

Quantum dissipation with conditional wave functions: Application to the realistic simulation of nanoscale electron devices

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Without access to the full quantum state, modeling dissipation in an open system requires approximations. The physical soundness of such approximations relies on using realistic microscopic models of dissipation that satisfy completely positive dynamical maps. Here we present an approach based on the use of the Bohmian conditional wave function that, by construction, ensures a completely positive dynamical map for either Markovian or non-Markovian scenarios while allowing the implementation of realistic dissipation sources. Our approach is applied to compute the current-voltage characteristic of a resonant tunneling device with a parabolic-band structure, including electron-lattice interactions. A stochastic Schrödinger equation is solved for the conditional wave function of each simulated electron. We also extend our approach to (graphenelike) materials with a linear band structure using Bohmian conditional spinors for a stochastic Dirac equation.

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I. INTRODUCTION

Although reversible dynamics in a closed system induce irreversibility into a smaller subsystem, the simulation of quantum dissipation cannot rely on the full quantum state, because it is computationally inaccessible. The solution is to deal only with the degrees of freedom of a smaller subsystem, referred as the open system [1], or simply the system. The remaining degrees of freedom constitute the environment. Most approaches for open systems revolve around the reduced density matrix constructed by tracing out the degrees of freedom of the environment [1]. A proper equation of motion of the reduced density matrix must lead to a dynamical map that satisfies complete positivity (CP) [2], which guarantees that such a reduced density matrix is always a positive operator. Some phenomenological treatments of the source of dissipation violate CP, such as the Boltzmann collision operator in the Liouville equation [3] or the seminal Caldeira-Leggett master equation [4]. For Markovian evolutions, the Lindblad master equation [5] preserves CP, but its connection to realistic practical scenarios and its extension beyond Markovian dynamics are still challenging [6,7].

Alternatively, inspired by the spontaneous collapse theories [8], Diósi, Gisin, and Strunz developed the stochastic Schrödinger equations (SSEs) to *unravel* the reduced density matrix in non-Markovian systems [9]. Continuous measurement theory allows the definition of a wave function of the open system conditioned on one *monitored* value associated with the environment [10–12]. This approach preserves positivity because the reduced density matrix is built from a sum of projectors associated with the states solution of a Schrödinger-like equation [1,7,10]. In practical applications, the non-Hermitian Hamiltonians can provoke states of the SSE to lose their norm and therefore their statistical relevance [1].

Here a discussion about the physical interpretation of the pure-state solution of the SSE is relevant. It is well recognized

that the continuous measurement of an open system with Markovian dynamics can be described by a SSE [1]. Therefore, the pure-state solution of a SSE can be interpreted as the state of the Markovian system while the environment is under (continuous) observation. However, such a physical interpretation cannot be given to the solutions of the SSE for non-Markovian systems [10–12]. In such non-Markovian systems, a continuous measurement requires a nontrivial interaction of the system with the environment so that the physical description of the continuously measured open system needs to be done through the reduced density matrix [1] (not through the pure state given by the non-Markovian SSE, which becomes just a numerical tool). The physical interpretation that one can assign to the solution of the non-Markovian SSE (conditioned to some environment value) is the following: the state of the open system at a given time if a measurement is performed in the environment at that time, yielding the mentioned value for the environment. Linking SSE states of the open system (or values of the environment) at different times is just a fiction.

In this work, we present an approach to deal with quantum dissipation based on the use of Bohmian conditional wave functions (CWFs) [13]. Such a CWF provides an unproblematic way of defining the wave function of a subsystem, from a computational and an interpretative points of view. By construction, within Bohmian mechanics, the CWF is always a well-defined physical state for Markovian and non-Markovian open systems, with continuous or non-continuous measurements. The general expression of the equations of motion of such a CWF with or without dissipation is mentioned in Ref. [17]. We anticipate the two main results of this work. First, since our approach deals directly with wave functions, it provides a CP map for either Markovian or non-Markovian dynamics with an unproblematic physical interpretation of the wave function of the open system at different times. Second, contrary to other CP methods, the numerical inclusion of different dissipative phenomena in the equation of motion of the CWF can be done straightforwardly with a microscopic and realistic implementation. These properties make the approach presented in this work very relevant for many different research

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fields. In this paper, we discuss its implementation for quantum transport with dissipation.

The article is structured as follows. After this Introduction, in Sec. II we present the basic elements of our general approach. In particular, we discuss its complete positivity in Sec. II A, the equation of motion of the CWF with dissipation in Sec. II B, and a comparison with similar techniques in Sec. II C. In Sec. III, as an example, we study quantum dissipation through electron-phonon interaction, with the definition of the conditional potential in Sec. III A. The application to tunneling nanodevices with parabolic- and linear-band structures is done in Secs. III B and III C, respectively. We conclude in Sec. IV. Finally, technical details are discussed in four Appendixes.

II. THE APPROACH

We consider an *isolated* (*closed*) quantum system described by a full many-body state $|\Psi\rangle$ solution of the unitary, reversible, and linear Schrödinger equation. We decompose the total Hilbert space of N particles as $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$, with $\vec{r} = \{\vec{r}_a, \vec{r}_b\}$ being \vec{r}_a the position of the a -particle and $\vec{r}_b = \{\vec{r}_1, \dots, \vec{r}_{a-1}, \vec{r}_{a+1}, \dots, \vec{r}_N\}$ the position of all other particles. Next, we present our approach, emphasizing that it provides a CP map for either Markovian or non-Markovian systems.

A. Complete positivity

The expectation value $\langle O_a \rangle \equiv \langle \Psi | \hat{O}_a \otimes \mathbb{1}_b | \Psi \rangle$ associated with an operator \hat{O}_a acting on the a -particle, with $\mathbb{1}_b$ being the identity operator for \mathcal{H}_b , can be computed as

$$\langle O_a \rangle = \int d\vec{r}_a O_a \rho(\vec{r}_a, \vec{r}'_a, t) |_{\vec{r}'_a = \vec{r}_a}, \quad (1)$$

where $\rho(\vec{r}_a, \vec{r}'_a, t)$ is the reduced density matrix:

$$\rho(\vec{r}_a, \vec{r}'_a, t) = \int d\vec{r}_b \Psi^*(\vec{r}'_a, \vec{r}_b, t) \Psi(\vec{r}_a, \vec{r}_b, t), \quad (2)$$

where $\Psi(\vec{r}_a, \vec{r}_b, t) \equiv \langle \vec{r}_a, \vec{r}_b | \Psi \rangle$ is the total wave function and O_a is the position representation of \hat{O}_a .

The same system can be described with the Bohmian theory [13,14] as follows. For each experiment, labeled by j , a Bohmian quantum state is defined by the same wave function $\Psi(\vec{r}_a, \vec{r}_b, t)$ plus a set of well-defined trajectories in physical space, $\{\vec{r}_1^j[t], \dots, \vec{r}_N^j[t]\}$. The velocity of each trajectory is [13]

$$\vec{v}_a^j[t] = \frac{d\vec{r}_a^j[t]}{dt} = \frac{\vec{J}_a(\vec{r}_a^j[t], \vec{r}_b^j[t], t)}{|\Psi(\vec{r}_a^j[t], \vec{r}_b^j[t], t)|^2}, \quad (3)$$

where $\vec{J}_a = \hbar \text{Im}(\Psi^* \nabla_a \Psi) / m_a$ is the (ensemble value of the) current density, with m_a the mass of the a th particle. The set of N positions $\{\vec{r}_1^j[t], \dots, \vec{r}_N^j[t]\}$ in different $j = 1, \dots, W$ experiments is distributed (in quantum equilibrium [13]) as

$$|\Psi(\vec{r}_a, \vec{r}_b, t)|^2 = \frac{1}{W} \sum_{j=1}^W \delta(\vec{r}_a - \vec{r}_a^j[t]) \delta(\vec{r}_b - \vec{r}_b^j[t]). \quad (4)$$

The identity in Eq. (4) requires $W \rightarrow \infty$. Numerically, we just require a large enough W .

The key element of our approach is the CWF associated with the a th particle in the open system during the j th

experiment, defined as $\psi_a^j(\vec{r}_a, t) \equiv \Psi(\vec{r}_a, \vec{r}_b^j[t], t)$. We emphasize that $\psi_a^j(\vec{r}_a, t)$ provides an unproblematic (Bohmian) definition of the wave function of an open system [13]. We compute a different CWF for each simulated particle of the open system and for each simulated experiment. In Sec. II B, we will discuss the equation of motion of such CWFs.

Next, we construct the reduced density matrix, Eq. (2), using the fundamental elements of the Bohmian theory to show that our approach based on CWFs is CP. We define the (tilde) CWF of the a th particle in the j th experiment as

$$\tilde{\psi}_a^j(\vec{r}_a, t) \equiv \frac{\Psi(\vec{r}_a, \vec{r}_b^j[t], t)}{\Psi(\vec{r}_a^j[t], \vec{r}_b^j[t], t)}. \quad (5)$$

Notice that the denominator $\Psi(\vec{r}_a^j[t], \vec{r}_b^j[t], t)$ is just a pure time-dependent term (without spatial dependence) that has no effect on the definition of the velocity in Eq. (3). The Bohmian velocity of the a -particle computed from $\tilde{\psi}_a^j(\vec{r}_a, t)$ is exactly the same value as the one we get from $\psi_a^j(\vec{r}_a, t)$. Putting Eq. (4) into $\langle O_a \rangle \equiv \langle \Psi | \hat{O}_a \otimes \mathbb{1}_b | \Psi \rangle$, integrating all degrees of freedom, and using the definition of the (tilde) CWF in Eq. (5), we get

$$\langle O_a \rangle = \sum_{j=1}^W [p_j \tilde{\psi}_a^{j*}(\vec{r}_a, t) O_a \tilde{\psi}_a^j(\vec{r}_a, t)]_{\vec{r}_a = \vec{r}_a^j[t]}, \quad (6)$$

where $p_j = 1/W$. Equation (6) allows us to compute $\langle O_a \rangle$ from Eq. (1) as

$$\langle O_a \rangle = \int d\vec{r}_a \left[O_a \sum_{j=1}^W p_j \tilde{\psi}_a^{j*}(\vec{r}'_a, t) \tilde{\psi}_a^j(\vec{r}_a, t) \right]_{\vec{r}'_a = \vec{r}_a = \vec{r}_a^j[t]}, \quad (7)$$

which directly allows the definition of the following density matrix [15]:

$$\rho(\vec{r}_a, \vec{r}'_a, t) = \sum_{j=1}^W p_j \tilde{\psi}_a^{j*}(\vec{r}'_a, t) \tilde{\psi}_a^j(\vec{r}_a, t). \quad (8)$$

The generalization to CWFs with an arbitrary number of particles is straightforward. The time evolution of Eq. (8) ensures, trivially, that the dynamical map associated with our approach is CP. In the position representation, the density operator $\hat{\rho} = \sum_{j=1}^W p_j |\tilde{\psi}_a^{j*}(t)\rangle \langle \tilde{\psi}_a^j(t)|$ gives $\langle \vec{r}_o | \hat{\rho} | \vec{r}_o \rangle = \sum_{j=1}^W p_j |\langle \vec{r}_o | \tilde{\psi}_a^j(t) \rangle|^2 \geq 0$ at any time [16] and at any position \vec{r}_o . The last step to conclude our CP demonstration is quite simple. If the density matrix in Eq. (8) is positive, then the diagonal elements of $\langle \vec{r}_o | \hat{\rho} | \vec{r}_o \rangle$ evaluated only at $\vec{r}_o = \vec{r}_a^j[t]$ and defined as $\langle \vec{r}_o | \hat{\rho} | \vec{r}_o \rangle_B \equiv \sum_{j=1}^W p_j |\langle \vec{r}_o | \tilde{\psi}_a^j(t) \rangle|^2 \delta(\vec{r}_o - \vec{r}_a^j[t]) \geq 0$ are, by construction, also positive.

In fact, the term $\langle \vec{r}_o | \hat{\rho} | \vec{r}_o \rangle_B$ has a very simple interpretation. For the j experiment, the tilde CWF in Eq. (5) evaluated at $\vec{r}_o = \vec{r}_a^j[t]$ is $\langle \vec{r}_a^j[t] | \tilde{\psi}_a^j(t) \rangle = \tilde{\psi}_a^j(\vec{r}_a^j[t], t) \equiv \Psi(\vec{r}_a^j[t], \vec{r}_b^j[t], t) / \Psi(\vec{r}_a^j[t], \vec{r}_b^j[t], t) = 1$. Then, since $p_j = 1/W$, we get $\langle \vec{r}_o | \hat{\rho} | \vec{r}_o \rangle_B \equiv \sum_{j=1}^W 1/W = W_B/W$, where W_B is just the number of experiments where the position of the trajectory $\vec{r}_a^j[t]$ coincides with \vec{r}_o . In conclusion, as far as we are dealing with CWF and Bohmian trajectories in the dynamical

description of the quantum systems with dissipation, the CP of our approach is always satisfied (the number W_B of trajectories with position $\vec{r}_o = \vec{r}_a^j[t]$ can be zero, but it cannot be negative).

