

Here the absolute value occurs, since the group velocity can also take negative values for positive q, e.g., for bands where the energy maximum is at $q=0$, while the resonant velocity is always positive.

A. Upper bound for the resonant tunneling velocity

In fact, by squaring the outer equality in Eq. (49), an improved inequality compared to Eq. (53) can be derived. We use that $|a|^2=|t|^{-2}\geqslant 1$. Additionally, inside an allowed band $\mathrm{Re}^2\{a\}\leqslant 1$ holds. Therefore, $0\leqslant 1-\mathrm{Re}^2\{a\}\leqslant \mathrm{Im}^2\{a\}$. Now, making use of the simple inequality $x/y\leqslant(x+z)/(y+z)$, which holds for $0\leqslant x\leqslant y$ and $0\leqslant z$, we obtain

$$\frac{1-\mathrm{Re}^2\{a\}}{\mathrm{Im}^2\{a\}} \leqslant \frac{1}{\mathrm{Im}^2\{a\}+\mathrm{Re}^2\{a\}} = |t|^2. \tag{54}$$

Finally, this proves

$$v_{\mathrm{res}} \leqslant |t||v_g|. \tag{55}$$

In both formulas, the equality holds for $\mathrm{Re}\{a\}=0$, i.e., for $q=\pi/2d$, which is in the middle of the band in q space. Equation (55) shows that the resonant tunneling velocity can be much smaller than the group velocity, given a sufficiently small transmission amplitude of the unit cell. Furthermore, towards the band edges where $\mathrm{Re}\{a\}$ approaches ± 1, the ratio v_{res}/v_g vanishes [see Eq. (49)]. Comparing with Eq. (10), taken from Ref. 2, we conclude that the matching of the wave functions at the ends of the system can reduce the velocity considerably.

B. Special case: Identity between v_{res} and $|v_g|$

From the outer equality in Eq. (49), we can conclude that the equality between v_{res} and $|v_g|$ holds if and only if $|a|=|t|^{-1}=1$, i.e., at energies E' with $|t(E')|=1$ *of the unit cell* of the periodic system:

$$v_{\mathrm{res}}(E') = |v_g(E')| \Leftrightarrow |t(E')| = 1. \tag{56}$$

A unit cell that is formed by a symmetric double-barrier resonant tunneling structure[39,40] possesses the property $|t(E')|=1$ at each transmission resonance energy $E'=E_n$. For this unit cell type, the resonant tunneling velocity v_{res} equals the magnitude of the group velocity v_g at all energies E_n. For energies different from the E_n, v_{res} is smaller than $|v_g|$. The only unit cell where v_{res} equals v_g for all energies is the trivial unit cell with $V(x)=0$, for $0\leqslant x\leqslant d$, since it has $|t(E)|=1$ for all energies.

Further, we can derive conditions from Eq. (49) for the identity between v_{res} and $|v_g|$, in terms of the coefficients $\alpha_q^{(n)}, \alpha_{-q}^{(n)}$:

$$v_{\mathrm{res}} = v_g \Leftrightarrow \alpha_{-q}^{(n)} = 0, \tag{57}$$

$$v_{\mathrm{res}} = -v_g \Leftrightarrow \alpha_{q}^{(n)} = 0. \tag{58}$$

The resonant tunneling velocity equals the magnitude of the group velocity if and only if the wave function has only one Bloch component.

Considering Eq. (56), this can also be written as

$$\alpha_{q}^{(n)} = 0 \vee \alpha_{-q}^{(n)} = 0 \Leftrightarrow |t| = 1, \tag{59}$$

yielding that the wave function inside a finite periodic potential consists of only one Bloch wave if and only if the transmission of the unit cell reaches unity. Therefore, we obtain the picture that the Bloch wave moving into the left direction is built up by a coherent superposition of the reflected parts of waves moving into the right direction.

