Linear Scaling Quantum Transport Methodologies

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In recent years, the role of predictive computational modeling has become a cornerstone for the study of fundamental electronic, optical, and thermal properties in complex forms of condensed matter, including Dirac and topological materials. The simulation of quantum transport in realistic materials calls for the development of linear scaling, or \( O(N) \), numerical methods, which then become enabling tools for guiding experimental research and for supporting the interpretation of measurements. In this review, we describe and compare different \( O(N) \) computational methods that have been developed during the past twenty years, and which have been intensively used to explore quantum transport phenomena in disordered media. We place particular focus on the electrical conductivities derived within the Kubo-Greenwood and Kubo-Streda formalisms, and illustrate the capabilities of these methods to tackle the quasi-ballistic, diffusive, and localization regimes of quantum transport. The fundamental issue of computational cost versus accuracy of various proposed numerical schemes is addressed in depth. We then extend the review to the study of spin dynamics and topological transport, for which efficient approaches of inspecting charge, spin, and valley Hall conductivities are outlined. The usefulness of these methods is illustrated by various examples of transport in disordered materials, such as polycrystalline and defected graphene models, 3D metals and Dirac semimetals, carbon nanotubes, and organic semiconductors.

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The study and development of new materials and devices often involves three complementary avenues of exploration—experiments, theory, and numerical simulations. Theory provides a framework to explain or predict material or device behavior, while numerical simulations are often needed to apply these theories to the complex situations that are encountered in experiments. In electronic devices, the understanding of the flow of electrons in response to an electric field is of central importance, and it is also a fundamental issue in condensed matter physics. The performance of devices in many applications in electronics, thermoelectrics, spintronics, optoelectronics, and photovoltaics is intricately connected to the material’s electrical conductivity or charge carrier mobility. To this end, there is a need for simulation tools that can accurately describe electronic transport in complex materials and devices, and do so in an efficient manner in order to reach the length scales typically seen in experiments.

In order to study electronic transport in disordered materials and devices on experimental length scales, one often needs to consider large systems consisting of many millions or billions of atoms. To simulate such systems accurately and efficiently, two basic ingredients are needed. The first is a realistic description of the structure and electronic properties of the material of interest. This can be achieved by using ab initio electronic structure methods such as density functional theory (DFT) (Hohenberg and Kohn, 1964; Jones, 2015; Kohn, 1999; Kohn and Sham, 1965). DFT has proven to be highly successful for describing the electronic, optical, and vibrational properties of a large number of materials. However, the computational cost of ab initio methods severely limits the size of the systems that can be studied. This limitation can be overcome with quasiparticle-based real-space tight-binding (TB) models, for which the Hamiltonian describing the electronic properties of the system becomes highly sparse, allowing for efficient numerical simulation. Therefore, using ab initio methods as a basis for the construction of appropriate TB models is currently the most successful approach for describing electronic and transport properties of large-area, spatially complex disordered or nanostructured materials.

The second ingredient needed to study large disordered systems is an efficient numerical method for simulating electronic transport. Ideally, to reach experimental length scales this method should be linear-scaling, i.e., its computational cost should be directly proportional to the number of atoms N. Such methods are also called order-N or O(N) methods. The development of stable O(N) algorithms for the calculation of spectral and transport quantities has been initiated by the seminal works of Roger Haydock (Haydock et al., 1972, 1975; Haydock, 1980) who first derived a real-space approach to compute spectral functions in disordered materials using the so-called recursion and continued fraction expansion technique. This was followed by the introduction of improved techniques for the computation of density of states, correlation functions, and transport coefficients in disordered materials. Techniques employing orthogonal polynomials, such as Chebyshev expansion-based algorithms (Leforestier et al., 1991; Petitfor and Weaire, 1985; Tal-Ezer and Kosloff, 1984) and the kernel polynomial method (KPM), have shown superior performance (Weiße et al., 2006) and are experiencing growing popularity for studying the dynamics of quantum systems (Fehske et al., 2009; Jing and Ma, 2007). Consequently, they find a considerable range of applications in chemistry and physics, including the fields of disordered systems, electron-phonon interactions, quantum spin systems, and strongly correlated quantum systems (Boehnke et al., 2011; Ganahl et al., 2014; Viswanath and Müller, 1994).

A fully quantum treatment of charge transport is undoubtedly a great asset and marks a significant advance over simpler classical models. However, under the proper conditions electronic transport is reminiscent of a clas-
sical system in which electrons in a material behave as point particles that are scattered by various sources, such as lattice defects, impurities, or phonons. In this semiclassical picture, the electrical conductivity is proportional to the momentum relaxation time, $\sigma \propto \tau_p$, which is the average time it takes for scattering processes to randomize an electron’s direction of motion. The conductivity is also independent of the system size in this regime. Each scattering process can be treated fully quantum mechanically, but between scattering events the electrons behave as point particles. This semiclassical picture is appropriate in the limit $k_F l_c \gg 1$, where $l_c$ is the average distance between scattering events, $k_F = 2\pi/\lambda_F$, and $\lambda_F$ is the Fermi wavelength of the electrons.

The limits of this semiclassical description are met when the wave nature of electrons starts to play a role, i.e., when $\lambda_F$ becomes comparable to $l_c$. In this regime, quantum interference effects can become important. In particular, constructive interferences in closed scattering loops can lead to the coherent localization of electrons, resulting in a decrease of the conductivity compared to its semiclassical value. The calculation of quantum corrections to the semiclassical conductivity was pioneered in 1979 by Abrahams et al. (Abrahams et al., 1979), who developed a scaling theory of localization in which the zero-temperature conductivity of a disordered material depends universally on its length scale $L$, and transitions smoothly from a logarithmic or slower decay to an exponential decay with increasing $L$. At the same time, the leading quantum corrections to the semiclassical conductivity were shown to be driven by coherent backscattering of electrons from momenta $k$ to $-k$ (Altshuler et al., 1980; Gor’kov et al., 1979). This phenomenon of weak localization has now been studied in many different materials and has been the topic of extensive reviews (Akkermans and Montambaux, 2010; Belitz and Kirkpatrick, 1994; Lee and Ramakrishnan, 1985; Rammer and Smith, 1986).

An important consequence of localization is that the conductivity becomes dependent on the system size. Thus, in low-dimensional materials and devices where localization effects are more pronounced, an accurate treatment of the impact of quantum effects on electronic transport is crucial. Over the past several decades, this has been revealed by the study of quantum interferences in low-dimensional semiconductor systems, including quantum wells, superlattices, and nanowires, as well as in a wide variety of organic systems (Charlier et al., 2007; Dasgupta et al., 2014; Laird et al., 2015; Rurali, 2010). More recently, the growing interest in low-dimensional materials such as carbon nanotubes, graphene, and transition metal dichalcogenides (Castro Neto et al., 2009; Das Sarma et al., 2011; Ferrari et al., 2015; Geim and Grigorieva, 2013; Mucciolo and Lewenkopf, 2010; Novoselov et al., 2016), among many others, also highlights the need for efficient ways to calculate the electrical conductivity while fully accounting for quantum effects.

There are several common approaches for simulating electronic transport, including the Boltzmann transport equation, the Landauer-Büttiker formalism, and the Kubo formula. The Boltzmann transport equation describes the dynamics of the electron distribution function, and is traditionally applied to the semiclassical regime of transport described above. However, with appropriate extensions it can also describe quantum interference effects, for example through the use of Wigner distribution functions (Bordone et al., 1999; Nedjalkov et al., 2004) or by introducing nonlocal terms into the collision integral (Hershfield and Ambegaokar, 1986). The Landauer-Büttiker formalism expresses the electrical conductance in terms of transmission probabilities, which are calculated from the full quantum mechanical scattering matrix, and thus naturally captures the impact of quantum effects on electron transport. Traditionally the Landauer-Büttiker formalism has been applied to devices with two or more electrical contacts (Büttiker et al., 1985; Landauer, 1957, 1970), but with the proper choice of self energies it can also handle bulk systems (Baranger and Stone, 1989; Nikolić, 2001; Stone and Szafer, 1988).

In this review, we focus on efficient numerical calculations of the Kubo and Kubo-Bastin formulas for the electrical and Hall conductivities. In its most general form, the Kubo formula describes the linear response of a system to a time-dependent perturbation. It does so by connecting the linear response to time-dependent correlation functions in the absence of the perturbation (Doniach and Sondheimer, 1974; Pines and Nozieres, 1989). In the case of electrical conductivity, it allows one to calculate the charge current response to an electric field through the current-current correlation function in the absence of the electric field. We note that by making a connection between (i) the response of an observable to an external perturbation, and (ii) its response to spontaneous system fluctuations, the Kubo formula is a manifestation of the fluctuation-dissipation theorem (Kubo, 1966; Kubo et al., 1985). It is also known as the Kubo-Greenwood approach for non-interacting electrons.

The calculation of the Kubo conductivity using $\mathcal{O}(N)$ techniques was pioneered by Thouless and Kirkpatrick in their study of a one-dimensional linear chain (Thouless and Kirkpatrick, 1981). A subsequent attempt to perform real-space calculations of the Kubo formula was made in higher-dimensional models (Bose et al., 1993), but an important step forward was accomplished by Mayou and Khanna who extended recursion methods to compute the frequency-dependent conductivity (Mayou, 1988; Mayou and Khanna, 1995). Roche and Mayou further combined real-space $\mathcal{O}(N)$ recursion techniques with time-propagation methods to evaluate the Kubo conductivity in its zero-frequency version (Roche, 1999; Roche and Mayou, 1997). One of the main advantages of such approaches is the ability to identify different regimes of
quantum transport – ballistic, diffusive, and localized – by following the time-dependent spatial spreading of quantum wavepackets. Similar types of methodology, as well as other algorithms using the KPM technique, have extended the capability of these methods to the study of other quantities such as the Hall conductivity (Garcia et al., 2015; Ortmann et al., 2015; Ortmann and Roche, 2013), spin dynamics (Cummings et al., 2017; Van Tuan et al., 2014; Vierimaa et al., 2017), and lattice thermal conductivity in disordered systems (Sevinçli et al., 2011; Li et al., 2010, 2011).

In recent years, the predictive power of such methodologies has been demonstrated in a large variety of realistic models of disordered graphene and two-dimensional materials (Ferreira and Mucciolo, 2015; Gargiulo et al., 2014; Trambly de Laissardière and Mayou, 2013; Lherbier et al., 2008b; Radchenko et al., 2013; Wehling et al., 2010; Yuan et al., 2010b; Zhao et al., 2015), multilayer graphene (Misasa et al., 2018; Yuan et al., 2010a), organic semiconductors (Fratini et al., 2017; Ishii et al., 2018, 2015, 2017; Ortmann and Roche, 2011) and conducting polymers (Adjizian et al., 2016; Ihnatsenka et al., 2015; Tomelé et al., 2019), quasicrystals and aperiodic systems (Trambly de Laissardière and Mayou, 2014; Roche et al., 1997; Roche and Mayou, 1997), silicon nanowires (Markussen et al., 2006; Persson et al., 2008), carbon nanotubes (Ishii et al., 2010b; Latil et al., 2004) and three-dimensional models of topological insulators (Cresti et al., 2016; Soriani et al., 2012; Wehling et al., 2014). Charge, spin and Hall transport coefficients have been numerically computed in different transport regimes, including the quasi-ballistic, diffusive, weak localization, weak antilocalization, and strong (Anderson) localization regimes, providing in-depth quantitative analysis directly comparable with experimental data. Today these approaches have become a cornerstone for the simulation of quantum transport in complex situations that are out of reach of analytical treatments and perturbative methods, especially in the presence of weak magnetic fields and for experimentally relevant disordered systems containing many millions of atoms.

This review covers more than twenty years of research dedicated to the numerical implementations of the Kubo formula for the electrical conductivity. Its purpose is to provide a comprehensive description of the most efficient linear-scaling algorithms for studying electronic transport in complex forms of disordered materials. The review is organized as follows. In Sec. II we derive a few forms of the single-particle Kubo formula, emphasizing those that are based on the velocity autocorrelation function and the mean-square displacement. Section III discusses the numerical implementations that enable linear-scaling calculations of quantum transport using these formulas, and we provide explicit examples to illustrate their similarities and differences with respect to accuracy and computational cost. Section IV summarizes and illustrates a variety of applications of this methodology to charge transport in disordered graphene, 3D metals and Dirac semimetals, carbon nanotubes, and organic semiconductors. Section V presents further extensions of this method to the calculations of the Hall conductivity and to spin dynamics, while Sec. VI describes how the linear-scaling techniques described in this review can be applied to the Landauer-Büttiker formalism. Finally, a summary and general conclusions are given in Sec. VII. This review is intended to communicate essential knowledge about physics and algorithms on equal footing, and we hope it will serve as a valuable resource for future developers and users of such methodologies, which can be applied to the large variety of materials of current interest for fundamental science and advanced technologies.

II. QUANTUM LINEAR RESPONSE THEORY AND KUBO FORMULAS

An important method for extracting information about the intrinsic properties of a system is to measure its response to an external perturbation. A perturbation can be, e.g., an electric field or a temperature gradient, and the response can be an electric current or a heat flux. In general, the response of a system can be very complex, but for perturbations that are small enough, one intuitively expects that the response will be proportional to the perturbation. This is the fundamental assumption of the linear response theory, and is the starting point of the work of Ryogo Kubo (Kubo, 1957), who showed under very general conditions that if the perturbation is applied sufficiently slowly such that the system always remains close to its equilibrium, one can express the response of the system in terms of its equilibrium properties. This result, currently known as the Kubo formula, is one of the pillars of modern quantum transport theory, and serves as the starting point for the different linear scaling quantum transport (LSQT) methodologies discussed in this review.

Although the Kubo formula can be used to extract transport coefficients under the presence of interactions (Bohr et al., 2006; Dugaev et al., 2005; Langer, 1962), we will focus only on its applications to non-interacting disordered systems. This choice is dictated by the fact that the LSQT methodologies have been developed and optimized for these systems, and their full capabilities are thus only attained when used within this context. On the other hand, the treatment of disordered systems is called for due to the unavoidable presence of defects and disorder in real materials. In this section, we will first outline a derivation of the general Kubo formula based on quantum linear response theory along the same lines as G. D. Mahan (Mahan, 2000). Then, we will proceed to derive a non-interacting Kubo formula that allows for defining the single-particle density matrix, which is useful for ob-
taining the expectation values of physical observables in systems out of equilibrium. After the general derivations, we will focus on the specific case of dissipative conductivity and derive different but equivalent representations of the non-interacting Kubo formula, which will serve as the starting points for the different LSQT methodologies. Finally, we will discuss the meaning of Green’s function regularization and its effect on the dissipative conductivity, as well as its relation to the different transport regimes. Such a discussion is crucial for understanding the numerical simulations that will appear in later sections.

A. Quantum linear response theory and the many-body Kubo formula

The Kubo formula is derived under four fundamental assumptions (Di Ventra, 2008; Mahan, 2000):

1. The system is at thermal equilibrium before the application of the perturbation.
2. The response is linear with respect to the perturbation strength.
3. The perturbation is turned on adiabatically.
4. The system is closed (although not isolated) and evolves under unitary Hamiltonian dynamics.

Although these assumptions can be relaxed, for example, by employing the Keldysh formalism (Rammer, 2007), they are sufficient for the systems we are dealing with in this review and allow for a general and rigorous derivation of the Kubo formula.

A general way to describe the state of a quantum system is by specifying its density matrix \( \hat{\rho} \), which can then be used to compute the expectation value \( \langle \hat{A}(t) \rangle \) of a general physical quantity described by the quantum mechanical operator \( \hat{A} \) at time \( t \) as (Sakurai and Napolitano, 2017)

\[
\langle \hat{A}(t) \rangle = \text{Tr} \left[ \hat{A} \hat{\rho}(t) \right],
\]

where \( \text{Tr}[...] \) denotes the trace over a complete basis set. Therefore, in order to determine the evolution of a certain observable, one must first determine the evolution of the density matrix \( \hat{\rho}(t) \) after the perturbation is turned on. The evolution of the density matrix can be described by the von Neumann equation, also called the quantum Liouville equation,

\[
\frac{\hbar}{i} \frac{d\hat{\rho}(t)}{dt} = [\hat{H}_{\text{tot}}(t), \hat{\rho}(t)],
\]

where \( \hat{H}_{\text{tot}}(t) \) is the total Hamiltonian of the system, generally time dependent, and the brackets represent a commutator.

Assumption 1 (above) states that at some long time in the past, the system is in an equilibrium state described by \( \hat{\rho}_{\text{eq}} \), which is obtained from the unperturbed Hamiltonian \( \hat{H} \). Then after some time, a perturbation \( \hat{H}' \) is switched on adiabatically from \( t = -\infty \) to the present time \( t \) (Di Ventra, 2008; Mahan, 2000). As long as this process is sufficiently slow, the exact time dependence of the perturbation is not very important and one can choose an arbitrary function to describe it. Here we assume an exponential increase of the perturbation with a rate of \( 1/\tau_\phi \) and add the perturbation to the equilibrium Hamiltonian to define the total Hamiltonian of the system

\[
\hat{H}_{\text{tot}}(t) = \hat{H} + \lim_{\tau_\phi \to \infty} e^{t/\tau_\phi} \hat{H}'.
\]

The limit \( \tau_\phi \to \infty \) has to be taken in order to force an adiabatic evolution in agreement with assumption 3. At this point, it is convenient to point out the importance of the order of the limits. Both \( \tau_\phi \) and \( t \) are meant to go to infinity, but in order to agree with the assumption that the perturbation vanishes at \( t = -\infty \), \( \lim_{t \to -\infty} \hat{H}_{\text{tot}}(t) = \hat{H} \), one must make sure that \( \tau_\phi \) goes to \( \infty \) at a slower rate than \( t \) goes to \( -\infty \).

In this review, we are interested in electrical responses and therefore, we will focus on the case where the perturbation is a small electric field. Due to gauge invariance, there is no unique way to introduce the electric field into the Hamiltonian. We choose to express the static electric field \( \mathbf{E}_0(r) \) in terms of a scalar potential \( \phi(r) = -\mathbf{r} \cdot \mathbf{E}_0 \), and write the perturbation as

\[
\hat{H}' = \int d^3r \rho(r) \phi(r).
\]

Here, \( \rho(r) \) is the charge density and the time dependence of the perturbation is assumed to be only embodied in the exponential function in Eq. (3). Additionally, this gauge also implies that we are neglecting any induced magnetic field due to the change of the electric field, a condition which is justified by the second and third assumptions.

Solving the von Neumann equation in Eq. (2) for the Hamiltonian in Eq. (3) is generally a challenging task. However, based on the second and third assumptions, we can assume that the density matrix is just slightly out of equilibrium and make an ansatz that it follows a similar time evolution as the perturbation,

\[
\hat{\rho}(t) = \hat{\rho}_{\text{eq}} + \lim_{\tau_\phi \to \infty} e^{t/\tau_\phi} \Delta \hat{\rho}(t).
\]

Here, \( \Delta \hat{\rho}(t) \) is a small deviation of the density matrix from its equilibrium value, which is assumed to vanish in the limit \( t \to -\infty \) and to be linearly proportional to \( \mathbf{E}_0(r) \), in the same way as the perturbation. By invoking Maxwell’s equations, substituting Eq. (3) and Eq. (5) into Eq. (2), and dropping terms that are nonlinear in \( \mathbf{E}_0(r) \) (assumption 2), one can obtain a solution for
\[ \Delta \rho(t) \]. We then substitute the solution into Eq. (1) to obtain an expression for the nonequilibrium expectation value of operator \( \hat{A} \) under the action of the external electric field \( \mathbf{E}_0(r) \) (Di Ventra, 2008; Mahan, 2000),

\[
\langle \hat{A} \rangle = \lim_{\tau_0 \to \infty} \Omega \int_0^{\infty} dt e^{-t/\tau_0} \int_0^\beta d\lambda \times \text{Tr} \left[ \hat{\rho}_{eq} \hat{A}(0) \hat{J}(t + i\hbar \lambda) \right] \cdot \mathbf{E}_0(r),
\]

(6)

where \( \Omega \) is the volume of the system and \( \beta = 1/k_B T \) is the inverse thermal energy. The time-dependent current density operator is defined in the interaction picture as

\[
\hat{J}_\alpha(t) = \hat{U}^\dagger(t) \hat{J}_\alpha \hat{U}(t),
\]

(7)

where

\[
\hat{U}(t) = e^{-i\hat{H}t/\hbar}
\]

(8)
is the time evolution operator associated with the unperturbed Hamiltonian \( \hat{H} \).

Equation (6) is the direct-current (DC) Kubo formula for electrical response. This formula was first derived by Kubo for computing the dissipative electrical conductivity (Kubo, 1957), for which \( \hat{A} \) is chosen as the current density \( \hat{J}_\alpha \) in the same direction \( \alpha \) as the electric field. Equation (6) then becomes

\[
\langle \hat{J}_\alpha \rangle = E_0(r) \left\{ \lim_{\tau_0 \to \infty} \Omega \int_0^{\infty} dt e^{-t/\tau_0} \int_0^\beta d\lambda \times \text{Tr} \left[ \hat{\rho}_{eq} \hat{J}_\alpha(0) \hat{J}_\alpha(t + i\hbar \lambda) \right] \right\},
\]

(9)

where \( E_0(r) \) is the magnitude of \( \mathbf{E}_0(r) \). According to Ohm’s law, the expression in the braces is just the DC electrical conductivity \( \sigma \). The Kubo formula can also be interpreted as a manifestation of the fluctuation-dissipation theorem (Kubo, 1966; Kubo et al., 1985), which states that the response of a system to a small external perturbation is equivalent to its spontaneous fluctuations at equilibrium. In this case, the response of the electrical current to an electric field is equivalent to the spontaneous fluctuations of the equilibrium current, captured by current-current correlation function \( [\hat{\rho}_{eq} \hat{J}_\alpha(0) \hat{J}_\alpha(t + i\hbar \lambda)] \).

### B. Kubo formulas for noninteracting electrons

In many situations, many-body effects driven by electron-electron interactions remain weaker than the effects of disorder. Therefore, it would be overkill and often impractical to use the general many-body Kubo formula. The noninteracting problem of \( N \) particles is equivalent to solving a single-particle problem and occupying the single-particle states with \( N \) particles with correct statistics. In the noninteracting approximation, all the many-body operators can be conveniently represented in second quantization notation (Mahan, 2000) using a complete set of orthonormal eigenvectors \( \{|n\}\) of the single-particle Hamiltonian \( \hat{H}, \hat{H}|n\rangle = E_n |n\rangle \). In this notation, any operator can be expressed as

\[
\hat{A} = \sum_{m,n} c_m^\dagger c_n \langle m | \hat{A} | n \rangle,
\]

(10)

where \( c_m^\dagger \) and \( c_n \) are the creation and annihilation operators of an electron in the single-particle eigenstates \( |m\rangle \) and \( |n\rangle \) respectively, and \( \langle m | \hat{A} | n \rangle \) is the matrix element of the single-particle operator. The time-dependent current density operator in Eq. (9) can then be expressed in second quantization notation as

\[
\hat{J}_\alpha(t + i\hbar \lambda) = \sum_{p,q} c_p^\dagger c_q \langle p | \hat{J}_\alpha | q \rangle e^{i(E_p - E_q)(t + i\hbar \lambda)/\hbar},
\]

(11)

where the exponential comes from the time evolution operator. Inserting Eqs. (10) and (11) into Eq. (6), making use of the identity (Allen, 2006)

\[
\text{Tr}[\hat{\rho}_{eq} c_m^\dagger c_n c_p^\dagger c_q] = \delta_{mq} \delta_{np} f(E_m)[1 - f(E_n)] + \delta_{mn} \delta_{pq} f(E_m)f(E_p),
\]

(12)

and performing the integration over \( \lambda \) and \( t \), one obtains the single-particle Kubo formula

\[
\langle \hat{A} \rangle = i\hbar \Omega \lim_{\tau_0 \to \infty} \sum_{m,n} \frac{f(E_m - \mu) - f(E_n - \mu)}{(E_n - E_m)(E_n - E_m + i\hbar/\tau_0)} \times \langle m | \hat{A} | n \rangle \langle n | \langle \hat{J} \cdot \mathbf{E}_0 | m \rangle ,
\]

(13)

where

\[
f(E_m - \mu) = \frac{1}{e^{E_m/(k_B T)} + 1}
\]

(14)
is the Fermi-Dirac distribution function, with \( \mu \) being the chemical potential or Fermi level.

Equation (13) expresses the conductivity in terms of the eigenvalues and eigenvectors of the Hamiltonian, which in general are difficult to obtain. Therefore, it is desirable to find an expression that depends solely on \( \hat{H} \) instead. This can be done by using the definition of the trace as well as the following identities (\( F \) is a general function):

\[
\int dE' F(E') \delta(E' - E_n) = F(E_n),
\]

\[
\sum_n F(E_n) |n\rangle \langle n| = F(\hat{H}).
\]

(15)

After some algebra, we can rewrite Eq. (13) as

\[
\langle \hat{A} \rangle = \lim_{\tau_0 \to \infty} -i\hbar \Omega \int dE' f(E' - \mu) \times \text{Tr} \left[ \delta(E' - \hat{H}) \hat{A} \frac{1}{(\hat{H} - E')(\hat{H} - E' - i\hbar/\tau_0)} (\hat{J} \cdot \mathbf{E}_0) - \text{h.c.} \right],
\]

(16)
where h.c. stands for the Hermitian conjugate of the preceding operator within the trace, and $\delta(E - \hat{H})$ is the projector onto the eigenstates of the Hamiltonian with energy $E$. Furthermore, one can express Eq. (16) in terms of Green’s functions, which will then allow its evaluation using Green’s function techniques. To this end, we first define the retarded ($G^r$) and advanced ($G^a$) regularized Green’s functions,

$$G^\pm(E; \tau_\phi, \tau) = \mp i \int_0^\tau d\tau' \frac{e^{\pm i(E - \hat{H} \pm i\hbar/\tau_\phi)\tau'/\hbar}}{E - \hat{H} \pm i\hbar/\tau_\phi},$$

(17)

where $\tau > 0$ and $\tau_\phi > 0$ are regularization parameters which can be interpreted as a finite evolution time and a finite quasi-particle lifetime, respectively. These functions can be used to obtain the exact Green’s functions through the limits

$$G^\pm(E) = \lim_{\tau_\phi \to \infty} \lim_{\tau \to \infty} G^\pm(E; \tau_\phi, \tau) = \lim_{\tau_\phi \to \infty} \frac{1}{E - \hat{H} \pm i\hbar/\tau_\phi},$$

(18)

where the order of the limits should be respected. Finally, using the identity

$$\lim_{\hbar \to 0} \frac{1}{x(x + \hbar)} = -\lim_{\hbar \to 0} \frac{d}{dx} \left( \frac{1}{x + \hbar} \right),$$

(19)

one can replace the energy factor in Eq. (16) by the retardation factor in Eq. (17) and the expression used in all the LSQT methodologies discussed in this review. Additionally, from this point onward, we will denote the velocity pointing in the same direction of the electric field as $\hat{V}$, which defines the diagonal elements of the conductivity tensor. Finally, by inserting $\hat{J} = q\hat{V}/\Omega$ into the Kubo-Bastin formula (Eq. (20)), setting $\hat{A} = \hat{J}$, and noting that $\langle \hat{J} \rangle = \sigma \hat{E}_0$, the DC conductivity $\sigma$ can be expressed in terms of the velocity operator as

$$\sigma(\mu, T) = \frac{i\hbar e^2}{\Omega} \int dE' f(E' - \mu) \times \text{Tr} \left[ \delta(E' - \hat{H}) \hat{V} \frac{dG^+(E')}{dE'} (\hat{J} \cdot \hat{E}_0) - \text{h.c.} \right].$$

(23)

### 1. Kubo-Greenwood and Chester-Thellung formulas

According to standard transport theories (Mahan, 2000; Rammer and Smith, 1986), the dissipative conductivity should depend only on the properties of the system around the Fermi level. However, the conductivity from the Kubo-Bastin formula seems to depend on the whole set of occupied states, as indicated by the presence of the

### C. The dissipative conductivity

In this section we will focus on the dissipative conductivity, which is one of the main probes of the electronic properties of materials. This section serves to prepare the reader for the numerical methods to be introduced in Sec. III. Therefore, we will clearly define the main quantities needed for calculating the dissipative conductivity. An important quantity here is the current density which, in the single-particle approximation, is proportional to the velocity operator $\hat{V}$, $\hat{J} = q\hat{V}/\Omega$, with $q$ being the charge of a single carrier ($q = -e$ for electrons). The velocity operator can be calculated by using the Heisenberg equation of motion,

$$\dot{\hat{V}} = \frac{i}{\hbar} [\hat{H}, \hat{R}],$$

(21)

where $\hat{R} \equiv (\hat{X}, \hat{Y}, \hat{Z})$ is the position operator. Equation (21) is of limited use when working in momentum space, but for disordered systems (such as those with defects or impurities) without translational symmetry, it is more convenient to use a real-space basis set, $\{ \{ \hat{R}_i \} \}$, where $| \hat{R}_i \rangle$ is a state centered at site $i$ of the system. Such a basis set can be, for example, formed by local atomic orbitals or Wannier functions. Using a real-space basis set, the matrix element of the velocity operator can be expressed in terms of the overlap integral $t_{ij} = \langle \hat{R}_i | \hat{H} | \hat{R}_j \rangle$ as

$$\langle \hat{R}_i | \dot{\hat{V}} | \hat{R}_j \rangle = -\frac{i}{\hbar} t_{ij} (\hat{R}_i - \hat{R}_j),$$

(22)

which is the expression used in all the LSQT methodologies discussed in this review. Additionally, from this point onward, we will denote the velocity pointing in the same direction of the electric field as $\hat{V}$, which defines the diagonal elements of the conductivity tensor. Finally, by inserting $\hat{J} = q\hat{V}/\Omega$ into the Kubo-Bastin formula (Eq. (20)), setting $\hat{A} = \hat{J}$, and noting that $\langle \hat{J} \rangle = \sigma \hat{E}_0$, the DC conductivity $\sigma$ can be expressed in terms of the velocity operator as

$$\sigma(\mu, T) = \frac{i\hbar e^2}{\Omega} \int dE' f(E' - \mu) \times \text{Tr} \left[ \delta(E' - \hat{H}) \hat{V} \frac{d(G^+(E') - G^-(E'))}{dE'} \hat{V} \right].$$

(23)
Fermi-Dirac distribution function in the integral. It was first shown by Streda (Streda, 1982) that this is indeed not the case and that the contribution from the occupied states (called the topological or Fermi sea contribution) vanishes for the dissipative conductivity. To show this, one first needs to use the following identity relating the Green’s functions to the Dirac delta function

\[ G^+(E) - G^-(E) = -2\pi i \delta(E - \hat{H}), \tag{24} \]

which implies the adiabatic limit \((\tau, \tau_\phi \to \infty)\). Using this identity and integrating by parts, the Kubo-Bastin formula can be rewritten as

\[
\sigma(\mu, T) = \frac{\pi \hbar e^2}{\Omega} \int dE' \left[ -\frac{\partial f(E' - \mu)}{\partial E'} \right] \times \text{Tr} \left[ \delta(E' - \hat{H}) \hat{V} \delta(E' - \hat{H}) \hat{V} \right].
\tag{25}
\]

The factor \(-\delta f(E' - \mu)/\partial E'\) is known as the Fermi energy window, which selects the energies close to the chemical potential. At zero temperature, the chemical potential \(\mu\) equals the Fermi energy \(E\) and this factor transforms into a Dirac delta function

\[
\lim_{\tau \to 0} \frac{\partial f(E' - \mu)}{\partial E'} = \delta(E' - E),
\tag{26}
\]

which allows us to identify

\[
\sigma(E) = \frac{\pi \hbar e^2}{\Omega} \text{Tr} \left[ \delta(E - \hat{H}) \hat{V} \delta(E - \hat{H}) \hat{V} \right]
\tag{27}
\]

as the zero temperature conductivity. This is known as the Kubo-Greenwood formula (Greenwood, 1958), and is at the core of different numerical (Ferreira and Mucciolo, 2015; Roche and Mayou, 1997) and diagrammatic (Rammer and Smith, 1986) methods for computing the conductivity. Additionally, this expression and Eq. (25) demonstrate that the role of temperature is to smear the zero-temperature conductivity across the Fermi window.