B. The equation of motion for the CWFs

Here we develop the equation of motion for the CWF, $\psi_a^j \equiv \psi_a^j(\vec{r}_a, t) \equiv \Psi(\vec{r}_a, \vec{r}_b^j[t], t)$. As we discussed, the Bohmian velocities obtained from $\tilde{\psi}_a^j$ and ψ_a^j are identical. It has been shown in Ref. [17] that the (non-tilde) CWF can be computed, in general, from the following single-particle Schrödinger-like equation in physical space:

$$i\hbar \frac{d\langle \vec{r} | \Psi \rangle}{dt} \Big|_{\vec{r}_b^j[t]} = \langle \vec{r} | \hat{\mathcal{H}} | \Psi \rangle \Big|_{\vec{r}_b^j[t]} \iff i\hbar \frac{d\psi_a^j}{dt} = H_a \psi_a^j, \quad (9)$$

where $\hat{\mathcal{H}}$ is the many-body Hamiltonian, and its relation to H_a will be explained next. First, we notice that the relation between $i\hbar d\langle \vec{r} | \Psi \rangle / dt \Big|_{\vec{r}_b^j[t]}$ and $i\hbar d\psi_a^j / dt$ on the right and left sides of Eq. (9) is the following:

$$\begin{aligned} i\hbar \frac{d\psi_a^j(\vec{r}_a, t)}{dt} &= i\hbar \frac{d\langle \vec{r}_a, \vec{r}_b^j[t] | \Psi(t) \rangle}{dt} \\ &= i\hbar \frac{d\langle \vec{r} | \Psi(t) \rangle}{dt} \Big|_{\vec{r}_b^j[t]} + i\hbar \sum_{k=1, k \neq a}^N \nabla_k \langle \vec{r} | \Psi(t) \rangle \Big|_{\vec{r}_b^j[t]} \vec{v}_k^j[t] \\ &= i\hbar \frac{d\langle \vec{r} | \Psi(t) \rangle}{dt} \Big|_{\vec{r}_b^j[t]} + iB_a(\vec{r}_a, \vec{r}_b^j[t], t), \end{aligned} \quad (10)$$

with the conditional imaginary potential iB_a defined as

$$B_a \equiv \hbar \sum_{k=1, k \neq a}^N \nabla_k \langle \vec{r} | \Psi(t) \rangle \Big|_{\vec{r}_b^j[t]} \vec{v}_k^j[t], \quad (11)$$

where $\vec{v}_k^j[t] = d\vec{r}_k^j[t]/dt$ is the Bohmian velocity of the k particle given by Eq. (3). Second, once we have defined B_a , the term H_a on the right-hand side of Eq. (9) can be defined as

$$H_a = \frac{\langle \vec{r} | \hat{\mathcal{H}} | \Psi(t) \rangle \Big|_{\vec{r}_b^j[t]} + iB_a}{\psi_a^j}. \quad (12)$$

In general, Eq. (9) is nonlinear because H_a in Eq. (12) depends on the wave function itself. In addition, the imaginary conditional potential iB_a indicates that the evolution of the CWF can be nonunitary. Equation (9) includes any type of evolution for the CWF (not only linear and unitary ones). In particular, Eq. (9) alone allows the description of irreversible dynamics (energy dissipation) in the open system as required in this work. Obviously, the full wave function $\Psi(\vec{r}_a, \vec{r}_b, t)$ satisfies unitary and linear dynamics, with conservation of the total energy [14].

The key computation for the practical application of our approach is the evaluation of H_a in Eq. (12), which allows us to determine an equation of motion for each CWF, ensuring the CP of our approach. The calculation of $\langle \vec{r} | \hat{\mathcal{H}} | \Psi(t) \rangle$ before conditioning depends on the full many-body wave function, and it requires educated guesses [17]. The potential B_a , which

contains many-body terms but does not depend directly on $\hat{\mathcal{H}}$, will be approximated following Ref. [17]. Stochasticity is introduced in Eq. (9) through the term H_a , which accounts for the effect of nonsimulated degrees of freedom of the environment in each experiment.

C. Comparison with other techniques

Several techniques use Bohmian trajectories as a mathematical/computational tool to solve some *reduced* equations of motion [18]. Here, on the contrary, Eq. (4) guarantees empirical equivalence between Bohmian and standard quantum (nonrelativistic) results in the whole closed system. This implies not only the correct description of any smaller portion of the closed system, i.e., our open systems, but also empirical equivalence in the measured values [13]. It is important to emphasize that Gambetta and Wiseman [10] pointed out that the only physical continuous-in-time interpretation of the wave-function solution of non-Markovian SSEs, i.e., with backaction from the environment to the system, has to be based on the Bohmian theory. In other words, in spite of its mathematical interest as a computational tool, the *improper* sum of wave functions of an open system in Eq. (8) has a problematic ontological meaning within standard quantum mechanics, as indicated by D'Espagnat [19,20]. On the contrary, the Bohmian theory allows a *proper* definition of a wave function of an open system with or without continuous measurements, for both Markovian and non-Markovian dynamics [13]. We can always interpret (part of) $\vec{r}_b^j[t]$ as the pointer of a measuring apparatus. Therefore, the Bohmian CWF $\psi_a^j(\vec{r}_a, t)$ can be thought of as the wave function of SSE conditioned to a continuous observation defined by the (part of) $\vec{r}_b^j[t]$ as the pointer.

To the best of our knowledge, we are the first to develop a practical SSE algorithm using CWF solutions of Eq. (9). In the Bohmian framework, the ensemble values can be directly computed from the trajectories and not from the CWF. Therefore, the technical problems of SSE due to norm degradation are avoided in our approach. It is a remarkable fact that the velocity of $\vec{r}_a^j[t]$ computed from $\psi_a^j(\vec{r}_a, t)$ gives the exact same value as if we use $\Psi(\vec{r}_a, \vec{r}_b^j[t], t)$. Thus, the velocity, as seen in Eq. (3), is totally independent of the norm of the CWF [13]. This explains why Eq. (9) deals with a non-normalized wave function.

Since we are dealing with a *realistic* definition (i.e., with a clear ontological meaning) of the wave function of an open system, $\psi_a^j(\vec{r}_a, t)$, a relevant advantage is that our approach allows a *realistic* description of the stochastic sources of dissipation (beyond the typical environmental noise sources introduced in SEE [1]) while maintaining CP. Below, as an example, we provide the stochastic conditioned potential of Eq. (9), which tackles the electron-lattice energy dissipation in tunneling devices.

III. APPLICATION TO ELECTRON-LATTICE INTERACTION

To analyze the electron-lattice interaction, here, we develop the exact expression for Eq. (9) for electrons interacting

with the lattice. For that purpose, we consider N_e electrons with positions $\vec{r} = \{\vec{r}_1, \dots, \vec{r}_{N_e}\}$ and N_h ions located at $\vec{R} = \{\vec{R}_1, \dots, \vec{R}_{N_h}\}$. Although not explicitly indicated, N_h includes also all additional particles required to deal with a closed system with the many-body wave function $\Psi(\vec{r}_a, \vec{r}_b, t) \equiv \langle \vec{r}_a, \vec{r}_b | \Psi \rangle$ mentioned in Sec. II A. To simplify the notation, hereafter we define $\vec{r} = \{\vec{r}_a, \vec{z}_a\}$ with $\vec{z}_a = \{\vec{r}_1, \dots, \vec{r}_{a-1}, \vec{r}_{a+1}, \dots, \vec{r}_{N_e}\}$. These new variables are related to previous ones through $\vec{r}_a = \vec{r}_a$ and $\vec{r}_b = \{\vec{z}_a, \vec{R}\}$, with $\vec{r} = \{\vec{r}_a, \vec{r}_b\}$.

We compute the evolution of the full wave function $\Psi(\vec{r}, \vec{R}, t) = \Psi(\vec{r}, t)$ under the effect of the full Hamiltonian $\hat{\mathcal{H}}$ in Eq. (9). The position representation of the Hamiltonian $\hat{\mathcal{H}}$ gives

$$H(\vec{r}, \vec{R}) = K_e(\vec{r}) + K_h(\vec{R}) + V_{ee}(\vec{r}) + V_{hh}(\vec{R}) + H_{ep}(\vec{r}, \vec{R}), \quad (13)$$

with $K_e(\vec{r})$ the electron kinetic energies, $K_h(\vec{R})$ the nucleus kinetic energies, $V_{ee}(\vec{r})$ the electron-electron interactions, $V_{hh}(\vec{R})$ the nucleus-nucleus interactions, and $H_{ep}(\vec{r}, \vec{R})$ the total electron-lattice interaction. The last term can be split into $H_{ep} = H_{ep, \vec{R}_0} + H_{ep, \vec{u}}$. The first term, H_{ep, \vec{R}_0} , corresponds to the interaction of the electrons with the fixed (equilibrium) positions of the ions \vec{R}_0 . The second one, $H_{ep, \vec{u}}$, includes the interaction of the electrons with the displacement of the ions, $\vec{u} = \vec{R} - \vec{R}_0 = \{\vec{u}_1, \dots, \vec{u}_{N_h}\}$, and it is the only term that prevents the exact separation of the many-particle wave function. Thus, we rewrite Eq. (13) as

$$H(\vec{r}, \vec{R}) = H_c(\vec{r}, \vec{R}) + H_{ep, \vec{u}}(\vec{r}, \vec{R}), \quad (14)$$

with $H_c(\vec{r}, \vec{R}) = K_e(\vec{r}) + K_h(\vec{R}) + V_{ee}(\vec{r}) + V_{hh}(\vec{R}) + H_{ep, \vec{R}_0}(\vec{r}, \vec{R}_0)$. Finally, the computation of H_a in Eq. (12) just requires the explicit evaluation of the terms

$$\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_{ep, \vec{u}} | \Psi(t) \rangle \Big|_{\vec{z}_a[t], \vec{R}^j[t]} \quad (15)$$

and

$$\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_c | \Psi(t) \rangle \Big|_{\vec{z}_a[t], \vec{R}^j[t]}. \quad (16)$$

The relevant interaction of the (conditional) wave packet with the moving lattice, present in $\hat{H}_{ep, \vec{u}}$, will be evaluated in Sec. III A in the second-quantization formalism. The less relevant interaction of the (conditional) wave packet with the fixed (equilibrium) lattice due to H_c present in Eq. (16) is discussed in Appendix B.

A. Electron-phonon stochastic potential

Assuming a small displacement of the ions $\vec{u}_h = \vec{R}_h - \vec{R}_{h,0}$ from their equilibrium positions $\vec{R}_{h,0}$, the electron-lattice Hamiltonian for small displacements of ions in the position representation can be written as $H_{ep, \vec{u}}(\vec{r}, \vec{R}) = \sum_{e,h} \vec{u}_h \partial U(\vec{r}_e - \vec{R}_h) / \partial \vec{R}_h |_{\vec{R}_{h,0}}$. The (second-quantization) electron-lattice Hamiltonian is then

$$\hat{\mathcal{H}}_{ep, \vec{u}} = \sum_{e,p} g_{\vec{k}_e}^{\vec{q}_p} \hat{c}_{\vec{k}_e + \vec{q}_p}^\dagger \hat{c}_{\vec{k}_e} (\hat{b}_{\vec{q}_p} + \hat{b}_{-\vec{q}_p}^\dagger), \quad (17)$$

with $\hat{b}_{\vec{q}_p}$ and $\hat{b}_{\vec{q}_p}^\dagger$ being the annihilation and creation operators of the atomic vibrational eigenstate $|\vec{q}_p\rangle$. Similarly, $\hat{c}_{\vec{k}_e}$ and

$\hat{c}_{\vec{k}_e}^\dagger$ are the corresponding operators of the (Bloch) eigenstate $\langle \vec{r}_e | \hat{c}_{\vec{k}_e}^\dagger | 0 \rangle = \langle \vec{r}_e | \vec{k}_e \rangle = \phi_{\vec{k}_e}(\vec{r}_e)$. The coupling constant $g_{\vec{k}_e}^{\vec{q}_p}$ specifies the transition between the eigenstates. The first-quantization explanation of the electron-lattice interaction and the definition of $g_{\vec{k}_e}^{\vec{q}_p}$ are given in Appendix A.