This also solves the puzzle we mentioned in Sec. I; namely, that the phase delay time and the group velocity both originate from a wave packet analysis, but lead to different results. Often the group velocity is used when, in good approximation, no reflection occurs inside the medium. In contrast, here, in the case that $|t|\neq 1$, there is reflection in each period. These reflections are the origin of the reduced velocity, compared to the group velocity.

VII. GaAs/AlGaAs SUPERLATTICE

All results presented are valid for arbitrary unit cells unless otherwise noted. In this section the results are applied to a periodic semiconductor heterostructure. Due to its widespread use, we choose a GaAs/AlGaAs superlattice (SL). Denoting the barriers (AlGaAs) with B and the well regions (GaAs) with A, we can give a short notation for the potential with n periods: $(BA)^n$. Assuming a stepwise constant potential function in each layer, the transfer matrix elements can be calculated analytically. To keep the focus on the main topic, we will use the following simplifications: (i) the effective mass m is approximated to be the same in GaAs and in AlGaAs, and (ii) the effective mass does not depend on the energy. These simplifications can be avoided, but this is left for future work. We present results for the lowest miniband. The analogous calculations for higher minibands will be discussed elsewhere.

For a SL of the form $(BA)^n$, we obtain the following expressions for the matrix elements of the unit cell (BA):[4]

$$\mathrm{Re}\{a_{\mathrm{SL}}\} = \cosh(\kappa L_b)\cos(kL_w) - c_2 \sinh(\kappa L_b)\sin(kL_w), \tag{60a}$$

$$\mathrm{Im}\{a_{\mathrm{SL}}\} = -\cosh(\kappa L_b)\sin(kL_w) - c_2 \sinh(\kappa L_b)\cos(kL_w), \tag{60b}$$

$$b_{\mathrm{SL}} = ic_1 \sinh(\kappa L_b)\exp(kL_w). \tag{60c}$$

Here L_b and L_w are the thicknesses of the barrier and the well layers, respectively:

$$\kappa = \hbar^{-1}[2m(V_b - E)]^{1/2}, \quad k = \hbar^{-1}(2mE)^{1/2},$$

are the decaying electron wave vector in the barrier layer and the electron wave vector in the well layer, respectively, and

$$c_{1,2} = \tfrac{1}{2}(k\kappa^{-1} \pm \kappa k^{-1}).$$

The energy and the conduction band offset between GaAs and AlGaAs are denoted as E and V_b, respectively.

The following SL parameters are chosen to be identical or nearly identical to systems that were studied experimentally and theoretically in the past.[4,27,34,41]

For the barrier and the well width, we choose $L_b = 2.5$ nm and $L_w = 6.5$ nm, respectively. The barriers consist of $Al_{0.3}Ga_{0.7}As$, the wells of GaAs. The number of periods is $n=6$. A schematic of the resulting conduction band is drawn in Fig. 2. The calculations are performed for the Γ valley of the conduction band for a temperature of 4 K. As the effective electron masses in both, GaAs and $Al_{0.3}Ga_{0.7}As$, we choose $m=0.072m_0$, where m_0 is the free electron mass. The conduction band offset is $V_b = 288$ meV.

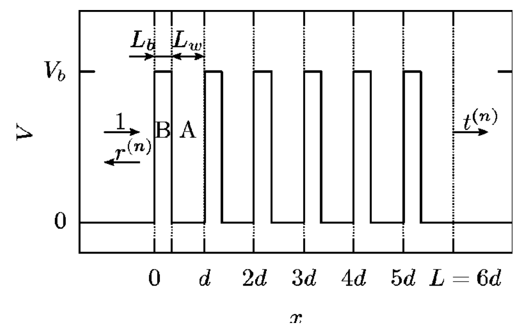

FIG. 2. Schematic potential of a SL of the form $(BA)^n$. The number of periods n is chosen to be 6.

Because of the strong interdependencies between the dispersion relation, transmission probability, group and resonant tunneling velocity, and the ratio of the amplitudes of the $+q$ and $-q$ Bloch waves, all are shown together in Fig. 3. All variables are plotted on the left as a function of the energy E and on the right as a function of the Bloch wave vector q.