At this point, it is important to point out that the two seemingly equivalent Dirac delta functions in the Kubo-Greenwood formula have different origins: one coming from the regularized Green’s function, and the other as a true delta function arising from the identities of Eq. (15). This can be seen explicitly in Eq. (23). Therefore, in order to use the Kubo-Greenwood formula for dissipative conductivity in numerical calculations, a regularization of one of the Dirac delta functions should be performed. Typically, a Gaussian or Lorentzian regularization is considered (Thouless and Kirkpatrick, 1981; Weiße et al., 2006). If one chooses a Lorentzian representation with width \(\hbar/\tau_\phi\) (corresponding to the limit \(\tau \to \infty\)),

\[
\delta(E - \hat{H}) = \frac{1}{\pi \tau_\phi} \lim_{\tau_\phi \to \infty} \frac{\hbar/\tau_\phi}{(E - \hbar)^2 + (\hbar/\tau_\phi)^2},
\tag{28}
\]

one can immediately identify the regularization parameter \(\tau_\phi\) as a dephasing time, which can be attributed to the coupling of the system to some external inelastic source such as the electric field. Although such a source of dephasing can be thought of as the effect of inelastic scattering at nonzero temperature in a real system, it must originate from uncorrelated random events, which is not entirely realistic (Thouless and Kirkpatrick, 1981). Nevertheless, under this regularization one can consider the limit \(\tau_\phi \to \infty\) as a convergence to the adiabatic limit.

An alternative regularization procedure can be done by using a finite time \(\tau\) and a vanishingly small dephasing rate \(1/\tau_\phi\). This process corresponds to time evolution toward the steady state. To show this, first replace one of the Dirac delta functions by its Fourier representation,

\[
\delta(E - \hat{H}) = \lim_{\tau \to \infty} \int_{-\tau}^{\tau} dt \frac{e^{i(E-\hat{H})t/\hbar}}{2\pi\hbar},
\tag{29}
\]

which is equivalent to taking the limits in Eq. (17) in the order \(\tau_\phi \to \infty\) and then \(\tau \to \infty\). Then, by using the identity,

\[
-\frac{\partial f(E - \mu)}{\partial E} = \frac{\partial f(E - \mu)}{\partial \mu}
\tag{30}
\]

and the identities in Eq. (15), we can obtain the following expression from Eq. (25):

\[
\sigma(\mu, T) = \lim_{\tau \to \infty} \frac{e^2}{2\Omega} \int_0^\tau dt \text{Tr} \left[ \frac{\partial f(\hat{H} - \mu)}{\partial \mu} \{\hat{V}(t), \hat{V}(0)\} \right],
\tag{31}
\]

where the braces represent the anti-commutator, and \(\hat{V}(t) \equiv e^{i\hat{H}t/\hbar} \hat{V} e^{-i\hat{H}t/\hbar}\) is the time-dependent velocity operator. This expression is known as the Chester-Thellung formula (Chester and Thellung, 1959, 1961).

Next, one can define a single-particle density matrix as

\[
\hat{\rho}_\text{eq}(\mu, T) = \frac{1}{\Omega} \frac{1}{\Omega} \frac{1}{\rho(\mu)} \frac{\partial f(\hat{H} - \mu)}{\partial \mu},
\tag{32}
\]

where

\[
\rho(\mu, T) = \frac{dn(\mu, T)}{d\mu} = \frac{1}{\Omega} \text{Tr} \left[ \frac{\partial f(\hat{H} - \mu)}{\partial \mu} \right]
\tag{33}
\]

is the density of states (DOS), and \(n(\mu, T) = \text{Tr}[f(\hat{H} - \mu)]/\Omega\) is the charge density. This definition of the single-particle density matrix allows the conductivity to be expressed as

\[
\sigma(\mu, T) = \lim_{\tau \to \infty} e^2 \rho(\mu) \int_0^\tau dt C_{vv}(t),
\tag{34}
\]

where we have defined the quantity

\[
C_{vv}(t) \equiv \frac{1}{2} \text{Tr} \left[ \hat{\rho}_\text{eq}(\hat{V}(t), \hat{V}(0)) \right]
= \text{Re} \left( \text{Tr} \left[ \hat{\rho}_\text{eq}(\hat{V}(t), \hat{V}(0)) \right] \right),
\tag{35}
\]
which is the velocity auto-correlation (VAC) function. Comparison to Eq. (9) shows that this expression for conductivity offers a direct connection between the single-particle Kubo formula and the fluctuation-dissipation theorem. The DOS in Eq. (34) appears as a consequence of multiple electrons taking part in the transport at the Fermi level.

Equation (32) indicates that the temperature dependence is embedded in $\rho_{eq}(\mu, T)$ and that its role is to smear the zero-temperature conductivity around the Fermi level. Therefore, the temperature dependence can be included later provided that one knows the zero-temperature conductivity at all energies. Due to this, from this point forward we will focus on explaining how to obtain the conductivity in this limit, and unless otherwise specified we will refer to the zero-temperature conductivity simply as the conductivity. The zero-temperature limit is achieved simply by using Eq. (26), which allows the density matrix and the DOS to be expressed as

$$\dot{\rho}_{eq}(E) = \frac{1}{\Omega} \frac{1}{\rho(E)} \delta(E - \hat{H}), \quad (36)$$

$$\rho(E) = \frac{1}{\Omega} \text{Tr} \left[ \delta(E - \hat{H}) \right], \quad (37)$$

while the rest of the formalism remains unchanged.

2. Relation between conductivity and diffusion

Starting from the Chester-Thellung formula, one can easily obtain the Einstein relation, which relates the conductivity to the diffusion coefficient. To this end, we first define the mean-square displacement (MSD) as

$$\Delta X^2(E, t) = \text{Tr} \left[ \dot{\rho}_{eq}(E)(\hat{X}(t) - \hat{X}(0))^2 \right]. \quad (38)$$

Using the identity

$$\frac{d^2 \Delta X^2(E, t)}{dt^2} = \text{Tr} \left[ \dot{\rho}_{eq}(E) \{V(t), V(0)\} \right], \quad (39)$$

we have

$$\sigma(E) = e^2\rho(E) \lim_{t \rightarrow \infty} \frac{1}{2} \frac{d\Delta X^2(E, t)}{dt}. \quad (40)$$

If we define

$$D(E) = \lim_{t \rightarrow \infty} D(E, t) = \lim_{t \rightarrow \infty} \frac{1}{2} \frac{d\Delta X^2(E, t)}{dt}, \quad (41)$$

we have $\sigma(E) = e^2\rho(E)D(E)$. The quantity $D(E)$ is called the diffusion coefficient and can be considered as one of the diagonal entries of the diffusion tensor as defined in (Nakajima, 1958). This result shows that choosing a regularization with time yields a formulation that is formally equivalent to semiclassical theory in the diffusive regime.

If instead of the time regularization we use the regularization provided by the dephasing time $\tau_\phi$, we can obtain a slightly different expression for $D(E)$, which nevertheless provides the correct results for $\tau_\phi \rightarrow \infty$. Using the regularized retarded Green’s function in Eq. (17) to represent one of the Dirac delta functions in Eq. (27), in a similar way as in the derivation of the Chester-Thellung formula, yields a diffusion coefficient that depends on both the evolution time $\tau$ and the dephasing time $\tau_\phi$,

$$D(E; \tau_\phi, \tau) = \int_0^\tau dt e^{-t/\tau_\phi} \frac{1}{2} \frac{d^2 \Delta X^2(E, t)}{dt^2}, \quad (42)$$

which when integrating by parts reduces to

$$D(E; \tau_\phi, \tau) = \frac{1}{2} e^{-t/\tau_\phi} \left[ \frac{d\Delta X^2(E, t)}{dt} + \frac{\Delta X^2(E, t)}{\tau_\phi} \right]_t^\tau + \frac{1}{2\tau_\phi} \int_0^\tau dt e^{-t/\tau_\phi} \Delta X^2(E, t). \quad (43)$$

If the limit $\tau_\phi \rightarrow \infty$ is taken first, we recover Eq. (41). Otherwise, if the limit $\tau \rightarrow \infty$ is taken first, we have

$$D(E) = \lim_{\tau_\phi \rightarrow \infty} D(E, \tau_\phi) = \lim_{\tau_\phi \rightarrow \infty} \frac{1}{2\tau_\phi} \int_0^\infty dt e^{-t/\tau_\phi} \Delta X^2(E, t). \quad (44)$$

The last expression shows that when we incorporate a finite dephasing time, the diffusion coefficient becomes essentially an average of $\Delta X^2(E, t)/2\tau_\phi$ over the time scale defined by $\tau_\phi$. Equations (41) and (44), although formally different, produce the same result when $\tau$ and $\tau_\phi$ are larger than the characteristic times of the system. This will be shown in the next section where we discuss the different transport regimes and the possible outcomes of these formulas.

3. Transport regimes and length scales

So far we have derived different representations of the Kubo formula that can be used to obtain the conductivity at a stationary state, i.e., in the limit of infinite time. However, these Kubo formulas can also be used to determine the behavior of the system in different transport regimes that occur at finite time. This is one of the benefits of using time-dependent approaches for quantum transport. To show this, we start with a discussion of the different transport regimes and some relevant physical quantities.

Consider a perfect crystal material, which by definition is a periodic array of atoms. An electron in this environment will be subjected to a periodic potential due to the Coulomb field of the atoms. By virtue of Bloch’s theorem, one can describe this system as a free electron gas whose components possess an effective mass accounting for the change in the group velocity due to a change
in the crystal momentum. Therefore, under the action of a small external electric field, the electrons will move freely along the direction of the electric field at an average speed of the Fermi velocity $v_F(E)$, leading to ballistic transport.

However, in disordered systems the electrons will be scattered by imperfections in the system. After some time $\tau_p(E)$, which is known as the momentum relaxation time, the system will have undergone many random scatterings that make it lose all memory about the initial conditions, leading to a steady state known as the diffusive regime. Finally, if the disorder is strong enough, a phenomenon known as Anderson localization will take place. In this situation, the electron’s wave function is no longer extended. Instead, due to quantum interference effects the wave function becomes localized within a volume whose radius is usually defined as the localization length $\xi(E)$. These are the canonical transport regimes, and in the following we will see how to identify each of these within quantum transport simulations. The first thing to address is how to compute the characteristic parameters of each regime: the Fermi velocity, momentum relaxation time, and localization length.

For ballistic transport, the MSD grows quadratically, $\Delta X^2(E, t) = v_F^2(E)t^2$. Inserting this into Eqs. (41) and (44) gives $D(E) = v_F^2\tau_p$ and $D(E) = v_F^2\tau_\phi$, respectively. This means that the conductivity diverges linearly with time, as expected for ballistic transport. Therefore, in the ballistic regime both regularization procedures give the same result, as illustrated in Fig. 1(b).

At longer time or length scales, the electrons will be scattered by imperfections and will lose the memory of their previous momenta after a time of order $\tau_p(E)$. In this limit the conductivity should be independent of length and time, which implies that it can be expressed in terms of a constant diffusion coefficient $D_{sc}(E)$, which is commonly referred to as the semiclassical (sc) diffusion constant. This is a consequence of a linearly increasing MSD, which in the diffusive regime is proportional to the diffusion constant

$$\Delta X^2(E, t) = 2D_{sc}(E)t.$$  \hspace{1cm} (45)

Inserting this into Eq. (41) gives directly what we expect

$$D(E) = D_{sc}(E).$$  \hspace{1cm} (46)

As for Eq. (44), one can divide the integral into two contributions given that before reaching the momentum relaxation time $\tau_p(E)$ the system behaves ballistically, while after reaching $\tau_p(E)$ the system enters the diffusive regime. For simplicity, let us assume a sharp transition at $t = \tau_p$ and write the diffusion coefficient as

$$D(E) = \lim_{\tau_\phi \to -\infty} \frac{1}{2\tau_\phi^2} \left( \int_0^{\tau_p} + \int_{\tau_p}^{\infty} \right) dt \ e^{-t/\tau_\phi} \Delta X^2(E, t).$$  \hspace{1cm} (47)

The first integral goes to zero as $\tau_\phi \to -\infty$ and the second integral gives the same expression as Eq. (46). This result can also be derived by assuming an exponentially decaying VAC (Beenakker and van Houten, 1991),

$$C_{\text{vac}}(t) = \frac{1}{2}v_F^2(E)e^{-t/\tau_p(E)},$$  \hspace{1cm} (48)

which leads to a connection between the diffusion constant and the momentum relaxation time,

$$D_{sc}(E) = \frac{1}{2}v_F^2(E)\tau_p(E).$$  \hspace{1cm} (49)

One can also define a mean free path

$$l_c(E) = v_F(E)\tau_p(E)$$  \hspace{1cm} (50)

and write $D_{sc}(E) = v_F(E)l_c(E)/2$. We see that the semiclassical electrical conductivity has the same form as that obtained from the Boltzmann equation within the relaxation time approximation (Ashcroft and Mermin, 1976). The equivalence between the two regularizations of the Green’s function in the diffusive limit is illustrated in Fig. 1(a).

Finally, in the weak and strong localization regimes the conductivity is expected to decay with increasing system length $L$ (Lee and Ramakrishnan, 1985). The weak localization regime is characterized by a logarithmic decay of
the conductivity, \( \sigma(E, L) - \sigma_{\text{sc}}(E) \propto -\ln(L/l_\text{c}(E)) \), while the strong localization regime is associated with an exponential decay of the conductivity, \( \sigma(E, L) \propto e^{-L/\xi(E)} \), where \( \xi(E) \) is the localization length. In the strong localization regime, the MSD saturates to a constant value and Eq. (41) predicts a zero diffusion coefficient and conductivity. The convergence towards this limit is usually assumed to be exponential with respect to the system length, and from this scaling the localization length can be obtained. One can also establish a relation between the localization length and the saturated value of the MSD \((\text{Triozon et al., 2000})\), which was found quantitatively to be \((\text{Uppstu et al., 2014})\)

\[
\xi(E) = \lim_{t \to \infty} \frac{\sqrt{\Delta X^2(E, t)}}{\pi}. \tag{51}
\]

This definition of localization length conforms with the standard definition in terms of the length scaling of conductance \((\text{Anderson et al., 1980})\) and is in accordance with the original definition of Anderson localization \((\text{Anderson, 1958})\), namely, the absence of diffusion.

Meanwhile, Eq. (44) gives a different convergence behavior. If we define \( \tau_\phi \) as the time after which strong localization dominates and impose the condition \( \tau_\xi/\tau_\phi \ll 1 \), we obtain a diffusion coefficient going to zero as the inverse dephasing time,

\[
D(E) = \lim_{\tau_\phi \to \infty} D(E, \tau_\phi) = \lim_{\tau_\phi \to \infty} \frac{\pi^2 \xi(E)^2}{2 \tau_\phi}. \tag{52}
\]

This difference in convergence behavior is demonstrated in Fig. 1(c). Nonetheless, \( 2\tau_\phi D(E, \tau_\phi) \) and the MSD converge to the same value \( \pi^2 \xi^2(E) \) in the limit of infinite time, as illustrated in Fig. 1(d). Therefore, the two regularizations of the Green’s function give the same results in the ballistic, diffusive, and localized limits.

Up to now, the discussion of the different transport regimes is based on a time parameter, \( \tau \) (or \( \tau_\phi \)). To make quantitative studies of charge transport in different transport regimes, one needs to consider length-dependent transport properties instead. In the LSQT methods, one usually considers a sufficiently large simulation cell and applies periodic boundary conditions. The length corresponding to the evolution time \( t \) is not the size of the simulation cell, but rather the propagation length associated with the MSD \((\text{Fan et al., 2014a; Lecoute et al., 2011; Lherbier et al., 2012; Roche and Saito, 2001; Roche et al., 2001})\),

\[
L(E, t) \equiv 2\sqrt{\Delta X^2(E, t)}, \tag{53}
\]

which can be considered as the average length that the electrons at energy \( E \) have propagated up to time \( t \).

This definition of length can be justified by considering the ballistic regime of transport. In this regime, the conductivity scales linearly with time, \( \sigma(E, t) = e^2 \rho(E) \nu^2(E) t \), and thus diverges. However, one can define the conductance \( g(E) \) as

\[
g(E) \equiv \frac{A}{L(E, t)} \sigma(E, t), \tag{54}
\]

where \( A \) is the cross-sectional area through which the current flows. The conductance is a geometry-dependent quantity and is therefore finite for finite systems. Using the definition of length in Eq. (53), we have \( L(E, t) = 2\nu_F(t) \) in the ballistic regime and

\[
g(E) = \frac{A}{2 \pi} e^2 \rho(E) \nu_F(E), \tag{55}
\]

which is independent of any length or time scale and is completely characterized by the DOS and Fermi velocity, consistent with the picture of ballistic transport. For a strictly one-dimensional system, the DOS is \( \rho(E) = 2/\pi \nu_F(E) \) and we finally get \( g(E) = 2e^2/h \). This is the expected conductance quantum for ballistic transport, as has been measured in quantum point contacts \((\text{van Wees et al., 1988; Wharam et al., 1988})\) and carbon nanotubes \((\text{Frank et al., 1998})\). The factor of two in Eq. (53) means that electrons propagate in two opposite directions. In early works \((\text{Roche and Saito, 2001; Roche et al., 2001})\), this factor of two was not included, but the conductivity was defined by substituting the derivative in Eq. (40) with division by \( t \), which exactly reduces the conductivity by half in the ballistic limit and results in the same ballistic conductance as in Eq. (55).

### III. LINEAR SCALING NUMERICAL TECHNIQUES

In Sec. II, we have presented three different representations of the Kubo formula for non-interacting electrons: the Kubo-Greenwood formula in Eq. (27), the VAC-based formula in Eq. (34), and the MSD-based formula in Eq. (40). The aim of this section is to review the various numerical techniques for efficiently evaluating these formulas. We will focus on dissipative transport in this section and discuss numerical evaluation of the Kubo-Bastin formula Eq. (20) in Sec. V, which can be used to compute other transport properties \((\text{García et al., 2015})\).

The major concern in numerical implementations is the scaling of the computational cost with respect to the Hamiltonian size \( N \). A common feature of the above Kubo formulas is that the trace can be evaluated using any complete set of single-particle wave functions that obey periodic boundary conditions \((\text{Chester and Thellung, 1959, 1961})\). An immediate choice would be to use the set of eigenvectors of the Hamiltonian, but this requires full diagonalization, which is usually prohibitive for large systems due to its \( O(N^3) \)-scaling computational cost with respect to the system size. To enable the study of large systems \((\text{e.g., } N > 10^6)\), a linear scaling, or
\(O(N)\) algorithm is mandatory. To achieve linear scaling, we avoid using the Hamiltonian’s eigenspace and instead work with a real-space tight-binding representation, where the basis functions are not eigenfunctions of the Hamiltonian but rather the electron orbitals around individual atoms. Because of this, the methods discussed in this review are usually referred to as real-space LSQT methods.

Before discussing the relevant numerical techniques for achieving linear scaling, we list the quantities to be calculated for each implementation. A prominent quantity is the DOS defined in Eq. (37), which contains information about the electronic structure of the system. In the Kubo-Greenwood representation, one directly evaluates the electrical conductivity as given in Eq. (27), but needs to represent one of the Dirac delta functions as a regularized Green’s function. In the VAC representation of Eq. (34), one first calculates the product of the DOS and the VAC,

\[
\rho(E)C_{vn}(E, t) = \frac{1}{\Omega} \text{Re} \left[ \text{Tr} \left( \hat{U}(t)\hat{V}\delta(E - \hat{H})\hat{U}^\dagger(t)\hat{V} \right) \right],
\]

and then performs a numerical time integration to obtain the running electrical conductivity \(\sigma(E, t)\). In the MSD representation of Eq. (40), one first calculates the product of the DOS and the MSD,

\[
\rho(E)\Delta X^2(E, t) = \frac{1}{\Omega} \text{Tr} \left[ \delta(E - \hat{H})(\hat{X}(t) - \hat{X})^2 \right],
\]

and then performs a numerical time derivative to obtain the running electrical conductivity \(\sigma(E, t)\). In periodic systems it is problematic to use the absolute position operator \(\hat{X}\). Instead, one can use the identity \(\hat{X}(t) - \hat{X} = \hat{U}^\dagger(t)[\hat{X}, \hat{U}(t)]\) to change the above equation to an equivalent one (Triozon et al., 2004, 2002),

\[
\rho(E)\Delta X^2(E, t) = \frac{1}{\Omega} \text{Tr} \left[ [\hat{X}, \hat{U}(t)]\delta(E - \hat{H})[\hat{X}, \hat{U}(t)] \right].
\]

After a polynomial expansion of the time evolution operator \(\hat{U}(t)\) (as discussed below), the commutator \([\hat{X}, \hat{U}(t)]\) only depends on the velocity operator, which only depends on the difference between the positions of the orbitals and is well defined in periodic systems.

There are some common features in these quantities: they are all represented as a trace and involve the quantum projection operator \(\delta(E - \hat{H})\), and the time evolution operator \(\hat{U}(t)\) appears in the VAC and MSD. Linear scaling techniques have been developed to evaluate these operators and we will discuss them in detail below.

A. Evaluating the trace using a stochastic approach

Recall that the trace of an operator \(\hat{A}\) is defined as

\[
\text{Tr}[\hat{A}] = \sum_{n=1}^{N} \langle n | \hat{A} | n \rangle,
\]

where \(\{|n\rangle\}_{n=1}^{N}\) is a complete basis set of the problem, which is taken as a real-space tight-binding basis set in this review. The operator \(\hat{A}\) relevant to this review will be essentially polynomials formed by the Hamiltonian and other quantities such as the velocity operator. What is important here is that even if \(\hat{A}\) is highly sparse, such that the operation \(\hat{A} | n \rangle\) scales linearly, the total computation still has an \(O(N^2)\) scaling, which is better than \(O(N^3)\) for a non-sparse \(\hat{A}\) but is still usually prohibitive. To achieve \(O(N)\) scaling, the trace must be approximated. A powerful method for approximating the trace of large matrices is to use random vectors, a stochastic approach that was developed along with the methods of calculating the spectral properties of large Hamiltonians (Drabold and Sankey, 1993; Silver and Röder, 1994; Silver et al., 1996; Skilling, 1989; Weiße et al., 2006).

In this stochastic method, one approximates the trace by using \(N_r\) random vectors \(\{|\phi_r\rangle\}_{r=1}^{N_r}\),

\[
\text{Tr}[\hat{A}] \approx \frac{1}{N_r} \sum_{r=1}^{N_r} \langle \phi_r | \hat{A} | \phi_r \rangle.
\]

Each random vector \(|\phi_r\rangle\) is constructed from \(N\) random coefficients,

\[
|\phi_r\rangle = \sum_{n=1}^{N} \xi_{rn} |n\rangle.
\]

Here, \(\xi_{rn} \in \mathbb{C}\) are independent identically distributed random variables which have zero mean and unit variance, which implies that each vector is normalized to \(\sqrt{N}\). It has been shown that (Itaka and Ebisuzaki, 2004; Weiße et al., 2006) the statistical error for the trace is proportional to \(1/\sqrt{N_rN}\), with the proportionality constant being related to the properties of the matrix \(\hat{A}\). The statistical accuracy can be systematically improved by increasing \(N_r\). In practice, for large \(N\) a small \(N_r\) on the order of unity is sufficient to achieve a high statistical accuracy.

For simplicity, we only use a single random vector \(|\phi\rangle\) to present the subsequent formulas. In practice, one needs to check the convergence of the results with respect to \(N_r\). Under the condition of sufficient average, in the following we use the \(\approx\) sign instead of the \(\approx\) sign as in Eq. (60). Using this, we can express the quantities that need to be calculated as the following inner products:

\[
\rho(E) = \frac{1}{\Omega} \langle \phi | \delta(E - \hat{H}) | \phi \rangle;
\]

\[
\sigma(E) = \frac{\pi \hbar e^2}{\Omega} \langle \phi | \delta(E - \hat{H})\hat{V}\delta(E - \hat{H})\hat{V} | \phi \rangle;
\]

\[
\rho(E)C_{vn}(E, t) = \frac{1}{\Omega} \text{Re} \left[ \langle \phi_{vn}^\text{vac}(t) | \delta(E - \hat{H}) | \phi_{vn}^\text{vac}(t) \rangle \right];
\]

\[
\rho(E)\Delta X^2(E, t) = \frac{1}{\Omega} \text{Tr} \left[ [\hat{X}, \hat{U}(t)]\delta(E - \hat{H})[\hat{X}, \hat{U}(t)] \right].
\]
\[ \rho(E)\Delta X^2(E, t) = \frac{1}{\Omega} \langle \phi_{L}^{\text{msd}}(t)|\delta(E - \hat{H})|\phi_{R}^{\text{msd}}(t) \rangle, \tag{65} \]

where
\[ |\phi_{L}^{\text{vac}}(t)\rangle = \hat{V}\tilde{U}(t)^{\dagger}|\phi\rangle; \quad |\phi_{R}^{\text{vac}}(t)\rangle = \tilde{U}(t)^{\dagger}\hat{V}|\phi\rangle; \tag{66} \]

\[ |\phi_{L}^{\text{msd}}(t)\rangle = |\phi_{R}^{\text{msd}}(t)\rangle = [\hat{X}, \tilde{U}(t)]|\phi\rangle. \tag{67} \]

The remaining task is to evaluate these inner products in a linear scaling way. We will discuss linear scaling numerical techniques related to the time evolution operator \( \tilde{U}(t) \) in Sec. III.C and those related to the quantum projection operator \( \delta(E - \hat{H}) \) in Sec. III.D. Before doing these, we first review a crucial numerical technique, namely the Chebyshev polynomial expansion.

B. Chebyshev polynomial expansion

We have presented different theoretical frameworks that can be used to determine the conductivity. We saw that a numerical evaluation of this quantity requires one to compute functions of the Hamiltonian matrix such as the time evolution operator and the quantum projection operator. We also discussed the need to choose an appropriate basis set so that the Hamiltonian can be represented as a sparse matrix. Therefore, if we want to exploit this feature we need to find a way to avoid explicit evaluation of these quantities, because an arbitrary function of a sparse matrix is generally not a sparse matrix. The use of polynomial expansion provides a way to achieve the goal of linear scaling computation. Among various polynomials, the Chebyshev polynomials are usually the optimal choice (Boyd, 2001).

The Chebyshev polynomials are a family of orthogonal polynomials which can be defined recursively. In this review we are using the Chebyshev polynomials of the first kind, \( \{T_{m}(x)\} \), which are defined as \( T_{m}(\cos(x)) = \cos(mx) \) and have the recurrence relation
\[
T_{0}(x) = 1; \quad T_{1}(x) = x; \\
T_{m}(x) = 2xT_{m-1}(x) - T_{m-2}(x) \quad (m \geq 2). \tag{68} \]

These polynomials form a complete basis for functions defined on the real axis within the interval \([-1, 1]\). As such, they can be used to expand a function \( f(x) \) defined within the same interval in a polynomial series
\[ f(x) = \sum_{m=0}^{\infty} \tilde{f}_{m} T_{m}(x), \tag{69} \]

where
\[ \tilde{f}_{m} = (2 - \delta_{m0}) \int_{-1}^{1} \frac{f(x)T_{m}(x)}{\pi \sqrt{1 - x^2}} dx \tag{70} \]

are the expansion coefficients and \( \delta_{m0} \) is the Kronecker delta.

In general, one deals with functions of the Hamiltonian \( \hat{H} \), whose energy spectrum may exceed the interval \([-1, 1]\) in a particular unit system. In order to use the Chebyshev polynomial expansion, one must first scale and shift \( \hat{H} \) such that the modified energy spectrum is in \([-1, 1]\). Specifically, this can be done by the linear transformation
\[ \tilde{H} = \frac{\hat{H} - E}{\Delta E}, \tag{71} \]

where \( \Delta E = (E_{\text{max}} - E_{\text{min}})/2 \) and \( E = (E_{\text{max}} + E_{\text{min}})/2 \), with \( E_{\text{max}} \) and \( E_{\text{min}} \) being the maximum and minimum eigenvalues of \( \hat{H} \). To avoid numerical problems, one usually makes \( \Delta E \) slightly larger than \((E_{\text{max}} - E_{\text{min}})/2\). Any function of \( \tilde{H} \) can thus be expanded in a manner similar to Eq. (69). To see this, we assume that \( \tilde{H} \) has the eigenvalues \( \{\tilde{E}_{n}\} \) and eigenvectors \( \{|n\rangle\} \). For a general function \( f(\tilde{H}) \), we have
\[ f(\tilde{H}) = \sum_{n} f(\tilde{H}) |n\rangle \langle n| = \sum_{n} f(\tilde{E}_{n}) |n\rangle \langle n| \]
\[ = \sum_{n} \sum_{m=0}^{\infty} \tilde{f}_{m} T_{m}(\tilde{E}_{n}) |n\rangle \langle n| \]
\[ = \sum_{m=0}^{\infty} \sum_{n} \tilde{f}_{m} T_{m}(\tilde{H}) |n\rangle \langle n| \]
\[ = \sum_{m=0}^{\infty} \tilde{f}_{m} T_{m}(\tilde{H}). \tag{72} \]

The inner products listed at the end of Sec. III.A are of the form \( \langle \phi_{L}|F(\tilde{H})|\phi_{R}\rangle \). These quantities can thus be evaluated iteratively by exploiting the recurrence relation of the Chebyshev polynomials and the whole computation breaks down to a number of sparse matrix-vector multiplications, which scale linearly with the vector length \( N \). In the next section, we discuss Chebyshev polynomial expansions of the time evolution operator and the regularized Green’s function.