The initial many-body (electron and lattice) quantum state is

$$\Psi(\vec{r}, \vec{R}, t_0) = \sum_{\vec{k}, \vec{q}} a(\vec{k}, \vec{q}, t_0) \Phi_{\vec{k}}(\vec{r}) \Phi_{\vec{q}}(\vec{R}), \quad (18)$$

with $a(\vec{k}, \vec{q}, t_0)$ accounting for an arbitrary superposition, $\Phi_{\vec{k}}(\vec{r}) \equiv \langle \vec{r} | \hat{c}_{\vec{k}_1}^\dagger \dots \hat{c}_{\vec{k}_{N_e}}^\dagger | 0 \rangle$ the Slater determinant with $\vec{k} = \{\vec{k}_1, \dots, \vec{k}_{N_e}\}$, and $\Phi_{\vec{q}}(\vec{R})$ the atomic part with $\vec{q} = \{\vec{q}_1, \vec{q}_2, \dots\}$ representing a phonon base. The Slater determinant of electrons can be expanded in minors giving

$$\Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) = \sum_{\vec{k}, \vec{q}} a(\vec{k}, \vec{q}, t) \Phi_{\vec{q}}(\vec{R}) \sum_{\vec{k}_w} \phi_{\vec{k}_w}(\vec{r}_a) s_{a,w} \times \langle \vec{z}_a | \hat{c}_{\vec{k}_1}^\dagger \dots \hat{c}_{\vec{k}_{w-1}}^\dagger \hat{c}_{\vec{k}_{w+1}}^\dagger \dots \hat{c}_{\vec{k}_N}^\dagger | 0 \rangle, \quad (19)$$

with $s_{a,w}$ the sign of the (a, w) cofactor. Then, the term in Eq. (17) acting on Eq. (19) is (for more details, see Appendix A)

$$\begin{aligned} & \langle \vec{r}_a, \vec{r}_b | \hat{\mathcal{H}}_{ep, \vec{u}} | \Psi(t) \rangle \\ &= \sum_{e,p} g_{\vec{k}_e}^{\vec{q}_p} \langle \vec{r}_a, \vec{r}_b | \hat{c}_{\vec{k}_e + \vec{q}_p}^\dagger \hat{c}_{\vec{k}_e} (\hat{b}_{\vec{q}_p} + \hat{b}_{-\vec{q}_p}^\dagger) | \Psi(t) \rangle \\ &= \sum_{e,p} g_{\vec{k}_e}^{\vec{q}_p} \sum_{\vec{k}, \vec{q}} a(\vec{k}, \vec{q}, t) \Phi_{\vec{q}}(\vec{R}) \sum_{\vec{k}_w} \phi_{\vec{k}_w + \vec{q}_p}(\vec{r}_a) s_{a,w} \\ & \times \langle \vec{z}_a | \hat{c}_{\vec{k}_1}^\dagger \dots \hat{c}_{\vec{k}_{w-1}}^\dagger \hat{c}_{\vec{k}_{w+1}}^\dagger \dots \hat{c}_{\vec{k}_N}^\dagger | 0 \rangle. \end{aligned} \quad (20)$$

We use $\Phi_{\vec{q}}(\vec{R})$ to account for the effect of the electron-lattice interaction in the atomic part.

When conditioning Eqs. (19) and (20) to $\{\vec{z}_a^j[t], \vec{R}^j[t]\}$, the variable \vec{q}_p^j is also fixed to some particular values in this j th experiment. The exact (deterministic) description of the electron-lattice interaction would require perfect knowledge of all ion dynamics through $\vec{R}^j[t]$. However, since ions are considered here as the *environment* of electrons (they are not explicitly simulated), we introduce their effect stochastically in the equation of motion of electrons in Eq. (9), ensuring that the probabilities of different phonon modes satisfy some well-known precomputed probabilities [21]. We assume that only one (or none) phonon mode \vec{q}_p^j becomes relevant at each time. Then, the (envelope) CWF before a collision $t < t_c$ is

$$\psi_a^j(\vec{r}_a, t) = \sum_{\vec{k}_w} f(\vec{k}_w, t) \phi_{\vec{k}_w}(\vec{r}_a). \quad (21)$$

Assuming that $g_{\vec{k}_a}^{\vec{q}_p^j} \approx g_{\vec{k}_{0a}}^{\vec{q}_p^j}$ with \vec{k}_{0a} the central wave vector of the a wave packet, the final (envelope) CWF in Eq. (20) after the collision $t > t_c$ is $\psi_a^j(\vec{r}_a, t) \equiv \langle \vec{r}_a, \vec{r}_b^j | \hat{\mathcal{H}}_{ep, \vec{u}} | \Psi(t) \rangle$, which

can be written as (see Appendix A)

$$\psi_a^j(\vec{r}_a, t) = g_{k_{0a}}^{\vec{q}_p} \sum_{\vec{k}_w} f(\vec{k}_w, t) \phi_{\vec{k}_w + \vec{q}_p}^{\vec{r}_a}, \quad (22)$$

where the \vec{r}_a dependence in Eqs. (21) and (22) is given by $\phi_{\vec{k}_a}(\vec{r}_a)$ and $\phi_{\vec{k}_w + \vec{q}_p}(\vec{r}_a)$, respectively, and $f(\vec{k}_w, t)$ includes all other terms evaluated at $\{\vec{z}_a^j[t], \vec{R}^j[t]\}$.

These results have a simple and intuitive explanation. During the collision, the (Bloch state) quasimomentum eigenstates that build the wave packet change from $|\vec{k}_a\rangle$ to $|\vec{k}_a + \vec{q}_p\rangle$, while its weight $f(\vec{k}_w, t)$ remains constant.

We notice that these collisions introduce not only stochastic dynamics in the evolution of the CWF, but also time-irreversibility in the whole simulation, since, in general, $g_{k_{0a}}^{\vec{q}_p} < g_{k_{0a} + \vec{q}_p}^{-\vec{q}_p}$, where positive (negative) \vec{q}_p means phonon absorption (emission).

B. Dissipative transport in parabolic-band structures

We apply our approach for the simulation of a typical GaAs/AlGaAs resonant tunneling device (RTD) when elastic (acoustic phonons and impurities) and inelastic (optical phonons) collisions are considered. In particular, it can be shown that the required evolution of the CWF ψ_a interacting with a phonon $\vec{q}_p = \{q_{px}, q_{py}, q_{pz}\}$ in a material with parabolic-band structure can be obtained from Eq. (9):

$$i\hbar \frac{\partial \psi_a}{\partial t} = \left[\frac{1}{2m^*} (\vec{p}_a + \vec{\lambda}_a \Theta_{t_c})^2 + V_a \right] \psi_a, \quad (23)$$

where $\vec{p}_a = -i\hbar \vec{\nabla}_a$, $m^* = 0.067m_e$ is the electron effective mass (m_e is the free-electron mass), $\vec{\lambda}_a = \hbar \vec{q}_p$, and $\Theta_{t_c} \equiv \Theta(t - t_c)$ is the Heaviside step function. In Appendix C, we prove that Eq. (23) exactly reproduces the transition of ψ_a from Eq. (21) to Eq. (22). Each electron $a = \{1, 2, \dots, N_e\}$ has its own Eq. (23) to compute ψ_a and $\vec{r}_a[t]$ by time-integrating its velocity in Eq. (3). The term V_a provides the Coulomb correlation among all simulated electrons, including the appropriate boundaries. The injection model locates the initial CWF outside the simulation box and defines it from typical Gaussian wave packets with a dispersion $\sigma = 40$ nm. The properties of the injected electrons are selected according to some well-defined assumptions. For example, the energies of the injected electrons from one contact (assumed in thermodynamical equilibrium) into the open system fulfill a Fermi-Dirac distribution. This randomness in the injection of electrons introduces another source of stochasticity in the description of the properties of the open system.

We compute the current as the net number of trajectories $\vec{r}_a[t]$ transmitted from one side to the other, divided by the total simulation time (5 ps). Identically, the dc current is also computed as the time average of the total (conduction plus displacement) current. Both types of dc computations provide the same value at each bias point, showing the accuracy of the simulation. Technically, the experiment is not repeated, but the numerical simulation takes so long that electrons are entering and leaving the active region many times, providing repeated scenarios. The number and type of collisions are obtained from the Fermi Golden Rule for GaAs

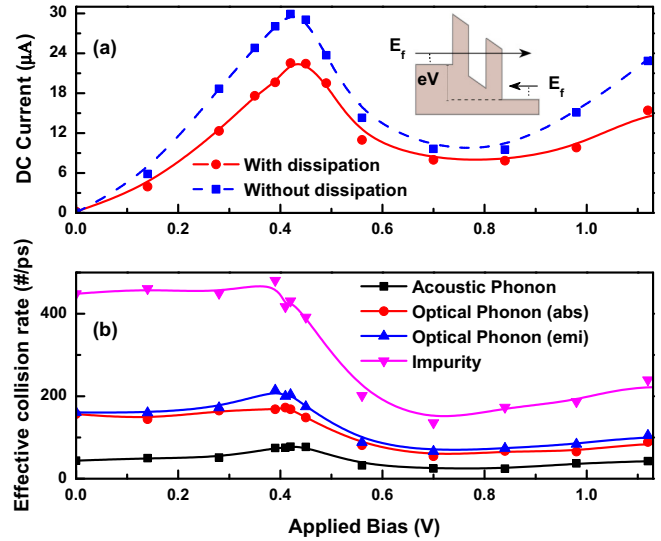


FIG. 1. (a) Current-voltage characteristic for a RTD with (solid red curve) and without (blue dashed curve) dissipation due to acoustic and optical phonons and impurities. The barrier height and width are 0.5 eV and 1.6 nm, and the well width is 2.4 nm. An n -type doping with a Fermi level of $E_f = 0.15$ eV above the conduction band is considered. (b) Effective collision rate as a function of bias. The optical phonons lead to an inelastic change of the electron energy of ± 0.036 eV.

materials [21]. We notice that the collision in Eq. (9) does not introduce any artificial decoherence. The expected reduction of the transmission [22] seen in Fig. 1(a) is because of the randomization of the momentum due to acoustic phonons and to the energy dissipation due to the emission of optical phonons. We see in Fig. 1(b) that the number of collisions at resonance is three times larger than that out of resonance, showing that the ballisticity of tunneling devices also depends on the electron transit time that varies from one voltage to another, due to different backactions of our non-Markovian (phonon) environment [6].

C. Dissipative transport in linear-band structures

Next, we present the Bohmian trajectories and CWF evolution of one electron during a collision with a phonon in graphene, with a richer band structure than GaAs. The whole development of the equation of motion in Eq. (9) and the inclusion of the collision needs to be redone for a conditional two-dimensional (2D) bispinor $\psi_a \equiv (\psi_{a,1}, \psi_{a,2})^T$ giving

$$i\hbar \frac{\partial \psi_a}{\partial t} = v_f \begin{pmatrix} V_a/v_f & p_a^- + \lambda_a^- \Theta_{t_c} \\ (p_a^+ + \lambda_a^+ \Theta_{t_c}) \chi_{t_c} & V_a \chi_{t_c}/v_f \end{pmatrix} \psi_a, \quad (24)$$

where $v_f = 10^6$ m/s is the Fermi velocity. We define $p_a^\pm = -i\hbar \partial_{x_a} \pm \hbar \partial_{y_a}$ and $\lambda_a^\pm = \lambda_{ax} \pm i\lambda_{ay}$ as the change in momentum $\vec{\lambda}_a = \hbar \vec{q}_p$ due to the interaction with a phonon with wave vector $\vec{q}_p = \{q_{px}, q_{py}\}$. When the interaction occurs, the term $\chi_{t_c} = e^{i(m\pi + \beta_{\vec{r}_{fa}} - \beta_{\vec{r}_{0a}})\Lambda_{t_c}}$ makes sure that the final state is either in the conduction band (positive energy branch) or in the valence band (negative energy states). If the electron changes from the conduction to the valence band (or vice versa), we use

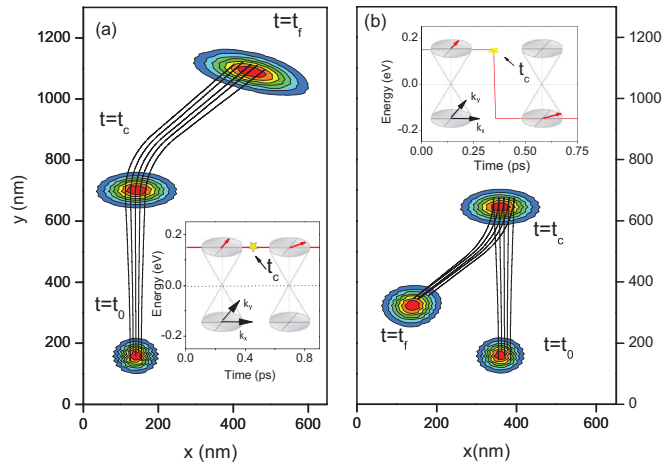


FIG. 2. (a) Time evolution of the modulus squared of the conditional bispinor for an electron initially at t_0 in the conduction band, with wave vector $(k_{0ax}, k_{0ay}) = (0, |\vec{k}_{0a}|)$, suffering an elastic collision at t_c with a phonon that provides a final wave vector $(k_{fax}, k_{fay}) = (|\vec{k}_{0a}|/\sqrt{2}, |\vec{k}_{0a}|/\sqrt{2})$. The associated Bohmian trajectories are also shown. Inset: electron energy conservation for the elastic collision. (b) Same change of wave vector as in (a) but with an inelastic collision that produces a final electron in the valence band (where velocity and momentum are opposite).