For the first miniband the resonance energies are given by the smallest solutions E_j of Eqs. (18) and (60a), i.e., by solving the transcendental equation

$$\cos(j\pi/n) = \cosh(\kappa L_b)\cos(kL_w) - c_2 \sinh(\kappa L_b)\sin(kL_w). \tag{61}$$

The diamonds in Fig. 3 mark the values at the resonance energies for the system with $n=6$ periods. Changing the number of periods n results in values that lie on the lines which connect the diamonds. In the limit $n\to\infty$, one would also obtain the continuous lines.

Figure 3(a) shows $q(E)$, and Fig. 3(b) shows its inverse, the dispersion relation $E(q)$. The dispersion relation is obtained from $\mathrm{Re}\{a_{\mathrm{SL}}\}=\cos(qd)$, where $\mathrm{Re}\{a_{\mathrm{SL}}\}$ is given by Eq. (60a).

In Figs. 3(c) and 3(d), the transmission probability $T^{(6)}$ [Eq. (17)] is plotted.

From the plots of $E(q)$ and $T^{(6)}(q)$ the equidistant behavior of the resonant levels, Eq. (19), in q space can be seen nicely. Of course, due to the nonlinear dispersion $E(q)$, this behavior is lost in energy space.

Next, in Figs. 3(e) and 3(f), the magnitude of the amplitude ratio of the $-q$ and $+q$ Bloch waves, $|\tilde{\alpha}_{-q}^{(n)}|$ [Eq. (47)] is shown. Towards the miniband edges this ratio approaches unity, and it drops to a minimum around the middle of the miniband.

Figs. 3(g) and 3(h) show the group velocity v_g [Eq. (26)] (solid line), and the resonant tunneling velocity v_{res} [Eq. (24)] (dashed line). For the $n=6$ case, the group velocity reaches its maximum in the fourth resonance, while the resonant tunneling velocity reaches its maximum in the third resonance. This shows again the fundamental difference between both velocities. It is interesting to note that the slope of $v_{\mathrm{res}}(q)$ is zero at $q=0,\pi/d$, while the slope of $v_g(q)$ has its maximum value there.