C. The time evolution operator and the regularized Green’s function

Both the VAC and MSD formalisms involve a time evolution operator \( \tilde{U}(t) \), and one of the Dirac delta functions \( \delta(E - \hat{H}) \) in the Kubo-Greenwood formula can be substituted by a regularized Green’s function. In this subsection, we discuss the expansion of the time evolution operator and the regularized Green’s function in terms of the Chebyshev polynomials.

In the VAC and MSD formalisms, after applying the random vector approximation for the trace we only need to evaluate the application of the time evolution operator on a vector, as can be seen from Eqs. (66) and (67). Because we need information at a discrete set of time points,
we need to construct an iterative scheme for evaluating the time evolution. The strategy is to divide the total correlation time into a number of steps. From time $t$ to time $t + \Delta t$ (the time steps $\Delta t$ need not to be uniform), we have the following iterative relations for the vectors defined in Eqs. (66) and (67):

\[
\hat{V}\hat{U}^\dagger(t + \Delta t)|\phi\rangle = \hat{V}\hat{U}^\dagger(\Delta t)\hat{U}^\dagger(t)|\phi\rangle; \quad (73)
\]

\[
\hat{U}^\dagger(t + \Delta t)\hat{V}|\phi\rangle = \hat{U}^\dagger(\Delta t)\hat{U}^\dagger(t)\hat{V}|\phi\rangle; \quad (47)
\]

\[
[\hat{X}, \hat{U}(t + \Delta t)]|\phi\rangle = \hat{U}(\Delta t)[\hat{X}, \hat{U}(t)]|\phi\rangle + [\hat{X}, \hat{U}(\Delta t)]\hat{U}(t)|\phi\rangle. \quad (75)
\]

Therefore, the task breaks down to evaluating the application of the operators $\hat{U}(\Delta t)$ and $[\hat{X}, \hat{U}(\Delta t)]$ on some vectors.

The Chebyshev polynomial expansion is particularly efficient when the expanded function is regular and differentiable. One of its first uses was the expansion of the time evolution operator $\hat{U}(\Delta t)$. Solving the integral in Eq. (70) for this operator leads to an expansion in the form of Eq. (72) (Tal-Ezer and Kosloff, 1984),

\[
\hat{U}(\Delta t) \approx \sum_{m=0}^{N_p} \hat{U}_m(\Delta t)T_m(\hat{H}), \quad (76)
\]

\[
\hat{U}_m(\pm \Delta t) = (2 - \delta_{m0})(-i)^m J_m(\omega_0 \Delta t), \quad (77)
\]

where $\omega_0 = \Delta E/\hbar$ and $J_m(x)$ is the $m$th-order Bessel function of first kind.

The operator $[\hat{X}, \hat{U}(\Delta t)]$ can be similarly expanded in terms of the Chebyshev polynomials,

\[
[\hat{X}, \hat{U}(\Delta t)] \approx \sum_{m=0}^{N_p} \hat{U}_m(\Delta t)[X, T_m(\hat{H})], \quad (78)
\]

where the commutator $[X, T_m(\hat{H})]$ can be calculated iteratively using the recurrence relation

\[
[\hat{X}, T_m(\hat{H})] = 2[\hat{X}, \hat{H}]T_{m-1}(\hat{H}) + 2\hat{H}[\hat{X}, T_{m-1}(\hat{H})] - [\hat{X}, T_{m-2}(\hat{H})]. \quad (79)
\]

Algorithms 1 and 2 give explicit steps for evaluating $|\phi_{\text{out}}\rangle = \hat{U}(\Delta t)|\phi_{\text{in}}\rangle$ and $|\phi_{\text{out}}\rangle = [\hat{X}, \hat{U}(\Delta t)]|\phi_{\text{in}}\rangle$. A demonstration of the accuracy of the Chebyshev expansion of the time evolution operator can be seen in Fig. 2. Panel (a) shows how $\hat{U}(\Delta t)$ quickly converges to its expected value after a finite number of iteration steps. Panel (b) indicates the number of Chebyshev polynomials $N_p$ needed to achieve a precision of $10^{-15}$ for a given time step $\Delta t$. In the limit of large $\Delta t$, $N_p \propto \Delta t$, as indicated by the dashed line.

**Algorithm 1 Evaluating $|\phi_{\text{out}}\rangle = \hat{U}(\Delta t)|\phi_{\text{in}}\rangle$**

1. $|\phi_0\rangle \leftarrow |\phi_{\text{in}}\rangle$
2. $|\phi_1\rangle \leftarrow \hat{H}|\phi_0\rangle$
3. $|\phi_{\text{out}}\rangle \leftarrow J_0(\omega_0 \Delta t)|\phi_0\rangle + 2(-i)J_1(\omega_0 \Delta t)|\phi_1\rangle$
4. $m \leftarrow 2$
5. while abs $[J_m(\omega_0 \Delta t)] > 10^{-15}$ do
6. $|\phi_2\rangle \leftarrow 2\hat{H}|\phi_1\rangle - |\phi_0\rangle$
7. $|\phi_{\text{out}}\rangle \leftarrow |\phi_{\text{out}}\rangle + 2(-i)^m J_m(\omega_0 \Delta t)|\phi_2\rangle$
8. $|\phi_0\rangle \leftarrow |\phi_1\rangle$
9. $|\phi_1\rangle \leftarrow |\phi_2\rangle$
10. $m \leftarrow m + 1$
11. end while

**Algorithm 2 Evaluating $|\phi_{\text{out}}\rangle = [\hat{X}, \hat{U}(\Delta t)]|\phi_{\text{in}}\rangle$**

1. $|\phi_0\rangle \leftarrow |\phi_{\text{in}}\rangle$
2. $|\phi_1\rangle \leftarrow \hat{H}|\phi_0\rangle$
3. $|\phi_{\text{out}}\rangle \leftarrow [\hat{X}, \hat{U}(\Delta t)]|\phi_{\text{in}}\rangle$
4. $m \leftarrow 2$
5. while abs $[J_m(\omega_0 \Delta t)] > 10^{-15}$ do
6. $|\phi_2\rangle \leftarrow 2\hat{H}|\phi_1\rangle - |\phi_0\rangle$
7. $|\phi_{\text{out}}\rangle \leftarrow |\phi_{\text{out}}\rangle + 2(-i)^m J_m(\omega_0 \Delta t)|\phi_2\rangle$
8. $|\phi_0\rangle \leftarrow |\phi_1\rangle$
9. $|\phi_1\rangle \leftarrow |\phi_2\rangle$
10. $m \leftarrow m + 1$
11. end while

**Panel (a)**

- **real-numerical**
- **imag-numerical**
- **cos(x*Delta t)**
- **sin(x*Delta t)**

**Panel (b)**

- **numerical**
- **fit**

**FIG. 2** Demonstration of the accuracy of the Chebyshev polynomial expansion of the time evolution operator using a simple function $U(\Delta t) = \exp(-ix\Delta t)$. (a) The real part $\cos(x\Delta t)$ and the imaginary part $-\sin(x\Delta t)$ of $U(\Delta t)$, calculated analytically (dashed lines) or by a numerical expansion (markers) similar to that in Eq. (76). Here, $x$ plays the role of the Hamiltonian in the time evolution operator and we choose $x = 0.5$ and $\Delta t = 100$. (b) The number of Chebyshev polynomials $N_p$ required for achieving a precision of $10^{-15}$ as a function of the time interval $\Delta t$. In the large $\Delta t$ limit, $N_p \propto \Delta t$, as indicated by the dashed line.
The Green’s functions are spectral quantities, and as such, can also be evaluated using the Chebyshev polynomial expansion. However, special care should be taken as they have singularities which carry physical information of the system. In Sec. II we defined a regularized version of the Green’s functions in Eq. (17), where we introduced an imaginary rate \(1/\tau_\phi\) and a finite time \(\tau\). These parameters broaden the singularities of the Green’s functions and serve as a mathematical regularization that enables the approximation of the Green’s functions to a given precision using a finite Chebyshev polynomial expansion. In the limit \(\tau \to \infty\), one can approximate the regularized retarded Green’s function as

\[
G^+ (\tilde{E}, \tau_\phi) = \frac{1}{\Delta E} \sum_m \tilde{G}_m^+ T_m (\tilde{H}.
\]

(80)

Here, \(\tilde{G}_m^+\) are the Chebyshev coefficients defined in Eq. (70), which can be evaluated using a Laplace transform of the Bessel function (Gradshteyn and Ryzhik, 1975) as

\[
\tilde{G}_m^+ = (2 - \delta_{m0}) i^{-1} \frac{(z - i\sqrt{1 - z^2})^m}{\sqrt{1 - z^2}},
\]

(81)

where \(z = (E + ih/\tau_\phi)/\Delta E\). This expansion has been used by Vijay et al. (Vijay et al., 2004) in the context of spectral filters and by Braun and Schmitteckert (Braun and Schmitteckert, 2014) to determine the impurity Green’s function of the interacting resonant level model. Recently, it was applied by Ferreira and Mucciolo for the first time to quantum transport, where it was dubbed the Chebyshev-polyomial Green’s function (CPGF) method (Ferreira and Mucciolo, 2015). One can also use analytic continuation of the logarithms to the complex plane to express Eq. (81) in terms of an exponential,

\[
\tilde{G}_m^+ = (2 - \delta_{m0}) i^{-1} \exp[-im \arccos(z)] / \sqrt{1 - z^2}.
\]

(82)

This shows that the CPGF method involves an analytic continuation of an expression previously obtained by other authors (Covaci et al., 2010; García et al., 2015; Weiße et al., 2006), where the singularities have been smoothed. In the limit of infinite \(\tau_\phi\), these coefficients do not decay but oscillate with increasing \(m\), and it is the presence of a finite dephasing time which provides a damping of the coefficients and forces the convergence of the expansion.

In the next subsection, we discuss different approaches to deal with singular functions in the context of approximating the quantum projection operator \(\delta (E - \tilde{H})\), a common factor in all the representations of the dissipative conductivity.

D. Evaluating the quantum projection operator

We now discuss the evaluation of the quantum projection operator \(\delta (E - \tilde{H})\) involved in all the conductivity formulas. There are several linear scaling techniques for approximating this operator, including the Lanczos recursion method (LRM) (Dagotto, 1994; Haydock et al., 1972, 1975; Haydock, 1980; Petitfor and Weaire, 1985), the Fourier transform method (FTM) (Alben et al., 1975; Feit et al., 1982; Hams and De Raedt, 2000), the kernel polynomial method (KPM) (Silver and Röder, 1994; Silver et al., 1996; Wang, 1994; Wang and Zunger, 1994; Weiße et al., 2006), and the maximum entropy method (MEM) (Drabold and Sankey, 1993; Silver and Röder, 1997; Skilling, 1989). We will only review the first three methods (LRM, FTM, and KPM), as the last one (MEM) has not been used in LSQT calculations. A comparison between the MEM and the KPM can be found in a previous review (Weiße et al., 2006). All of these methods have been used recently to compute transport properties in different systems (Cummings et al., 2017; Fan et al., 2014a; Ferreira et al., 2011; García et al., 2015; Weiße et al., 2006; Yuan et al., 2010a,b; Zhao et al., 2015). Although we have a few different quantities to calculate, it suffices to discuss these methods in terms of the DOS as given in Eq. (62). Generalizations to other quantities are straightforward.

1. The Lanczos recursion method

The LRM is based on the Lanczos algorithm (Lanczos, 1950) for tridiagonizing sparse Hermitian matrices. The Lanczos algorithm is usually used to obtain extremal eigenvalues and the corresponding eigenstates (Cullum and Willoughby, 1985), but it can also be used to calculate spectral properties (Haydock et al., 1972, 1975; Haydock, 1980; Petitfor and Weaire, 1985).

The first step of the LRM is to project the Hamiltonian onto an orthogonal basis in a Krylov subspace, generating

\begin{algorithm}
\caption{Evaluating \(|\phi_{\text{out}}\rangle = [\tilde{X}, \tilde{U}(\Delta t)]|\phi_{\text{in}}\rangle\)}
\begin{algorithmic}[1]
  \State \(|\phi_0\rangle \leftarrow |\phi_{\text{in}}\rangle\)
  \State \(|\phi_0^n\rangle \leftarrow 0\)
  \State \(|\phi_1\rangle \leftarrow \tilde{H}|\phi_0\rangle\)
  \State \(|\phi_i^+\rangle \leftarrow [\tilde{X}, \tilde{H}]|\phi_0\rangle\)
  \State \(|\phi_{\text{out}}\rangle \leftarrow 2(-i)^j (\omega_0 \Delta t) |\phi_i^+\rangle\)
  \State \(m \leftarrow 2\)
  \While {abs \([J_m (\omega_0 \Delta t)] > 10^{-15}\)}
    \State \(|\phi_2\rangle \leftarrow 2\tilde{H}|\phi_1\rangle - |\phi_0\rangle\)
    \State \(|\phi_0^n\rangle \leftarrow 2[\tilde{X}, \tilde{H}]|\phi_1\rangle + 2\tilde{H}|\phi_2\rangle - |\phi_0^n\rangle\)
    \State \(|\phi_{\text{out}}\rangle \leftarrow |\phi_{\text{out}}\rangle + 2(-i)^m J_m (\omega_0 \Delta t) |\phi_2^+\rangle\)
    \State \(|\phi_0\rangle \leftarrow |\phi_1\rangle\)
    \State \(|\phi_1\rangle \leftarrow |\phi_2\rangle\)
    \State \(|\phi_0^n\rangle \leftarrow |\phi_1^+\rangle\)
    \State \(|\phi_i^+\rangle \leftarrow |\phi_2^+\rangle\)
    \State \(m \leftarrow m + 1\)
  \EndWhile
\end{algorithmic}
\end{algorithm}
a tridiagonal matrix
\[
T = \begin{pmatrix}
a_1 & b_2 & 0 & \cdots & 0 \\
b_2 & a_2 & b_3 & \ddots & 0 \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & 0 \\
0 & \cdots & 0 & b_{M} & a_{M}
\end{pmatrix}.
\] (83)

The dimension \(M\) of the tridiagonal matrix can be much smaller than the dimension \(N\) of the original matrix. The matrix elements \(\{a_n\}\) and \(\{b_n\}\) are obtained from a Lanczos algorithm. There are multiple versions of the Lanczos algorithm and the most numerically stable one is given in Algorithm 3 (Saad, 2003). The computational effort of the LRM is thus proportional to \(NM\), which is \(O(N)\) when \(M \ll N\).

**Algorithm 3** Lanczos algorithm (Saad, 2003)

Require: |\(\phi\rangle = |\phi\rangle\) is the normalized random vector
1: \(b_1 \leftarrow 0\)
2: \(|\phi_0\rangle \leftarrow 0\)
3: for \(m = 1\) to \(M\) do
4: \(|\psi_m\rangle \leftarrow H|\phi_m\rangle - b_m|\phi_{m-1}\rangle\)
5: \(a_m \leftarrow \langle \psi_m|\phi_m\rangle\)
6: \(|\psi_m\rangle \leftarrow |\psi_m\rangle - a_m|\phi_m\rangle\)
7: \(b_{m+1} \leftarrow \sqrt{|\psi_m\rangle}\langle \psi_m|\psi_m\rangle\)
8: \(|\phi_{m+1}\rangle \leftarrow |\psi_m\rangle/b_{m+1}\)
9: end for

The second step of the LRM is to calculate the first element of the retarded Green’s function \(G^+ (E) = (E + i\eta - \hat{H})^{-1}\) in the Lanczos basis \(|\phi_m\rangle\) using the continued fraction
\[
\langle \phi | G^+ (E) | \phi \rangle = \frac{1}{E + i\eta - a_1 - \frac{b_2^2}{E + i\eta - a_2 - \cdots}}.
\] (84)

The DOS of Eq. (62) can then be calculated using the relation between the quantum projection operator and the Green’s function given in Eq. (24). The computation time for the second step is proportional to \(MN\), where \(N_e\) is the number of energy points considered in the calculation. Usually, \(N_e \ll N\), and the computation time for the second step is thus negligible compared to the first step. Because of this, the overall computational effort almost does not scale with respect to \(N_e\). We can say that the algorithm is parallel in energy, which is a common feature for all the methods presented below.

An important issue is the energy resolution \(\delta E\) achievable using a given number of recursion steps \(M\). The energy resolution is actually set by the imaginary energy \(i\eta\) in the Green’s function, i.e., \(\delta E = \eta\). One should therefore make sure that a sufficiently large \(M\) is used to ensure converged results. However, it is well known that in its basic forms such as that presented in Algorithm 3, the Lanczos algorithm can become numerically unstable when \(M\) is large, due to the loss of orthogonality in the Lanczos basis vectors. The Lanczos basis vectors can be explicitly orthogonalized (Saad, 2003), but this will increase the computational complexity of the algorithm, making it less efficient than other methods.

2. The Fourier transform method

The FTM is very simple conceptually: it is based on the Fourier transform of the Dirac \(\delta\) function as given by Eq. (29). Ideally, the time integral is over the whole real axis, but in practice one can only reach a finite time with a finite time step \(\Delta \tau\). Therefore, one should be satisfied with a truncated discrete Fourier transform,
\[
\delta(E - \hat{H}) \approx \frac{\Delta \tau}{2\pi\hbar} \sum_{m=-M}^{M} e^{i(E - \hat{H})m\Delta \tau/\hbar}.
\] (85)

A direct expansion in this way leads to Gibbs oscillations, and a window function is usually used to suppress them. A frequently used one is the Hann window
\[
w_m = \frac{1}{2} \left[ 1 + \cos \left( \frac{\pi m}{M + 1} \right) \right],
\] (86)

where \(M\Delta \tau\) represents the upper limit of the time integral in Eq. (29). Using the discrete Fourier transform, we can write the DOS in Eq. (62) as
\[
\rho(E) \approx \frac{\Delta \tau}{2\pi\hbar\Omega} \sum_{m=-M}^{M} e^{iE m\Delta \tau/\hbar} w_m F_m,
\] (87)

where
\[
F_m = \langle \phi | e^{-i\hat{H} m\Delta \tau/\hbar} | \phi \rangle = \langle \phi | \hat{U}(m\Delta \tau) | \phi \rangle
\] (88)
is the \(m\)th Fourier moment.

Based on the formulas above, we can see that the FTM consists of the following two steps: (1) construct a set of Fourier moments \(\{F_m\}\) as defined in Eq. (88), and (2) calculate physical properties such as the DOS from the Fourier moments through a discrete Fourier transform as given by Eq. (87). Similar to the case of the LRM, the computation time for the second step is negligible compared to the first one and the algorithm is essentially parallel in energy.

As the Fourier moments are the expectation values of the time evolution operator, this method is also usually called the equation of motion method (Alben et al., 1975) or the time-dependent Schrödinger equation method (Feit et al., 1982; Hams and De Raedt, 2000). Note that we have used \(\Delta \tau\) here to distinguish it from the correlation time step \(\Delta t\) in the VAC and MSD formalisms. Based on the Nyquist sampling theorem, which states that the sampling rate must be no
less than the Nyquist rate $2f_{\text{max}}$ to perfectly reconstruct a signal with a spectrum between 0 and $f_{\text{max}}$, the optimal value of $\Delta \tau$ can be determined to be $\Delta \tau = \pi h/\Delta E$, giving $\omega_0 \Delta \tau = \pi$. Using this $\Delta \tau$, the energy resolution is given by $\delta E \sim \Delta E/M$ (Feit et al., 1982).

3. The kernel polynomial method

In Sec. III.B we introduced the Chebyshev polynomial expansion as a useful tool for approximating regular functions and discussed additionally the problem of expanding a singular function such as the Green’s function using the CPGF method (Ferreira and Mucciolo, 2015). There, the singularity in the Green’s function was regularized by introducing a small imaginary energy $i\eta$. There is another widely used approach to handle the singularity in the function to be expanded in terms of Chebyshev polynomials, which is called the kernel polynomial method (KPM) (Silver and Röder, 1994; Silver et al., 1996; Wang, 1994; Wang and Zunger, 1994; Weiße et al., 2006).

When the expansion in Eq. (69) is truncated to a finite order $M$, there will be Gibbs oscillations near the points where the expanded function $f(x)$ is not continuously differentiable. These can be damped by a convolution of the function with a kernel $K(x)$ (Silver et al., 1996; Weiße et al., 2006). The advantage of the Chebyshev polynomials is that this convolution can be included by multiplying the Chebyshev coefficients with a damping factor $g_m$, transforming Eq. (69) into

$$f(x) \approx \sum_{m=0}^{M} \tilde{f}_m g_m T_m(x). \quad (89)$$

To derive an expression for the DOS using the KPM, we start by exploiting the following scaling property of the function $g_m$ multiplying the Chebyshev coefficients with a damping factor $g_m$ defined in Eq. (95), the Lorentz damping factor $g_m^L(\lambda = 4)$ defined in Eq. (96), and the Hann window function $w_m$ defined in Eq. (86).

$$C_m^{\text{DOS}} = \langle \phi | T_m(\tilde{H}) | \phi \rangle \quad (94)$$

are the Chebyshev moments for the DOS.

Up to this point we showed that the DOS can be approximated using Chebyshev polynomials, but we have not specified any choice for the kernel, which will vary with the specific application. For the expansion of the quantum resolution operator, which is essentially a set of delta peaks, the Jackson kernel with the damping factor

$$g_m^J = \frac{(M + 1 - m) \cos \left(\frac{\pi m}{M+1}\right) + \sin \left(\frac{\pi m}{M+1}\right) \cot \left(\frac{\pi}{M+1}\right)}{M + 1} \quad (95)$$

has been found to be optimal (Silver et al., 1996; Weiße et al., 2006), as it produces the smallest broadening for a given value of $M$. If one considers the Green’s function, the Lorentz kernel with the damping factor

$$g_m^L(\lambda) = \frac{\sinh[\lambda(1 - m/M)]}{\sinh(\lambda)} \quad (96)$$

may offer a better choice ($\lambda$ is a parameter which is usually chosen to be 3-5) due to the fact that it regularizes the imaginary part of the Green’s function into a Lorentzian, which is closer to physical reality.

In Fig. 3 we plot the Jackson and Lorentz damping factors along with the Hann window function, where the expansion order is chosen as $M = 10^4$. To demonstrate the performance of the different damping factors and the window function, we use them to approximate the function $\delta(x)$. The results obtained by using the KPM with
different damping factors are shown in Fig. 4. Also shown are the results obtained with the Fourier expansion and the CPGF method (Ferreira and Mucciolo, 2015). For the same value of $M = 10^4$, the Jackson damping gives a narrower shape compared to the Lorentz damping and therefore has finer resolution, while the CPGF method is essentially equivalent to the KPM with the Lorentz damping ($\lambda = 4$) when the resolution parameter in the CPGF method is chosen as $4/M$. Although CPGF and KPM with a Lorentz kernel behave similarly, it is important to note that CPGF provides a uniform energy resolution, contrary to KPM with a Lorentz kernel, whose resolution is energy-dependent. Furthermore, CPGF allows for approximating the Green’s function up to an arbitrary precision, and is thus a better choice when the physical origin of the $\delta$-function is a Green’s function. We also note that while the Gibbs oscillations can be effectively suppressed using the KPM, they persist in the case of the FTM. Apart from being less effective in suppressing Gibbs oscillations, the FTM has also been shown to be less computationally efficient as compared to the KPM (Fan et al., 2014a). This comparison and the comparison between the KPM and the LRM (Silver et al., 1996; Weiße et al., 2006) indicate that the KPM with the Jackson damping factor is the optimal approach for approximating the quantum projection operator $\delta(E - \hat{H})$.

**Algorithm 4** Evaluating the Chebyshev moments

$$\langle \phi_L T_m (\hat{H}) \phi_R \rangle$$

1: $|\phi_0\rangle \leftarrow |\phi_R\rangle$
2: $C_0 \leftarrow \langle \phi_L | \phi_0 \rangle$
3: $|\phi_1\rangle \leftarrow \hat{H} |\phi_0\rangle$
4: $C_1 \leftarrow \langle \phi_L | \phi_1 \rangle$
5: for $m = 2$ to $M$ do
6: $|\phi_2\rangle \leftarrow 2\hat{H} |\phi_1\rangle - |\phi_0\rangle$
7: $C_m \leftarrow \langle \phi_L | \phi_2 \rangle$
8: $|\phi_3\rangle \leftarrow |\phi_1\rangle$
9: $|\phi_4\rangle \leftarrow |\phi_2\rangle$
10: end for

We can now summarize the procedure of the KPM: (1) construct a set of Chebyshev moments $\{C_m\}$ (see Algorithm 4), and (2) calculate physical properties such as the DOS from the Chebyshev moments through a finite-order Chebyshev polynomial summation as given by Eq. (93). Similar to the case of the LRM and the FTM, the construction of the Chebyshev moments dominates the computation time and the algorithm is parallel in energy. The energy resolution achieved in the KPM is $\delta E \sim \Delta E/M$ (Weiße et al., 2006), similar to the case of the FTM.

**E. Numerical examples**

In this section, we use some numerical examples to illustrate the formalisms and techniques discussed above. We consider the Anderson model (Anderson, 1958), implemented as a nearest-neighbor tight-binding model defined on a cubic lattice with lattice constant $a$ and dimension $N = N_x \times N_y \times N_z$. The Hamiltonian can be written as

$$\hat{H} = \sum_{ij} (\gamma) c^\dagger_i c_j + \sum_i U_i c^\dagger_i c_i,$$

where $-\gamma$ is the hopping integral between neighboring sites and $U_i$ are the on-site potentials. The on-site potentials are uniformly distributed in an interval $[-W/2, W/2]$, where $W$ is called the Anderson disorder strength. Without loss of generality, we consider transport in the $x$ direction, which has periodic boundary conditions. The boundary conditions in the other directions will be chosen according to the specific application. Note that the two-fold spin degeneracy in this model is not included in the equations but is considered in the results shown in the relevant figures.

1. **Formalisms to be compared**

We compare three representations of the Kubo conductivity, including the VAC representation of Eq. (34), the MSD representation of Eq. (40), and the KG representation of Eq. (27). See Table I for a summary of
the explicit formulas and the computational cost for each method. For the VAC and MSD representations, we use the KPM with Jackson damping for the quantum projection operator. The quantity to be calculated in the VAC representation is the product of the DOS and the VAC

\[ \rho(E)C_{vv}(E, t) = \frac{1}{\pi \Omega \Delta E \sqrt{1 - E^2}} \sum_{m=0}^{M} (2 - \delta_{m0}) \times g_m T_m(\tilde{E}) C_{m}^{\text{vac}}(t), \]  

(98)

where

\[ C_{m}^{\text{vac}}(t) = \text{Re} \left[ \langle \phi_{L}^{\text{vac}}(t)|T_m(\tilde{H})|\phi_{R}^{\text{vac}}(t) \rangle \right] \]  

(99)

are the Chebyshev moments of \( \rho(E)C_{vv}(E, t) \). The quantity to be calculated in the MSD representation is the product of the DOS and the MSD

\[ \rho(E)\Delta X^2(E, t) = \frac{1}{\pi \Omega \Delta E \sqrt{1 - E^2}} \sum_{m=0}^{M} (2 - \delta_{m0}) \times g_m T_m(\tilde{E}) C_{m}^{\text{msd}}(t), \]  

(100)

where

\[ C_{m}^{\text{msd}}(t) = \langle \phi_{L}^{\text{msd}}(t)|T_m(\tilde{H})|\phi_{R}^{\text{msd}}(t) \rangle \]  

(101)

are the Chebyshev moments of \( \rho(E)\Delta X^2(E, t) \). We call these the VAC-KPM and MSD-KPM methods. For the Kubo-Greenwood formalism, we consider a numerical implementation based on the Chebyshev polynomial expansion for the Green’s function according to Eq. (80), which we call the KG-CFGP method (Ferreira and Mucciolo, 2015). Following Ferreira and Mucciolo, we change both of the Dirac delta functions in the Kubo-Greenwood formula to the regularized Green’s function and rewrite the Kubo-Greenwood conductivity in Eq. (63) as

\[ \sigma(E, \eta) = \frac{\hbar e^2}{\pi \Omega} \langle \phi | V \text{Im}[G^+(E)] V \text{Im}[G^+(E)] | \phi \rangle. \]  

(102)

Here, we have highlighted the \( \eta \)-dependence (\( \eta = \hbar / \tau_{\phi} \)) of the conductivity. Then, using the Chebyshev expansion of the Green’s function in Eq. (80), we have

\[ \sigma(E, \eta) = \frac{\hbar e^2}{\pi \Omega (\Delta E)^2} \sum_{m=0}^{M} \sum_{n=0}^{M} \text{Im}[G_m^+(z)] \text{Im}[G_n^+(z)] C_{mn}^{\text{kg}} \]  

(103)

where \( G_m^+(z) \) is given in Eq. (81) and

\[ C_{mn}^{\text{kg}} = \langle \phi | V T_m(\tilde{H}) V T_n(\tilde{H}) | \phi \rangle. \]  

(104)

An efficient “single-energy” algorithm for evaluating this conductivity has been proposed (Ferreira and Mucciolo, 2015):

\[ \sigma(E, \eta) = \frac{\hbar e^2}{\pi \Omega (\Delta E)^2} \langle \phi_L | \phi_R \rangle, \]  

(105)

\[ |\phi_L\rangle = \sum_{m=0}^{M} \text{Im}[g_m(z)] T_m(\tilde{H}) V |\phi\rangle, \]  

(106)

\[ |\phi_R\rangle = \sum_{n=0}^{M} \text{Im}[g_n(z)] \tilde{V} T_n(\tilde{H}) |\phi\rangle. \]  

(107)

In addition to algorithmic improvements, increasing computing power has played an important role in advancing quantum transport simulations. If large-memory computational nodes are available, high-resolution spectral calculations of DOS and DC conductivity using CPGF can be carried out in very large systems (Ferreira and Mucciolo, 2015). This RAM-intensive approach inspired the recent open-source KITE initiative (available at www.quantum-KITE.com) for real-space calculations of electronic structure and quantum transport (João et al., 2019). We compare the above LSQT methods with the Landauer-Büttiker (LB) method (Datta, 1995; Ferry and Goodnick, 1997), when appropriate. In tight-binding calculations of the LB method, the recursive Green’s function formalism (Lewenkopf and Mucciolo, 2013) is usually used. The contacts are modeled as ballistic semi-infinite leads and the conductance \( g(E) \) is obtained from the transmission function \( T(E) \),

\[ g(E) = \frac{2e^2}{h} T(E). \]  

(108)

For a single-mode system, the transmission function equals the probability of a charge carrier to transmit
one contact to another. If there are several transport modes involved, the transmission function equals the sum of the transmission probabilities for the different modes. There are many equivalent forms for the transmission function, and here we adopt the Caroli form (Caroli et al., 1971),

$$T(E) = \text{Tr}[G(E)\Gamma_L G^\dagger(E)\Gamma_R],$$  \hspace{1cm} (109)

where $G(E)$ is the advanced Green’s function of the device, $G^\dagger(E)$ is the retarded Green’s function, and $\Gamma_L/\Gamma_R$ describe the coupling of the device to the leads. The advanced Green’s function for a system attached to two leads is

$$G(E) = \frac{1}{E - H - \Sigma_L(E_L) - \Sigma_R(E_R)},$$  \hspace{1cm} (110)

where $\Sigma_L(E_L)$ is the self-energy of the left lead at Fermi energy $E_L$ and $\Sigma_R(E_R)$ is the self-energy of the right lead at Fermi energy $E_R$. The Fermi energies $E_L$ and $E_R$ of the leads can be set to the same value as in the device, $E$, or to an arbitrary value. In the calculations below, we set $E_L = E_R = E$. The self-energy matrices can be obtained through different methods, e.g., using an iterative method (Sancho et al., 1985). The coupling matrices $\Gamma_L$ and $\Gamma_R$ are the imaginary part of the self energies,

$$\Gamma_{L/R} = i\left(\Sigma_{L/R} - \Sigma_{L/R}^\dagger\right) = -2\text{Im}\left[\Sigma_{L/R}\right].$$  \hspace{1cm} (111)

2. Ballistic regime

As discussed in Sec. II.C.3, the VAC and MSD formalisms capture the essential physics of ballistic transport. To illustrate this, we consider a narrow ribbon with $N_y = 2$ and $N_z = 1$, and hard-wall boundary conditions in the $y$ and $z$ directions. To achieve high accuracy in the random vector approximation, we set $N_x = 5 \times 10^6$ in the transport direction and average the results over $N_e = 10$ random vectors. The total number of tight binding orbitals is thus $N = N_x N_y N_z = 10^7$. We use the KPM with $M = 3000$.