$m = 1$ and if there is no change of band $m = 0$, with $e^{i\beta_{k_{0a}}} = (k_{0ax} + ik_{0ay})/|\vec{k}_{0a}|$, where \vec{k}_{0a} (\vec{k}_{fa}) is the central initial (final) wave vector and $e^{i\beta_{k_{fa}}}$ having the same definition. χ_{t_c} is only relevant at t_c , i.e., $\Lambda_{t_c} \equiv \Lambda_{t_c}(t) = 0$ except $\Lambda_{t_c}(t = t_c) = 1$. In Appendix D, we prove that Eq. (24) produces the transition of the 2D bispinor ψ_a from Eq. (21) to Eq. (22).

We present in Figs. 2 and 3 numerical results for the electron-phonon collisions in graphene, whose dynamics near the Dirac points are given by Eq. (24). The initial state in

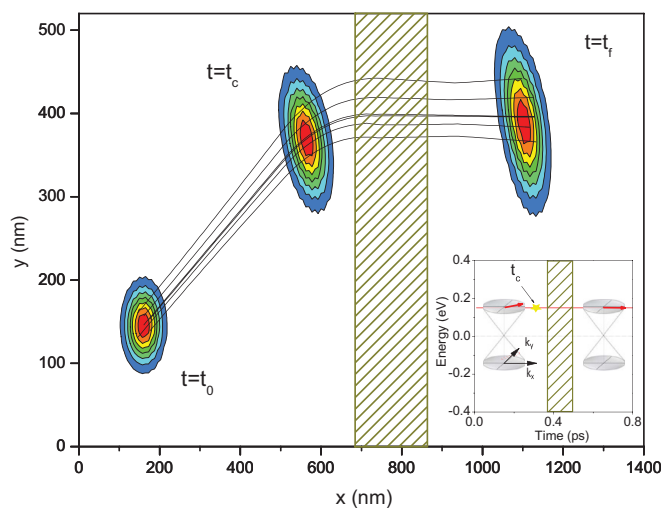


FIG. 3. Time evolution of the modulus squared of the conditional bispinor for an electron that impinges on a 0.4 eV barrier with a width of 200 nm. The initial $t = t_0$ direction is $\beta_0 = \pi/6$, so Klein tunneling should be minimal. At $t = t_c$, an elastic collision deviates the electron in a perpendicular direction to the barrier maximizing the Klein tunneling.

both examples is a Gaussian wave packet with dispersion $\sigma = 40$ nm and wave vector $|\vec{k}_{0a}| = 2.27 \times 10^8 \text{ m}^{-1}$, whose initial pseudospin lies in the conduction band.

IV. CONCLUSIONS

In this paper, we present an approach to analyze quantum dissipation. It is based on Bohmian CWFs that preserves CP and allows a realistic consideration of dissipative sources. Formally, our approach follows the SSE technique [9] for non-Markovian scenarios [7,10,12], but allowing a physical interpretation of the output results under a continuous measurement. The open-system techniques mentioned in the Introduction are rarely applied to the simulation of electron devices (with exceptions such as the Wigner-Boltzmann approach, which has problems of CP [2,3], or other density matrix approaches that have difficulties in being adapted to spatially well-defined models respecting the different spatial regions (with well-defined boundaries) typical in electron devices [23,24]). Typically, dissipation in quantum electron transport is simulated through a partition of the full Hilbert space into smaller spaces where sets of eigenstates are perfectly determined. Interactions (dissipation) between different spaces are introduced through coupling constants [25]. The solution of such models implicitly involves an improper mixture of states [19] that, in spite of its computational interest, has no ontological definition within standard quantum mechanics [20]. The Bohmian CWFs provide a *unproblematic* way to define the wave function of an open system [10], and we have shown that it allows a realistic simulation of quantum dissipation in electron devices with linear and parabolic-band structures. With the accurate inclusion of quantum dissipation in the evolution of CWFs, the *general* and *accurate* quantum-trajectory approach [26] presented here is the best candidate to substitute the old Monte Carlo solution of the Boltzmann equation for semiclassical systems [21] in the new nanoelectronics/atomtronics quantum scenarios.

ACKNOWLEDGMENTS

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APPENDIX A: EVALUATION OF THE TERM

$$(\vec{r}_a, \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_{ep, \vec{u}} | \Psi(t)) |_{\vec{z}_a^j(t), \vec{R}^j(t)} \text{ IN EQ. (15)}$$

We evaluate the effect of the $\hat{\mathcal{H}}_{ep, \vec{u}}$ on the wave packet $\Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t)$. For that purpose, we develop the explicit expression of $\hat{\mathcal{H}}_{ep, \vec{u}}$ and then we define an initial many-body wave packet $\Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t)$.

1. Definition of the electron-phonon Hamiltonian

The term H_{ep} in Eq. (13) can be written as $H_{ep} = H_{ep, \vec{R}_0} + H_{ep, \vec{u}} = \sum_{e,h} V_{ep}(\vec{r}_e - \vec{R}_h)$. We decompose $V_{ep}(\vec{r}_e - \vec{R}_h)$ in

a Taylor expansion around the equilibrium position of the h ions $\vec{R}_{h,0}$ as

$$\begin{aligned} & \sum_{e,h} V_{ep}(\vec{r}_e - \vec{R}_h) \\ & \approx \sum_{e,h} V_{ep}(\vec{r}_e - \vec{R}_{h,0}) + (\vec{R}_h - \vec{R}_{h,0}) \cdot \nabla_h V_{ep}(\vec{r}_e - \vec{R}_h)|_{\vec{R}_h = \vec{R}_{h,0}} \\ & = \sum_{e,h} V_{ep}(\vec{r}_e - \vec{R}_{h,0}) + \vec{u}_h \cdot \nabla_h V_{ep}(\vec{r}_e - \vec{R}_h)|_{\vec{R}_h = \vec{R}_{h,0}} \\ & = H_{ep,\vec{R}_0} + H_{ep,\vec{u}}. \end{aligned} \quad (\text{A1})$$

The term $V_{ep}(\vec{r}_e - \vec{R}_{h,0})$ will become relevant later for the electronic band structure, while $\vec{u}_h \cdot \nabla_h V_{ep}(\vec{r}_e - \vec{R}_h)|_{\vec{R}_h = \vec{R}_{h,0}}$ provides the interaction of the electron \vec{r}_e with the ion \vec{R}_h (neglecting second-order Taylor terms in the atomic displacements expansion). Instead of dealing with individual displacements \vec{u}_h , we consider the normal coordinate $\vec{Q}_{\vec{q}_p}$ defined from the Fourier transform:

$$\vec{u}_h = \sum_{\vec{q}_p} \vec{Q}_{\vec{q}_p} e^{i\vec{q}_p \cdot \vec{R}_{h,0}}, \quad (\text{A2})$$

where \vec{q}_p is a wave vector in the reciprocal space that labels each of the possible collective solutions of the movement of ions. Then we perform the Fourier transform of the potential $V_{ep}(\vec{r}_e - \vec{R}_h)$:

$$V_{ep}(\vec{r}_e - \vec{R}_h) = \sum_{\vec{v}} e^{i\vec{v}(\vec{r}_e - \vec{R}_h)} U_{\vec{v}}, \quad (\text{A3})$$

where \vec{v} is another wave vector in the reciprocal space, and $U_{\vec{v}}$ is the Fourier coefficients of the potential. Notice that $\sum_h V_{ep}(\vec{r}_e - \vec{R}_h)$ is a periodic potential, while $V_{ep}(\vec{r}_e - \vec{R}_h)$ alone is essentially a Coulomb potential with corrections due to screening. Then, the gradient of the potential in Eq. (A1) can be written as

$$\nabla_h V_{ep}(\vec{r}_e - \vec{R}_h)|_{\vec{R}_h = \vec{R}_{h,0}} = \sum_{\vec{v}} (-i\vec{v}) e^{i\vec{v}(\vec{r}_e - \vec{R}_{h,0})} U_{\vec{v}}. \quad (\text{A4})$$

Putting Eq. (A4) and Eq. (A2) altogether for all electrons and ions, we obtain finally

$$\begin{aligned} H_{ep,\vec{u}} & = \sum_e H_{ep,\vec{u},\vec{r}_e} = \sum_e \sum_h \vec{u}_h \cdot \nabla_h V_{ep}(\vec{r}_e - \vec{R}_h)|_{\vec{R}_h,0} \\ & = \sum_e \sum_h \sum_{\vec{q}_p} e^{i\vec{q}_p \cdot \vec{R}_{h,0}} \vec{Q}_{\vec{q}_p} \sum_{\vec{v}} (-i\vec{v}) e^{i\vec{v}(\vec{r}_e - \vec{R}_{h,0})} U_{\vec{v}}. \end{aligned} \quad (\text{A5})$$

Before discussing the interaction through the term $H_{ep,\vec{u}}$, we define the initial electron-lattice wave packet.

2. Definition of the many-body wave packet $\Psi(\vec{r}, \vec{R}, t)$

The many-body wave packet $\Psi(\vec{r}, \vec{R}, t) = \langle \vec{r}_a, \vec{z}_a, \vec{R} | \Psi(t) \rangle$ can be written as

$$\Psi(\vec{r}, \vec{R}, t) = \sum_{\vec{k}, \vec{q}} a(\vec{k}, \vec{q}, t) \Phi_{\vec{k}}(\vec{r}) \Phi_{\vec{q}}(\vec{R}), \quad (\text{A6})$$

with $a(\vec{k}, \vec{q}, t)$ accounting for an arbitrary superposition of the many-body electron base $\Phi_{\vec{k}}(\vec{r})$ and many-body phonon base $\Phi_{\vec{q}}(\vec{R})$. The vector $\vec{k} = \{\vec{k}_1, \vec{k}_2, \dots, \vec{k}_{N_e}\}$ represents the

many-body index of the electronic (Bloch states) base, and $\vec{q} = \{\vec{q}_1, \vec{q}_2, \dots\}$ is the index of the ionic base. We define $\Phi_{\vec{k}}(\vec{r}) \equiv \sum_{n=1}^{N_e!} \prod_{i=1}^{N_e} \phi_{\vec{k}_i}(\vec{r}_{p(n)}) s_n$, with $\vec{p}(n) = \{p(n)_1, \dots, p(n)_{N_e}\}$ the n -permutation vector, and s_n is its sign. We have also used the single-particle Bloch eigenstate:

$$\phi_{\vec{k}_e}(\vec{r}_e) = \langle \vec{r}_e | \vec{k}_e \rangle = e^{i\vec{k}_e \cdot \vec{r}_e} u_{\vec{k}_e}(\vec{r}_e), \quad (\text{A7})$$

where $u_{\vec{k}_e}(\vec{r}_e)$ is periodic with respect to lattice translations (which includes the appropriate normalizing constant) and \vec{k}_e is the electron (quasi) wave vector related to the quasi (or crystal) momentum $\vec{p}_e = \hbar \vec{k}_e$.