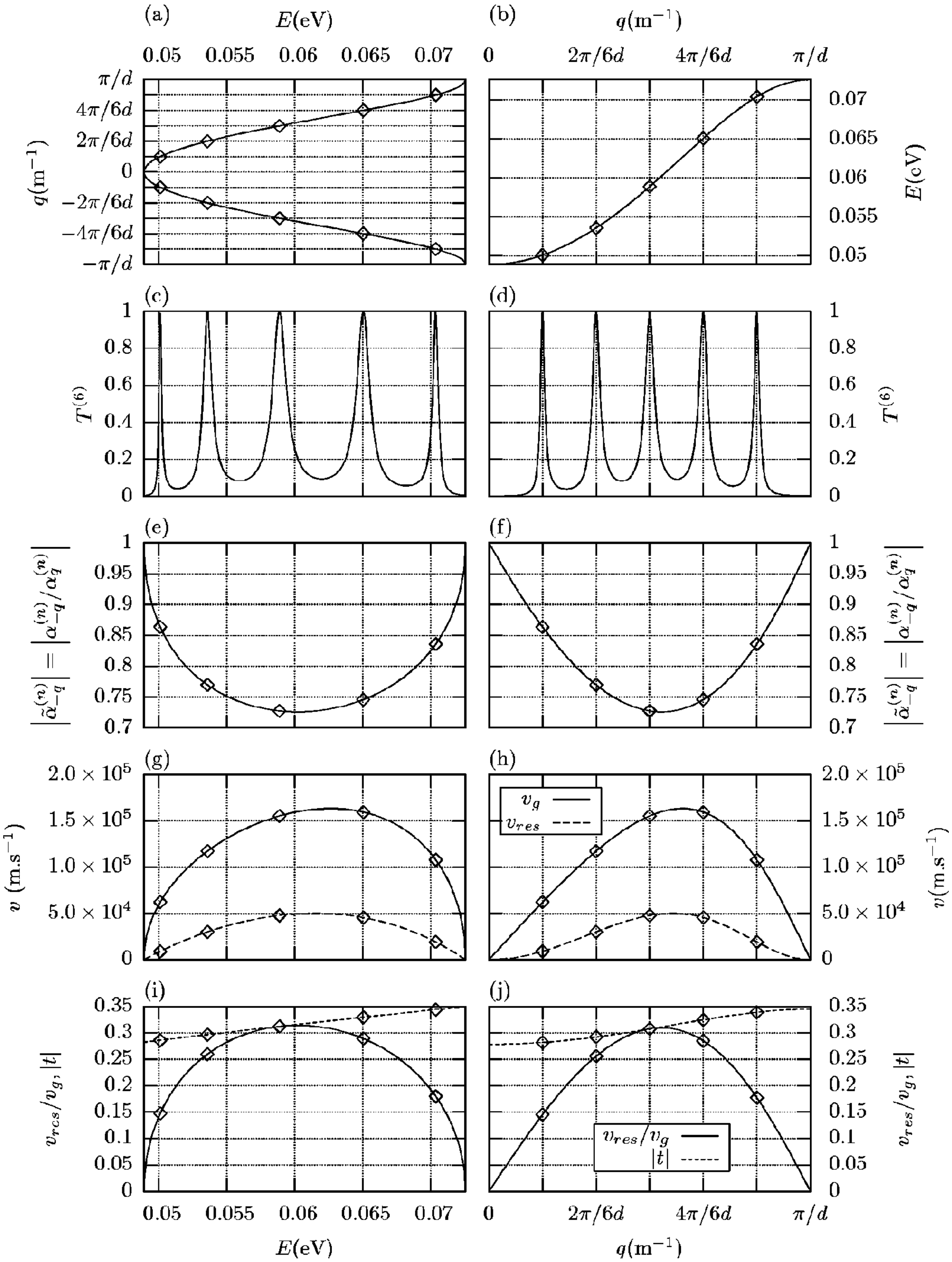

FIG. 3. Shown are relevant physical properties of superlattices. In the left column, all functions are plotted vs energy E, and in the right column vs Bloch wave vector q. Diamonds mark the positions of the resonant levels for $n=6$ periods (band structure given in Fig. 2). By changing the number of periods n, the lines connecting the diamonds are formed. The dispersion relation $q(E)$ and $E(q)$, the transmission probability $T^{(6)}$, the normalized coefficient of the backwards propagating Bloch wave $|\tilde{\alpha}_{-q}^{(n)}|$, the group velocity v_g, the resonant tunneling velocity v_{res}, and the ratio of resonant tunneling and group velocity of the periodic system together with the magnitude of the unit cell transmission amplitude $|t|$ are shown.

In Figs. 3(i) and 3(j), the ratio v_{res}/v_g and the magnitude of the unit cell transmission amplitude $|t|$ are plotted. The velocity ratio is always smaller than the single-cell transmission, except for $q=\pi/2d$ when both are equal [see Eq. (55)]. For the given parameters, the velocity ratio is below one-third.

VIII. DISCUSSION

The group velocity is often used as the speed of the electrons inside a SL. Strictly speaking, the group velocity is the expectation value of the velocity operator applied to only a single Bloch wave. We showed that the solution of the

Schrödinger equation, which fulfills the boundary conditions of the open system, is not given by a single Bloch wave. Instead, the solution is given by a superposition of two Bloch waves traveling in opposite directions. This inevitable (except for singular energies at which $|t|=1$ holds for the unit cell) second Bloch wave is the reason that the physically significant expectation value of the velocity of the composed wave function is reduced compared to the velocity of the single Bloch wave; i.e., the group velocity. The velocity of a single Bloch wave is not a directly observable entity in periodic systems (except again for $|t|=1$), but can be used as an upper bound for the resonant tunneling velocity. The presented results support the numerical findings of Ref. 27.