The VAC at the band center $E = 0$ is a constant, $v_F^2 = 3a^2 \gamma^2 / h^2$, as shown in Fig. 5(a). Consequently, the MSD in Fig. 5(b) is a quadratic function of the correlation time, $\Delta X^2(E, t) = v_F^2(E)t^2$. In other words, the electrons are propagating at a constant velocity without scattering. The DOS $\rho(E)$ is shown Fig. 5(c), and the group velocity $v_F(E)$, which is the square root of the VAC at zero correlation time, is shown in Fig. 5(d). From these we can calculate the ballistic conductance according to Eq. (55), as given by the solid line in Fig. 6. For comparison, we also show the conductance calculated with the LB method, which is represented by the dashed line. The VAC-KPM and MSD-KPM methods clearly produce the correct conductance plateaus. Around the Van Hove singularity points at $E = \pm \gamma$, however, these methods overshoot the conductance plateau, as has been noticed in a variety of studies (Charlier et al., 2007; Fan et al., 2014a; Markussen et al., 2006). The overshooting originates from a mixing of the densities of states from different bands around the band edges, which results in an overestimation of the group velocity, as clearly demonstrated by Markussen et al (Markussen et al., 2006). When the system contains some disorder, deviating the conduction
regime from purely ballistic motion, the MSD formalism becomes extremely suitable for calculating length-dependent conductance, as largely illustrated in applications to carbon nanotubes (Charlier et al., 2007; Roche and Saito, 2001; Roche et al., 2001). The KG-CPGF method has so far not been used in the ballistic regime.

3. Diffusive regime

We next consider a disordered system and closely compare the different LSQT methods as well as the LB method in the ballistic-to-diffusive crossover regime. As a generic case, and to make the computation feasible for the LB method, we take a square lattice with width $N_y = 50$ ($N_z = 1$) and an Anderson disorder strength $W = \gamma$. In the LSQT calculations, $N_x = 2 \times 10^5$, $N_L = 10$, and $M = 3000$. In the LB method, we increase the system length from $L = a$ to $100a$ and calculate the conductance $g(E, L)$ iteratively. We average over 100 disorder realizations in the LB calculations.

![Fig. 7 Results for the $E = 0$ energy point in a square lattice with $N_y = 50$ ($N_z = 1$) and $W = \gamma$. (a) VAC, (b) MSD, and (c) running electrical conductivity as a function of the evolution time $t$ for the VAC-KPM and MSD-KPM methods or the dephasing time $\tau_\phi = \hbar/\eta$ for the KG-CPGF method. (d) Semiclassical conductivity $\sigma_{sc}$ as a function of energy $E$ from the various methods. Because the LB method is not parallel in energy, only a few energy points were considered.](image)

Results for the $E = 0$ energy point are shown in Fig. 7. As expected, the VAC decays exponentially with increasing evolution time $t$ [Fig. 7(a)] and the MSD changes from a quadratic to a linear function of $t$ [Fig. 7(b)]. The running electrical conductivities calculated from the VAC and MSD (via a time integration) and the MSD (via a time derivative) are equivalent, as can be seen in Fig. 7(c).

Figure 7(c) also shows the evolution of the electrical conductivity calculated using the KG-CPGF method as a function of the dephasing time $\tau_\phi = \hbar/\eta$. As we have discussed in the previous section, the dephasing time $\tau_\phi$ and the evolution time $t$ are associated with different regularizations of the Green’s function, resulting in different time dependence, as shown previously in Fig. 1(a) and here in Fig. 7(c). However, they can lead to the same diffusion constant and semiclassical conductivity $\sigma_{sc}(E)$ in the diffusive regime. This is shown in Fig. 7(d). Here, $\sigma_{sc}(E)$ is taken as the maximum value of the scale-dependent electrical conductivity, which is the conductivity attained in the system before coherent backscattering and quantum interference come into play. In the LB method, we calculate the semiclassical conductivity based on the ballistic-to-diffusive transition formula (Datta, 1995)

$$\frac{1}{g(E, L)} = \frac{1}{\sigma_{sc}(E)} \frac{L}{N_y a} + \frac{1}{g_0(E)} ,$$

where $g_0(E)$ is the ballistic conductance at energy $E$. As shown in Fig. 7(d), this coincides with each of the other polynomial expansion-based methods.

4. Localized regime

It is well known that any amount of disorder is enough to localize electrons in the low-dimensional Anderson model (Anderson, 1958). In this example, we consider a square lattice with the same width $N_y = 50$ ($N_z = 1$ and $N_x = 2 \times 10^5$) as the one we considered for diffusive transport above, but with a larger disorder strength $W = 5\gamma$. Among the different LSQT methods, only the MSD-KPM method has been quantitatively compared to the LB method in the localized regime. Here, we choose $N_L = 10$, and $M = 3000$ in the MSD-KPM method and convert the computed conductivity to conductance using the standard definition given by Eq. (54). The length $L$ is calculated using Eq. (53). In the LB method, we average over 5000 disorder realizations to obtain the typical conductance (Anderson et al., 1980)

$$g_{typ}(E, L) = \exp[\langle \ln g(E, L) \rangle] .$$

Figure 8 shows the conductance at $E = 0$. As expected, the conductance decays exponentially in the large length limit in the LB formalism. This provides a definition of the localization length $\xi(E)$,

$$g_{typ}(E, L) \sim \exp[-L/\xi(E)] .$$

The localization length at $E = 0$ is fitted to be $\xi \approx 16a$. The conductance calculated from the MSD is very close
and dashed line indicates the value of 2\(\pi\xi(E)\), where \(\xi(E)\) is calculated from the LB method. The propagation length will approach \(2\pi\xi(E)\) in the long-time limit.

to the LB conductance down to \(g \approx 0.1e^2/h\), highlighting this method’s ability to capture the strong localization regime. Below \(g \approx 0.1e^2/h\), the conductance calculated from the MSD decays super-exponentially (Fan et al., 2014a). This is the result of the propagation length \(L(E,t)\) as defined in Eq. (53) having an upper limit \(2\pi\xi(E)\), as pointed out in Eq. (51). This definition has been discussed in Refs. (Fan et al., 2014b; Uppstu et al., 2014) and shown to be equivalent to that given by Eq. (114). This can be seen in the inset of Fig. 8, where \(L(E,t) \rightarrow 2\pi\xi(E)\) at long times. This saturation of the propagation length corresponds exactly to the absence of diffusion as in the definition of Anderson localization (Anderson, 1958).

In principle, the VAC-KPM method can also be used in the localized regime. However, it is less practical than the MSD-KPM method because the time integration in the localized regime. The method by Yuan et al. (Yuan et al., 2010a,b; Zhao et al., 2015) is based on the VAC formalism and the Fourier transform method for approximating both the quantum resolution operator and the time evolution operator. Therefore, a fixed time step of \(\Delta t = \pi/\omega_0\) (determined by the Nyquist sampling theorem) is chosen together with a certain value of \(N_t\). However, we note that using a fixed \(N_t\) for the whole spectrum might be insufficient for a quantitative study of quantum transport when different energy states exhibit different transport timescales. Finally, a quantitative extraction of the localization length has never been carried out with the KG-CPGF formalism.

5. Computational cost, convergence, and method comparison

Although all the methods give consistent results for the semiclassical conductivity, they have different scalings of the computational cost with respect to the different simulation parameters. Here, we quantitatively analyze the computational complexities of these methods. In the MSD-KPM method, the evaluations of the time evolution and the quantum projection operator are decoupled. According to Fig. 2(b), it takes about \(3\omega_0\tau_{\text{max}}\) iterations to evaluate the time evolution operator \([X,U(t_{\text{max}})]\), where \(t_{\text{max}}\) is the maximum correlation time and \(\alpha\) is a numerical factor of the order of 1. According to Algorithm 2, the number of matrix-vector multiplies (MVMs) for each iteration is 3 and the number of MVMs for the time evolution part is thus \(3\alpha\omega_0\tau_{\text{max}}\). According to Algorithm 4, the number of MVMs for evaluating the quantum projection operator using the KPM is \(MN_t\), where \(N_t\) is the number of time intervals. Each MVM costs \(\sim WN\) multiplication operations, where \(W\) is the bandwidth of the Hamiltonian. For simplicity, we omit the factor \(W\) that is common to all the methods. Then the total computational cost of the MSD-KPM method can be written as \(\sim N(MN_t + 3\alpha\omega_0\tau_{\text{max}})\). The computational cost in the VAC-KPM method can be determined to be the same. In the KG-CPGF method, the number of MVMs for a fixed energy \(E\) and a fixed energy resolution \(\eta = 2M\). If one considers \(N_e\) energy points and \(N_e\) energy resolution values for each energy point (needed for checking the \(\eta\)-dependence of the conductivity), the overall computational cost is \(\sim N(2N_eN_\eta M)\). Because the maximum dephasing time \(\tau_\phi\), or equivalently, the minimum energy resolution \(\eta = \hbar/\tau_\phi\) achievable with a given \(M\) in the KG-CPGF method (Ferreira and Mucciolo, 2015) is \(\eta = 4\Delta E/\hbar\), we can transform \(M\) to \(4\omega_0\tau_\phi\), where \(\omega_0 = \Delta E/\hbar\), and write the computational cost in this method as \(\sim N(8N_eN_\eta\omega_0\tau_\phi)\). The computational cost of each method is summarized in Table I.

Next we illustrate the convergence properties of the LSQT methods in the diffusive regime, with respect to the number of random vectors \(N_t\) and the number of Chebyshev polynomials \(M\). For this we consider a 3D cubic lattice with periodic boundaries in all three directions. We set \(N_x = 250\), \(N_y = N_z = 200\) and consider transport in the \(x\) direction. The Anderson disorder strength is chosen as \(W = 2\gamma\). As we have demonstrated the equivalence of all the LSQT methods for diffusive transport, we only choose the MSD-KPM method in this example.
The main panel of figure 9 shows the semiclassical conductivity for the whole energy spectrum. We have performed ten independent simulations, each with a different random vector, as shown by the gray lines. The statistical error is quite small, on the order of 1%. As we have remarked before, the overall statistical error is proportional to \(1/\sqrt{N_r N} \), which is a very appealing feature of the LSQT methods: when \(N\) is large, a small \(N_r\) is sufficient to achieve a high level of accuracy. To demonstrate the effects of the value of \(M\) on the results, we show in the inset of Fig. 9 the differences in the semiclassical conductivity between the cases with \(M = 1000\) to 3000 and the case with \(M = 4000\). In the inset, the results for each value of \(M\) were obtained using ten random vectors.

The energy spectrum is insensitive to the order \(M\) in the KPM or \(\eta\) in the CPGF expansion, similar to that shown in Fig. 9, treating the two Dirac delta functions equally or differently does not make much difference; otherwise, there can be nontrivial differences between the two approaches, as we will point out in Sec. IV.A.3.

Finally, we would like to note that while the focus of this review is on the calculation of DC transport, one can also derive an expression for the AC electrical conductivity \(\sigma(\omega)\) in the spirit of Sec. II. Several works have used KPM or FTM methods to study optical conductivity numerically (Cysne et al., 2016; Weisse, 2004; Yuan et al., 2011), and in principle it should reduce to the DC conductivity \(\sigma_{\text{DC}}\) in the limit \(\omega \rightarrow 0\). To the best of our knowledge, nobody has directly compared the numerical implementations of DC and AC conductivity, but one group has published two independent papers in which they calculate these quantities for graphene with 0.4% of vacancy defects (Cysne et al., 2016; Ferreira and Mucciolo, 2015). A comparison of these papers shows that the DC and AC implementations give identical results at finite doping levels, but at the graphene Dirac point \(\sigma(\omega \rightarrow 0)\) is about 20% smaller than \(\sigma_{\text{DC}}\). It is unclear why this discrepancy exists at the Dirac point, but as will be discussed in Sec. IV.A.3, the exact value of the conductivity here is still a matter of some debate, with different numerical implementations of \(\sigma\) giving different results.

6. Implementations

Implementations of all the algorithms presented in this review will be distributed within the open-source C++ package TB-TK (available at http://secondtech.com/wordpress/index.php/tbtk/).

In addition, an implementation based on graphics processing units was used to obtain the results presented in this section and has been distributed as an open-source code named GPUQT (Fan et al., 2018).

Finally, a pedagogical Python implementation of the VAC-KPM and MSD-KPM methods using a Jupyter notebook is also available (https://github.com/brucefan1983/LSQT-Jupyter).

IV. APPLICATIONS TO DISSIPATIVE TRANSPORT IN DISORDERED MATERIALS

After presenting the LSQT methodologies for dissipative electronic transport, we are now in a position to discuss the various applications made during the last two decades. The LSQT method based on the MSD was first developed to study electronic transport in quasicrystals (Roche and Mayou, 1997), structures with a fivefold symmetry in the absence of translational invari-
A. Applications to disordered graphene

Ever since its discovery (Novoselov et al., 2004, 2005b), graphene research has included an intense focus on the impact of disorder on its transport properties. Many studies have considered either realistic or simplified theoretical models, and have been inspired by the plethora of observed defects generated during material fabrication and its integration into practical devices. Studying quantum transport in graphene and two-dimensional disordered materials is of particular interest given the large variety of physical scattering sources such as long-range charged impurities and screening effects (electron-hole puddle formation), short-range static defects, thermal disorder, as well as many-body effects. The quantum transport theory of massless Dirac fermions in the presence of such disorder is extremely rich in novel phenomena such as Klein tunneling, the minimum conductivity at the Dirac point, weak antilocalization, and the anomalous quantum Hall effect, all of which have been widely studied and presented in excellent reviews (Castro Neto et al., 2009; Das Sarma et al., 2011; Peres, 2010). Here we will focus on a few representative cases of defects and their implication in electrical transport. For further background and reviews on the electronic and transport properties of graphene, see (Castro Neto et al., 2009; Das Sarma et al., 2011; Mucciolo and Lewenkopf, 2010; Peres, 2009, 2010; Torres et al., 2014).

1. Anderson disorder

Anderson disorder (Anderson, 1958), as introduced in the last section, is the canonical disorder model for studying quantum transport in different materials. Although this is not a very realistic disorder model for graphene, it is still of theoretical importance. One advantage of this disorder model is that analytical results (Ostrovsky et al., 2006; Shon and Ando, 1998) can be obtained in the weak-disorder limit based on perturbation theory such as the self-consistent Born approximation (SCBA). LSQT calculations of the transport properties of graphene with Anderson disorder were first performed by Lherbier et al (Lherbier et al., 2008a). With the presence of Anderson disorder, the electronic DOS at the charge neutrality point is enhanced and the Van Hove singularities are smoothed, which is consistent with the prediction from SCBA (Shon and Ando, 1998). The semiclassical conductivity from LSQT calculations has a minimum at the charge neutrality point, which approaches the so-called minimum conductivity $4e^2/\pi h$ in the strong-disorder limit but remains generally larger in the weak-disorder limit. In the weak-disorder limit, the LSQT results can be well fitted by the SCBA prediction (Roche et al., 2012). Meanwhile, in the strong-disorder limit the SCBA fails to quantitatively describe the conductivity because of the neglect of quantum interference and hence localization effects. In both cases, the semiclassical Boltzmann transport equation approach fails to capture the energy dependence of the conductivity. This comparison highlights the necessity of employing fully quantum mechanical and nonperturbative calculations for a complete description of the transport physics of disordered graphene and related materials.

Beyond the diffusive regime, the conductivity decreases with increasing time or length (Fan et al., 2014b; Lherbier et al., 2008a), experiencing weak and strong localization effects consecutively. The weak localization regime is characterized by a logarithmic decay of the conductivity with respect to the length $L(E)$,

$$\sigma(E, L) = \sigma_{sc}(E) - \frac{G_0}{\pi} \ln \left[ \frac{L(E)}{l_c(E)} \right],$$

where $G_0 = 2e^2/h$ and $l_c(E)$ is the mean free path. This has been confirmed numerically with LSQT calculations (Fan et al., 2014b). In the scaling theory of Anderson localization (Abrahams et al., 1979; Lee and Ramakrishnan, 1985), one assumes that $L(E)$ reaches the localization length $\xi(E)$ when the weak localization correction $(G_0/\pi)\ln[L(E)/l_c(E)]$ equals the semiclassical conductivity $\sigma_{sc}(E)$. This gives an expression of the two-dimensional localization length

$$\xi(E) = l_c(E) \exp \left[ \frac{\pi \sigma_{sc}(E)}{G_0} \right].$$

It has been demonstrated (Fan et al., 2014b) that the two-dimensional localization length calculated in this way is consistent with that calculated based on the one-parameter scaling of localization length in quasi-one-dimensional systems (Kramer and MacKinnon, 1993; MacKinnon and Kramer, 1981). Graphene with Ande-
son disorder fully follows the one-parameter scaling theory of localization (Abrahams et al., 1979) and there is no extended state in the absence of decoherence. However, as remarked initially, the Anderson disorder model is not a satisfactory description of defects in real materials, and the study of more realistic disorder models become fundamental for any quantitative analysis of experimental measurements.

2. Charged impurities

One realistic disorder model is a long-range potential model accounting for the effects of charged impurities trapped in the substrate beneath graphene. It has been argued (Rycerz et al., 2007) that the bare Coulomb potential is not suitable for describing the potential induced by charged impurities. A standard model considering screening effects is obtained by replacing the bare Coulomb potential with the smoother Gaussian function, although more complex charged impurity models have been studied using the LSQT approach (Radchenko et al., 2013). Under this disorder model, the electrostatic potential energy at position \( r \) is given in real space by

\[
U(r) = \sum_{k=1}^{N_{\text{imp}}} U_k \exp \left[ -\frac{|r - r_k|^2}{2\xi^2} \right],
\]

where \( N_{\text{imp}} \) is the number of screened charge impurities, \( U_k \) is the strength of the \( k \)th impurity located at \( r_k \), and \( \xi \) is the effective range of the potential (here we distinguish this from the localization length discussed in previous sections). The ratio \( n_{\text{imp}} = N_{\text{imp}}/N \), with \( N \) being the number of atoms, defines the impurity concentration. The potential heights \( U_k \) are assumed to be uniformly distributed in the interval \([-W/2, W/2]\). \( W \) is the strength of the potential, which plays a similar role as in the Anderson disorder model. Actually, this charged impurity model reduces to the Anderson disorder model in the limit \( \xi \to 0 \) and \( n_{\text{imp}} \to 1 \). By tuning the value of \( \xi \) across the lattice constant, both short-range and long-range potentials can be realized. A dimensionless quantity which is frequently used to quantify the disorder strength when \( n_{\text{imp}} \ll 1 \) is given by (Rycerz et al., 2007)

\[
K_0 \approx 40.5 \times n_{\text{imp}} \left( \frac{W}{2\gamma_0} \right)^2 \left( \frac{\xi}{a} \right)^4,
\]

where \( a \approx 2.46 \text{ Å} \) is the lattice constant of graphene.

Graphene with long-range disorder shows diverse transport regimes. The Gaussian-shaped potential can induce two kinds of scattering: intervalley scattering which mixes the states in the two valleys of reciprocal space, and intravalley scattering which does not. The dependence of the ratio between the amplitudes of the two scatterings on the disorder strength has been studied numerically (Zhang et al., 2009). When intervalley scattering is completely excluded by considering a single-valley Dirac Hamiltonian, the conductivity follows a one-parameter scaling, either with (Ostrovsky et al., 2007) or without (Bardarson et al., 2007; Nomura et al., 2007) an unstable fixed point. In this case, the \( \beta \) function \( \beta(\sigma) = d \ln \sigma/d \ln L \) is positive (metallic), indicating weak antilocalization. On the other hand, using the full \( \pi \)-orbital tight-binding model and considering the long-range potential with \( \xi = \sqrt{3}a \), the conductivity follows a one-parameter scaling with a negative \( \beta \) function (Zhang et al., 2009), which is associated with the weak localization regime.

![FIG. 10 Conductivity \( \sigma \) at the charge neutrality point in graphene with Gaussian-shaped disorder as a function of length \( L \). The dimensionless strength is fixed to \( K_0 = 2 \) and the impurity concentration is fixed to \( n_{\text{imp}} = 2\% \). Four disorder ranges (\( \xi = a \) to \( 4a \)) are considered and the parameter \( W \) is thus determined from Eq. (118). The horizontal dashed line indicates the critical conductivity \( \sigma_{\text{Sp}}^* \approx 4 \times 1.42e^2/h \) where the factor 4 comes from spin and valley degeneracies (Markos and Schweitzer, 2006). The results were obtained by using the MSD-KPM method with \( M = 3000 \) moments, \( N_c = 10 \) random vectors, and \( N = 10^7 \) orbitals.](image)

The above scenario can be fully captured using the linear-scaling quantum transport approach in the MSD formalism. Figure 10 shows the calculated electrical conductivity \( \sigma \) of graphene with Gaussian-shaped disorder at the charge neutrality point as a function of the propagation length. Four sets of disorder parameters are considered, where the impurity concentration is fixed to \( n_{\text{imp}} = 1\% \) and the dimensionless disorder strength is fixed to \( K_0 = 2 \), while the disorder range changes from \( \xi = a \) to \( 4a \) and the \( W \) parameter is determined according to Eq. (118). In all cases, the conductivity first increases from zero to a plateau value (the
plateau for the case of $\xi = a$ cannot be seen clearly in this figure), which corresponds to the ballistic-to-diffusive transition. However, there are diverse behaviors beyond the diffusive regime. When $\xi = a$, $\sigma$ is smaller than $G_0 = 2e^2/h$ and decreases exponentially with increasing length, which is expected for strong (Anderson) localization. When $\xi = 2a$, $\sigma$ is larger than $G_0$ but decreases logarithmically, which is a weak localization behavior. When $\xi = 3a$ and $4a$, $\sigma$ keeps a value of about $\sigma_{St}^\alpha \approx 4 \times 1.42e^2/h$ (Markos and Schweitzer, 2006) for a wide range of length and then increases with increasing length. This unusual increase in $\sigma$ is a sign of antilocalization as predicted by considering a single-valley Dirac Hamiltonian (Bardarson et al., 2007; Nomura et al., 2007; Ostrovsky et al., 2007). The conductivity scaling in the presence of Gaussian-shaped disorder has also been studied using the Landauer-Büttiker approach (Lewenkopf et al., 2008). Using the full π-orbital tight-binding model, it was found that the conductivity at the charge neutrality point exhibits a metallic $\beta$ function of the form (Lewenkopf et al., 2008) $\beta \approx 0.17(2e^2/h)/\sigma$. However, a close comparison between Fig. 2 of (Lewenkopf et al., 2008) and Fig. 10 here reveals that what has been demonstrated in (Lewenkopf et al., 2008) is not weak antilocalization, but the ballistic-to-diffusive transition. The maximum conductivity reached in (Lewenkopf et al., 2008) is only about $2e^2/h$, which is still far below the critical point $\sigma_{St}^\alpha \approx 4 \times 1.42e^2/h$. Both localization and antilocalization are quantum corrections to the diffusive (semiclassical) conductivity caused by coherent multiple scattering.

Experimentally, quantum corrections to the conductivity can be explored by measuring the low temperature magnetoresistance, or equivalently, the magnetococonductance $\Delta \sigma(B) = \sigma(B) - \sigma(B = 0)$, where $\sigma(B)$ is the conductivity in the presence of a magnetic field $B$. A diagrammatic theory of quantum interference in disordered graphene (Fal’ko et al., 2007; Kechedzhi, K. et al., 2007; McCann et al., 2006) has been developed and provides a possible quantitative analysis of magnetococonductance data. Both positive (weak localization) and negative (weak antilocalization) magnetoconductance can be obtained, depending on the relative strength between the intravalley scattering time, the intervalley scattering time, and the coherence time. A transition from localization to antilocalization has been demonstrated experimentally (Tikhonenko et al., 2009) and similar results have been obtained from numerical calculations based on the LSQT method in the MSD formalism (Ortmann et al., 2011). It should be noted that the introduced intravalley and intervalley scattering times are beyond the reach of experimental analysis, making the simulations and comparison with measurements essential.

Away from the charge neutrality point, localization and antilocalization become less prominent and semiclassical Boltzmann transport theory (Das Sarma et al., 2011) has been successfully applied to study the transport properties of graphene with long-range disorder. The most important result is that the conductivity scales linearly with respect to the carrier density, giving a constant mobility. This transport fingerprint has been confirmed by using the LSQT method with the MSD formalism (Fan et al., 2017), as shown in Fig. 11. Here, long-range disorder ($\xi = 10a$ to $20a$) with fixed $W = \gamma/2$ is used as well as a set of values for $n_{imp}$ and $\xi$ that are comparable to experimental situations (Das Sarma et al., 2011). The reported conductivity is chosen as the value where the propagating length reaches 2 microns. At this length, the system is in the diffusive regime for all energies except for a small energy window around the charge neutrality point where weak antilocalization occurs, as discussed above. Both the mean free path and the scattering time scale as $n^{1/2}$ (Fan et al., 2017). Meanwhile, a sub-linear relationship between conductivity and carrier concentration has been obtained (Zhao et al., 2015) by using a LSQT method based on the Fourier transform (Yuan et al., 2010a,b), which might be related to the fact that a fixed total evolution time is used for all the energy states.

3. Point-like defects

Point-like structural defects have also been observed in graphene and have been shown to greatly affect transport properties (Cresti et al., 2008; Roche et al., 2012). Be-
yond those induced by material and device fabrication, point-like defects can also be deliberately created using ion irradiation or chemical treatments for tailoring the conduction regime (Nakaharai et al., 2013). Chemical substitution of carbon with nitrogen or boron atoms has been experimentally observed (Zhao et al., 2011), and numerical studies using the LSQT approach have discovered the emergence of mobility gaps (Biel et al., 2009; Lherbier et al., 2008b, 2013), which can help in fabricating p-type or n-type graphene-based transistors (Marconcini et al., 2012).

A generic and common defect that is found in any material is the missing lattice atom. Single vacancies in graphene have been produced and characterized by transmission electron microscopy (Meyer et al., 2008) and scanning tunneling microscopy (Ugeda et al., 2010). This type of disorder has a dramatic impact on the electronic structure of graphene with the formation of bands (also called zero-energy modes) which are localized at the Dirac point and which display a wavefunction decay following a power law (Pereira et al., 2008). The impact of such anomalous localization behavior on quantum transport properties for a random distribution of vacancies of varying density has been the subject of an intense debate in the literature.

For vacancies distributed roughly equally on both sublattices in a random fashion and for low density, one expects short-range scattering and localization effects to emerge. Such an effect was found by Cresti et al. (Cresti et al., 2013) and Fan et al. (Fan et al., 2014b), although the numerical simulations differ in the downscaling behavior of the quantum conductivity with system size. While Anderson localization is obtained in (Fan et al., 2014b), the authors of (Cresti et al., 2013) extract \( \sigma \sim 1/L^\beta \) with \( \beta \sim 2 \), although a fit of the scaling behavior with an exponential decay could also be numerically possible. The authors favored the power law scaling to be consistent with the power law localization of the wavefunctions. However, in Fig. 12, one can see that the Anderson localization regime and estimated localization length of Eq. (116) are confirmed by an independent calculation using the one-parameter scaling of localization length (Kramer and MacKinnon, 1993; MacKinnon and Kramer, 1981), albeit with some discrepancy around the charge neutrality point. This discrepancy originates from the fact that the semiclassical conductivity around the charge neutrality point is not well defined due to a sharp peak of the running conductivity, making it hard to identify the diffusive regime. However, Fig. 12 shows clearly that the conductivity around the charge neutrality point decays exponentially with increasing length and the extracted localization length from this conductivity decay agrees excellently with that predicted from the one-parameter scaling theory (Kramer and MacKinnon, 1993; MacKinnon and Kramer, 1981). This strongly supports the existence of an Anderson localization regime at the Dirac point in the presence of vacancies (a result also confirmed with a different implementation of the Kubo formula (Trambly de Laissardi`ere and Mayou, 2013)).