In the language of the second quantization, the Slater determinant of the electrons can be written as $\Phi_{\vec{k}}(\vec{r}) \equiv \langle \vec{r} | \hat{c}_{\vec{k}_1}^\dagger \dots \hat{c}_{\vec{k}_{N_e}}^\dagger | 0 \rangle$. To explicitly write the dependence of $\Phi_{\vec{k}}(\vec{r})$ on \vec{r}_e , we expand the Slater determinant of electrons by minors as $\langle \vec{r}_e, \vec{z}_e | \hat{c}_{\vec{k}_1}^\dagger \dots \hat{c}_{\vec{k}_{N_e}}^\dagger | 0 \rangle = \sum_{w=1}^{N_e} \phi_{\vec{k}_w}(\vec{r}_e) s_{e,w} \langle \vec{z}_e | \hat{c}_{\vec{k}_1}^\dagger \dots \hat{c}_{\vec{k}_{w-1}}^\dagger \hat{c}_{\vec{k}_{w+1}}^\dagger \dots \hat{c}_{\vec{k}_{N_e}}^\dagger | 0 \rangle$, with $s_{e,w}$ the sign of the (e, w) cofactor. Then

$$\begin{aligned} \Psi(\vec{r}_e, \vec{z}_e, \vec{R}, t) & = \sum_{\vec{k}, \vec{q}} a(\vec{k}, \vec{q}, t) \Phi_{\vec{q}}(\vec{R}) \sum_{\vec{k}_w} \phi_{\vec{k}_w}(\vec{r}_e) s_{e,w} \\ & \quad \times \langle \vec{z}_e | \hat{c}_{\vec{k}_1}^\dagger \dots \hat{c}_{\vec{k}_{w-1}}^\dagger \hat{c}_{\vec{k}_{w+1}}^\dagger \dots \hat{c}_{\vec{k}_N}^\dagger | 0 \rangle. \end{aligned} \quad (\text{A8})$$

3. Evaluation of $H_{ep,\vec{u}}(\vec{r}, \vec{R}, t) \Psi(\vec{r}, \vec{R}, t)$

The term $H_{ep,\vec{u}} = \sum_e H_{ep,\vec{u},\vec{r}_e}$ in Eq. (A5) is a sum over terms that depend on a unique \vec{r}_e , so that when conditioning $H_{ep,\vec{u}}(\vec{r}, \vec{R}, t) \Psi(\vec{r}, \vec{R}, t)$ to $\{\vec{z}_a^j[t], \vec{R}^j[t]\}$, all terms except one do not depend on \vec{r}_a . We have

$$\begin{aligned} & H_{ep,\vec{u}}(\vec{r}, \vec{R}, t) \Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) \Big|_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ & = \left(\sum_e H_{ep,\vec{u},\vec{r}_e}(\vec{r}_e, \vec{R}, t) \right) \Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) \Big|_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ & = \left(\sum_{e \neq a} H_{ep,\vec{u},\vec{r}_e}(\vec{r}_e^j[t], \vec{R}^j[t], t) \right) \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) \\ & \quad + H_{ep,\vec{u},\vec{r}_a}(\vec{r}_a, \vec{R}^j[t], t) \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t). \end{aligned} \quad (\text{A9})$$

The term $\sum_{e \neq a} H_{ep,\vec{u},\vec{r}_e}(\vec{r}_e^j[t], \vec{R}^j[t], t)$ is a constant value without dependence on \vec{r}_a . This pure time-dependent term only provides a global phase on the conditional wave function that can be omitted without any effect [17]. The only term that we have to compute explicitly is $H_{ep,\vec{u},\vec{r}_a}(\vec{r}_a, \vec{R}, t) \Psi(\vec{r}, \vec{R}, t) = \langle \vec{r}, \vec{R} | \hat{\mathcal{H}}_{ep,\vec{u},\vec{r}_a} | \Psi(t) \rangle$. Using the identities $\int_{\vec{r}} d\vec{r} |\vec{r}\rangle \langle \vec{r}| = \mathbb{1}$ and $\int_{\vec{R}} d\vec{R} |\vec{R}\rangle \langle \vec{R}| = \mathbb{1}$, the fact that $\hat{\mathcal{H}}_{ep,\vec{u},\vec{r}_a}$ is diagonal in the position representation, and the identity $\sum_{\vec{k}_a} |\vec{k}_a\rangle \langle \vec{k}_a| = \mathbb{1}$, we can write

$$\begin{aligned} & \langle \vec{r}, \vec{R} | \hat{\mathcal{H}}_{ep,\vec{u},\vec{r}_a} | \Psi(t) \rangle \\ & = \langle \vec{r}, \vec{R} | \hat{\mathcal{H}}_{ep,\vec{u},\vec{r}_a} | \vec{r}, \vec{R} \rangle \langle \vec{r}, \vec{R} | \Psi(t) \rangle \\ & = \sum_{\vec{k}_a} \sum_{\vec{k}_a''} \langle \vec{r}_a | \vec{k}_a'' \rangle \langle \vec{k}_a'', \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_{ep,\vec{u},\vec{r}_a} | \vec{k}_a, \vec{z}_a, \vec{R} \rangle \langle \vec{k}_a, \vec{z}_a, \vec{R} | \Psi(t) \rangle \\ & = \sum_{\vec{k}_a} \sum_{\vec{k}_a''} \mathcal{T}(\vec{k}_a'', \hat{\mathcal{H}}_{ep,\vec{u},\vec{r}_a}, \vec{k}_a) \langle \vec{r}_a | \vec{k}_a'' \rangle \langle \vec{k}_a, \vec{z}_a, \vec{R} | \Psi(t) \rangle, \end{aligned} \quad (\text{A10})$$

where we have defined $\mathcal{T}(\vec{k}_a'', \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a}, \vec{k}_a) \equiv \langle \vec{k}_a'', \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a} | \vec{k}_a, \vec{z}_a, \vec{R} \rangle$ as the electron-phonon Hamiltonian in the momentum (Bloch state) representation. This term can be rewritten as

$$\mathcal{T}(\vec{k}_a'', \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a}, \vec{k}_a) = \int_{\vec{r}_a} d\vec{r}_a \langle \vec{k}_a'' | \vec{r}_a \rangle \langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a} | \vec{r}_a, \vec{z}_a, \vec{R} \rangle \langle \vec{r}_a | \vec{k}_a \rangle, \quad (\text{A11})$$

and using the final expression of the electron-phonon Hamiltonian in the position representation, Eq. (A5), we obtain

$$\begin{aligned} \mathcal{T}(\vec{k}_a'', \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a}, \vec{k}_a) &= \int_{\vec{r}_a} d\vec{r}_a e^{-i\vec{k}_a'' \vec{r}_a} u_{\vec{k}_a''}(\vec{r}_a) e^{i\vec{k}_a \vec{r}_a} u_{\vec{k}_a}(\vec{r}_a) \\ &\quad \times \langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a} | \vec{r}_a, \vec{z}_a, \vec{R} \rangle \\ &= \int_{\vec{r}_a} d\vec{r}_a e^{-i\vec{k}_a'' \vec{r}_a} u_{\vec{k}_a''}(\vec{r}_a) e^{i\vec{k}_a \vec{r}_a} u_{\vec{k}_a}(\vec{r}_a) \\ &\quad \times \sum_h \sum_{\vec{q}_p} e^{i\vec{q}_p \vec{R}_{h,0}} \bar{Q}_{\vec{q}_p} \sum_{\vec{v}} (-i\vec{v}) \\ &\quad \times e^{i\vec{v}(\vec{r}_a - \vec{R}_{h,0})} U_{\vec{v}}. \end{aligned} \quad (\text{A12})$$

We take away from the integral those elements that do not depend on \vec{r}_a :

$$\begin{aligned} \mathcal{T}(\vec{k}_a'', \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a}, \vec{k}_a) &= \sum_h \sum_{\vec{q}_p} e^{i\vec{q}_p \vec{R}_{h,0}} \bar{Q}_{\vec{q}_p} \sum_{\vec{v}} (-i\vec{v}) e^{-i\vec{v} \vec{R}_{h,0}} U_{\vec{v}} \\ &\quad \times \int_{\vec{r}_a} d\vec{r}_a e^{-i\vec{k}_a'' \vec{r}_a} u_{\vec{k}_a''}(\vec{r}_a) e^{i\vec{k}_a \vec{r}_a} u_{\vec{k}_a}(\vec{r}_a) e^{i\vec{v} \vec{r}_a}. \end{aligned} \quad (\text{A13})$$

Due to the periodicity of $u_{\vec{k}_a}(\vec{r}_a)$, we can use the change of variable $\vec{r}_a = \vec{r}'_a + \vec{R}_{m,0}$, where \vec{r}'_a integrates only inside the first Brillouin zone. We get

$$\begin{aligned} \mathcal{T}(\vec{k}_a'', \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a}, \vec{k}_a) &= \sum_h \sum_{\vec{q}_p} \bar{Q}_{\vec{q}_p} \sum_{\vec{v}} (-i\vec{v}) e^{i\vec{R}_{h,0}(\vec{q}_p - \vec{v})} U_{\vec{v}} \left(\sum_m e^{i\vec{R}_{m,0}(-\vec{k}_a'' + \vec{v} + \vec{k}_a)} \right) \\ &\quad \times \int_{\vec{r}'_a} d\vec{r}'_a e^{-i\vec{k}_a'' \vec{r}'_a} u_{\vec{k}_a''}(\vec{r}'_a) e^{i\vec{k}_a \vec{r}'_a} u_{\vec{k}_a}(\vec{r}'_a) e^{i\vec{v} \vec{r}'_a}. \end{aligned} \quad (\text{A14})$$

The sum over $\vec{R}_{h,0}$ in $\sum_h e^{i\vec{R}_{h,0}(\vec{q}_p - \vec{v})}$ imposes the condition $\vec{G} = \vec{q}_p - \vec{v}$, and the sum over $\vec{R}_{m,0}$ in $\sum_m e^{i\vec{R}_{m,0}(-\vec{k}_a'' + \vec{v} + \vec{k}_a)}$ imposes that $\vec{G}' = -\vec{k}_a'' + \vec{v} + \vec{k}_a$, with \vec{G} and \vec{G}' two vectors of the reciprocal lattice. For simplicity, although umklapp scattering can also be considered, we assume that all momentum vectors can be considered in the first Brillouin zone, $\vec{G} = 0$ and $\vec{G}' = 0$, so that $\vec{k}_a'' = \vec{q}_p + \vec{k}_a$. Therefore,

$$\mathcal{T}(\vec{k}_a'', \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a}, \vec{k}_a) = \sum_{\vec{q}_p} \delta(\vec{k}_a'' - \vec{q}_p - \vec{k}_a) g_{\vec{k}_a}^{\vec{q}_p}. \quad (\text{A15})$$

All other terms in Eq. (A14) are included into the coupling constant $g_{\vec{k}_a}^{\vec{q}_p}$ defined as

$$\begin{aligned} g_{\vec{k}_a}^{\vec{q}_p} &= -i \bar{Q}_{\vec{q}_p} \bar{q}_p U_{\vec{q}_p} \int_{\vec{r}'_a} d\vec{r}'_a e^{-i(\vec{k}_a + \vec{q}_p) \vec{r}'_a} \\ &\quad \times u_{\vec{k}_a + \vec{q}_p}(\vec{r}'_a) e^{i\vec{k}_a \vec{r}'_a} u_{\vec{k}_a}(\vec{r}'_a) e^{i\vec{v} \vec{r}'_a}. \end{aligned} \quad (\text{A16})$$

We emphasize that we did not include any dependence on the n band we are dealing with, since usually phonon energies are smaller than band gaps and then phonons cannot make band transitions. However, for materials with small band gaps, these multiband transitions can be included straightforwardly. In fact, when dealing with graphene bispinors, we include the dependence of the coupling constant on the energy branches. We introduce Eq. (A15) into Eq. (A10), and we conclude

$$\begin{aligned} H_{ep, \vec{u}, \vec{r}_a}(\vec{r}_a, \vec{z}_a, \vec{R}, t) \Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) &= \sum_{\vec{k}_a} \sum_{\vec{k}_a''} \langle \vec{r}_a | \vec{k}_a'' \rangle \mathcal{T}(\vec{k}_a'', \hat{\mathcal{H}}_{ep, \vec{u}, \vec{r}_a}, \vec{k}_a) \langle \vec{k}_a, \vec{z}_a^j[t], \vec{R}^j[t] | \Psi(t) \rangle \\ &= \sum_{\vec{q}_p} \sum_{\vec{k}_a} g_{\vec{k}_a}^{\vec{q}_p} \langle \vec{r}_a | \vec{k}_a + \vec{q}_p \rangle \langle \vec{k}_a, \vec{z}_a, \vec{R} | \Psi(t) \rangle. \end{aligned} \quad (\text{A17})$$

4. Conditional (envelope) wave packet before the collision

The conditional wave packet before the collision can be obtained from Eq. (A8) by fixing $\vec{z}_a = \vec{z}_a^j[t]$ and $\vec{R} = \vec{R}^j[t]$, where these positions correspond to one j experiment. Then

$$\begin{aligned} \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) &= \sum_{\vec{k}, \vec{q}} a(\vec{k}, \vec{q}, t) \Phi_{\vec{q}}(\vec{R}^j[t]) \sum_{\vec{k}_w} \phi_{\vec{k}_w}(\vec{r}_a) s_{a,w} \\ &\quad \times \langle \vec{z}_a^j[t] | \hat{c}_{\vec{k}_1}^\dagger \cdots c_{\vec{k}_{w-1}}^\dagger c_{\vec{k}_{w+1}}^\dagger \cdots \hat{c}_{\vec{k}_N}^\dagger | 0 \rangle. \end{aligned} \quad (\text{A18})$$