In this context, the often used relation "mean free path equals group velocity times scattering time" seems questionable. We suggest that in open mesoscopic structures, (see Fig. 1 and Fig. 2) where the mean free path exceeds the length of the periodic structure, it should be replaced by "*mean free path equals resonant tunneling velocity multiplied by scattering time*."

The commutator of the observable that measures the event of transmission and the tunneling time operator does not vanish,[23] as already mentioned. We showed that the expectation value of the velocity is in general complex for nonzero reflection. Thus, in some sense, we presented a different argumentation that this problem is not well defined and that asking for the velocity of the (transmitted) electrons is only a valid question if the transmission probability of the periodic system, $|t^{(n)}|^2$, is unity. Therefore, we restricted our calculations to this case.

In calculating the velocity expectation value we obtained the average over a set of identical velocity measurements but no information of the time-dependent behavior of the process. The solutions of the time-dependent Schrödinger equation can be studied in addition. Nevertheless, it has been pointed out that arriving wave packet peaks do not turn into transmitted peaks among other difficulties[2] in the wave packet approach. Despite that, in the light of our results, we suggest the analysis of periodic wave packets composed of a discrete set of resonant states. In contrast to any tunneling wave packet simulation we are aware of, the *reflection is exactly zero* for these packets. Therefore, we would expect some new insights.

IX. CONCLUSIONS

We calculated the resonant tunneling electron velocity in finite periodic structures embedded in regions of constant potential in two different ways and proved their identity.

The first method was based on the fact that $|t^{(n)}|=1$ leads to a coincidence of all tunneling time definitions, turning up in the literature. We used the phase time $\tau_{\text{phase}}=\hbar\partial \arg t/\partial E$ and the natural definition $v=L/\tau$ to calculate the velocity in terms of the unit cell transfer matrix elements and the unit cell transmission amplitude, respectively, yielding Eqs. (24) and (25).

Bloch's theorem was combined with the transfer matrix approach to separate the wave function into two Bloch waves, which propagate in opposite directions [Eq. (39a)] together with either Eq. (47) or Eq. (48). After proving that the velocity operator is real at resonance, we calculated its expectation value [Eq. (49)] as the second method.

Both results are completely identical, showing the physical equivalence of the two approaches. The resonant tunneling velocity is in any case smaller or equal to the group velocity. In addition, the resonant tunneling velocity is smaller than or equal to the product of the group velocity and the magnitude of the transmission amplitude of the unit cell. Thus for unit cells with a small transmission amplitude both velocities can differ considerably. We discussed that the Bloch wave moving in the opposite direction of the incident electrons is due to reflections inside all unit cells. These reflections are the reason for the reduced velocity compared to the group velocity. At energies, where the unit cell has a transmission of unity, only one Bloch wave remains. Consequently, the resonant tunneling velocity equals the group velocity.

We intentionally avoided studying the problem of the tunneling time and velocity for nonzero reflection. However, as stated above, certain wave packet analysis might help to complete the picture. We believe that the identity of the tunneling time and velocity expectation value approach will hold also for nonperiodic systems with zero reflection. This topic is considered for future investigation.

Electron waves have been used throughout this paper. In analogy the main results hold for the propagation of light waves, of phonons waves, and so on, in periodic structures.