Other numerical results have claimed a different regime and assign a critical state at the Dirac point. Ostrovsky and coworkers found a saturation of the conductivity at a value of \( 4e^2/\pi \hbar \) when increasing the vacancy density, a behavior suggesting the suppression of localization phenomena and the formation of a critical state (Ostrovsky et al., 2010). This picture is supported by field-theoretical calculations showing the absence of weak localization corrections at the band center of 2D disordered systems with chiral symmetry (Gade, 1993; Gade and Wegner, 1991), suggesting that the localization length diverges at \( E = 0 \) in chiral-symmetric disordered graphene (class BDI, in the case of graphene with vacancies) (Ostrovsky et al., 2010). These results were however not obtained in the bulk limit but in a situation where boundary conditions are likely to introduce direct tunneling between evanescent states, whose density increases with the number of vacancies. Additionally, Ferreira and Mucciolo developed and employed the KG-CPGF method and also obtained a conductivity of \( 4e^2/\pi \hbar \) at the Dirac point over a wide range of dilute vacancy concentrations (Ferreira and Mucciolo, 2015). From the discussion in the

![FIG. 12 Conductivity \( \sigma \) as a function of length \( L \) in graphene with 1% of vacancy defects. The inset shows the localization length as a function of the Fermi energy calculated from the one-parameter scaling of localization length (Kramer and MacKinnon, 1993; MacKinnon and Kramer, 1981) (solid line), from the semiclassical conductivity using Eq. (116) (dashed line), and from an exponential fit to the conductivity shown in the main frame (markers). To be consistent with the conventions in Ref. (Fan et al., 2014b), the localization length here is twice that defined in Eq. (114). The results were obtained by using the MSD-KPM method with \( M = 3000 \) moments, \( N_r = 10 \) random vectors, and \( N = 10^7 \) orbitals. Adapted from Fan et al. (2014b).]
FIG. 13 (a) Summary of the values of grain boundary resistivity ($\rho_{GB}$) extracted from the literature. Open circles are measurements at the charge neutrality point, closed circles are measurements far from the charge neutrality point, and stars are for measurements where the position of the Fermi level is unknown. (b) Summary of the values of graphene sheet resistance, as a function of grain size, extracted from the literature. The solid gray line illustrates the scaling law of Eq. (119), assuming $R_s^G = 300 \ \Omega/\square$ and $\rho_{GB} = 0.3 \ \text{k}\Omega \ \mu\text{m}$. In both panels, the spread of simulation results is due to the impact of chemical functionalization of the grain boundaries, as depicted in the insets. In the simulations, system sizes ranged from $\sim$140,000 to $\sim$280,000 atoms, the semiclassical conductivity was calculated using the Lanczos expansion of the MSD with 1000 moments and an energy broadening of $\sim$100 meV, and the diffusive regime was reached after a simulation time of 0.1-0.3 ps. Adapted from Isacsson et al. (2017).

previous two sections, we know that the major difference between the KG-CPGF method and the MSD-based method is that while the two Dirac delta functions in the Kubo-Greenwood formula are interpreted differently in the MSD-based method (one for quantum projection and the other for time evolution), they are treated on an equal footing in the KG-CPGF method, i.e., the dephasing time $\tau_\phi$ in the KG-CPGF method controls both the transport regime and the energy resolution ($\eta = \hbar/\tau_\phi$). This difference could be the source of the differing results, but more dedicated simulations are needed to assess these two approaches.

4. Large-scale structural defects

Beyond point-like or electrostatic disorder, the methods presented in this review are also readily applicable to large-scale lattice defects such as grain boundaries (GBs) or graphene antidots (Bai et al., 2010; Lherbier et al., 2011; Pedersen et al., 2008). Grain boundaries are a natural result of chemical vapor deposition (CVD), which is the most useful approach for the large-scale production of graphene (Zhang et al., 2013b). During the CVD growth process, graphene grains nucleate and grow at random positions and orientations, resulting in a polycrystalline structure when growth is complete (Arjmandi-Tash et al., 2018). The grain boundaries that form at the interface of the graphene grains typically consist of disordered arrays of carbon pentagons, heptagons, and octagons. Experiments based on scanning tunneling microscopy or quantum transport have shown that GBs are strong charge scatterers, and can thus limit the electronic transport properties of large-area CVD-grown graphene (Isacsson et al., 2017).

A variety of numerical simulations, based on the methods presented in this review, have been carried out to quantify the impact that GBs have on charge transport in CVD-grown graphene (Barrios-Vargas et al., 2017; Cummings et al., 2014a,b; Seifert et al., 2015; Van Tuan et al., 2013). By applying Eq. (40) to realistic models of polycrystalline graphene generated by molecular dynamics simulations, Van Tuan et al. showed that the semiclassical conductivity $\sigma_{sc}$ of these materials scales linearly with the average grain size (Van Tuan et al., 2013). Subsequent work quantified the impact of GBs through the scaling relation (Cummings et al., 2014b)

$$R_s = R_s^G + \rho_{GB}/l_G,$$

(119)

where $R_s \equiv 1/\sigma_{sc}$ is the sheet resistance of the polycrystalline graphene, $R_s^G$ is the sheet resistance within the graphene grains, $l_G$ is the average graphene grain size, and $\rho_{GB}$ is the GB resistivity. By calculating $R_s$ for polycrystalline samples with a variety of grain sizes and fitting to Eq. (119), Cummings et al. extracted an intrinsic GB resistivity of $\rho_{GB} = 0.07 \ \text{k}\Omega \ \mu\text{m}$ (Cummings
et al., 2014b). This value is on the low end of those obtained experimentally. However, as shown in Fig. 13(a), the value of $\rho_{GB}$ depends significantly on the measurement technique, doping level, material quality, and degree of chemical functionalization (Isacsson et al., 2017). Indeed, the spread of simulation results indicates that $\rho_{GB}$ can be tuned by more than one order of magnitude by varying the concentration of chemical adsorbates on the GBs.

The impact of GBs on the electrical properties of CVD graphene can be seen in Fig. 13(b), where we show a summary of the values of graphene sheet resistance, as a function of grain size, extracted from the experimental literature. Simulation results are shown as open squares, with the spread of values resulting from different degrees of chemical functionalization of the GBs. Overall, the measurements follow the scaling trend described by Eq. (119), and the crossover between GB-dominated and grain-dominated transport occurs for grain sizes in the range of 1–10 µm.

Apart from GBs, large-scale lattice defects can also be intentionally engineered. A graphene antidot lattice (Pedersen et al., 2008), also called a graphene nanomesh (Bai et al., 2010), is a graphene sheet containing a pattern of nanometer-sized holes. These structures have been proposed to create a band gap in otherwise gapless graphene. However, deviations from a perfect superlattice structure are usually present in real experimental situations. The effects of geometrical disorder, modeled as fluctuations in the antidot radius and location (Power and Jauho, 2014), have been studied using the LSQT method. It was shown that the band gap in a perfect antidot lattice vanishes with the introduction of sufficiently strong geometrical disorder, and a transport gap can be induced via Anderson localization (Fan et al., 2015), in accordance with experimental results (Eroms and Weiss, 2009; Giesbers et al., 2012; Zhang et al., 2013a). The charge carrier mobilities are found to be very small compared to values found in graphene without antidots, and quantitative agreement with experiments has been obtained (Zhang et al., 2013a). In a model of anisotropic geometrical disorder, a coexistence of ballistic conduction and Anderson localization in different directions have also been predicted using the LSQT method (Pedersen et al., 2014).

B. 3D metals and semimetals

1. Electrical conductivity in liquid transition metals

Early studies of electron transport in disordered metallic systems have been conducted for liquid phase 3d transition metals such as Cr, Mn, Fe, Co and Ni with the so-called tight-binding linear muffin-tin orbital (TB-LMTO) recursion method (Bose et al., 1993). This method is an illustrative example of the connection between ab initio electronic structure approaches and linear-scaling quantum transport methods.

The TB-LMTO method divides the real space into atomic and interstitial regions by muffin-tin spheres that are centered at the atomic sites $\mathbf{R}$. Within these spheres, orbitals are defined with a collective angular momentum index $l = (l, m)$ for which $s$, $p$ and $d$ orbitals are included in this approach. The TB parameters for these orbitals are obtained from DFT calculations, thus providing a self-consistent description of the electronic properties at the Kohn-Sham level, which describes the general wave functions by orbitals

$$\chi_{RL}(\mathbf{r}_R) = \phi_{RL}(\mathbf{r}_R) + \sum_{R'L'} \phi_{RL'}(\mathbf{r}_R) h_{RL',RL}^{\alpha}$$

in the TB representation $\alpha$. Here $\phi_{RL}(\mathbf{r}_R)$ are reference wave functions inside a sphere of radius $s_R$ at $\mathbf{R}$ for a particular reference energy $E_{F,RL}$. Inside the sphere the potential is calculated with DFT and additional functions $\phi_{RL'}(\mathbf{r}_R)$ related to the energy derivative of $\phi_{RL}(\mathbf{r}_R)$ at the reference energy enter with expansion coefficients $h_{RL',RL}^{\alpha}$. These expansion coefficients typically vanish for the second neighbor shell in close-packed structures. This short-range nature makes the application of the Lanczos approach particularly efficient.

The geometry of the liquid metals was modeled by clusters with a size of 600 particles, which were generated with a Monte Carlo method. This leads to a disordered configuration of the metal atoms deviating from their fcc or bcc crystal structure. Strength and type of disorder are reflected in the matrix elements $h_{RL',RL}^{\alpha}$ that can intermix different angular momentum components of the muffin-tin orbitals.

In a preliminary step towards calculating electronic transport, Bose et al. (Bose et al., 1993) analyzed the momentum and angular momentum-resolved spectral functions as

$$n_k^j(E) = -\frac{1}{\pi} \lim_{\epsilon \to 0^+} \text{Im} \left\{ \sum_m \left| u_{k,m}^j \right|^2 G(E + i\epsilon) \left| u_{k,m}^j \right| \right\}$$

with $\left| u_{k,m}^j \right| = \sum_j e^{i\mathbf{kR}_j} \chi_{RL,t,m}^{\alpha}$ being the Fourier-transform of the muffin-tin orbitals in $\mathbf{k}$-space. In Fig. 14, the spectral function $n_k^j(E)$ for liquid Fe obtained with the TB-LMTO recursion method is plotted. The spectral function is used to study residual dispersion and the effect of disorder on the $s$, $p$, and $d$ orbitals in the liquid phase.

Subsequently real-space calculations of the electrical conductivity were performed with the Kubo-Greenwood formula in the form

$$\sigma_{jj} = \frac{e^2}{4\pi} n(E_F) D(E_F)$$

(122)
They turned out to be substantial for these liquid metal systems reaching the conductivities of the conventional channels however with opposite sign. Hence, the orbital mixing strongly impacts the conductivity and impedes the conduction process.

Finally, the work compared the electrical resistivities to experimental results with good quantitative agreement (except for liquid Ni) which corroborates the TB-LMTO recursion method. Further studies of the electrical conductivity with the Kubo-Greenwood formula extended the application of the TB-LMTO recursion approach to a larger number of systems including liquid La, Hg, and metallic glasses (Bose, 1998, 1999; Bose et al., 1994).

2. Localization transitions in disordered Dirac semimetals

In recent years LSQT approaches have also been used to theoretically study higher-dimensional materials such as three-dimensional Dirac semimetals (Pixley et al., 2015, 2016) or disordered Weyl fluids (Pixley et al., 2017, 2018; Wilson et al., 2017). In general, a Dirac semimetal is a condensed matter system where twofold degenerate conduction and valence bands touch each other. These materials can be described with a massless Dirac equation in the infrared limit. In the undoped case the Fermi level lies exactly at the Dirac point where the bands touch each other. Examples for Dirac semimetals are Cd$_3$As$_2$, Na$_3$Bi, Bi$_{1-x}$Sb$_x$, BiTl(S$_{1-x}$Se$_x$)$_2$, (Bi$_{1-x}$In$_x$)$_2$Se$_3$, or Pb$_{1-x}$Sn$_x$Te.

Dirac semimetals can be modeled by a massless Dirac Hamiltonian in its non-covariant form that additionally involves a disorder potential. The underlying Dirac Hamiltonian is defined by

$$ H = \frac{1}{2} \sum_{\mathbf{r}, \mu} (i\hbar) \hat{V} \psi_\mu \psi_{\mathbf{r} + \mathbf{e}_\mu} + H.c.) + \sum_{\mathbf{r}} V(\mathbf{r}) \psi_\mathbf{x}^\dagger A W \psi_\mathbf{x}, $$

(124)

where $\psi_\mathbf{x} = (c_{\mathbf{r}, \uparrow}, c_{\mathbf{r}, \downarrow}, c_{\mathbf{r}, \cdasharrow}, c_{\mathbf{r}, \cdashldownarrow})^T$ denotes the four components of a Dirac spinor referring to an electron at site $\mathbf{r}$ with parity ($\pm$) and spin ($\uparrow/\downarrow$); $\mathbf{e}_\mu$ (with $\mu = \hat{x}, \hat{y}, \hat{z}$) refers to a unit vector pointing to the nearest neighbor; and $\hat{V} = \sigma_\mu \otimes I_2$ are the $4 \times 4$ Dirac matrices that obey the anti-commutation relation $\{ \alpha_\mu, \alpha_\nu \} = 2\delta_{\mu\nu} I_4$ according to the anti-commutation relations of the $2 \times 2$ Pauli spin matrices $\sigma_\mu$. The type of the disorder (symmetry of the disorder) is given by $A W$. In case it is diagonal in the spinor components ($A W = I_4$), the disorder potential is just a scalar potential and $V(\mathbf{r})$ describes a random scalar potential at site $\mathbf{r}$ with strength $V(\mathbf{r}) \in [W/2, W/2]$. Off-diagonal terms are also studied, e.g., with an axial chemical potential $A W = \gamma_5 = i\alpha_1 \alpha_2 \alpha_3$. The model study in (Pixley et al., 2015) determined the quantum phase transition of a Dirac semimetal into a conventional diffusive metal. At larger disorder the

FIG. 14 Momentum resolved spectral functions $n_\mathbf{k}^\alpha(E)$ for the $s$-orbitals in (a) and the $d$-orbitals in (b) in liquid Fe obtained with the TB-LMTO recursion method. The $k$ values range from zero to $2\pi/a$ with the lattice parameter $a$ of fcc Fe at the density, $0.0756/\text{Å}^3$, of liquid Fe. The results were obtained for a cubic cluster with 600 particles.

From Bose et al. (1993).
latter experiences a further phase transition towards an Anderson insulator. These quantum phase transitions were obtained through the analysis of the average DOS given by

\[ \rho_a(E) = \left\langle \frac{1}{4N_s} \sum_{i=1}^{N_s} \sum_{\alpha=1}^{4} \delta(E - E_{i\alpha}) \right\rangle, \]  

(125)

with site index \( i \) and orbital index \( \alpha \) at eigenenergy \( E_{i\alpha} \). \( N_s \) is the size of the system and \( \langle \ldots \rangle \) represents the average over several realizations of disorder. Furthermore, they introduced the typical DOS as

\[ \rho_t(E) = \exp \left( \frac{1}{4N_s} \sum_{i=1}^{N_s} \sum_{\alpha=1}^{4} \left( \log \rho_{i\alpha}(E) \right) \right) \]  

(126)

with

\[ \rho_{i\alpha}(E) = \sum_{k_{i\beta}} |\langle k, \beta | i, \alpha \rangle|^2 \delta(E - E_{k\beta}). \]  

(127)

The above quantities for the average DOS and the typical DOS were calculated with the KPM. The strength of the disorder determines the corresponding phase transition of the model. For a system size of \( N_s = 60^3 \), model simulations of the average DOS and the typical DOS were performed with \( N_c = 1028 \) Chebyshev polynomials for the average DOS and \( N_c = 8192 \) Chebyshev polynomials for the typical DOS.

![Graph of quantum phase transitions](image)

**FIG. 15** Quantum phase transitions of a three-dimensional Dirac semimetal (DSM) to a conventional diffusive metal (CDM) and to an Anderson insulator (AI). Left: average DOS \( \rho_a(0) \) and typical DOS \( \rho_t(0) \) for a cubic system of size \( N_s = 60^3 \) at the Dirac point \( E = 0 \) as a function of the disorder strength \( W \). For the average DOS the KPM-methods was used with 1028 moments whereas the typical DOS required 8192 moments. From Pixley et al. (2015).

Further analysis involved the evaluation of the inverse participation ratio of the wave function as an indicator of the localization transition. The average participation ratio is defined as

\[ P_{\text{avg}} = \left\langle \frac{\sum_{i,\alpha} |\psi_{i\alpha}(r_i)|^2}{\sum_{i,\alpha} |\psi_{i\alpha}(r_i)|^4} \right\rangle^2, \]  

(128)

and was calculated for much smaller system sizes than used for the DOS calculation. From the inverse participation ratio \( P_{\text{avg}}^{-1} \), the localization transition was obtained in full accordance with KPM-based results, which corroborates the approach. In essence, the authors in (Pixley et al., 2015) studied transport properties via the density of states of disordered Dirac semimetals and compared the results to the inverse participation ratio leading to the same findings for the localization transitions.

Subsequent publications were dedicated to further analyze localization transitions in Dirac semimetals (Pixley et al., 2016) and Weyl semimetals (Pixley et al., 2018; Wilson et al., 2017) as well as the investigation of spectral properties of disordered Weyl fluids (Pixley et al., 2017) that could be tested by appropriate ARPES or STM measurements in undoped compounds dominated by neutral defects.

### C. Quantum transport in nanotubes and crystalline organic semiconductors with electron-phonon coupling

Electron-phonon coupling (EPC) (Ginstein, 2017) plays a crucial role in many transport properties, notably in conventional superconductivity (Bardeen et al., 1957) and temperature-dependent electrical resistivity. Although EPC and electrical conductivity can be studied using first principles calculations combined with the Boltzmann transport equation, this method is computationally formidable for complex systems. EPC can also be rigorously taken into account in quantum transport calculations based on the LB method, but various approximations (Frederiksen et al., 2007; Lusier and Klimeck, 2009; Rhyner and Lusier, 2014) have to be used in practical calculations and the computation is generally very expensive.

Phonons are lattice vibrations which are associated with deviations of the atom from their equilibrium positions \( R_i^0 \). In the TB formalism, the hopping integral \( \gamma_{ij} \) between atoms \( i \) and \( j \) is affected by the variation of the bond length between two atoms \( R_{ij}(t) = |R_j(t) - R_i(t)| \). A simple relation between \( \gamma(R_{ij}) \) and \( R_{ij} \) is \( \gamma_{ij} \propto 1/R_{ij}^2 \) (Harrison, 1989), although more sophisticated models (Porezag et al., 1995) can be constructed in specific materials. Based on the idea of distance-dependent hopping integrals, Roche et al. proposed a method to take the EPC into account in the MSD formalism (Roche et al., 2005a,b). In this approach, the EPC is encoded in a time-dependent TB Hamiltonian \( H\{\{R(t)\}\} \), where the time dependence of the atom positions \( R_i(t) \) is induced by phonon modes (labeled by the phonon branch \( \nu \) and wave vector \( \mathbf{q} \)) with amplitude \( A_{\nu}(\mathbf{q}) \), frequency \( \omega_{\nu}(\mathbf{q}) \), and polarization \( e_{\nu}(\mathbf{q}) \),

\[ R_i(t) = R_i^0 + A_{\nu}(\mathbf{q}) e_{\nu}(\mathbf{q}) \cos(\mathbf{q} \cdot \mathbf{R}_i^0 + \omega_{\nu}(\mathbf{q}) t). \]  

(129)

The total correlation time in the MSD formalism is di-
vided into a number of time intervals which are about one-tenth of the oscillation period of the considered phonon mode. The electron Hamiltonian is kept constant during each time interval and is updated after each time interval according to the updated atom positions. In this way, the electron wave propagation is coupled to the phonons. Dynamical off-diagonal disorder for electrons can also be modeled by combining the quantum evolution of the electronic wave function and the classical evolution of the lattice sites (Troisi and Orlandi, 2006). An approach combining the MSD approach and molecular dynamics (MD) simulations has also been developed (Ishii et al., 2010a, 2009), where the atom positions are updated according to interatomic forces from an empirical potential. Using these methods, the impact of EPC on quantum decoherence in carbon nanotubes has been quantified (Ishii et al., 2010b; Roche et al., 2007, 2005a,b).

While dynamical disorder from EPC is responsible for decoherence, a static disorder approximation can be used when the purpose is to compute the phonon-limited electron mobility. Based on the Born-Oppenheimer approximation, the electrons essentially experience a static potential profile associated with an instantaneous atomic configuration. In this approximation, one only needs to use MD simulations to generate a few equilibrated configurations and calculate the transport properties for each one separately. When the simulation system is large, the results from different configurations should not differ significantly. This approach has been used to study the phonon-limited electrical conductivity and mobility in suspended single-layer graphene with large-scale ripples spontaneously formed at room temperature (Fan et al., 2017). It was found that the semiclassical conductivity is a constant and the mobility is inversely proportional to the carrier density, in good agreement with results obtained by using the many-body perturbative GW approximation (Li and Das Sarma, 2013). A similar static disorder approximation has also been used in the LB approach, where harmonic lattice dynamics (Liu et al., 2015) or classical MD simulations (Markussen et al., 2017) are used to generate equilibrated configurations at a given temperature, and the electron transmissions in these systems are then calculated by combining DFT and nonequilibrium Green’s function calculations. Instead of using MD simulations or stochastic sampling, Gunst et al. showed that a single “special thermal displacement” (STD) of the atoms in a large supercell can give the correct thermal average of the LB conductance and phonon-assisted current (Gunst et al., 2017). This STD method would be an optimal way to include EPC in linear scaling quantum transport methods for large systems.

As an example of the application of the static disorder approximation for EPC, we show results (Fan et al., 2018) for electron transport in a single-walled metallic (14,14)-CNT with a diameter of about 1.8 nm, which is comparable to that reported in prior experiments (Park et al., 2004). Figure 16(a) shows σ(E, t) calculated using the MSD-KPM method. We see that for the whole energy spectrum, the conductivity converges well up to a correlation time of 3 ps. The ballistic-to-diffusive transition is clearly seen in Fig. 16(b), where the resistance (the inverse of the conductance defined in Eq. (55)) at E = 0 (corresponding to the low-bias situation in the experiments) as a function of the channel length is shown. In the short-length limit, the resistance approaches the bal-

![Graph](image-url)
listic value of \(1/(2G_0) = h/4e^2 = 6.45 \text{ k}\Omega\) (there are two conducting channels at the charge neutrality point). In the long-length limit, the resistance scales linearly with the channel length, which is the expected diffusive behavior. The good agreement with experiments demonstrates the applicability of the static disorder approximation in this case and the predictive power of the MSD-based LSQT method.

More complex systems where LSQT approaches have been applied are organic semiconductor crystals, which are used for instance in organic transistors (Gershenson et al., 2009). While charge transport in organic crystals has been studied extensively over the last few decades, the microscopic picture of transport and the crossover between different mechanisms is still not fully clear. The higher complexity in such systems compared to CNTs stems from the large number of molecular vibrations and from the electronic anisotropy. The former influence the electronic properties in different ways depending on temperature, while the latter induces an anisotropic transport behavior. To understand how EPC affects charge transport beyond simple models is a key requirement for predicting the electrical conductivity of crystalline organic semiconductors, and the efficiency of LSQT approaches makes them a useful tool for tackling such complexity in the limit of coherent electronic transport.

Different theoretical approaches exist to include the EPC for intra- and intermolecular vibrational modes in the Kubo transport framework based on the LSQT methods reviewed in this article. The EPC of high-frequency modes can be treated within polaron theories (Ortmann et al., 2011; Ishii et al., 2012; Troisi and Orlandi, 2006). This mixed description is often referred to as the adiabatic limit as the nuclei are treated classically.

The work of Ortmann and Roche (Ortmann and Roche, 2011) used a non-perturbative description of the EPC in organic crystals via a polaron transformation that takes into account their full quantum mechanical nature with a non-adiabatic approach, while other implementations of the EPC use a mixed classical-quantum mechanical description (Ciuchi et al., 2011; Ishii et al., 2012; Troisi and Orlandi, 2006). This mixed description is often referred to as the adiabatic limit as the nuclei are treated semiclassically.

In Fig. 17 we show the time-dependent diffusion constant and the energy-resolved mean free path of a three-dimensional cubic model of an organic crystal, parametrized as shown in the inset. At high enough temperature and disorder strength, the transport regime changes from diffusive to localized, as seen in Fig. 17. The diffusion constant depends on the polaronic bandwidth, and thus the carrier mobility varies with temperature through the temperature dependence of the bandwidth. In addition, disorder-induced localization is apparent at low temperatures and is reduced with increasing temperature. The combination of both of these effects may induce a transition of the transport regime from band-like to hopping transport with increasing temperature.

Troisi et al. (Troisi and Orlandi, 2006) have presented a transport approach based on a microscopic description of dynamical lattice disorder within the adiabatic regime. In the adiabatic approximation, the electronic transfer integral is assumed to exceed typical vibrational frequencies by one order of magnitude (or at least a large factor) and thus leads to a semiclassical treatment of the vibrational modes and the EPC. The carrier’s MSD and the diffusion constant for a coherently-propagated electronic wave packet can then be calculated based on a mixed quantum-classical description employing Ehrenfest equations.
A related numerical approach utilizing LSQT methods has been applied to organic semiconductors by other authors (Ishii et al., 2012), where several transport scenarios have been investigated based on a pentacene model system including intra- and intermolecular EPC and the effects of static disorder. Their numerical approach (referred to as time-dependent wave packet diffusion, TD-WPD) is an extension of the approach that was successfully applied to CNTs and graphene nanoribbons. During the propagation of the electronic wave packet the system Hamiltonian is updated in each individual time step according to the molecular dynamics of the vibrational modes within the single propagation step. As described above the approach considers the modes dynamically, leading to polaronic effects of the initial electronic wave packet. Additional static disorder effects and the interplay with the EPC are studied in this work.

In the same spirit, Ciuchi et al. (Ciuchi et al., 2011) demonstrated that the lattice dynamics of low-frequency intermolecular modes lead to a localization of the charge carriers on the time scale below a vibration period, at which the lattice is assumed to be frozen. Here rubrene is taken as the reference system, which has been intensively studied as a prototype compound in recent years (Girlando et al., 2010; Machida et al., 2010; Ordejón et al., 2017; Podzorov et al., 2004; Sundar et al., 2004; Troisi, 2007). The results from their LSQT-based method suggest that charge carriers (after an initial localization) remain in a diffusive transport regime with diffusion constant \( D \) leading to finite carrier mobilities according to \( \mu(T) = eD/k_B T \). Implementing this idea, they proposed an exponential decay of the velocity correlation function over time with an inelastic scattering time \( \tau_{\text{in}} \) that is on the order of the vibrational period of a typical intermolecular mode, i.e., \( \tau_{\text{in}} \propto \omega_{\text{inter}}^{-1} \).

This relaxation time approach is designed to counteract the localization phenomenon, which eventually results in finite mobilities, in contrast to the semiclassical Ehrenfest method proposed earlier. Indeed, it has been shown that the latter suffers from an increase of the velocity correlation function, leading to an increase of the time-dependent diffusion constant at time scales above the period of the inter-molecular vibrations, which results in diverging carrier mobilities. Employing the relaxation time approach, the diffusion constant is obtained from the so called transient localization length and the inelastic scattering time via \( D = L^2(\tau_{\text{in}})/2\tau_{\text{in}} \). Recently this approach has been applied to charge transport properties in two-dimensional herringbone structures (Fratini et al., 2017). The anisotropy of the electronic coupling (distribution of transfer integrals) was studied and connected to the localization behavior and the carrier mobility.

The emerging picture from these various studies using LSQT approaches is that there is a partial localization of charge carriers induced by disorder that can have vibrational or static origin. The spatial extent, or localization length, is still difficult to predict, since it is influenced both by high-frequency molecular vibrations leading to polaronic effects and by semiclassical dynamical disorder leading to localization. Since each can enhance the other, a combination of different approaches including those for high frequencies and low frequencies is desirable. The present success of the efficient numerical approaches in these studies suggests that future developments might emerge based on similar methods.

V. HALL AND SPIN TRANSPORT

A. Topological and Fermi surface contributions

In the previous sections, we explained how to combine different numerical techniques to compute the diagonal conductivity from different representations of the Kubo-Greenwood formula in a linear scaling way. However, it is nontrivial to extend this approach to study other transport properties such as the Hall conductivity. The reason is that the Kubo-Greenwood formula only captures the Fermi level properties of the system, and as shown by Thouless et al. in their seminal work (Thouless et al., 1982), some quantities are defined in terms of the topology of the electronic structure, and therefore depend on the whole energy spectrum. This means that in order to compute a general observable, one should first determine whether the topological contributions are negligible and choose the appropriate methodology accordingly.

![FIG. 18 Spin Hall conductivity for the Kane-Mele model using a SOC strength \( \lambda = 0.178 \gamma \), where \( \gamma \) is the nearest-neighbor transfer integral. The full spin Hall conductivity obtained from the Kubo-Bastin formula (black solid line) overlaps with the sum (red dashed line) of the Fermi level contribution (blue solid line) and the Fermi sea contribution (green dotted line). The simulation was performed on a system containing four million atoms, and the Green’s functions were approximated using the KPM with 2000 moments.](image)

The Hall conductivity is a quantity for which topological effects are prominent. In Sec. II we demonstrated that the Kubo-Bastin formula Eq. (20) is the single-particle...
approximation of the general Kubo formula, and as such, should contain both the topological and the Fermi level contributions. Indeed, the electrical response $A \equiv \langle \hat{A} \rangle$ of an arbitrary operator $\hat{A}$ can separated into two different contributions

$$A = A^{FS} + A^T,$$

by following Streda’s procedure (Crépieux and Bruno, 2001; Streda, 1982), originally developed for the Hall conductivity and later extended to an arbitrary operator (Cresti et al., 2016). In Eq. (130),

$$A^{FS} = \hbar \Omega \int_{-\infty}^{\infty} dE' \frac{dG(E' - \mu)}{dE'} \times \Im \left( \text{Tr} \left[ \delta(\hat{H} - E') \hat{A} G^+(E') (\hat{J} \cdot \mathbf{E}_0) \right] \right)$$

is what is called the Fermi surface contribution, while

$$A^T = \frac{\hbar \Omega}{2\pi} \text{Re} \left( \int_{-\infty}^{\infty} dE f(\varepsilon, H, T) \text{Tr}[\hat{B}] \right)$$

is the topological or Fermi sea contribution, where

$$\hat{B} = \left\{ G^+(E') \hat{A} \frac{dG^+(E')}{dE'} - \frac{dG^+(E')}{dE'} \hat{A} G^+(E') \right\} \hat{J} \cdot \mathbf{E}_0.$$  

The latter is responsible for, e.g., the quantized conductivity arising from the quantum Hall and quantum spin Hall effects. In Fig. 18 we show the calculated spin Hall conductivity for the Kane-Mele model (Kane and Mele, 2005), an example of a system possessing both Fermi level and Fermi sea contributions. This model describes the electronic behavior of a system composed of a honeycomb lattice with nearest-neighbor hoppings and strong intrinsic spin-orbit coupling (SOC) characterized by a strength $\lambda_1$. This system behaves as a topological insulator, with a bulk gap and topological edge states for $|E| < \lambda_1$, leading to a quantized spin Hall conductivity for the same range of Fermi energies. This calculation was performed using a system of four million orbitals and the KPM, following the methodology developed by García et al. (García et al., 2015), which will be discussed in detail in the next subsection. As one can see, the decomposition by Streda allows for separating purely topological features from Fermi sea contributions. It should be noted that the decomposition by Streda reduces to Aoki’s formula when used for the Hall conductivity (Aoki and Ando, 1981; Aoki, 1985),

$$\sigma_{\mu\nu} = -\lim_{\eta \to 0} \frac{i\hbar}{\Omega} \sum_{m,n} f(E_m) \frac{\langle E_m | \hat{J}_\mu | E_n \rangle \langle E_n | \hat{J}_\nu | E_m \rangle}{E_m - E_n + i\eta} + \text{h.c},$$

which is commonly used to compute the topological conductivity through exact diagonalization.