The dependence on \vec{r}_a of the conditional wave packet in Eq. (A18) appears because of the Bloch state $\phi_{\vec{k}_w}(\vec{r}_a) \equiv \langle \vec{r}_a | \vec{k}_w \rangle$. Therefore, it can be compactly rewritten as

$$\begin{aligned} \psi_a(\vec{r}_a, t) &\equiv \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) \\ &= \sum_{\vec{k}_w} f_a(\vec{k}_w, \vec{z}_a^j[t], \vec{R}^j[t], t) \phi_{\vec{k}_w}(\vec{r}_a) \\ &= \sum_{\vec{k}_w} f_a(\vec{k}_w, t) \phi_{\vec{k}_w}(\vec{r}_a), \end{aligned} \quad (\text{A19})$$

where $f_a(\vec{k}_w, t) \equiv f_a(\vec{k}_w, \vec{z}_a^j[t], \vec{R}^j[t], t) \equiv \langle \vec{k}_w, \vec{z}_a^j[t], \vec{R}^j[t] | \Psi(t) \rangle$, appearing in Eq. (21) and Eq. (22) in the text, is defined here as

$$\begin{aligned} f_a(\vec{k}_w, t) &= \sum_{\vec{q}} \sum_{\vec{k}, \vec{k}_e \neq \vec{k}_w} a(\vec{k}, \vec{q}, t) \Phi_{\vec{q}}(\vec{R}^j[t]) s_{a,w} \\ &\quad \times \langle \vec{z}_a^j[t] | \hat{c}_{\vec{k}_1}^\dagger \cdots c_{\vec{k}_{w-1}}^\dagger c_{\vec{k}_{w+1}}^\dagger \cdots \hat{c}_{\vec{k}_N}^\dagger | 0 \rangle. \end{aligned} \quad (\text{A20})$$

Under the standard envelope approximation in which the wave packet is centered around $\vec{k}_a \approx \vec{k}_{0a}$, we can rewrite the Bloch states as $\langle \vec{r}_a | \vec{k}_a \rangle = \phi_{\vec{k}_a}(\vec{r}_a) \approx e^{i\vec{k}_a \vec{r}_a} u_{\vec{k}_{0a}}(\vec{r}_a)$ and rewrite Eq. (A19) as

$$\begin{aligned} \psi_a(\vec{r}_a, t) &= u_{\vec{k}_{0a}}(\vec{r}_a) \sum_{\vec{k}_w} e^{i\vec{k}_w \vec{r}_a} \langle \vec{k}_w, \vec{z}_a^j[t], \vec{R}^j[t] | \Psi(t) \rangle \\ &= u_{\vec{k}_{0a}}(\vec{r}_a) \sum_{\vec{k}_w} e^{i\vec{k}_w \vec{r}_a} f_a(\vec{k}_w, t). \end{aligned} \quad (\text{A21})$$

We notice that $f(\vec{k}_a, t)$ includes now an (irrelevant) normalization constant. Finally, we notice that we will use the same symbol $\psi_a(\vec{r}_a, t)$ to refer to the conditional wave packet and to

the envelope conditional wave function defined, by ignoring the atomic periodicity $u_{\vec{k}_{0a}}(\vec{r}_a)$, as

$$\begin{aligned}\psi_a(\vec{r}_a, t) &= \sum_{\vec{k}_w} e^{i\vec{k}_w \vec{r}_a} \langle \vec{k}_w, \vec{z}_a^j[t], \vec{R}^j[t] | \Psi(t) \rangle \\ &= \sum_{\vec{k}_w} e^{i\vec{k}_w \vec{r}_a} f_a(\vec{k}_w, t).\end{aligned}\quad (\text{A22})$$

The ensemble momentum of the initial envelope wave packet $\psi_a(\vec{r}_a, t)$ in Eq. (A22), at $t = t_{c1}$ before the collision, can be written as

$$\langle \vec{p}_a \rangle_{t_{c1}} = \sum_{\vec{k}_w} \hbar \vec{k}_w |f_a(\vec{k}_w, t)|^2. \quad (\text{A23})$$

5. Conditional (envelope) wave packet after the collision

Conditioning the many-body wave function $\Psi(\vec{r}_a, \vec{z}_e, \vec{R}, t)$ to the particular values of $\vec{z}_a^j[t]$ and $\vec{R}^j[t]$ belonging to the j experiment means that we are considering only one event of the many available in the wave function. In particular, from all phonon modes present in Eq. (A17), we consider that, in a particular j experiment, only one $\vec{q}_p^j[t]$ (or none) is relevant at each time t (if more than one phonon mode is relevant simultaneously, then we can assume two single-phonon collisions simultaneously, each one with only one type of phonon mode). In addition, we consider that the involved wave packets are narrow enough in momentum space so that $g_{\vec{k}_{0a}}^{\vec{q}_p, j}[t] \approx g_{\vec{k}_{0a}}^{\vec{q}_p, j}[t]$, with \vec{k}_{0a} the central wave vector of the a wave packet. Then, Eq. (A17) conditioned to the value of $\vec{z}_a^j[t]$ and $\vec{R}^j[t]$ can be written as

$$\begin{aligned}H_{ep, \vec{u}, \vec{r}_a}(\vec{r}_a, \vec{z}_a, \vec{R}, t) \Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) \Big|_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ = g_{\vec{k}_{0a}}^{\vec{q}_p^j}[t] \sum_{\vec{k}_w} \langle \vec{r}_a | \vec{k}_w + \vec{q}_p \rangle \langle \vec{k}_w, \vec{z}_a^j[t], \vec{R}^j[t] | \Psi(t) \rangle.\end{aligned}\quad (\text{A24})$$

The coupling constant $g_{\vec{k}_{0a}}^{\vec{q}_p^j}[t]$ in the j experiment will imply an interaction of the \vec{r}_a electron with the phonon mode \vec{q}_p during a collision time interval, starting at t_{c1} and ending at t_{c2} . In a later time, $g_{\vec{k}_{0a}}^{\vec{q}_p^j}[t]$ will indicate a collision with another phonon mode. The exact (deterministic) description of $g_{\vec{k}_{0a}}^{\vec{q}_p^j}[t]$ would require perfect knowledge of the dynamics of $\vec{R}^j[t]$. Since we do not explicitly simulate the dynamics of the ions (which are understood as the environment of the electrons), we can only introduce their effects in a stochastic way ensuring that the probabilities of different phonon modes given by $g_{\vec{k}_{0a}}^{\vec{q}_p^j}[t]$ satisfy some precomputed values. This is the origin of the stochasticity in Eq. (9) due to the environment.

In one particular j experiment, during one collision, the term $g_{\vec{k}_{0a}}^{\vec{q}_p^j}[t]$ becomes irrelevant (the Bohmian velocity only depends on the dependence of the phase on \vec{r}_a , not on the norm), and the final wave packet in Eq. (A24), at time $t > t_{c2}$

after the collision, can be written as

$$\begin{aligned}\psi_a(\vec{r}_a, t) &\equiv \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) \\ &= \sum_{\vec{k}_w} f_a(\vec{k}_w, \vec{z}_a^j[t], \vec{R}^j[t], t) \phi_{\vec{k}_w + \vec{q}_p}(\vec{r}_a) \\ &= \sum_{\vec{k}_w} f_a(\vec{k}_w, t) \phi_{\vec{k}_w + \vec{q}_p}(\vec{r}_a),\end{aligned}\quad (\text{A25})$$

where $f_a(\vec{k}_w, t) = \langle \vec{k}_w, \vec{z}_a^j[t], \vec{R}^j[t] | \Psi(t) \rangle$ remains equal to the value in Eq. (A20) before the collision.

After the collision at $t = t_{c2}$, the (pseudo)momentum base changes from $|\vec{k}_e\rangle$ to $|\vec{k}_e + \vec{q}_p^j\rangle$, so that the final ensemble momentum of the envelope conditional wave packet in Eq. (A25) is

$$\begin{aligned}\langle \vec{p}_a \rangle_{t_{c2}} &= \sum_{\vec{k}_w} \hbar(\vec{k}_w + \vec{q}_p^j) |f_a(\vec{k}_w, t)|^2 \\ &= \langle \vec{p}_a \rangle_{t_{c1}} + \hbar \vec{q}_p^j.\end{aligned}\quad (\text{A26})$$

Let us emphasize that Eqs. (A23) and (A26) provide the expected role of the electron-phonon interaction: such a collision generates a change of momentum $\hbar \vec{q}_p^j$ in the conditional wave packet during a time interval $t_{c2} - t_{c1}$. We notice that we are considering a collision with a finite duration. As will be later explained, for simplicity in practical applications, we have considered instantaneous collisions in the text.

APPENDIX B: EVALUATION OF THE TERM

$\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_c | \Psi(t) \rangle \Big|_{\vec{z}_a^j[t], \vec{R}^j[t]}$ IN EQ. (16)

The term $\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{\mathcal{H}}_c | \Psi(t) \rangle \Big|_{\vec{z}_a^j[t], \vec{R}^j[t]} = \langle \vec{r}_a, \vec{z}_a, \vec{R} | K_e(\vec{r}) + K_h(\vec{R}) + V_{ee}(\vec{r}) + V_{hh}(\vec{R}) + H_{ep, \vec{R}_0}(\vec{r}, \vec{R}_0) | \Psi(t) \rangle \Big|_{\vec{z}_a^j[t], \vec{R}^j[t]}$ can be evaluated as follows. First, we divide $V_{ee}(\vec{r}) = V_{ee, \vec{r}_a}(\vec{r}_a) + V_{ee, \vec{z}_a}(\vec{z}_a)$ as the terms with an explicit dependence on \vec{r}_a , plus the terms without it. Similarly, $H_{ep, \vec{R}_0}(\vec{r}, \vec{R}_0) = H_{ep, \vec{R}_0, \vec{r}_a}(\vec{r}_a, \vec{R}_0) + H_{ep, \vec{R}_0, \vec{z}_a}(\vec{z}_a, \vec{R}_0)$.

1. Evaluation of $\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{V}_{hh} + \hat{V}_{ee, \vec{z}_a} + \hat{H}_{ep, \vec{R}_0, \vec{z}_a} | \Psi(t) \rangle \Big|_{\vec{z}_a^j[t], \vec{R}^j[t]}$

We have

$$\begin{aligned}\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{V}_{hh} + \hat{V}_{ee, \vec{z}_a} + \hat{H}_{ep, \vec{R}_0, \vec{z}_a} | \Psi(t) \rangle \Big|_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ = (V_{hh}(\vec{R}^j[t]) + V_{ee, \vec{z}_a}(\vec{z}_a^j[t]) + H_{ep, \vec{R}_0, \vec{z}_a}(\vec{z}_a^j[t], \vec{R}_0)) \\ \times \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t),\end{aligned}\quad (\text{B1})$$

where $V_{hh}(\vec{R}^j[t]) + V_{ee, \vec{z}_a}(\vec{z}_a^j[t]) + H_{ep, \vec{R}_0, \vec{z}_a}(\vec{z}_a^j[t], \vec{R}_0)$ are pure time-dependent terms, without an \vec{r}_a dependence, and then it only contributes to an arbitrary pure time-dependent angle that can be directly ignored; see Ref. [17].

2. Evaluation of $\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{V}_{ee, \vec{r}_a} | \Psi(t) \rangle |_{\vec{z}_a^j[t], \vec{R}^j[t]}$

Similarly, we write

$$\begin{aligned} & \langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{V}_{ee, \vec{r}_a} | \Psi(t) \rangle |_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ &= V_{ee, \vec{r}_a}(\vec{r}_a, \vec{z}_a^j[t]) | \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) \rangle \\ &= u_{\vec{k}_{0a}}(\vec{r}_a) V_{ee, \vec{r}_a}(\vec{r}_a, \vec{z}_a^j[t]) \psi_a(\vec{r}_a, t), \end{aligned} \quad (\text{B2})$$

where $V_{ee, \vec{r}_a}(\vec{r}_a, \vec{z}_a^j[t])$ can be easily known once the set of $\vec{r}^j[t]$ trajectories are known. Later we will use $V_a \equiv V_{ee, \vec{r}_a}(\vec{r}_a, \vec{z}_a^j[t])$.