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APPENDIX A: EVALUATION OF $\langle\Psi_{\text{FPS}}^{(n)}|\hat{v}\hat{P}_{\text{FPS}}|\Psi_{\text{FPS}}^{(n)}\rangle$

First, we consider the case in which $q=q_{\text{res}}$. Expanding the integral with the help of Eqs. (30) and (31) leads to

$$\langle\Psi_{\text{FPS}}^{(n)}|\hat{v}\hat{P}_{\text{FPS}}|\Psi_{\text{FPS}}^{(n)}\rangle = |\alpha_q^{(n)}|^2\langle\Psi_q^B|\hat{v}\hat{P}_{\text{FPS}}|\Psi_q^B\rangle + |\alpha_{-q}^{(n)}|^2\langle\Psi_{-q}^B|\hat{v}\hat{P}_{\text{FPS}}|\Psi_{-q}^B\rangle - \frac{i\hbar}{m}\left\{\alpha_q^{(n)}\alpha_{-q}^{(n)*}\int_0^L dx\, u_q(x)e^{iqx}\frac{\partial}{\partial x}[u_q(x)e^{iqx}] + \text{c.c.}\right\}. \tag{A1}$$

If the Bloch wave vector q is given by Eq. (19), i.e., $q_j^{\text{res}}=j\pi/L$, the last integral vanishes:

$$\int_0^L dx\, u_q(x)e^{iqx}\frac{\partial}{\partial x}[u_q(x)e^{iqx}] = \left[\frac{1}{2}u_q^2(x)e^{i2qx}\right]_0^L = 0, \tag{A2}$$

due to the periodicity of both, the $u_q(x)$ and the complex exponential function. Using the fact[42] that

$$\langle\Psi^B_{\pm q}|\hat{v}|\Psi^B_{\pm q}\rangle/\langle\Psi^B_{\pm q}|\Psi^B_{\pm q}\rangle = v_g(\pm q) = \pm v_g(q), \qquad \text{(A3)}$$

the normalization (31) leads finally to Eq. (36).

For the second case, i.e., $|t|=1$, we use Eq. (51). This means that there is only one Bloch wave and either $\alpha_q^{(n)}$ or $\alpha_{-q}^{(n)}$ is zero. Equation (A3) and the normalization (31) then give Eq. (36) directly.

APPENDIX B: EVALUATION OF $\langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle$

First, we consider again the case in which $q=q_{\mathrm{res}}$. Expanding the integral with the help of Eqs. (30) and (31) leads to

$$\begin{aligned}\langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle &= |\alpha_q^{(n)}|^2\langle\Psi^B_q|\hat{P}_{\mathrm{FPS}}|\Psi^B_q\rangle \\ &\quad + |\alpha_{-q}^{(n)}|^2\langle\Psi^B_{-q}|\hat{P}_{\mathrm{FPS}}|\Psi^B_{-q}\rangle \\ &\quad + \left(\alpha_q^{(n)}\alpha_{-q}^{(n)*}\int_0^L dx\, u_q^2(x)e^{i2qx} + \text{c.c.}\right).\end{aligned} \qquad \text{(B1)}$$

Due to the periodicity of $u_q(x)$ and considering that $q_j^{\mathrm{res}} = j\pi/nd$, the last integral vanishes:

$$\begin{aligned}\int_0^{nd} dx\, u_q^2(x)e^{i2qx} &= \left(\sum_{l=0}^{n-1}\exp(i2qld)\right)\int_0^d u_q^2(x)e^{i2qx}dx \\ &= \sum_{l=0}^{n-1}[\exp(i2\pi j/n)]^l\int_0^d u_q^2(x)e^{i2qx}dx = 0,\end{aligned} \qquad \text{(B2)}$$

where the last identity is due to the vanishing of the geometric sum. Together with the normalization (31), we end up with Eq. (37).

For the second case, i.e., $|t|=1$, we use Eq. (51). This means that there is only one Bloch wave and either $\alpha_q^{(n)}$ or $\alpha_{-q}^{(n)}$ is zero. The normalization (31) then gives Eq. (37) directly.