### B. Numerical implementations of the Kubo-Bastin formula

Previously, we showed how to use the KPM and the time evolution approaches for approximating the Dirac delta function and the Green’s function. These approximations can also be applied to the Kubo-Bastin formula. The simplest approach is to expand the Green’s function in terms of a polynomial series and regularize it by either using the KPM or by including a finite but small broadening $\eta$. The advantage of this approach is that the energy derivative, present in the Kubo-Bastin formula, only affects the Chebyshev coefficients and therefore can be done analytically. After insertion of the Chebyshev series into Eq. (20) and the application of the corresponding derivative to the Chebyshev coefficients in Eq. (82), one obtains the following expression for Kubo-Bastin formula (García et al., 2015),

$$\langle \hat{A} \rangle = \hbar \Omega E_\alpha \int_{-1}^{1} d\tilde{E} f(\tilde{E}) \sum_{m,n} \Gamma_{m,n}(\tilde{E}) \mu_{mn}^\alpha,$$

where

$$\mu_{mn}^\alpha = g_m g_n \text{Tr} \left[ \hat{J}_\alpha T_m(\tilde{H}) \hat{A} T_n(\tilde{H}) \right]$$

are the multi-dimensional version of the Chebyshev moments (Weiße et al., 2006) and

$$\Gamma_{m,n}(\tilde{E}) = \frac{1}{\Delta E^2 (1 - \tilde{E}^2)^2 (1 + \delta_{m0})(1 + \delta_{n0})} \times \left( (\tilde{E} - i\eta) \sqrt{1 - \tilde{E}^2} e^{im\arccos(\tilde{E})} T_m(\tilde{E}) + (\tilde{E} + i\eta) \sqrt{1 - \tilde{E}^2} e^{-im\arccos(\tilde{E})} T_n(\tilde{E}) \right)$$

are energy-dependent Chebyshev coefficients.

The second approach is based on Lanczos recursion and the time-dependent Kubo-Bastin formula presented in Eq. (20), and has been called the time-evolution Kubo (TEK) approach. Although the simulation time for the transversal components of the DC conductivity is increased compared to the simulation time for the longitudinal components (by a factor of about 500-5000 depending on the number of Lanczos vectors), the time evolution of the studied quantity usually provides more physical insight into the mechanism leading to the stationary state, as already discussed in Sec. II. The core of this method lies in the approximation of the completeness relation by random-phase vectors (Ortmann et al., 2015; Ortmann and Roche, 2013),

$$1 \approx \sum_{j=1}^{N_R} |\phi_j\rangle \langle \phi_j|,$$

where $N_R$ is the number of Lanczos recursion steps and the set $\{|\phi_j\rangle\}$ are random phase vectors as defined in
Sec. III.A. This identity can then be inserted into Eq. (20) in order to obtain an alternative representation of Eq. (135),

$$\langle \hat{A} \rangle = 4E_0\Omega \lim_{\eta \to 0^+} \int_0^{t_c} \frac{dt}{2\pi} e^{-\eta t/\hbar} \int_{-\infty}^\infty dE f(E, \mu, T)$$

$$\times \sum_{j=0}^{N_R} \text{Im} [\kappa_j(E)] \text{Re} \left[ \langle \phi_j | E_0 \cdot jG^+(E) \hat{A}(t) | \phi_1 \rangle \right] ,$$

(139)

where

$$\kappa_j(E) = \langle \phi_j | G^+(E) | \phi_1 \rangle$$

(140)

are the elements of the first column of the matrix-valued Green’s function. This numerical implementation avoids the tedious computation of the eigensystem by using a combination of $O(N)$ techniques. The conductivity can then be obtained from numerical simulations using the formerly introduced Lanczos algorithm and continued fraction expansion for the calculation of the $\kappa_j(E)$. The $\kappa_j(E)$ are defined recursively with the initial element $\kappa_1(E) = \langle \phi_1 | G^+(E) | \phi_1 \rangle$ being related to the DOS $\rho(E)$ of the system via

$$\frac{1}{\pi} \text{Im} [\kappa_1(E)] = \rho(E).$$

(141)

In the second step, $\kappa_2(E)$ is

$$\kappa_2(E) = \frac{1}{b_1} (-1 + (E - a_1 + i\eta)\kappa_1(E)) .$$

(142)

For $n > 2$, we find the recursion relation

$$\kappa_{n+1}(E) = \frac{1}{b_n} (-b_{n+1}\kappa_{n-1}(E) + (E - a_n + i\eta)\kappa_n(E)) .$$

(143)

In Eqs. (142) and (143), the coefficients $a_n$ and $b_n$ are the matrix elements of the tridiagonal matrix obtained from the Lanczos algorithm for the initial random phase vector $| \phi_1 \rangle$. In addition, the Chebyshev polynomial expansion method is used for the time evolution operator $\hat{U}(t)$ as explained in Sec. III. This approach will be illustrated in the next subsection for graphene.

C. Quantum Hall effect

One canonical example where the topological contribution plays a dominant role is the quantum Hall effect. When a two-dimensional system is subjected to a perpendicular homogeneous magnetic field, under appropriate conditions the electrons will move in degenerate orbitals which for certain Fermi energies will produce bulk insulating behavior and quantized edge currents, both originating from the topology of the band structure. This effect, and the interaction of the topological states with disorder, has been studied numerically using the two implementations of the Kubo-Bastin formula presented in the above subsection (García et al., 2015; Ortmann et al., 2015).

As an example, we discuss the quantum Hall effect in disordered graphene. The Hamiltonian for this system is

$$\hat{H} = \sum_i V_i \hat{c}_i^\dagger \hat{c}_i - \sum_{ij} \gamma e^{-i\phi_{ij}} \hat{c}_i^\dagger \hat{c}_j$$

(144)

with the nearest neighbor transfer integral $\gamma = \gamma_0 = 2.7$ eV. To include disorder, we use an uncorrelated Anderson model with matrix elements $V_i$ taken at random from the interval $[-W\gamma_0/2, W\gamma_0/2]$. The strength of the disorder in units of the nearest neighbor transfer integral is given by $W$.

The constant magnetic field $B = \nabla \times A$ is implemented via a Peierls phase (Luttinger, 1951), leading to an additional phase evolution $\phi_{ij}$ that modifies the transfer integral between the sites $i$ and $j$ as

$$\phi_{ij} = \frac{\hbar}{e} \int_{r_i}^{r_j} dr \cdot A .$$

(145)

FIG. 19 Hall conductivity of graphene with Anderson disorder (dashed curves, exact diagonalization; solid curves, TEK) at different magnetic fields (main frame). Effect of increasing disorder for high field 964 T (upper inset) and intermediate field 45 T (lower inset). From Ortmann et al. (2015). The simulation was performed in a system of 10 million atoms, using one random vector and the Lanczos algorithm with a broadening of 0.002$\gamma_0$ and at least 1000 Lanczos recursion steps.

The numerical results for the Hall conductivity $\sigma_{xy}$, which is obtained by replacing $\hat{A} = \hat{J}_y$ in the Kubo-Bastin formula, are shown in Fig. 19. The quantization of the Hall conductivity, following the sequence of steps according to $\sigma_{xy} = \pm 4 \left( \frac{1}{2} + n \right) \frac{e^2}{\pi} \hbar$, reproduces experimental measurements (Novoselov et al., 2005a; Zhang et al.,
The results are plotted for large and intermediate magnetic field strengths. A comparison of our method with the results from exact diagonalization yields high quantitative agreement.

Using LSQT methods, Ortmann et al. also examined the impact that sublattice-dependent disorder can have on the quantum Hall effect in graphene (Ortmann et al., 2015). This was done by including an additional sublattice-symmetry breaking potential according to $V_i \rightarrow (V_i + V_{AB} (\delta_{iA} - \delta_{iB}))$ with $V_{AB} = 0.2\gamma_0$ and this modification applied randomly to $p = 2.5\%$ of the sites in the sample. As shown in Fig. 20, a zero-energy Landau level splitting is clearly visible and corresponds to a plateau onset energy of $pV_{AB} = 0.005\gamma_0$ (indicated by the dotted vertical line).

**D. Quantum valley Hall effect**

Another phenomenon where topology plays an important role is the quantum valley Hall effect. Honeycomb structures are characterized by a linear energy dispersion centered at two inequivalent Brillouin zone points, usually denoted as $K^+$ and $K^-$, or equivalently, $K$ and $K'$. However, when these systems become massive an anomalous Hall effect is predicted to occur, but with opposite sign in each valley as imposed by the system's inversion symmetry (Sinitsyn et al., 2006). Moreover, similarly to the previously discussed quantum Hall effect, a periodically strained system will behave as if it were subjected to a pseudomagnetic field, producing Landau levels (Levy et al., 2010) and a valley quantum Hall effect (Settnes et al., 2017). Here we show that by using the Kubo-Bastin formula and an adequate definition of the valley current operator, one can obtain appropriate transport coefficients for graphene under uniform strain and propose an experimental way to detect valley polarized currents.

For modeling graphene under uniform strain we use a first-nearest-neighbor TB model where strain is included through a modification of the hopping parameters, while the external magnetic field is added using the standard Peierls substitution described in the previous subsection. In the Dirac approximation the strain is described by a gauge field $\pm A_S$, where $\pm$ denote the two valleys. This gauge field is related to the strain tensor $\epsilon_{ij}$ through $A_S \propto (\epsilon_{xx} - \epsilon_{yy}, -2\epsilon_{xy})$ (Fujita et al., 2011; Guinea et al., 2010; Vozmediano et al., 2010), and the pseudomagnetic field becomes $B_S = \nabla \times A_S$. From this, it is straightforward to show that a triaxial deformation $u(x, y) = u_0(2xy, x^2-y^2)$ induces a constant pseudomagnetic field. Uniaxial tensile strain has also been shown to generate a constant pseudomagnetic field (Zhu et al., 2015).

In order to resolve each valley, one needs to remember that in linear response theory one is computing the average of a microscopic operator, which for charge transport is the current operator. Therefore, we need to find an appropriate microscopic valley current operator. This can be achieved by taking inspiration from the spin current operator, which is in general defined as

$$\tilde{J}_\alpha = \frac{1}{2} \{ \tilde{J}_\alpha, s_z \},$$

where $\tilde{J}_\alpha$ is the single-particle current operator in the $\alpha$ direction as defined in Sec. II, and $s_z$ is the spin operator in the $z$ direction. Then, by expressing $s_z$ in terms of its eigenvector projectors $P^\pm_s = |\pm\rangle \langle \pm |$, we have

$$\tilde{J}_s^z = \frac{1}{2} ( P^+_s \tilde{J}_\alpha P^+ - P^-_s \tilde{J}_\alpha P^- ),$$

and from this expression we conclude that the spin current operator is nothing but the difference between the projections of the current operator in each spin subspace. From here the extension is obvious; we define the valley projector operators as $P^\pm_v = |K^\pm\rangle \langle K^\pm |$, and define the valley current operator as

$$\tilde{J}_\alpha^v = \frac{1}{2} ( P^+_v \tilde{J}_\alpha P^+ - P^-_v \tilde{J}_\alpha P^- ).$$

Different from the case of spin, there is no valley operator in the full tight-binding Hamiltonian, and therefore it is in general impossible to find $P^\pm$ using the same approach. However, from a numerical perspective one can consider the projector as a filter of electrons with momentum not belonging to the $K^\pm$ valley, or in explicit terms

$$P^\pm_v = \sum_k \theta(|k - K^\pm| - R) |k\rangle \langle k |$$

where $\theta$ is the Heaviside step function.
where $\theta(x)$ the Heaviside function and $R$ is a valley cutoff which in general is defined by the disorder energy scale and can be chosen to be for example $R = |M - K^\pm|$.

$B_M = B_0 \quad B_S = 0 \quad (a)$

$B_M = 0 \quad B_S = B_0 \quad (b)$

$B_S = B_0 \quad B_M = B_0 \quad (c)$

(E) Spin transport physics

Spintronics, or spin electronics, involves the study of spin information transfer as well as the manipulation of spin degrees of freedom in solid-state systems (Žutić et al., 2004). Spin transport differs from charge transport in that spin is generally a nonconserved quantity in type of valley mixing as we only consider a bulk effect in the part of the sample with a constant pseudomagnetic field. The results remain qualitatively unchanged as long as a sufficiently large part of the sample experiences a uniform field.

FIG. 22 Transport in graphene with compensating pseudo- and real magnetic fields. (a) The Hall conductivity, showing a quantum Hall effect in one valley and not in the other. (b) Valley polarization $\zeta = (\sigma_{Kxx} - \sigma_{K'xx})/\sigma_{xx}$ of the dissipative longitudinal current. Inset: Illustration of valley Hall effect in $K$ and standard diffusive transport for $K'$ in the longitudinal direction. From Settnes et al. (2017). The simulation was performed in a system of half a million atoms, with 200 random vectors and the KPM for expanding the Green’s functions with 4000 moments.

In Fig. 21 we show the density of states of graphene for the cases with magnetic field, pseudomagnetic field, and a combination of both with the same strength. We see the formation of Landau levels in the first two cases, and for the third one we see a perfect cancellation of fields for one of the valleys, leading to the typical metallic state. This is because due to inversion symmetry, the pseudomagnetic field has opposite sign in each valley and will add to or subtract from the real magnetic field.

Next we compute the Hall conductivity in the situation where the pseudomagnetic field compensates the real magnetic field. This is shown in Fig. 22. In this scenario, we can see that the system behaves exactly as expected for the quantum Hall effect discussed previously, but with a Hall conductivity reduced to half because only one of the valleys is carrying the current. Moreover, because the system is metallic the longitudinal current is fully valley polarized, which is key for valleytronic applications.
solids due to spin-orbit and hyperfine coupling. An essential metric to characterize spin transport is given by the upper limits of time or distance over which spin signals can be measured or manipulated. To evaluate the corresponding spin lifetime (or relaxation time) and spin diffusion length in disordered materials, one can either use a semiclassical spin Bloch transport equation (Fabian et al., 2007), or compute numerically the time evolution of the spin polarization of propagating wavepackets. As shown below, real-space $\mathcal{O}(N)$ methods provide a new tool for exploring spin dynamics, spin relaxation and spin transport phenomena (such as the spin Hall effect) in complex materials.

1. Spin relaxation time

To study spin dynamics and spin relaxation using the numerical methods presented above, it suffices to calculate the energy- and time-dependent spin polarization

$$S(E, t) = \frac{1}{2} \frac{\langle \phi(t) | \hat{\delta}(E - \hat{H}) | \phi(t) \rangle + \text{h.c.}}{\langle \phi(t) | \hat{\delta}(E - \hat{H}) | \phi(t) \rangle},$$

(150)

where $\hat{s}$ are the spin Pauli matrices, “h.c.” is the Hermitian conjugate, and $| \phi(t) \rangle = \hat{U}(t) | \phi(0) \rangle$ is the time-evolved initial state of the system. This initial state is spin polarized along axis $\hat{j}$ according to

$$| \phi(0) \rangle = \frac{1}{2} (\mathbb{I}_{2N} + \hat{j} \cdot \hat{s}) | \phi_t \rangle,$$

(151)

where $\mathbb{I}_{2N}$ is the $2N \times 2N$ identity matrix and $| \phi_t \rangle$ is the random-phase state defined in Eq. (61) with the replacement $N \rightarrow 2N$ to account for spin.

With a bit of knowledge about spin relaxation mechanisms and the nature of the system under investigation, the spin relaxation time can be extracted from the time-dependent spin polarization. For example, the typical Elliott-Yafet (EY) and D’yakonov-Perel’ (DP) spin relaxation mechanisms give $S(t) = S(0) \exp(-t/\tau_s)$, where $\tau_s$ is the spin relaxation time (D’yakonov and Perel’, 1971; Elliott, 1954; Yafet, 1963). When outside the motional narrowing regime or in the presence of a uniform magnetic field, the DP mechanism changes to $S(t) = S(0) \exp(-t/\tau_s) \cos(\omega_s t)$, where $\omega_s$ is the spin precession frequency (Gridnev, 2001). Meanwhile, more complicated dephasing mechanisms can lead to different behaviors (Cummings and Roche, 2016; Van Tuan et al., 2014).

An example of spin dynamics and relaxation is shown in Fig. 23(a). Here we plot the time dependence of spins oriented in (blue symbols) or out of (red symbols) the graphene plane, for graphene on a WSe$_2$ substrate in the presence of weak electron-hole puddles (Cummings et al., 2017). Here we see that the in-plane spins undergo precession plus relaxation, while the out-of-plane spins undergo simple exponential decay. Lines show the fits to these numerical results.

The methodology presented in Eqs. (150) and (151) has been applied to the study of spin dynamics and relaxation in a wide variety of graphene-based systems. The first studies using this methodology revealed the role that spin-pseudospin entanglement has on spin relaxation in graphene with gold impurities (Van Tuan et al., 2014), graphene on typical SiO$_2$ or hBN substrates (Cummings and Roche, 2016; Van Tuan et al., 2016b), or graphene functionalized with fluorine adatoms (Van Tuan and Roche, 2016). An example of this can be seen in Figs. 23(c) and (d), which show calculations of
the spin lifetime in graphene on a SiO$_2$ or hBN substrate for different defect densities. For graphene on SiO$_2$, the spin lifetime increases with increasing defect density, indicating the presence of DP spin relaxation. Meanwhile, graphene on hBN shows the opposite scaling behavior, indicating a transition out of the motional narrowing regime of spin dynamics due to the much weaker scattering induced by the hBN substrate. In all cases, a minimum in the spin lifetime at the charge neutrality point is a signature of spin-pseudospin entanglement in graphene systems dominated by Rashba spin-orbit coupling (Cummings and Roche, 2016; Van Tuan et al., 2016b, 2014).

Recent work investigated spin relaxation in graphene on transition metal dichalcogenide (TMDC) substrates, and predicted the presence of giant spin lifetime anisotropy, with in-plane spins relaxing much faster than out-of-plane spins (Cummings et al., 2017). This is depicted in Fig. 23(b), which shows the simulated spin lifetime in a graphene/WSe$_2$ system. In the presence of intervalley scattering the spin lifetime anisotropy can reach values of several tens, while for graphene on typical SiO$_2$ substrates this value is on the order of one (Raes et al., 2016). These results have been supported and generalized using a time-dependent perturbative treatment to derive the spin Bloch equations governing the spin dynamics at high electronic density (Offidani and Ferreira, 2018). The predicted giant spin lifetime anisotropy has also been verified experimentally (Benítez et al., 2018; Ghasi et al., 2017), confirming the strong impact that TMDC substrates can have on spin transport in graphene.

Beyond the aforementioned examples, spin relaxation in graphene functionalized with thallium or hydrogen atoms has also been studied with these methods (Cresti et al., 2014; Soriano et al., 2015), as has the impact of local magnetism coupled with electron-hole puddles (Vierimaa et al., 2017).

2. Spin Hall effect

The spin Hall effect (SHE) is another phenomenon where the Fermi sea contribution is highly relevant. It consists of the generation of a spin current that is transverse to an applied electric field due to the presence of spin-orbit coupling (D’yakonov and Perel’, 1971; Hirsch, 1999). There are two mechanisms behind the emergence of SHE. The first is named the intrinsic SHE since it occurs solely due to the spin-orbit coupling encoded in the band structure of the materials, whereas the extrinsic SHE stems from an interplay between disorder and the states at the Fermi level (Sinova et al., 2015). In general, the spin Hall effect measured experimentally is usually a combination of both, and there are even situations where these two effects exactly cancel (Inoue et al., 2004; Milletari et al., 2017; Mishchenko et al., 2004). The intrinsic SHE can be considered as the time-reversal generalization of the quantum Hall effect, in the sense that it is the sum of the Berry curvature of each band that determines the behavior of the system (Sinova et al., 2015). For metallic systems, there are methods for mapping Fermi sea problems into Fermi surface problems (Haldane, 2004; Wang et al., 2007). Still, these methods do not allow for obtaining quantized topological invariant for insulators, emphasizing the need for efficient spectral approaches.

The Kubo formula for bulk conductivity allows one to define the main figure of merit of the SHE, namely the spin Hall angle (SHA), which measures how much pure spin current is produced by a charge current, and is connected to transport coefficients through (Cresti et al., 2016)

$$\theta_{\text{SH}} = \frac{\sigma_{xy}}{\sigma_{xx}},$$

where $\sigma_{xy}$ is the SH conductivity and $\sigma_{xx}$ is the longitudinal charge conductivity. The formal expression of the spin Hall conductivity $\sigma_{\text{SH}}$ used in numerical simulations is (Sinova et al., 2015)

$$\sigma_{\text{SH}} = \frac{e\hbar}{\Omega} \sum_{m,n} \frac{f(E_m) - f(E_n) \Im \left[ J_z / n \right] \left\langle \langle n | v_y | m \rangle \right\rangle}{E_m - E_n + i\eta},$$

where $J_z = \frac{i}{2} \left\{ s_z, v_x \right\}$ is the spin current operator and $s_z$ is the $z$-component of the Pauli matrices. This formula can be understood as a generalization of Aoki’s formula (Aoki and Ando, 1981; Aoki, 1985), presented in Eq. (134). This formula becomes computationally prohibitive for large systems given that it requires the full spectrum of eigenvalues and eigenvectors of the Hamiltonian. However, the Kubo-Bastin formula and its variants remain valid given that it is derived for an arbitrary Hermitian operator, a condition that the spin current operator satisfies. This approach has been used used to determine the SHA of spin-orbit-enhanced graphene in recent years (van den Berg et al., 2011; García et al., 2015; García and Rappoport, 2016; Van Tuan et al., 2016a). One illustrative example of the SHA computed for graphene with random adsorbed gold adatoms is shown in Fig. 24, where a large SHA is observed when gold adatoms are deposited randomly on the graphene surface, while atomic segregation into clusters affects its energy dependence substantially (Van Tuan et al., 2016a).

An additional example is shown in Fig. 25, where the intrinsic spin Hall conductivity is computed for graphene on different graphene/transition metal dichalcogenide (TMD) substrates. In this particular work it was shown that this methodology can capture both the intrinsic and extrinsic contributions, because the intrinsic SHE is effectively canceled by an opposite extrinsic SHE originating from disorder-induced intervalley scattering. This suppression was studied as a function of the intervalley scattering rate in (García et al., 2017, 2018). The recent
FIG. 24 Spin Hall angle $\theta_{\text{si}}$ for two cases of 15% gold adatoms distributed onto graphene: scattered (in black) and clustered distributions (in red), as illustrated in the insets. From Van Tuan et al. (2016a). The simulation was done in a system consisting of 4 million atoms, with one random vector and the KPM for expanding the Green’s functions using 1500 moments and the Jackson kernel.

Experimental confirmation of the SHE induced by proximity effects in graphene/TMD heterostructures (Safeer et al., 2019) opens a new playground to search for the upper limit of SHE efficiency, a task which can be supported by the simulation methods presented here.

Others studies combining $\mathcal{O}(N)$ bulk Kubo approaches with multiterminal Landauer-Büttiker quantum transport methods have revealed more complexity in understanding the physics of the SHE than can be obtained from a simple theoretical interpretation of experimental data. For instance, Gregersen and coworkers have demonstrated how geometrical effects allow finite samples to display transverse resistances that are reminiscent of the SHE, but which disappear in the bulk limit (Gregersen et al., 2018). Another important finding concerns the parasitic background contributions that appear when calculating the nonlocal resistance of chemically functionalized graphene systems, which can mask spin effects or mislead the interpretation of experiments (Van Tuan et al., 2016a). Importantly, this type of theoretical analysis has recently refuted the claim that topological valley Hall currents (Beconcini et al., 2016; Song et al., 2015) carried by the Fermi sea can explain large nonlocal resistance measured at the Dirac point for certain graphene/hBN interfaces (Gorbachev et al., 2014). A complete analysis of bulk and multiterminal quantum transport reveals a limit of the direct connection between the valley Hall conductivity and nonlocal resistance, and shows that non-topological dispersive edge states, resilient to (weak) disorder, give a more solid explanation for the large nonlocal resistance (Cresti et al., 2016; Marmolejo-Tejada et al., 2018).

VI. LANDAUER-BÜTTIKER QUANTUM TRANSPORT METHODOLOGY

Transport properties at the nanoscale in open systems (with electrodes in a device geometry) are conveniently described by the Landauer-Büttiker (Büttiker et al., 1985; Landauer, 1957, 1970) and the nonequilibrium Green’s function formalisms (Haug and Jauho, 1996; Kadanoff and Baym, 1962; Keldysh, 1965; Rammer and Smith, 1986). The Landauer-Büttiker formalism expresses the current response of a multi-port conductor in terms of transmission matrices, and is also derivable straightforwardly from linear response theory (Baranger and Stone, 1989; Stone and Szafer, 1988).

In the Landauer-Büttiker formalism, efficient numerical methods based on recursive Green’s functions (Ferry and Goodnick, 1997) have been developed and are routinely used. As matrix inversion is at the heart of this approach, the computational cost generally scales cubically with respect to the cross-sectional area of the system, making it computationally prohibitive for large and disordered two-dimensional and three-dimensional systems. Despite this limitation, it is still possible to implement density-functional methods in the nonequilibrium transport formalism (Brandbyge et al., 2002), and to investigate low-dimensional nanostructures such as disordered semiconducting nanowires (Markussen et al., 2017; Persson et al., 2008) or chemically functionalized nanotubes with lengths reaching the micrometer scale (Lopez-Bezanilla et al., 2009). A recent study of quantum transport in carbon nanotubes confirms for instance...
the universality of the single-parameter scaling Anderson localization for realistic models of disordered systems (Lopez-Bezanilla et al., 2018).

Interestingly, a wave function formulation of the quantum scattering problem in the Landauer–Büttiker formalism (available in the KWANT code (https://kwant-project.org/) can actually reduce the computational time to some degree, compared to the recursive Green’s function formulation, but at the cost of increased memory footprint (Groth et al., 2014). For nanostructures, a self-contained description of such type of wave-function matching method has been shown to bring the number of operations to scale linearly with the number of sites of the studied system ($N_s$), or more precisely following a computational cost as $N_s \times N_p$ ($N_p$ the number of open channels in the asymptotic leads region) for large $N_s$, faster than previously claimed (Santos et al., 2019).

A. Lanczos method for computing off-diagonal Green’s functions

A fully order-$N$ method for the calculation of the Landauer–Büttiker conductance has also been proposed (Triozon and Roche, 2005). This method is based on a bi-orthogonalization process that generalizes the Lanczos approach to nonsymmetric matrices, and which is essential to cope with device geometries including open boundaries. The basic approach is to rewrite the transmission function of Eq. (109) as

$$T(E) = \sum_{\alpha, \beta, \alpha', \beta'} \langle \beta | \Gamma_R | \alpha \rangle \langle \alpha | G^\dagger | \alpha' \rangle \langle \alpha' | \Gamma_L | \beta' \rangle \langle \beta' | G | \beta \rangle,$$

(154)

where $\alpha, \beta$ ($\alpha', \beta'$) are the interface localized states that run over the orbitals coupled to the left (right) electrode. The self-energies of the leads can be calculated efficiently using standard recursion techniques (Sancho et al., 1985), while an order-$N$ method is needed for evaluating the Green’s functions. The off-diagonal elements of the Green’s functions can be expressed as a sum of three diagonal elements

$$\langle \alpha | G^\dagger | \alpha' \rangle = \frac{1}{2} \left[ (1 + i) \langle \psi_+ | G^\dagger | \psi_+ \rangle + (i - 1) \langle \psi_- | G^\dagger | \psi_- \rangle - 2i \langle \psi_i | G^\dagger | \psi_i \rangle \right],$$

(155)

where $| \psi_{\pm} \rangle = (| \alpha \rangle \pm | \alpha' \rangle) / \sqrt{2}$ and $| \psi_i \rangle = (| \alpha \rangle + i | \alpha' \rangle) / \sqrt{2}$. The problem thus reduces to the order-$N$ evaluation of $\langle \psi_i | G^\dagger | \psi_i \rangle$.

The Green’s function is obtained from an effective Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \Sigma_L + \Sigma_R$, which is non-Hermitian due to the presence of the left and right leads. This Hamiltonian can be written in tridiagonal form via a bi-orthogonal expansion similar to the Lanczos recursion method,

$$\psi_{n+1} = \mathcal{H} \psi_n - a_{n+1} \psi_n - b_n \psi_{n-1},$$

(156)

$$\langle \phi_{n+1} | = \langle \phi_n | \mathcal{H} - \langle \phi_n | a_{n+1} - \langle \phi_{n-1} | b_n, \langle \psi_n \rangle = \langle \phi_0 | \psi_0 \rangle,$$

(157)

with the initial conditions $| \psi_{-1} \rangle = | \phi_{-1} \rangle = 0$, and the bi-orthogonality condition $\langle \phi_n | \psi_m \rangle = 0$ if $n \neq m$. This last condition is equivalent to the following relations for $a_n$ and $b_n$:

$$a_{n+1} = \frac{\langle \psi_n | \mathcal{H} | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle},$$

(158)

$$b_n = \frac{\langle \psi_{n-1} | \mathcal{H} | \psi_n \rangle}{\langle \psi_{n-1} | \psi_n \rangle} = \frac{\langle \phi_n | \psi_n \rangle}{\langle \phi_{n-1} | \psi_{n-1} \rangle}.$$ (159)

In the basis $\{|\psi_n\rangle\}$, $\mathcal{H}$ can be written as

$$\mathcal{H} = \begin{pmatrix} a_1 & b_1 & & \\
1 & a_2 & b_2 & \\
& 1 & a_3 & b_3 & \\
& & & \ddots & \ddots \end{pmatrix}. \quad (160)$$

The quantity $\langle \psi | G^\dagger (z = E \pm i0^+) | \psi \rangle = \langle \phi_0 | \frac{1}{z - \mathcal{H}} | \psi_0 \rangle$ can then be computed by the continued fraction method. This quantity is equal to the first diagonal element of $(z - \mathcal{H})^{-1}$, where $\mathcal{H}$ is the tridiagonal matrix in Eq. (160). Let us call this matrix element $G_0(z)$ and define $G_n(z)$ to be the first diagonal element of the matrix $(z - \mathcal{H}_n)^{-1}$, with $\mathcal{H}_n$ the matrix $\mathcal{H}$ without its $n$ first lines and columns,

$$G_0(z) = \frac{1}{z - a_1 - b_1 G_1(z)}, \quad (162)$$

and repeating this algorithm leads to a continued fraction expansion of $G_0(z)$,

$$G_0(z) = \frac{1}{z - a_1 - \frac{b_1}{z - a_2 - \frac{b_2}{z - \ldots}}}. \quad (163)$$

However, one should note that in contrast with the standard Lanczos recursion, the coefficients $a_n$ and $b_n$ do not show any simple behavior for large $n$, but simple truncation of the continued fraction at sufficiently large $n$ was found to yield reasonably good convergence. This method was tested on carbon nanotube-based heterojunctions (Triozon and Roche, 2005), with perfect agreement with the decimation techniques.
Finally one mentions that Istas, Groth and Waintal have recently proposed an approach to cope with “mostly translationally invariant systems” (Istas et al., 2018), i.e., systems with weak disorder. With this method, systems of complex geometries are decomposed into two parts: one fully periodic part that is stitched with another part containing the disorder potential and electrodes. This approach becomes truly order-N, which opens promising perspective to study in particular quantum transport at surfaces of large systems, such as 3D topological insulators or Weyl semimetals.