3. Evaluation of $\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{K}_{e, \vec{z}_a} + \hat{K}_h | \Psi(t) \rangle |_{\vec{z}_a^j[t], \vec{R}^j[t]}$

The kinetic energy of ions \hat{K}_h and the kinetic energy of the rest of electrons, different from \vec{r}_a , defined as \hat{K}_{e, \vec{z}_a} with $\hat{K}_e = \hat{K}_{e, \vec{r}_a} + \hat{K}_{e, \vec{z}_a}$, can be written as

$$\begin{aligned} & \langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{K}_{e, \vec{z}_a} + \hat{K}_h | \Psi(t) \rangle |_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ &= \sum_{e=1, e \neq a}^{N_e} K_{e, \vec{r}_a} \Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) |_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ &+ \sum_{h=1}^{N_h} \frac{-\hbar^2}{2m_h} \nabla_h^2 \Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) |_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ &= A(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) \\ &= u_{\vec{k}_{0a}}(\vec{r}_a) A_a(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) \psi_a(\vec{r}_a, t), \end{aligned} \quad (\text{B3})$$

where K_{e, \vec{r}_a} is the kinetic energy of each \vec{z}_a electron and where we have introduced the real potential A_a as

$$\begin{aligned} A_a &\equiv A_a(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t) \\ &= \frac{\sum_{e=1, e \neq a}^{N_e} K_{e, \vec{r}_a} \Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) |_{\vec{z}_a^j[t], \vec{R}^j[t]}}{\Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t)} \\ &+ \frac{\sum_{h=1}^{N_h} \frac{-\hbar^2}{2m_h} \nabla_h^2 \Psi(\vec{r}_a, \vec{z}_a, \vec{R}, t) |_{\vec{z}_a^j[t], \vec{R}^j[t]}}{\Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t)}. \end{aligned} \quad (\text{B4})$$

This constant A_a includes other correlations (different from the electron-lattice correlations that we treat exactly apart from the stochastic approximation for ions dynamics), and it will be approximated later according to Ref. [17].

4. Evaluation of $\langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{K}_{e, \vec{r}_a} + \hat{H}_{ep, \vec{R}_0, \vec{r}_a} | \Psi(t) \rangle |_{\vec{z}_a^j[t], \vec{R}^j[t]}$

The last terms that have to be evaluated from \hat{H}_c in Eq. (15) are $\hat{K}_{e, \vec{r}_a} + \hat{H}_{ep, \vec{R}_0, \vec{r}_a}$. They determine the electronic band structure:

$$\begin{aligned} & \langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{K}_{e, \vec{r}_a} + \hat{H}_{ep, \vec{R}_0, \vec{r}_a} | \Psi(t) \rangle |_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ &= \left(K_{e, \vec{r}_a} + \sum_h V_{ep}(\vec{r}_a - \vec{R}_{h,0}) \right) \Psi(\vec{r}_a, \vec{z}_a^j[t], \vec{R}^j[t], t), \end{aligned} \quad (\text{B5})$$

where K_{e, \vec{r}_a} corresponds to the kinetic energy of the conditioned a electron, and $H_{ep, \vec{R}_0, \vec{r}_a} = \sum_h V_{ep}(\vec{r}_a - \vec{R}_{h,0})$ is the periodic potential seen by this a electron. From here, and after a tight binding and the approximation for low-energy

excitations (small \vec{k}), depending on the system we will end up with a band structure $E(\vec{p})$ either with linear or parabolic shape. Therefore,

$$\begin{aligned} & \langle \vec{r}_a, \vec{z}_a, \vec{R} | \hat{K}_{e, \vec{r}_a} + \hat{H}_{ep, \vec{R}_0, \vec{r}_a} | \Psi(t) \rangle |_{\vec{z}_a^j[t], \vec{R}^j[t]} \\ &\approx u_{\vec{k}_{0a}}(\vec{r}_a) E(\vec{p}) \psi_a(\vec{r}_a, t), \end{aligned} \quad (\text{B6})$$

where $\psi_a(\vec{r}_a, t)$ is the (conditional) envelope wave packet already defined in Eq. (A21).

APPENDIX C: SCHRÖDINGER (PARABOLIC-BAND) EQUATION

In the parabolic case, $E(\vec{p}_a)$ appearing in Eq. (B6) is $E(\vec{p}_a) = \frac{|\vec{p}_a|^2}{2m^*}$ with m^* an isotropic effective mass. After the collision, $t = t_{c2}$, regarding Eq. (A25) the state $|\vec{k}_e\rangle$ changes to $|\vec{k}_e + \vec{q}_p^j\rangle$. Under the mentioned envelope approximation, the Bloch states are $\langle \vec{r}_a | \vec{k}_a \rangle = \phi_{\vec{k}_a}^-(\vec{r}_a) \approx e^{i\vec{k}_a \vec{r}_a} u_{\vec{k}_{0a}}^-(\vec{r}_a)$. Then, the conditional wave packet at t_{c2} in Eq. (A25) can be related to the initial wave packet at t_{c1} given by Eq. (A22) as

$$\begin{aligned} \psi_a(\vec{r}_a, t_{c2}) &= \sum_{\vec{k}_w} e^{i(\vec{k}_w + \vec{q}_p) \vec{r}_a} \langle \vec{k}_w, \vec{z}_a^j[t_{c2}], \vec{R}^j[t_{c2}] | \Psi(t_{c2}) \rangle \\ &= \sum_{\vec{k}_w} e^{i(\vec{k}_w + \vec{q}_p) \vec{r}_a} f_a(\vec{k}_w, t_{c2}) = e^{i\vec{q}_p \vec{r}_a} \psi_a(\vec{r}_a, t_{c1}). \end{aligned} \quad (\text{C1})$$

Therefore, since Bloch states are energy eigenstates, the ensemble energy before the collision $\langle E(\vec{k}_a) \rangle_{t_{c1}}$ changes to the value $\langle E(\vec{k}_a + \vec{q}_p) \rangle_{t_{c2}}$ after the collision.

Putting together Eqs. (B2), (B3), (B6), and (10) into the original Eq. (15), and removing $u_{\vec{k}_{0a}}^-(\vec{r}_a)$, we get

$$i\hbar \frac{\partial \psi_a(\vec{r}_a, t)}{\partial t} = \left[\frac{1}{2m^*} (\vec{p}_a)^2 + V_a + A_a + iB_a \right] \psi_a(\vec{r}_a, t), \quad (\text{C2})$$

where the terms A_a and B_a in Eqs. (B4) and (11) are approximated by a zero-order Taylor expansion (i.e., no dependence on \vec{r}_a) so that they can be neglected when computing Bohmian velocities. See Ref. [17] for a discussion of such an approximation. Therefore, the time-evolution operator (propagator) from the initial time t_0 until a time before the collision $t < t_{c1}$ is just $\hat{U}_a(t, t_0) = e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}_{ca}(t') dt'}$, with $H_{ca} = \frac{1}{2m^*} (\vec{p}_a)^2 + V_a$, where H_c is conditioned at $\vec{z}_a^j[t]$.

The time evolution of the wave packet due to the collision with the phonon has to reproduce the condition given by Eq. (C1). The time-evolution operator (propagator) from $t = t_0$ until a time $t > t_{c2}$ after the collision is then

$$\begin{aligned} \hat{U}_a(t, t_0) &= e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}_{ca}(t') dt'} e^{-\frac{i}{\hbar} \int_{t_{c1}}^{t_{c2}} \hat{H}_{epa}(t') dt'} \\ &e^{-\frac{i}{\hbar} \int_{t_0}^{t_{c1}} \hat{H}_{ca}(t') dt'} = e^{-\frac{i}{\hbar} \int_{t_0}^{t_{c2}} \hat{H}_{ca}(t') dt'} e^{i \frac{\vec{q}_p \vec{r}_a}{\hbar}} e^{-\frac{i}{\hbar} \int_{t_0}^{t_{c1}} \hat{H}_{ca}(t') dt'}, \end{aligned} \quad (\text{C3})$$

where $\hat{H}_{epa} = -\hbar \vec{\lambda}_a \vec{r}_a \delta(t - t_c)$ is the previously mentioned total electron-lattice interaction \hat{H}_{ep} conditioned at $\vec{z}_a^j[t]$.

For a small time interval, Δt , we have $\hat{U}_a(t + \Delta t, t) = (1 - \frac{i}{\hbar} \Delta t \hat{H}_{ca})$. Then, it can be proven that $(1 -$

$\frac{i}{\hbar} \Delta t H_{ca} e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} \psi_a(\vec{r}_a, t_{c1}) = e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} (1 - \frac{i}{\hbar} \Delta t H_{ca+\lambda}) \psi_a(\vec{r}_a, t_{c1})$,
 where $H_{ca+\lambda} = \frac{(\vec{p}_a + \vec{\lambda}_a)^2}{2m^*} + V_a$. The demonstration of this result just requires us to show that

$$\begin{aligned}
 (\vec{p})^2 e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} \psi_a(\vec{r}_a, t) &= -\hbar^2 \vec{\nabla}^2 e^{-i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} \psi_a(\vec{r}_a, t) \\
 &= \vec{\lambda}_a^2 e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} \psi_a(\vec{r}_a, t) \\
 &\quad - 2i \hbar \vec{\lambda}_a e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} \vec{\nabla} \psi_a(\vec{r}_a, t) \\
 &\quad - \hbar^2 e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} \vec{\nabla}^2 \psi_a(\vec{r}_a, t) \\
 &= e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} (\vec{p} + \vec{\lambda}_a)^2 \psi_a(\vec{r}_a, t). \quad (C4)
 \end{aligned}$$

Therefore, the time evolution of the conditional wave packet at any time $t = t_{c2} + n \Delta t$ can be computed by applying the previous property n times and then

$$\begin{aligned}
 &\left(1 - \frac{i}{\hbar} \Delta t H_{ca}\right) \cdots \left(1 - \frac{i}{\hbar} \Delta t H_{ca}\right) e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} \psi_a(\vec{r}_a, t_{c1}) \\
 &= e^{i \frac{\vec{\lambda}_a \vec{r}_a}{\hbar}} \left(1 - \frac{i}{\hbar} \Delta t H_{ca+\lambda}\right) \cdots \left(1 - \frac{i}{\hbar} \Delta t H_{ca+\lambda}\right) \psi_a(\vec{r}_a, t_{c1}). \quad (C5)
 \end{aligned}$$

Finally, we can combine the time evolution of the envelope conditional wave packet $\psi_a(\vec{r}_a, t)$ before and after the collision in a unique equation of motion as

$$i \hbar \frac{\partial \psi_a}{\partial t} = \left[\frac{1}{2m^*} (\vec{p}_a + \vec{\lambda}_a \Theta_t)^2 + V_a \right] \psi_a, \quad (C6)$$

where $\Theta_t(t)$ can be any function that accomplishes $\Theta_t(t) = 0$ before the collision ($t < t_{c1}$) and $\Theta_t(t) = 1$ after the collision ($t > t_{c2}$). For practical purposes, and to facilitate computations, in the numerical results we consider $\Theta_t \equiv \Theta_{t_c}$ to be the Heaviside step function, $t = t_c$ is the time when the interaction occurs, t_{c2} is a time infinitely small after t_c , and t_{c1} is a time infinitely small before t_c . The time interval $t_{c2} - t_{c1}$ can be roughly estimated from time-energy uncertainty relations, and it gives a value on the order of a few fs. If a more slow/adiabatic evolution of the collision is required in some practical implementations, the equation of motion in Eq. (C6) can be easily adapted to a slower or more adiabatic collision process by just splitting the whole momentum exchange taking place during one time step of the simulation into more steps but with smaller momentum exchange. This equation of motion of the conditional wave function reproduces Eq. (23) for the conditional wave packet suffering an electron-lattice interaction with parabolic energy bands. We emphasize that the stochasticity is introduced into Eq. (C6) because the exact (Bohmian) path of the ions $\vec{R}^j[t]$ is not explicitly simulated. Their effect is introduced into the dynamics of the electron $\vec{r}_a^j[t]$ through the random selection of collision times and phonon modes satisfying some *well-known* probability distributions.

By construction, the time evolution of $\psi(\vec{r}_a, t)$ before and after the collision is fully coherent. The main and important difference is the change of momentum. For example, in a double barrier, a collision adding and subtracting the momentum $\vec{\lambda}_a = \hbar \vec{q}_p$ in the wave function $\psi(\vec{r}_a, t)$ can convert a nonresonant state into a resonant one or vice versa. Until here,

only collisions within a unique band have been considered. The implementation in electron-phonon multiband models [already indicated below Eq. (A16)] or other types of collision could be straightforwardly done.

APPENDIX D: DIRAC (LINEAR-BAND) EQUATION

In the linear case, $E(\vec{p}_a) = \pm v_f |\vec{p}_a|$, with v_f the Fermi velocity. The same development done for the Schrödinger equation can be followed here for the evolution of the 2D bispinor solution of the Dirac equation, with a slight difference appearing because the wave function is a bispinor wave function. The Bloch energy eigenstates $|\vec{k}_a\rangle$ defined in Eq. (A7) have to be substituted by $|\vec{k}_a, s_a\rangle$ defined as

$$\phi_{\vec{k}_a, s_a} = \langle \vec{r}_a | \vec{k}_a, s_a \rangle = \frac{u_{\vec{k}_a}}{\sqrt{2}} \begin{pmatrix} 1 \\ s_a e^{i\beta_{\vec{k}_a}} \end{pmatrix}, \quad (D1)$$

where s_a indicates if the electron is in the conduction ($s_a = 1$) or valence ($s_a = -1$) band, with positive or negative energies, respectively. We have defined $e^{i\beta_{\vec{k}_i}} = \frac{k_{ix} + ik_{iy}}{\sqrt{k_{ix}^2 + k_{iy}^2}}$, and $\beta_{\vec{k}_i}$ is the angle of the \vec{k}_i wave vector.