APPENDIX C: SIMPLIFIED CALCULATION OF THE WAVE FUNCTION IN THE FPS

As a supplementary result, once $\tilde{\alpha}_{-q}^{(n)}$ is calculated from Eq. (45), the values of $\Psi^{(n)}_{\mathrm{FPS}}(x)$ *in one period*, e.g., obtained with the transfer matrix approach, allows us to calculate the periodic function $\tilde{u}_q(x)$. Solving Eq. (39a) for $\tilde{u}_q(x)$ we obtain

$$\tilde{u}_q(x) = \frac{\Psi^{(n)}_{\mathrm{FPS}}(x) - \tilde{\alpha}_{-q}^{(n)}(\Psi^{(n)}_{\mathrm{FPS}})^*(x)}{1-|\tilde{\alpha}_{-q}^{(n)}|^2}\exp(-iqx). \qquad \text{(C1)}$$

Using Eqs. (39a) and (45), the wave function in the *entire FPS* can be obtained easily.

APPENDIX D: DERIVATION OF AN IDENTITY AND CALCULATION OF $\alpha_q^{(n)}$ AND $\alpha_{-q}^{(n)}$

1. Identity—first method

From Eqs. (52), (35), and (23),

$$\frac{L}{\tau^{(n)}_{\mathrm{res}}} = v^{(n)}_{\mathrm{res}} = \frac{\langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{v}\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle}{\langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle}, \qquad \text{(D1)}$$

and Eqs. (5) and (7),

$$\tau^{(n)}_{\mathrm{res}} = \frac{1}{j_{\mathrm{in}}}\langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle, \qquad \text{(D2)}$$

we derive the interesting identity, valid at resonance,

$$L = \frac{1}{j_{\mathrm{in}}}\langle\Psi^{(n)}_{\mathrm{FPS}}|\hat{v}\hat{P}_{\mathrm{FPS}}|\Psi^{(n)}_{\mathrm{FPS}}\rangle, \qquad \text{(D3)}$$

where the incoming probability current is given by $j_{\mathrm{in}} = \hbar k/m$.

2. Identity—second method

This equation can also be derived directly from the conservation of electrical charge in the form

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 + \frac{\partial}{\partial x}j(x,t) = 0, \qquad \text{(D4)}$$

where j is the one-dimensional probability current given by

$$j(x,t) = \mathrm{Re}\left[\Psi^*\left(-\frac{i\hbar}{m}\frac{\partial}{\partial x}\right)\Psi\right]. \qquad \text{(D5)}$$

Since in our case $|\Psi|^2$ and j do not depend on time, Eq. (D4) simplifies to

$$j(x,t) = \text{const}. \qquad \text{(D6)}$$

Now we integrate the constant probability current density [Eq. (D5)], first for the wave function to the left, i.e., $\Psi_L(x)=\exp(ikx)$, and second for the wave function at resonance inside the FPS, i.e., $\Psi^{(n)}_{\mathrm{FPS}}(x)$, both over the interval $[0,L]$. Equations (D6) and (34) then yield identity (D3).

3. Calculation of $\alpha_q^{(n)}$ and $\alpha_{-q}^{(n)}$

Making use of Eqs. (36), (D3), and (39a), we can calculate $\alpha_q^{(n)}$ and $\alpha_{-q}^{(n)}$. Choosing the (arbitrary) phase of $\alpha_q^{(n)}$, so that $\alpha_q^{(n)}$ is real and positive, we obtain

$$\alpha_q^{(n)} = \left[\frac{2\pi j_{\mathrm{in}}}{(1-|\tilde{\alpha}_{-q}^{(n)}|^2)v_g}\right]^{1/2}, \qquad \text{(D7)}$$

$$\alpha_{-q}^{(n)} = \tilde{\alpha}_{-q}^{(n)}\alpha_q^{(n)}, \qquad \text{(D8)}$$

where $\tilde{\alpha}_{-q}^{(n)}$ is given by Eq. (45).

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$$\begin{pmatrix} A_R^+ \\ A_R^- \end{pmatrix} = \hat{\mathbf{M}} \begin{pmatrix} A_L^+ \\ A_L^- \end{pmatrix},$$

for example, used in Ref. 3. Of course, $\hat{\mathbf{M}} = \mathbf{M}^{-1}$. The reader is asked to check carefully which definition is used when he consults the literature, since both occur frequently.
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