VII. SUMMARY AND CONCLUSIONS

This paper has reviewed the development of linear-scaling numerical methods applied to quantum transport based on the Kubo-Greenwood and Kubo-Streda formalisms. These methods provide insight into the transport physics in the ballistic, diffusive, and localized regimes, as well as in topological regimes such as the quantum Hall effect.

The fundamental issue of computational cost versus numerical accuracy of various proposed numerical schemes has been addressed in detail, illustrating the capabilities and limitations of each. The usefulness of the time-propagation methods has been shown for the calculation of the dissipative conductivity, since it allows one to track the conduction regime in which the quantum conductivity is computed. This is actually critical for disordered systems since the onset of localization effects will reveal the downscaling behavior of the conductivity. Meanwhile, the implementations based on KPM-type of polynomial expansions become much more practical in the presence of topological gaps when compared with time-propagation methods, and allow for a faster convergence of the results. Finally, we have illustrated the applicability of such approaches to spin and valley Hall conductivities as well as to the time evolution of spin densities, while some references to the efforts to improve the scaling behavior of computational approaches for the Landauer–Büttiker conductance were also outlined.

Today, linear-scaling quantum transport methodologies stand as unique computational methodologies to explore many emerging and complex quantum transport phenomena in modern condensed matter physics, including disordered topological materials such as topological Anderson insulators (Groth et al., 2009; Li et al., 2009; Zhang et al., 2012), three-dimensional models of Dirac semimetals (Kobayashi et al., 2014; Louvet et al., 2018; Pixley et al., 2015; Young et al., 2012), and topological insulators (Araki et al., 2019; Chiu et al., 2016; Fu et al., 2007; Hasan and Kane, 2010; Kobayashi et al., 2014; Liao et al., 2015; Soriano et al., 2012), which all display nontrivial transport features difficult to fully tackle with perturbative approaches and simplified effective models.

We hope that interested readers will harness such enabling tools to investigate unexplored quantum transport phenomena in complex matter, and that the clarification of the capabilities of such methods, as well as their dissemination through various dedicated open sources, will also promote their use in machine learning strategies (Schleder et al., 2019), therefore taking part in the global efforts to bring materials simulation to its highest level of predictability.

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REFERENCES

Abrahams, E. P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan (1979), “Scaling Theory of Localization: Absence of Quantum Diffusion in Two Dimensions,” Phys. Rev. Lett. 42, 673–676.

Adjizian, Jean-Joseph, Aurélien Lherbier, Simon M.-M. Dubois, André Rafael Botello-Méndez, and Jean-Christophe Charlier (2016), “The electronic and transport properties of two-dimensional conjugated polymer networks including disorder,” Nanoscale 8, 1642–1651.

Akkermans, Eric, and Gilles Montambaux (2010), Meso-scopic Physics of Electrons and Photons (Cambridge University Press).

Alben, R. M. Blume, H. Krakauer, and L. Schwartz (1975), “Exact results for a three-dimensional alloy with site diagonal disorder: comparison with the coherent potential approximation,” Phys. Rev. B 12, 4090–4094.

Allen, P. B. (2006), “Electron transport,” in Conceptual Foundations of Materials, Volume 2: A Standard Model for Ground- and Excited-State Properties (Contemporary Con-
cepts of Condensed Matter Science), edited by S. Louie and M. Cohen, Chap. 6 (Elsevier Science) pp. 165–218.

Altschuler, BL, D. Khmel’nit’zkii, A.I. Larkin, and P.A. Lee (1980), “Magnetoresistance and hall effect in a disordered two-dimensional electron gas,” Phys. Rev. B 22, 5142–5153.

Anderson, P W (1958), “Absence of Diffusion in Certain Random Lattices,” Phys. Rev. 109, 1492–1505.

Anderson, P W, D. J. Thouless, E. Abrahams, and D. S. Fisher (1980), “New method for a scaling theory of localization,” Phys. Rev. B 22, 3519–3526.

Aoki, H, and T. Ando (1981), “Effect of localization on the hall conductivity in the two-dimensional system in strong magnetic fields,” Solid State Commun. 38, 1079 – 1082.

Aoki, Hideo (1985), “Aharonov-Bohm Effect for the Quantum Hall Conductivity on a Disordered Lattice,” Phys. Rev. Lett. 55, 1136–1139.

Araki, Hiromu, Tomonari Mizoguchi, and Yasuhiro Hatsugai (2019), “Phase diagram of a disordered higher-order topological insulator: A machine learning study,” Phys. Rev. B 99, 085406.

Arjmandi-Tash, Hadi, Dipankar Kalita, Zheng Han, Shan Jiang, Yu Huang, and Xiangfeng Duan (2010), “Graphene nanomesh,” Nat. Nanotechnol. 5, 190.

Baranger, Harold U, and A. Douglas Stone (1989), “Electrical linear-response theory in an arbitrary magnetic field: A new fermi-surface formation,” Phys. Rev. B 40, 8169–8193.

Baradonna, J H, J. Tworzydlo, P. W. Brouwer, and C. W. J. Beenakker (2007), “One-Parameter Scaling at the Dirac Point in Graphene,” Phys. Rev. Lett. 99, 106801.

Bardeen, J, L. N. Cooper, and J. R. Schrieffer (1957), “The theory of superconductivity,” Phys. Rev. 108, 1175–1204.

Barrios-Vargas, José Eduardo, Bohayra Mortazavi, Aron W. Cummings, Rafael Martinez-Gordillo, Miguel Pruneda, Luciano Colombo, Timon Rabczuk, and Stephan Roche (2017), “Electrical and Thermal Transport in Coplanar Polycrystalline GrapheneBN Heterostructures,” Nano Lett. 17, 1660–1664.

Bastin, A, C. Lewiner, O. Betheder-matibet, and P. Nozieres (1971), “Quantum oscillations of the hall effect of a fermion gas with random impurity scattering,” J. Phys. Chem. Solids 32, 1811–1824.

Beconcini, Michael, Fabio Taddei, and Marco Polini (2016), “Nonlocal topological valley transport at large valley hall angles,” Phys. Rev. B 94, 121408.

Beenakker, CWJ, and H. van Houten (1991), “Quantum Transport in Semiconductor Nanostructures,” in Semiconductor Heterostructures and Nanostructures, Solid State Physics, Vol. 44, edited by Heny Ehrenreich and David Turnbull (Academic Press) pp. 1 – 228.

Bellitz, D, and T. R. Kirkpatrick (1994), “The Anderson-Mott transition,” Rev. Mod. Phys. 66, 261–380.

Benítez, L Antonio, Juan F. Sierra, Williams Savero Torres, Aloís Arriighi, Frédéric Bonell, Marius V. Costache, and Sergio O. Valenzuela (2018), “Strongly anisotropic spin relaxation in graphene-transition metal dichalcogenide heterostructures at room temperature,” Nat. Phys. 14, 303–308.

van den Berg, T L, L. Raymond, and A. Verga (2011), “Dynamical spin hall conductivity in a magnetic disordered system,” Phys. Rev. B 84, 245210.

Biel, Blanca, François Triozon, X. Blase, and Stephan Roche (2009), “Effect of the Chemical Functionalization on Charge Transport in Carbon Nanotubes at the Mesoscopic Scale,” Nano Lett. 9, 2725–2729.

Boehnke, Lewin, Hartmut Hafermann, Michel Ferrero, Frank Lechermann, and Olivier Parcollet (2011), “Orthogonal polynomial representation of imaginary-time green’s functions,” Phys. Rev. B 84, 075145.

Bohr, D, P Schmitteckert, and P Wölfle (2006), “DMRG evaluation of the Kubo formula - Conductance of strongly interacting quantum systems,” EPL 73, 246–252.

Bordone, P, M. Pascoli, R. Brunetti, A. Bertoni, C. Jacoboni, and A. Abramov (1999), “Quantum transport of electrons in open nanostructures with the wigner-function formalism,” Phys. Rev. B 59, 3060–3069.

Bose, S K (1998), “Electronic structure and related properties of metallic glasses: Linear muffin-tin orbital approach,” Metall. Mater. Trans. A 29, 1853.

Bose, S K (1999), “Electronic structure of liquid mercury,” J. Phys. Condens. Matter 11, 4597–4615.

Bose, S K, O. Jepsen, and O. K. Andersen (1993), “Real-space calculation of the electrical resistivity of liquid 3d transition metals using tight-binding linear muffin-tin orbitals,” Phys. Rev. B 48, 4265–4275.

Bose, S K, O. Jepsen, and O. K. Andersen (1994), “An electronic structure and resistivity calculation for liquid La,” J. Phys. Condens. Matter 6, 2145–2158.

Boyd, J P (2001), Chebyshev and Fourier Spectral Methods: Second Revised Edition (Dover Books on Mathematics) (Dover Publications).

Brandbyge, Mads, José-Luis Mozos, Pablo Ordejón, Jeremy Taylor, and Kurt Stokbro (2002), “Density-functional method for nonequilibrium electron transport,” Phys. Rev. B 65, 165401.

Braun, A, and P. Schmitteckert (2014), “Numerical evaluation of green’s functions based on the chebyshev expansion,” Phys. Rev. B 90, 165112.

Büttiker, M., Y. Imry, R. Landauer, and S. Pinhas (1985), “Generalized many-channel conductance formula with application to small rings,” Phys. Rev. B 31, 6207–6215.

Caroli, C, R Combescot, P Nozieres, and D Saint-James (1971), “Direct calculation of the tunneling current,” J. Phys. C: Solid State Phys. 4, 916.

Castro Neto, A H, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim (2009), “The electronic properties of graphene,” Rev. Mod. Phys. 81, 109–162.

Sevinçli, H. W., L. N. Mingo, G. Cuniberti, and S. Roche (2011), “Effects of domains in phonon conduction through hybrid boron nitride and graphene sheets,” Phys. Rev. B 84, 205444.

Nikolić, Branislav K (2001), “Deconstructing kubo formula usage: Exact conductance of a mesoscopic system from weak to strong disorder limit,” Phys. Rev. B 64, 165303.
Chiu, Ching-Kai, Jeffrey C. Y. Teo, Andreas P. Schnyder, G. V., and A. Thellung (1961), “The Law of Wiedemann-Franz,” J. Chem. Phys. 128, 114713.

Chester, G. V., and A. Thellung (1959), “On the Electrical Conductivity of Metals,” Proc. Phys. Soc. 73, 745.

Chester, G. V., and A. Thellung (1961), “The Law of Wiedemann and Franz,” Proc. Phys. Soc. 77, 1005.

Chiu, Ching-Kai, Jeffrey C. Y. Teo, Andreas P. Schnyder, and Shinsei Ryu (2014), “Classification of topological quantum matter with symmetries,” Rev. Mod. Phys. 88, 035005.

Cirelli, S., S. Fratini, and D. Mayou (2011), “Transient localization in crystalline organic semiconductors,” Phys. Rev. B 83, 081202.

Covaci, L., F. M. Peeters, and M. Berciu (2010), “Efficient Numerical Approach to Inhomogeneous Superconductivity: The Chebyshev-Bogoliubov–de Gennes Method,” Phys. Rev. Lett. 105, 167006.

Crépieux, A., and P. Bruno (2001), “Theory of the anomalous Hall effect from the Kubo formula and the Dirac equation,” Phys. Rev. B 64, 014410.

Cresti, A. B. K., Nikiolić, J. H. García, and S. Roche (2016), “Charge, spin and valley Hall effects in disordered graphene,” Riv. Nuovo Cimento 39, 587.

Cresti, Alessandro, Norbert Nemec, Blanca Biel, Gabriel Niebler, François Troizon, Gianluca Cuniberti, and Stephan Roche (2008), “Charge transport in disordered graphene-based low dimensional materials,” Nano Res. 1, 361–394.

Cresti, Alessandro, Frank Ortmann, Thibaud Louvet, Dinh Van Tuan, and Stephan Roche (2013), “Broken Symmetries, Zero-Energy Modes, and Quantum Transport in Disordered Graphene: From Supermetallic to Insulating Regimes,” Phys. Rev. Lett. 110, 196601.

Cresti, Alessandro, Dinh Van Tuan, David Soriano, Aron W. Cummings, and Stephan Roche (2014), “Multiple Quantum Phases in Graphene with Enhanced Spin-Orbit Coupling: From the Quantum Spin Hall Regime to the Spin Hall Effect and a Robust Metallic State,” Phys. Rev. Lett. 113, 246603.

Cullum, J. K., and R. A. Willoughby (1985), Lanczos Algorithms for Large Symmetric Eigenvalue Computations (Birkhäuser).

Cummings, Aron W., Alessandro Cresti, and Stephan Roche (2014a), “Quantum Hall effect in polycrystalline graphene: The role of grain boundaries,” Phys. Rev. B 90, 164401.

Cummings, Aron W., Dinh Loc Duong, Van Luan Nguyen, Dinh Van Tuan, Jani Kotakoski, Jose Eduardo Barrios Vargas, Young Hee Lee, and Stephan Roche (2014b), “Charge Transport in Polycrystalline Graphene: Challenges and Opportunities,” Adv. Mater. 26, 5079–5094.

Cummings, Aron W., Jose H. Garcia, Jaroslav Fabian, and Stephan Roche (2017), “'Giant Spin Lifetime Anisotropy in Graphene Induced by Proximity Effects,'” Phys. Rev. Lett. 119, 206601.

Cummings, Aron W., and Stephan Roche (2016), “Effects of Dephasing on Spin Lifetime in Ballistic Spin-Orbit Materials,” Phys. Rev. Lett. 116, 086602.

Cysne, T. P., T. G. Rappoport, A. Ferreira, J. M. Viana Parente Lopes, and N. M. R. Peres (2016), “Numerical calculation of the Casimir-Polder interaction between a graphene sheet with vacancies and an atom,” Phys. Rev. B 94, 235405.

Dagotto, E. (1994), “Correlated electrons in high-temperature superconductors,” Rev. Mod. Phys. 66, 763–840.

Das Sarma, S., Shaffleque Adam, E. H. Hwang, and Enrico Rossi (2011), “Electronic transport in two-dimensional graphene,” Rev. Mod. Phys. 83, 407–470.

Dasgupta, Neil P., Jianwei Sun, Chong Liu, Sarah Brittman, Sean C. Andrews, Jongwoo Lim, Hanwei Gao, Ruoxue Yan, and Peidong Yang (2014), “25th Anniversary Article: Semiconductor Nanowires Synthesis, Characterization, and Applications,” Adv. Mater. 26, 2137–2184.

Datta, S. (1995), Electronic transport in mesoscopic systems (Cambridge University Press).

Di Ventra, M. (2008), Electrical transport in nanoscale systems (Cambridge University Press).

Doniach, S., and E. H. Sondheimer (1974), Greens Functions for Solid State Physicists (Addison-Wesley).

Drabold, D., and Otto F. Sankey (1993), “Maximum entropy approach for linear scaling in the electronic structure problem,” Phys. Rev. Lett. 70, 3631–3634.

Dugaev, V. K., P. Bruno, M. Taillefumier, B. Canals, and C. Lacroix (2005), “Anomalous Hall effect in a two-dimensional electron gas with spin-orbit interaction,” Phys. Rev. B 71, 224423.

D’yakonov, M. I., and V. I. Pervel’ (1971), “Spin Orientation of Electrons Associated with the Interband Absorption of Light in Semiconductors,” Zh. Eksp. Teor. Fiz. 60, 1954–1965.

Elliott, R. J. (1954), “Theory of the effect of spin-orbit coupling on magnetic resonance in some semiconductors,” Phys. Rev. 96, 266–270.

Eroms, J., and D. Weiss (2009), “Weak localization and transport gap in graphene antidot lattices,” New J. Phys. 11, 095021.

Fabian, F., A. Mataos-Abiague, C. Ertler, P. Stano, and I. Zutic (2007), “Semiconductor spintronics,” Acta Phys. Slovaca 57, 565.

Fal’ko, Vladimir I., K. Khechedzhi, E. McCann, B. L. Altshuler, H. Suzuura, and T. Ando (2007), “Weak localization in graphite,” Solid State Commun. 143, 33 – 38.

Fan, Z., A. Uppstu, and A. Harju (2015), “Electronic and transport properties in geometrically disordered graphene antidot lattices,” Phys. Rev. B 91, 125434.

Fan, Z., A. Uppstu, T. Siro, and A. Harju (2014a), “Efficient linear-scaling quantum transport calculations on graphics processing units and applications on electron transport in graphene,” Comput. Phys. Commun. 185, 28 – 39.

Fan, Zheyong, Andreas Uppstu, and Ari Harju (2014b), “Anderson localization in two-dimensional graphene with short-range disorder: One-parameter scaling and finite-size effects,” Phys. Rev. B 89, 245422.

Fan, Zheyong, Andreas Uppstu, and Ari Harju (2017), “Dominant source of disorder in graphene: charged impurities or ripples?” 2D Mater. 4, 025004.

Fan, Zheyong, Ville Vierimaa, and Ari Harju (2018), “GPUQT: An efficient linear-scaling quantum transport code fully implemented on graphics processing units,” Comput. Phys. Commun. 230, 113 – 120.

Fehske, Holger, Jens Schleede, Gerald Schubert, Gerhard Wellein, Vladimir S. Filinov, and Alan R. Bishop (2009),
“Numerical approaches to time evolution of complex quantum systems,” Phys. Lett. A 373, 2182 – 2188.

Feit, MD, J.A Fleck, and A Steiger (1982), “Solution of the Schrodinger equation by a spectral method,” J. Comp. Phys. 47, 412 – 433.

Ferrari, Andrea C, Francesco Bonaccorso, Vladimir Fal’ko, Konstantin S. Novoselov, Stephan Roche, Peter Boggild, Stefano Borini, Frank H. L. Koppens, Vincenzo Palermo, Nicola Pugno, José A. Garrido, Roman Sordan, Alberto Blanco, Laura Ballerini, Maurizio Prato, Elefterios Lidorikis, Jani Kivioja, Claudio Marinelli, Tapani Rychänen, Alberto Morpurgo, Jonathan N. Coleman, Valeria Nicolosi, Luigi Colombo, Albert Fert, Mar García-Hernández, Adrian Bachtold, Grégory F. Schneider, Francisco Guinea, Ces Decker, Matteo Barbone, Zhipei Sun, Costas Galiotis, Alexander N. Grigorenko, Gerasimos Konstantatos, Andras Kis, Mikhail Katsnelson, Lieven Vandersypen, Annick Loiseau, Vittorio Morandi, Daniel Neumaier, Emanuele Treossi, Vittorio Pellegrini, Marco Polini, Alessandro Tredicucci, Gareth M. Williams, Byung Hee Hong, Jong-Hyun Ahn, Jung Min Kim, Herbert Zirath, Bart J. van Wees, Herre van der Zant, Luigi Occhipinti, Andrea Di Matteo, Ian A. Kinloch, Thomas Seyller, Etienne Quezel, Xinliang Feng, Ken Teo, Nalin Rupesinghe, Perti Hakonen, Simon R. T. Neil, Quentin Tannock, Tomas Löfwander, and Jari Kinaret (2015), “Science and technology roadmap for graphene, related two-dimensional crystals, and hybrid systems,” Nanoscale 7, 4598–4810.

Ferreira, Aires, and Eduardo R. Mucciolo (2015), “Critical Delocalization of Chiral Zero Energy Modes in Graphene,” Phys. Rev. Lett. 115, 106601.

Ferreira, Aires, J. Viana-Gomes, Johan Nilsson, E. R. Mucciolo, N. M. R. Peres, and A. H. Castro Neto (2011), “Unified description of the dc conductivity of monolayer and bilayer graphene at finite densities based on resonant scatterers,” Phys. Rev. B 83, 165402.

Ferry, D K, and S. M. Goodnick (1997), Transport in nanosstructures (Cambridge University Press).

Frank, Stefan, Philippe Poncharal, Z. L. Wang, and Walt A. de Heer (1998), “Carbon Nanotube Quantum Resistors,” Science 280, 1744–1746.

Fratini, S, S. Ciuchi, D. Mayou, G. Trambly de Laissardi`ere, and A. Troisi (2017), “A map of high-mobility molecular semiconductors,” Nat. Mater. 16, 908, article.

Frederiksen, Thomas, Magnus Paulsson, Mads Brandbyge, and Antti-Pekka Jauho (2007), “Inelastic transport theory from first principles: Methodology and application to nanoscale devices,” Phys. Rev. B 75, 205413.

Fu, Liang, C. L. Kane, and E. J. Mele (2007), “Topological insulators in three dimensions,” Phys. Rev. Lett. 98, 106803.

Fujita, T, M. B. A. Jalil, S. G. Tan, and S. Murakami (2011), “Gauge fields in spintronics,” J. Appl. Phys. 110, 121301.

Gade, Renate (1993), “Anderson localization for sublattice models,” Nucl. Phys. B 398, 499 – 515.

Gade, Renate, and Franz Wegner (1991), “The n = 0 replica limit of u(n) and u(n)so(n) models,” Nucl. Phys. B 360, 213 – 218.

Ganahl, Martin, Patrik Thunström, Frank Verstraete, Karsten Held, and Hans Gerd Evertz (2014), “Chebyshev expansion for impurity models using matrix product states,” Phys. Rev. B 90, 045144.

García, Jose H, Lucian Covaci, and Tatiana G. Rappoport (2015), “Real-Space Calculation of the Conductivity Tensor for Disordered Topological Matter,” Phys. Rev. Lett. 114, 116602.

García, Jose H, Aron W. Cummings, and Stephan Roche (2017), “Spin hall effect and weak antilocalization in graphene/transition metal dichalcogenide heterostructures,” Nano Lett. 17, 5078–5083.

García, Jose H, and Tatiana G Rappoport (2016), “Kubo-Bastin approach for the spin Hall conductivity of decorated graphene,” 2D Mater. 3, 024007.

García, Jose H, Marc Vila, Aron W Cummings, and Stephan Roche (2018), “Spin transport in graphene/transition metal dichalcogenide heterostructures,” Chem. Soc. Rev. 47, 3359–3379.

Gargiulo, Fernando, Gabriel Autès, Naumidh Virk, Stefan Barthel, Malte Rössner, Lisa R. M. Toller, Tim O. Wehling, and Oleg V. Yazyev (2014), “Electronic transport in graphene with aggregated hydrogen adatoms,” Phys. Rev. Lett. 113, 246601.

Geim, A K, and I. V. Grigorieva (2013), “Van der Waals heterostructures,” Nature 499, 419.

Gershenson, M E V Podzorov, and A. F. Morpurgo (2006), “Colloqium: Electronic transport in single-crystal organic transistors,” Rev. Mod. Phys. 78, 973–989.

Ghiasi, Taliel S, Josep Ingl` a-Ayn` es, Alexey A. Kaverzin, and Bart J. van Wees (2017), “Large Proximity-Induced Spin Lifetime Anisotropy in Transition-Metal Dichalcogenide/Graphene Heterostructures,” Nano Lett. 17, 7528–7532.

Giesbers, A J M E. C. Peters, M. Burghard, and K. Kern (2012), “Charge transport gap in graphene antidot lattices,” Phys. Rev. B 86, 054454.

Girlando, Alberto, Luca Grisanti, Matteo Masino, Ivano Bilotti, Aldo Brillante, Raffaele G. della Valle, and Elisabetta Venuti (2010), “Peierls and Holstein carrier-phonon coupling in crystalline rubrene,” Phys. Rev. B 82, 035208.

Giustino, Feliciano (2017), “Electron-phonon interactions from first principles,” Rev. Mod. Phys. 89, 015003.

Gorbachev, R V, J. C. W. Song, G. L. Yu, A. V. Kretinin, F. Withers, Y. Cao, A. Mishchenko, I. V. Grigorieva, K. S. Novoselov, L. S. Levitov, and A. K. Geim (2014), “Detecting topological currents in graphene superlattices,” Science 346, 448–451.

Gor’kov, LP, A.I. Larkin, and D.E. Khmel’nitskii (1979), “Particle conductivity in a two-dimensional random potential,” JETP Lett. 30, 228.

Gradishney, I S, and I. M. Ryzhik (1975), Table of Integrals, Series, and Products, 7th Edition (Elsevier, Academic Press).

Greenwood, D A (1958), “The Boltzmann Equation in the Theory of Electrical Conduction in Metals,” Proc. Phys. Soc. 71, 585.

Gregersen, Sren Schou, Jose H García, Antti-Pekka Jauho, Stephan Roche, and Stephen R Power (2018), “Charge and spin transport anisotropy in nanopatterned graphene,” J. Phys. Mater. 1, 015005.

Gridnev, V N (2001), “Theory of Faraday rotation beats in crystalline rubrene,” J. Phys. B 34, 121301.

Gusarov, L, J. V. Vorontsov, and Xavier Waintal (2014), “Kwant: a software package for quantum transport,” New J. Phys. 16(6), 063065.
Guinea, F., M. I. Katsnelson, and A. K. Geim (2010), “Energy gaps and a zero-field quantum Hall effect in graphene by strain engineering,” *Nat. Phys.*, 6, 30–33.

Gunst, Tue, Troels Markussen, Mattias L. N. Palsgaard, Kurt Stokbro, and Mads Brandbyge (2017), “First-principles electron transport with phonon coupling: Large scale at low cost,” *Phys. Rev. B* 96, 161404.

Haldane, F DM (2004), “Berry curvature on the fermi surface: Anomalous hall effect as a topological fermi-liquid property,” *Physical Review Letters* 93 (20), 206602.

Hans, Anthony, and Hans De Raedt (2000), “Fast algorithm for finding the eigenvalue distribution of very large matrices,” *Phys. Rev. E* 62, 4365–4377.

Hannewald, K., and P. A. Bobbert (2004), “Anisotropy effects in phonon-assisted charge-carrier transport in organic molecular crystals,” *Phys. Rev. B* 69, 075212.

Harrison, Walter A (1989), *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond* (Dover Publications).

Hasan, M Z, and C. L. Kane (2010), “Colloquium: Topological insulators,” *Rev. Mod. Phys.* 82, 3045–3067.

Haug, Hartmut, and Antti-Pekka Jauho (1996), *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer-Verlag).

Haydock, R, V Heine, and M J Kelly (1972), “Electronic structure based on the local atomic environment for tight-binding bands,” *J. Phys. C: Solid State Phys.* 5, 2845.

Haydock, R, V Heine, and M J Kelly (1975), “Electronic structure based on the local atomic environment for tight-binding bands. II.” *J. Phys. C: Solid State Phys.* 8, 2591.

Ishii, Hiroyuki, Keisuke Honma, Nobuhiko Kobayashi, and Kenji Hirose (2010b), “Inelastic Transport in Vibrating Disordered Carbon Nanotubes: Scattering Times and Temperature-Dependent Decoherence Effects,” *Phys. Rev. Lett.* 104, 116801.

Ishii, Hiroyuki, François Triozon, Nobuhiko Kobayashi, Kenji Hirose, and Stephan Roche (2009), “Charge transport in carbon nanotubes based materials: a Kubo-Greenwood computational approach,” *Compt. Rendus Phys.* 10, 283–296.

Istas, Mathieu, Christoph Groth, and Xavier Waintal (2018), “A general algorithm for computing bound states in infinite tight-binding systems,” *SciPost Phys.* 4, 026.

Jones, R O (2015), “Density functional theory: Its origins, rise to prominence, and future,” *Rev. Mod. Phys.* 87, 897–923.

Kadanoff, L P, and G. Baym (1962), *Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Nonequilibrium Problems* (Benjamin, New York).

Kane, C L, and E J Mele (2005), “Quantum Spin Hall Effect in graphene,” *Phys. Rev. Lett.* 95 (22), 226801.

Kenji Hirose (2010b), “Inelastic Transport in Vibrating Disordered Carbon Nanotubes: Scattering Times and Temperature-Dependent Decoherence Effects,” *Phys. Rev. Lett.* 104, 116801.

Knoch, R, J M. Toberer (2008), “Order-N electron transport calculations from ballistic to diffusive regimes by a time-dependent wave-packet diffusion method: Application to transport properties of carbon nanotubes,” *Phys. Rev. B* 82, 085435.

Kohn, W, and L. J. Sham (1965), “Self-Consistent Equations Involving Exchange and Correlation Effects,” *Phys. Rev.* 140, A1133–A1138.

Kramer, B., and A MacKinnon (1993), “Localization: theory and experiment,” *Rep. Prog. Phys.* 56, 1469.
Laird, Edward A, Ferdinand Kuemmeth, Gary A. Steele, Kubo, Ryogo (1957), “Statistical-Mechanical Theory of Inverse Processes. I. General Theory and Simple Applications to Magnetic and Conduction Problems,” J. Phys. Soc. Jpn. 12, 570–586.

Landauer, Rolf (1970), “Electrical resistance of disordered one-dimensional lattices,” Phil. Mag. 21, 863–867.

Langer, J S (1962), “Evaluation of Kubo’s formula for the irreversible Processes. I. General Theory and Simple Applications to Magnetic and Conduction Problems,” J. Phys. Soc. Jpn. 12, 570–586.

Lanczos, C (1950), “An iteration method for the solution of the eigenvalue problem of linear differential and integral operators,” J. Res. Natl. Bur. Stand. 45, 255–282.

Landauer, R (1957), “Spatial Variation of Currents and Fields Due to Localized Scatterers in Metallic Conduction,” IBM J. Res. Dev. 1, 223–231.

Landauer, Rolf (1970), “Electrical resistance of disordered one-dimensional lattices,” Phil. Mag. 21, 863–867.

Langer, J S (1962), “Evaluation of Kubo’s formula for the impurity resistance of an interacting electron gas,” Phys. Rev. 127, 5–16.

Latil, Sylvain, Stephan Roche, Didier Mayou, and Jean-Christophe Charlier (2004), “Mesoscopic Transport in Chemically Doped Carbon Nanotubes,” Phys. Rev. Lett. 92, 256805.

Leconte, N. A, Lherbier, F. Varchon, P. Ordejon, S. Roche, and J.-C. Charlier (2011), “Quantum transport in chemically modified two-dimensional graphene: From minimal conductivity to Anderson localization,” Phys. Rev. B 84, 235420.

Lee, Patrick A, and T. V. Ramakrishnan (1985), “Disordered electronic systems,” Rev. Mod. Phys. 57, 287–337.

Leforestier, C, R H Bisseling, C Cerjan, M.D Feit, R Friesner, A Guldberg, A Hammerich, G Jolicard, W Karrlein, H-D Meyer, N Lipkin, O Roncero, and R Kosloff (1991), “A comparison of different propagation schemes for the time dependent Schrödinger equation,” J. Comp. Phys. 94, 59 – 80.

Levy, N, S. A. Burke, K. L. Meaker, M. Panlasigui, A. Zettl, F. Guinea, A. H. C. Neto, and M. F. Crommie (2010), “Strain-Induced Pseudo-Magnetic Fields Greater Than 300 Tesla in Graphene Nanobubbles,” Science 329, 544–547.