All developments done previously for a parabolic band can be reproduced here by just introducing the appropriate index s_a and the bispinor. In particular, the initial conditional envelope wave packet before the collision in Eq. (A22) is rewritten here as

$$\begin{aligned}
 \psi_a(\vec{r}_a, t) &= \begin{pmatrix} \psi_{a,1}(\vec{r}_a, t) \\ \psi_{a,2}(\vec{r}_a, t) \end{pmatrix} = \sum_{\vec{k}_w} \begin{pmatrix} 1 \\ s_a e^{i\beta_{\vec{k}_w}} \end{pmatrix} f_a(\vec{k}_w, t) e^{i\vec{k}_w \vec{r}_a} \\
 &\approx \begin{pmatrix} 1 \\ s_{0a} e^{i\beta_{\vec{k}_{0a}}} \end{pmatrix} \sum_{\vec{k}_w} f_a(\vec{k}_w, t) e^{i\vec{k}_w \vec{r}_a}, \quad (D2)
 \end{aligned}$$

where we have assumed again that $\vec{k}_w \approx \vec{k}_{0a}$ and $s_a \approx s_{0a}$, with s_{0a} indicating that the initial wave packet belongs to the conduction ($s_{0a} = 1$) or valence ($s_{0a} = -1$) band. Identically, the coupling constant defined in Eq. (A16) has to be substituted by the new one:

$$\begin{aligned}
 g_{\vec{k}_a, s_a, s'_a}^{\vec{q}_p} &= -i \vec{Q}_{\vec{q}_p} \vec{q}_p U_{\vec{q}_p} \int_{\vec{r}'_a} d\vec{r}'_a e^{-i(\vec{k}_a + \vec{q}_p) \vec{r}'_a} u_{\vec{k}_a + \vec{q}_p}(\vec{r}'_a) \\
 &\quad \times e^{i\vec{k}_a \vec{r}'_a} u_{\vec{k}_a}(\vec{r}'_a) e^{i\vec{v} \vec{r}'_a} \left(\frac{1 + s_a s'_a e^{i(\beta_{\vec{k}_a} - \beta_{\vec{k}_a + \vec{q}_p})}}{2} \right), \quad (D3)
 \end{aligned}$$

which contains the information of the transition from the initial energy branch s_a to the final branch s'_a . We assume again that, in a particular experiment j , only one $\vec{q}_p[t]$ (or none) is relevant at each time, and that $g_{\vec{k}_a, s_a, s'_a}^{\vec{q}_p, j}[t] \approx g_{\vec{k}_{0a}, s_{0a}, s'_{fa}}^{\vec{q}_p, j}[t]$, where s'_{fa} indicates that the final wave packet is in the conduction ($s'_{fa} = 1$) or valence ($s'_{fa} = -1$) band (more exotic collisions with final presence of the wave packet at both energy branches can be considered by two collisions with the one final-branch-collision process mentioned here). Then, the condition given in Eq. (C1) between the envelope conditional wave packet before and after the collision with parabolic energy bands can

be straightforwardly rewritten here as

$$\begin{aligned} \psi_a(\vec{r}_a, t_{c2}) &= \sum_{\vec{k}_w} \left(s_{fa} e^{i\beta_{\vec{k}_w + \vec{q}_p}} \right) f_a(\vec{k}_w, t_{c1}) e^{i\vec{k}_w \vec{r}_a} e^{i\vec{q}_p \vec{r}_a} \\ &= e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} \sum_{\vec{k}_w} \left(s_{fa} s_{0a} e^{i(\beta_{\vec{k}_w + \vec{q}_p} - \beta_{\vec{k}_w})} s_{0a} e^{i\beta_{\vec{k}_w}} \right) f_a(\vec{k}_w, t_{c1}) e^{i\vec{k}_w \vec{r}_a} \\ &\approx e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\alpha_a} \end{pmatrix} \begin{pmatrix} 1 \\ s_{0a} e^{i\beta_{\vec{k}_w}} \end{pmatrix} \sum_{\vec{k}_w} f_a(\vec{k}_w, t_{c1}) e^{i\vec{k}_w \vec{r}_a}, \quad (\text{D4}) \end{aligned}$$

where we have introduced $s_{0a} s_{0a} = 1$ and $e^{-i\beta_{\vec{k}_w}} e^{i\beta_{\vec{k}_w}} = 1$. We define $s_{fa} s_{0a} = e^{im\pi}$, where $m\pi$ reflects the changing from one branch to the other due to the absorption/emission of the phonon ($m = 1$) or the collision without changing ($m = 0$). We have finally defined $\alpha_a = m\pi + \beta_{\vec{k}_{fa}} - \beta_{\vec{k}_{0a}}$. We can then rewrite Eq. (D4) compactly as

$$\begin{aligned} \psi_a(\vec{r}_a, t_{c2}) &= \begin{pmatrix} \psi_{a,1}(\vec{r}_a, t_{c2}) \\ \psi_{a,2}(\vec{r}_a, t_{c2}) \end{pmatrix} \\ &\approx e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} \begin{pmatrix} \psi_{a,1}(\vec{r}_a, t_{c1}) \\ e^{i\alpha_a} \psi_{a,2}(\vec{r}_a, t_{c1}) \end{pmatrix}. \quad (\text{D5}) \end{aligned}$$

With the same development done for the parabolic band, we know that the time evolution of $\psi_a(\vec{r}_a, t)$ before the collision is given by the 2D Dirac equation as

$$\begin{aligned} i\hbar \frac{\partial \psi_a}{\partial t} &= (v_f \hat{\sigma}_x p_{ax} + v_f \hat{\sigma}_y p_{ay} + (V_a + A_a + iB_a) \hat{I}) \psi_a \\ &= \begin{pmatrix} V_a + A_a + iB_a & v_f p_a^- \\ v_f p_a^+ & V_a + A_a + iB_a \end{pmatrix} \psi_a, \quad (\text{D6}) \end{aligned}$$

with $\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\hat{\sigma}_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$ the Pauli matrices, $\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ the identity matrix, $\vec{p} = \{p_{ax}, p_{ay}\} = \{-i\hbar \partial_x, -i\hbar \partial_y\}$, and $p_a^\pm = -i\hbar \partial_{x_a} \pm \hbar \partial_{y_a}$. With the same approximations used in Eq. (C2) for A_a and B_a based on Ref. [17], we get the following time-evolution operator (propagator) from the initial time $t = t_0$ until a time before the collision $t < t_{c1}$ as $\hat{U}_a(t, t_0) = e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{\mathcal{H}}_{ca}(t') dt'}$ with $H_{ca} = v_f (\hat{\sigma}_x p_{ax} + \hat{\sigma}_y p_{ay}) + V_a \hat{I}$. Again we can define the time-evolution operator for any time larger than the collision $t > t_{c2}$ as

$$\begin{aligned} \hat{U}_a(t, t_0) &= e^{-\frac{i}{\hbar} \int_{t_{c2}}^t \hat{\mathcal{H}}_{ca}(t') dt'} e^{-\frac{i}{\hbar} \int_{t_{c1}}^{t_{c2}} \hat{\mathcal{H}}_{epa}(t') dt'} \\ &\quad \times e^{-\frac{i}{\hbar} \int_{t_{c1}}^{t_{c2}} \hat{\mathcal{H}}_{sa}(t') dt'} e^{-\frac{i}{\hbar} \int_{t_0}^{t_{c1}} \hat{\mathcal{H}}_{ca}(t') dt'}, \quad (\text{D7}) \end{aligned}$$

with the interacting Hamiltonian given by $\mathcal{H}_{epa} = -\hbar \lambda_a \vec{r}_a \delta(t - t_c) \hat{I}$ and $\mathcal{H}_{sa} = -\hbar \delta(t - t_c) \begin{pmatrix} 1 & 0 \\ 0 & \alpha_a \end{pmatrix}$. With this time-dependent Hamiltonian, it can be easily demonstrated that Eq. (D5) is

satisfied:

$$\begin{aligned} \psi_a(\vec{r}_a, t_{c2}) &= \begin{pmatrix} e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} \psi_{a,1}(\vec{r}_a, t_{c1}) \\ e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} e^{i\alpha_a} \psi_{a,2}(\vec{r}_a, t_{c1}) \end{pmatrix} \\ &= e^{-\frac{i}{\hbar} \int_{t_{c1}}^{t_{c2}} \hat{\mathcal{H}}_{epa}(t') dt'} e^{-\frac{i}{\hbar} \int_{t_{c1}}^{t_{c2}} \hat{\mathcal{H}}_{sa}(t') dt'} \psi_a(\vec{r}_a, t_{c1}). \quad (\text{D8}) \end{aligned}$$

It can also be demonstrated that $(p_a^+) e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} \psi_{a,1}(\vec{r}_a, t) = e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} (p_a^+ + \lambda_a^+) \psi_{a,1}(\vec{r}_a, t)$. Identically, $(p_a^-) e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} \psi_{a,2}(\vec{r}_a, t) = e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} (p_a^- + \lambda_a^-) \psi_{a,2}(\vec{r}_a, t)$, where we have defined $\lambda_a^\pm = \lambda_{ax} \pm i\lambda_{ay}$. Therefore, we have proved for the bispinor

$$\begin{aligned} &\left(1 - \frac{i}{\hbar} \Delta t \hat{\mathcal{H}}_{ca}\right) \cdots \left(1 - \frac{i}{\hbar} \Delta t \hat{\mathcal{H}}_{ca}\right) e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} \psi_a(\vec{r}_a, t_{c1}) \\ &= e^{i\frac{\lambda_a \vec{r}_a}{\hbar}} \left(1 - \frac{i}{\hbar} \Delta t \hat{\mathcal{H}}_{ca+\lambda}\right) \cdots \left(1 - \frac{i}{\hbar} \Delta t \hat{\mathcal{H}}_{ca+\lambda}\right) \psi_a(\vec{r}_a, t_{c1}), \quad (\text{D9}) \end{aligned}$$

with $\hat{\mathcal{H}}_{ca+\lambda} = v_f [\hat{\sigma}_x (p_{ax} + \lambda_{ax}) + \hat{\sigma}_y (p_{ay} + \lambda_{ay})] + V_a \hat{I}$. Notice that we have still not considered the effect of the term $e^{-\frac{i}{\hbar} \int_{t_{c1}}^{t_{c2}} \hat{\mathcal{H}}_{sa}(t') dt'}$. It includes an angle $e^{i\alpha_a}$ in the second element of the bispinor at time $t = t_{c1}$. As discussed in Appendix C, in most practical applications, for simplicity, we assume an instantaneous collision. A slower or more adiabatic collision process is also easily implementable. Finally, the global equation of motion of the conditional bispinor that includes all mentioned dynamics and is valid for any time, either before or after the collision, is

$$\begin{aligned} i\hbar \frac{\partial \psi_a(\vec{r}_a, t)}{\partial t} &= v_f \begin{pmatrix} V_a/v_f & p_a^- + \lambda_a^- \Theta_{tc} \\ (p_a^+ + \lambda_a^+ \Theta_{tc}) \chi_{tc} & V_a \chi_{tc}/v_f \end{pmatrix} \\ &\quad \times \psi_a(\vec{r}_a, t). \quad (\text{D10}) \end{aligned}$$

As we explained below, the term $\chi_{tc} = \exp[i(m\pi + \beta_{\vec{k}_{fa}} - \beta_{\vec{k}_{0a}}) \Lambda_{tc}]$ projects the general bispinor into positive or negative energy states, and for practical purposes in the numerical results we chose Θ_{tc} to be the Heaviside step function. This equation of motion exactly reproduces Eq. (24). We emphasize again that the stochasticity is introduced into Eq. (D6) because the exact (Bohmian) path of the ions $\vec{R}^j[t]$ is not explicitly simulated. Their effect is introduced into the dynamics of the electron $\vec{r}_a^j[t]$ through the random selection of collision times and phonon modes satisfying some *well-known* probability distributions.

We achieve the same conclusion as in the Schrödinger case: the time evolution of $\psi(\vec{r}_a, t)$ before and after the collision is fully coherent. For example, as is shown in the text, if a collision occurs with an initial electron whose direction was not perpendicular to a potential barrier (and therefore will not suffer Klein tunneling) and that collision changes the electron direction appropriately, the electron can experience the full Klein tunneling effect.

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