Lewenkopf, C H, E. R. Mucciolo, and A. H. Castro Neto (2008), “Numerical studies of conductivity and Fano factor in disordered graphene,” Phys. Rev. B 77, 081410.

Lewenkopf, Caio H., and Eduardo R. Mucciolo (2013), “The recursive Green’s function method for graphene,” J. Comput. Electron. 12, 203–231.

Lherbier, Aurélien, Blanca Biel, Yann-Michel Niquet, and Stephan Roche (2008a), “Transport Length Scales in Disordered Graphene-Based Materials: Strong Localization Regimes and Dimensionality Effects,” Phys. Rev. Lett. 100, 036803.

Lherbier, Aurélien, X. Blase, Yann-Michel Niquet, François Troizon, and Stephan Roche (2008b), “Charge Transport in Chemically Doped 2D Graphene,” Phys. Rev. Lett. 101, 036808.

Lherbier, Aurélien, Andrés Rafael Botello-Méndez, and Jean-Christophe Charlier (2013), “Electronic and Transport Properties of Unbalanced Sublattice N-Doping in Graphene,” Nano Lett. 13, 1446–1450.

Lherbier, Aurélien, Simon M.-M. Dubois, Xavier Declerck, Yann-Michel Niquet, Stephan Roche, and Jean-Christophe Charlier (2012), “Transport properties of graphene containing structural defects,” Phys. Rev. B 86, 075402.

Lherbier, Aurélien, Simon M.-M. Dubois, Xavier Declerck, Stephan Roche, Yann-Michel Niquet, and Jean-Christophe Charlier (2011), “Two-dimensional graphene with structural defects: Elastic mean free path, minimum conductivity, and Anderson transition,” Phys. Rev. Lett. 106, 046803.

Liu, Jian, Rui-Lin Chu, J. K. Jain, and Shun-Qing Shen (2009), “Topological anderson insulator,” Phys. Rev. Lett. 102, 136806.

Liu, Yi, Xin, Akihiro Funakoshi, Naoki Ogawa, Satoshi Kera, Nobuo Ueno, and Hisao Ishii (2010), “Highest-Occupied-Molecular-Orbital Band Dispersion of Rubrene Single Crystals as Observed by Angle-Resolved Ultraviolet Pho-
toelectron Spectroscopy,” Phys. Rev. Lett. 104, 156401.
MacKinnon, A., and B. Kramer (1981), “One-Parameter Scaling of Localization Length and Conductance in Disordered Systems,” Phys. Rev. Lett. 47, 1546–1549.
Mahan, Gerald D (2000), Many-Particle Physics (Plenum Press).
Marconcini, Paolo, Alessandro Cresti, François Tpiozon, Gianluca Fiori, Blanca Biel, Yann-Michel Niquet, Massimo Macucci, and Stephan Roche (2012), “Atomicistic Boron-Doped Graphene Field-Effect Transistors: A Route toward Unipolar Characteristics,” ACS Nano 6, 7942–7947.
Markos, P., and L Schweitzer (2006), “Critical regime of two-dimensional Ando model: relation between critical conductance and fractal dimension of electronic eigenstates,” J. Phys. A 39, 3221.
Markussen, Troels, Mattias Palsgaard, Danièle Stradi, Tue Gunst, Mads Brandbyge, and Kurt Stokbro (2017), “Electron-phonon scattering from Green’s function transport combined with molecular dynamics: Applications to mobility predictions,” Phys. Rev. B 95, 245210.
Markussen, Troels, Riccardo Rulari, Mads Brandbyge, and Antti-Pekka Jauho (2006), “Electronic transport through Si nanowires: Role of bulk and surface disorder,” Phys. Rev. B 74, 245313.
Marmolejo-Tejada, J. M., J H García, M D Petrović, P-H Chang, X-L Sheng, A Cresti, P Plechac, S Roche, and B K Nikolić (2018), “Deciphering the origin of nonlocal resistance in multiterminal graphene on hexagonal-boron-nitride with ab initio quantum transport: Fermi surface edge currents rather than fermi sea topological valley currents,” J. Phys. Mater. 1, 015006.
Mayou, D. (1988), “Calculation of the Conductivity in the Short-Mean-Free-Path Regime,” EPL 6, 549.
Mayou, D., and S. Khanna (1995), “A Real-Space Approach to Electronic Transport,” J. Phys. I 5, 1199–1211.
McCann, E K, Kechedzhi, Vladimir I. Fal’ko, H Suzuura, T. Ando, and B L Altshuler (2006), “Weak-Localization Magnetoconductance and Valley Symmetry in Graphene,” Phys. Rev. Lett. 97, 146805.
Meyer, Jannik C, C. Kisielowski, R. Erni, Marta D. Rossell, M. F. Crommie, and A. Zettl (2008), “Direct Imaging of Lattice Atoms and Topological Defects in Graphene Membranes,” Nano Lett. 8, 3582–3586.
Milletari, Mirco, Manuel Offidani, Aires Ferreira, and Roberto Raimondi (2017), “Covariant conservation laws and spin Hall effect in the Dirac-Rashba model,” Phys. Rev. Lett. 119, 246801.
Mishchenko, E G, A. V. Shytov, and B. I. Halperin (2004), “Spin current and polarization in impure two-dimensional electron systems with spin-orbit coupling,” Phys. Rev. Lett. 93, 226602.
Missous, Ahmed, Jouda Jemaa Khabthani, Nejm-Eddine Jaidane, Didier Mayou, and Guy Trambly de Laissardière (2018), “Mobility gap and quantum transport in a functionalized graphene bilayer,” J. Phys. Condens. Matter 30, 195701.
Muccioni, E R, and C H Lewenkopf (2010), “Disorder and electronic transport in graphene,” J. Phys. Condens. Matter 22, 273201.
Nakaharaï, Shinichi Ogawa, Shingo Suzuki, Song-Lin Li, Kazuhito Tsukagoshi, Shintaro Sato, and Naoki Yokoyama (2013), “Conduction Tuning of Graphene Based on Defect-Induced Localization,” ACS Nano 7, 5694–5700.
Nakajima, Sadao (1958), “On Quantum Theory of Transport Phenomena,” Prog. Theor. Phys. 20, 948–959.
Nedjalkov, M, H. Kosina, S. Selberherr, C. Ringhofer, and D. K. Ferry (2004), “Unified particle approach to wigner-boltzmann transport in small semiconductor devices,” Phys. Rev. B 70, 115319.
Nomura, Kentaro, Mikito Koshino, and Shinsei Ryu (2007), “Topological Delocalization of Two-Dimensional Massless Dirac Fermions,” Phys. Rev. Lett. 99, 146806.
Novoselov, K. S. A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov (2005a), “Two-dimensional gas of massless Dirac fermions in graphene,” Nature 438, 197–200.
Novoselov, K S., A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov (2004), “Electric Field Effect in Atomically Thin Carbon Films,” Science 306, 666–669.
Novoselov, K. S., D. Jiang, F. Schedin, T. J. Booth, V. V. Khotkevich, S. V. Morozov, and A. K. Geim (2005b), “Two-dimensional atomic crystals,” Proc. Natl. Acad. Sci. U.S.A. 102, 10451–10453.
Novoselov, K S., A. Mishchenko, A. Carvalho, and A. H. Castro Neto (2016), “2D materials and van der Waals heterostructures,” Science 353, aac9439.
Offidani, Manuel, and Aires Ferreira (2018), “Microscopic theory of spin relaxation anisotropy in graphene with proximity-induced spin-orbit coupling,” Phys. Rev. B 98, 245408.
Ordejón, P., D. Boskovic, M. Panhans, and F. Ortmann (2017), “Ab initio study of electron-phonon coupling in rubrene,” Phys. Rev. B 96, 035202.
Ortmann, Frank, Friedhelm Bechstedt, and Karsten Hannewald (2009), “Theory of charge transport in organic crystals: Beyond Holstein’s small-polaron model,” Phys. Rev. B 79, 235206.
Ortmann, Frank, Alessandro Cresti, Gilles Montambaux, and Stephan Roche (2011), “Magnetoconductance in disordered graphene: The role of pseudospin and dimensionality effects unraveled,” EPL 94, 47006.
Ortmann, Frank, Nicolas Leconte, and Stephan Roche (2015), “Efficient linear scaling approach for computing the Kubo Hall conductivity,” Phys. Rev. B 91, 165117.
Ortmann, Frank, and Stephan Roche (2011), “Polaron transport in organic crystals: Temperature tuning of disorder effects,” Phys. Rev. B 84, 180302.
Ortmann, Frank, and Stephan Roche (2013), “Splitting of the Zero-Energy Landau Level and Universal Dissipative Conductivity at Critical Points in Disordered Graphene,” Phys. Rev. Lett. 110, 086602.
Ostrovsky, P M, I. V. Gornyi, and A. D. Mirlin (2006), “Electron transport in disordered graphene,” Phys. Rev. B 74, 235443.
Ostrovsky, P M, I. V. Gornyi, and A. D. Mirlin (2007), “Quantum criticality and minimal conductivity in graphene with long-range disorder,” Phys. Rev. Lett. 98, 256801.
Ostrovsky, P M., M. Titov, S. Bera, I. V. Gornyi, and A. D. Mirlin (2010), “Diffusion and Criticality in Undoped Graphene with Resonant Scatterers,” Phys. Rev. Lett. 105, 266803.
Park, Ji-Yong, Sami Rosenblatt, Yuval Yaish, Vera Sazonova, Hande stnel, Stephan Braig, T. A. Arias, Piet W. Brouwer, and Paul L. McEnen (2004), “Electron-Phonon Scattering in Metallic Single-Walled Carbon Nanotubes,” Nano Lett. 4, 517–520.
Pedersen, Jesper Goor, Aron W. Cummings, and Stephan Roche (2014), “Anisotropic behavior of quantum transport in graphene superlattices: Coexistence of ballistic conduction with Anderson insulating regime,” Phys. Rev. B 89, 165401.

Pedersen, Thomas G, Christian Flindt, Jesper Pedersen, Niels Asger Mortensen, Anti-Pekka Jauho, and Kjeld Pedersen (2008), “Graphene Antidot Lattices: Designed Defects and Spin Qubits,” Phys. Rev. Lett. 100, 136804.

Pereira, Vitor M, J. M. B. Lopes dos Santos, and A. H. Castro Neto (2008), “Modeling disorder in graphene,” Phys. Rev. B 77, 115109.

Peres, N M R (2009), “The transport properties of graphene,” J. Phys. Condens. Matter 21, 323201.

Peres, N M R (2010), “Colloquium: The transport properties of graphene: An introduction,” Rev. Mod. Phys. 82, 2673–2700.

Persson, Martin P, Aurélien Lherbier, Yann-Michel Niquet, François Trizion, and Stephan Roche (2008), “Orientational Dependence of Charge Transport in Disordered Silicon Nanowires,” Nano Lett. 8, 4146–4150.

Petitfor, DG, and D.L. Weaire (1985), Recursion Method and its Applications (Springer Series in Solid States Sciences, Vol. 58) (Springer Verlag, Berlin).

Pines, D, and P. Nozieres (1969), The Theory of Quantum Liquids (Addison-Wesley, California).

Pixley, J H, Yang-Zhi Chou, Pallab Goswami, David A. Huse, Rahul Nandkishore, Leo Radzihovsky, and S. Das Sarma (2017), “Single-particle excitations in disordered weyl fluids,” Phys. Rev. B 95, 235101.

Pixley, J H, Pallab Goswami, and S. Das Sarma (2015), “Anderson localization and the quantum phase diagram of three dimensional disordered dirac semimetals,” Phys. Rev. Lett. 115, 076601.

Pixley, J H, Pallab Goswami, and S. Das Sarma (2016), “Disorder-driven itinerant quantum criticality of three-dimensional massless dirac fermions,” Phys. Rev. B 93, 085103.

Pixley, J H, Justin H. Wilson, David A. Huse, and Sarang Gopalakrishnan (2018), “Weyl semimetal to metal phase transitions driven by quasiperiodic potentials,” Phys. Rev. Lett. 120, 207604.

Podzorov, V, E. Menard, A. Borisov, V. Kryukhlin, J. A. Rogers, and M. E. Gershenson (2004), “Intrinsic Charge Transport on the Surface of Organic Semiconductors,” Phys. Rev. Lett. 93, 086602.

Porezag, D, Th. Frauenheim, Th. Köhler, G. Seifert, and R. Kaschner (1995), “Construction of tight-binding-like potentials on the basis of density-functional theory: Application to carbon,” Phys. Rev. B 51, 12947–12957.

Power, Stephen R, and Antti-Pekka Jauho (2014), “Electronic transport in disordered graphene antidot lattice devices,” Phys. Rev. B 90, 115408.

Radchenko, T M, A. A. Shylau, and I. V. Zozoulenko (2012), “Influence of correlated impurities on conductivity of graphene sheets: Time-dependent real-space Kubo approach,” Phys. Rev. B 86, 035418.

Radchenko, T M, A. A. Shylau, I. V. Zozoulenko, and Aires Ferreira (2013), “Effect of charged line defects on conductivity in graphene: Numerical Kubo and analytical Boltzmann approaches,” Phys. Rev. B 87, 195448.

Raes, Bart, Jeroen E. Scheerder, Marius V. Costache, Frédéric Bonell, Juan F. Sierra, Jo Cuppens, Joris Van de Vondel, and Sergio O. Valenzuela (2016), “Determination of the spin-lifetime anisotropy in graphene using oblique spin precession,” Nat. Commun. 7, 11444.

Rammer, J, and H. Smith (1986), “Quantum field-theoretical methods in transport theory of metals,” Rev. Mod. Phys. 58, 323–359.

Rammer, Jorgen (2007), Quantum Field Theory of Nonequilibrium States (Cambridge University Press, Cambridge).

Rhyner, Reto, and Mathieu Luisier (2014), “Atomistic modeling of coupled electron-phonon transport in nanowire transistors,” Phys. Rev. B 89, 235311.

Roche, S (1999), “Quantum transport by means of O(N) real-space methods,” Phys. Rev. B 59, 2284–2291.

Roche, S, G. Trambly de Laissardiére, and D. Mayou (1997), “Electronic transport properties of quasicrystals,” J. Math. Phys. 38, 1794–1822.

Roche, S, and D. Mayou (1997), “Conductivity of Quasiperiodic Systems: A Numerical Study,” Phys. Rev. Lett. 79, 2518–2521.

Roche, Stephan, Jie Jiang, Luis E Foa Torres, and Riichiro Saito (2007), “Charge transport in carbon nanotubes: quantum effects of electron-phonon coupling,” J. Phys. Condens. Matter 19, 183203.

Roche, Stephan, Jie Jiang, François Trizion, and Riichiro Saito (2005a), “Conductance and coherence lengths in disordered carbon nanotubes: Role of lattice defects and phonon vibrations,” Phys. Rev. B 72, 113410.

Roche, Stephan, Jie Jiang, François Trizion, and Riichiro Saito (2005b), “Quantum Dephasing in Carbon Nanotubes due to Electron-Phonon Coupling,” Phys. Rev. Lett. 95, 076803.

Roche, Stephan, Nicolas Leconte, Frank Ortman, Aurélien Lherbier, David Soriano, and Jean-Christophe Charlier (2012), “Quantum transport in disordered graphene: A theoretical perspective,” Solid State Commun. 152, 1404 – 1410.

Roche, Stephan, and Riichiro Saito (2001), “Magnetoresistance of Carbon Nanotubes: From Molecular to Mesoscopic Fingerprints,” Phys. Rev. Lett. 87, 246803.

Roche, Stephan, François Trizion, Angel Rubio, and Didier Mayou (2001), “Conduction mechanisms and magnetotransport in multiwalled carbon nanotubes,” Phys. Rev. B 64, 121401.

Rurali, Riccardo (2010), “Colloquium: Structural, electronic, and transport properties of silicon nanowires,” Rev. Mod. Phys. 82, 427–449.

Ryczek, A, J. Tworzydlo, and C. W. J. Beenakker (2007), “Anomalously large conductance fluctuations in weakly disordered graphene,” EPL 79, 57003.

Saad, Y (2003), Iterative Methods for Sparse Linear Systems (Society for Industrial and Applied Mathematics).

Safaeer, C K, Josep Inglada-Aynés, Franz Herling, José H. García, Marc Vila, Nerea Ontoso, M. Reyes Calvo, Stephan Roche, Luis E. Hueso, and Flix Casanova (2019), “Room-temperature spin hall effect in graphene/mos2 van der waals heterostructures,” Nano Lett. 19, 1074–1082.

Sakurai, J J, and Jim Napolitano (2017), Modern Quantum Mechanics, 2nd ed. (Cambridge University Press).

Sanco, M P Lopez, J M Lopez Sancho, J M I Sancho, and J Rubio (1985), “Highly convergent schemes for the calculation of bulk and surface Green functions,” J. Phys. F 15, 851.

Santos, Tatiane P, Leandro R.F. Lima, and Caio H. Lewenkopf (2019), “An order n numerical method to effi-
ciently calculate the transport properties of large systems: An algorithm optimized for sparse linear solvers,” Journal of Computational Physics 394, 440 – 455.

Schleder, Gabriel R, Antonio C M Padilha, Carlos Mera Acosta, Marcio Costa, and Adalberto Fazzio (2019), “From DFT to machine learning: recent approaches to materials science—a review,” J. Phys. Mater. 2, 032001.

Schleede, J. G. Schubert, and H. Fehske (2010), “Comment on Anderson transition in disordered graphene by Amini M. et al.” EPL 90, 17002.

Seifert, Max, Jose E B Vargas, Marco Bobinger, Matthias Sachsenhauser, Aron W Cummings, Stephan Roche, and Jose A Garrido (2015), “Role of grain boundaries in tailoring electronic properties of polycrystalline graphene by chemical functionalization,” 2D Mater. 2, 024008.

Settnes, Mikkel, Jose H Garcia, and Stephan Roche (2017), “Valley-polarized quantum transport generated by gauge fields in graphene,” 2D Mater. 4, 031006.

Shechtman, D. I. Blech, D. Gratias, and J. W. Cahn (1984), “Metallic Phase with Long-Range Orientational Order and No Translational Symmetry,” Phys. Rev. Lett. 53, 1951–1953.

Shon, NguyenHong, and Tsuneyu Ando (1998), “Quantum Transport in Two-Dimensional Graphite System,” J. Phys. Soc. Jpn. 67, 2421–2429.

Silver, R N, and H Röder (1994), “Densities of States of Mega-Dimensional Hamiltonian Matrices,” Int. J. Mod. Phys. C 05, 735–753.

Silver, R N, and H. Röder (1997), “Calculation of densities of states and spectral functions by Chebyshev recursion and maximum entropy,” Phys. Rev. E 56, 4822–4829.

Silver, RN, H. Roeder, A.F. Votier, and J.D. Kress (1996). “Kernel Polynomial Approximations for Densities of States and Spectral Functions,” J. Comp. Phys. 124, 115 – 130.

Sinitsyn, N A, J. E. Hill, Hongki Min, Jairo Sinova, and A. H. MacDonald (2006), “Charge and spin hall conductivity in metallic graphene,” Phys. Rev. Lett. 97, 1–4.

Sinova, Jairo, Sergio O. Valenzuela, J. Wunderlich, C. H. Back, and T. Jungwirth (2015), “Spin hall effects,” Rev. Mod. Phys. 87, 1213–1260.

Skilling, J (1989), “The eigenvalues of mega-dimensional matrices,” in Maximum Entropy and Bayesian Methods (An International Book Series on The Fundamental Theories of Physics: Their Clarification, Development and Application), edited by J. Skilling (Springer, Dordrecht) pp. 455–466.

Song, Justin C W, Polnip Samutpraphoot, and Leonid S. Levitov (2015), “Topological bloch bands in graphene superlattices,” Proc. Natl. Acad. Sci. U.S.A. 112, 10879–10883.

Soriano, David, Frank Ortmann, and Stephan Roche (2012), “Three-dimensional models of topological insulators: Engineering of dirac cones and robustness of the spin texture,” Phys. Rev. Lett. 109, 266805.

Soriano, David, Dinh Van Tuan, Simon M-M Dubois, Martin Gmitra, Aron W Cummings, Denis Kochan, Frank Ortmann, Jean-Christophe Charlier, Jaroslav Fabian, and Stephan Roche (2015), “Spin transport in hydrogenated graphene,” 2D Mater. 2, 022002.

Stone, S Douglas, and Aaron Szafer (1988), “What is Measured when You Measure a Resistance? – The Landauer Formula Revisited,” IBM J. Res. Dev. 32 (3), 384–413.

Streda, P (1982), “Theory of quantised Hall conductivity in two dimensions,” J. Phys. C: Solid State Phys. 15, L717–L721.

Sundar, Vikram C, Jana Zauamseil, Vitaly Podzorov, Etienne Menard, Robert L. Willett, Takao Someya, Michael E. Gershenson, and John A. Rogers (2004), “Elastomeric Transistor Stamps: Reversible Probing of Charge Transport in Organic Crystals,” Science 303, 1644–1646.

Tal-Ezer, H, and R. Kosloff (1984), “An accurate and efficient scheme for propagating the time dependent Schrödinger equation,” J. Chem. Phys. 81, 3967–3971.

Thouless, D J, and S Kirkpatrick (1981), “Conductivity of the disordered linear chain,” J. Phys. C: Solid State Phys. 14, 235.

Thouless, D J M. Kohmoto, M. P. Nightingale, and M. den Nijs (1982), “Quantized Hall Conductance in a Two-Dimensional Periodic Potential,” Phys. Rev. Lett. 49, 405–408.

Tikhonenko, F V, A. A. Kozikov, A. K. Savchenko, and R. V. Gorbachov (2009), “Transition between Electron Localization and Antilocalization in Graphene,” Phys. Rev. Lett. 103, 226801.

Tonnél, Claire, Anton Pershin, Sai Manoj Gali, Aurélien Lherbier, Jean-Christophe Charlier, Frédéric Castet, Luca Muccioli, and David Beljonne (2019), “Atomic simulations of charge transport in photoswitchable organic–graphene hybrids,” J. Phys. Mater. 2, 035001.

Torres, L E F Foa, S. Roche, and J.-C. Charlier (2014), Introduction to graphene-based nanomaterials (Cambridge University Press).

Triozon, F, and S. Roche (2005), “Efficient linear scaling method for computing the landauer-büttiker conductance,” Eur. Phys. J. B 46, 427–431.

Triozon, F S, Roche, and D. Mayou (2000), “Wave-packet dynamics by optimized polynomials methods,” RIKEN Rev. 29, 73.

Triozon, François, Stephan Roche, Angel Rubio, and Didier Mayou (2004), “Electrical transport in carbon nanotubes: Role of disorder and helical symmetries,” Phys. Rev. B 69, 121410.

Triozon, François, Julien Vidal, Rémy Mosseri, and Didier Mayou (2002), “Quantum dynamics in two- and three-dimensional quasiperiodic tilings,” Phys. Rev. B 65, 220202.

Troisi, A (2007), “Prediction of the Absolute Charge Mobility of Molecular Semiconductors: the Case of Rubrene,” Adv. Mater. 19, 2000–2004.

Troisi, Alessandro, and Giorgio Orlandi (2006), “Charge-Transport Regime of Crystalline Organic Semiconductors: Diffusion Limited by Thermal Off-Diagonal Electronic Disorder,” Phys. Rev. Lett. 96, 086601.

Ugeda, M M, I. Brihuega, F. Guinea, and J. M. GómezRodriguez (2010), “Missing Atom as a Source of Carbon Magnetism,” Phys. Rev. Lett. 104, 096804.

Uppstu, A, Z Fan, and A Harju (2014), “Obtaining localization properties efficiently using the Kubo-Greenwood formalism,” Phys. Rev. B 89, 075420.

Van Tuan, D. J. Marmolejo-Tejada, X. Waintal, B. K. Nikolić, S. O. Valenzuela, and S. Roche (2016a), “Spin hall effect and origins of nonlocal resistance in adatom-decorated graphene,” Phys. Rev. Lett. 117, 176602.

Van Tuan, Dinh, Jani Kotakoski, Thibaud Louvet, Frank Ortmann, Jannik C. Meyer, and Stephan Roche (2013), “Scaling Properties of Charge Transport in Polycrystalline Graphene,” Nano Lett. 13, 1730–1735.
Van Tuan, Dinh, Frank Ortman, Aron W. Cummings, David Soriano, and Stephan Roche (2016), “Spin dynamics and relaxation in graphene dictated by electron-hole puddles,” Sci. Rep. 6, 21046.

Van Tuan, Dinh, Frank Ortman, David Soriano, Sergio O. Valenzuela, and Stephan Roche (2014), “Pseudospin-driven spin relaxation mechanism in graphene,” Nat. Phys. 10, 857–863.

Van Tuan, Dinh, and Stephan Roche (2016), “Spin Manipulation in Graphene by Chemically Induced Pseudospin Polarization,” Phys. Rev. Lett. 116, 106601.

Vierimaa, V, Z Fan, and A Harju (2017), “Scattering from spin-polarized charged impurities in graphene,” Phys. Rev. B 95, 041401.

Vijay, Amrendra, Donald J. Kouri, and David K. Hoffman (2004), “Scattering and Bound States: A Lorentzian Function-Based Spectral Filter Approach,” J. Phys. Chem. A 108, 8987–9003.

Viswanath, VS, and G. Müller (1994), The Recursion Method: Application to Many-Body Dynamics (Lectures Notes in Physics, Vol. 23) (Springer Verlag, Berlin).

Vozmediano, M.AH, M. I. Katsnelson, and F. Guinea (2010), “Gauge fields in graphene,” Phys. Rep. 496, 109–148.

Wang, Lin-Wang (1994), “Calculating the density of states and optical-absorption spectra of large quantum systems by the plane-wave moments method,” Phys. Rev. B 49, 10154–10158.

Wang, Lin-Wang, and Alex Zunger (1994), “Dielectric Constants of Silicon Quantum Dots,” Phys. Rev. Lett. 73, 1039–1042.

Wang, Xinjie, David Vanderbilt, Jonathan R. Yates, and Ivo Souza (2007), “Fermi-surface calculation of the anomalous Hall conductivity,” Physical Review B - Condensed Matter and Materials Physics 76 (19), 195109.

van Wees, B J, H. van Houten, C. W. J. Beenakker, J. G. Williamson, L. P. Kouwenhoven, D. van der Marel, and C. T. Foxon (1988), “Quantized conductance of point contacts in a two-dimensional electron gas,” Phys. Rev. Lett. 60, 848–850.

Wehling, T O, S. Yuan, A. I. Lichtenstein, A. K. Geim, and M. I. Katsnelson (2010), “Resonant scattering by realistic impurities in graphene,” Phys. Rev. Lett. 105, 056802.

Wehling, TO, A.M. Black-Schaffer, and A.V. Balatsky (2014), “Dirac materials,” Adv. Phys. 63, 1–76.

Weisse, A (2004), “Chebyshev expansion approach to the AC conductivity of the Anderson model,” Eur. Phys. J. B 40, 125–128.

Weiße, Alexander, Gerhard Wellein, Andreas Alvermann, and Holger Fehske (2006), “The kernel polynomial method,” Rev. Mod. Phys. 78, 275–306.

Wharam, D A, T J Thornton, R Newbury, M Pepper, H Ahmed, J E F Frost, D G Hasko, D C Peacock, D A Ritchie, and G A C Jones (1988), “One-dimensional transport and the quantisation of the ballistic resistance,” J. Phys. C: Solid State Phys. 21, L209.

Wilson, Justin H, J. H. Pixley, Pallab Goswami, and S. Das Sarma (2017), “Quantum phases of disordered three-dimensional majorana-weyl fermions,” Phys. Rev. B 95, 155122.

Yafet, Y (1963), “g Factors and Spin-Lattice Relaxation of Conduction Electrons,” in Solid State Physics, Vol. 14, edited by Frederick Seitz and David Turnbull (Academic Press) pp. 1 – 98.

Young, S M, S. Zaheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, and A. M. Rappe (2012), “Dirac semimetal in three dimensions,” Phys. Rev. Lett. 108, 140405.

Yuan, S, R. Roldán, H. De Raedt, and M.I. Katsnelson (2011), “Optical conductivity of disordered graphene beyond the Dirac cone approximation,” Phys. Rev. B 84, 195418.

Yuan, Shengjun, Hans De Raedt, and Mikhail I. Katsnelson (2010a), “Electronic transport in disordered bilayer and trilayer graphene,” Phys. Rev. B 82, 235409.

Yuan, Shengjun, Hans De Raedt, and Mikhail I. Katsnelson (2010b), “Modeling electronic structure and transport properties of graphene with resonant scattering centers,” Phys. Rev. B 82, 115448.

Zhang, Haijing, Jianming Lu, Wu Shi, Zhe Wang, Ting Zhang, Mingyuan Sun, Yuan Zheng, Qihong Chen, Ning Wang, Juhn-Jong Lin, and Ping Sheng (2013a), “Largescale Mesoscopic Transport in Nanostructured Graphene,” Phys. Rev. Lett. 110, 066805.

Zhang, Yan-Yang, Rui-Lin Chu, Fu-Chun Zhang, and Shuming Shen (2012), “Localization and mobility gap in the topological anderson insulator,” Phys. Rev. B 85, 035107.

Zhang, Yan-Yang, Jiangping Hu, B. A. Bernevig, X. R. Wang, X. C. Xie, and W. M. Liu (2009), “Localization and the Kosterlitz-Thouless Transition in Disordered Graphene,” Phys. Rev. Lett. 102, 106401.

Zhang, Yi, Luyao Zhang, and Chongwu Zhou (2013b), “Review of Chemical Vapor Deposition of Graphene and Related Applications,” Acc. Chem. Res. 46, 2329–2339.

Zhang, Yuanbo, Yan-Wen Tan, Horst L. Stormer, and Philip Kim (2005), “Experimental observation of the quantum Hall effect and Berry’s phase in graphene,” Nature 438, 201–204.

Zhao, Liuyan, Rui He, Kwang Taeg Rim, Thaeane Schiro, Keun Soo Kim, Hui Zhou, Christopher Gutiérrez, S. P. Chockalingam, Carlos J. Argüello, Lucia Pálová, Dennis Nordlund, Mark S. Hybertsen, David R. Reichman, Tony F. Heinz, Philip Kim, Aron Pinczuk, George W. Flynn, and Abhay N. Pasupathy (2011), “Visualizing Individual Nitrogen Dopants in Monolayer Graphene,” Science 333, 999–1003.

Zhao, Pei-Liang, Shengjun Yuan, Mikhail I. Katsnelson, and Hans De Raedt (2015), “Fingerprint of disorder source in graphene,” Phys. Rev. B 92, 045437.

Zhu, Shuzhe, Joseph A. Stroscio, and Teng Li (2015), “ProgrammableExtreme Pseudomagnetic Fields in Graphene by a Uniaxial Stretch,” Phys. Rev. Lett. 115, 245501.