Quantum transport by means of O(N) real-space methods

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Quantum transport is investigated by a suitable development of the Kubo formula on a basis of orthogonal polynomials and by using real-space recursion principle. The general method enables us to treat aperiodic systems close to metal-insulator transitions. For quantum Hall systems, results in the context of universal relations between transport coefficients are reported. The RKKY mesoscopic interaction is also evaluated for generally inhomogeneously disordered compounds and exemplified on two-dimensional quasiperiodic systems. Finally, insight of the potential perspectives for large-scale computational applications are given. [S0163-1829(98)06748-4]

I. INTRODUCTION

Quantum transport in high-dimensional nonperiodic systems is usually investigated by way of scaling analysis through diagonalization of a periodic Hamiltonian. However, if N is the number of states, exact diagonalization requires a CPU time scaling as $O(N^3)$, and memory scaling as $O(N^2)$. For sparse Hamiltonians, the use of a Lanczos algorithm reduces memory and CPU time requirements to $O(N)$.[1,2] In the present work, quantum transport in the presence of magnetic field using a development of the Kubo formula on orthogonal polynomials is investigated. This approach has been developed in the context of strongly disordered,[3] quasiperiodic[4] and inhomogeneous systems where electronic susceptibility and diagonal conductivity were successfully estimated.[5] The key point of the algorithm is to rescale the density of states after an evaluation of the upper and lower bounds on energy and then to make a polynomial expansion of the associated Kubo formula. In principle, any orthogonal polynomials may be used, but it turns out that manipulations of Chebyshev polynomials are particularly suitable as they are isomorphic to the Fourier series.[6]

In two-dimensional systems, the study of localization in a magnetic field enables us to address problems related to the quantum Hall effect and metal-insulator transitions.[7] A magnetic field in a pure system introduces further topological complication of the electronic spectrum, which turns out to be a degenerate ensemble of discrete Landau levels. For disordered systems, in the limit of strong magnetic field, perturbational, numerical, and field theoretical approaches have depicted a comprehensive view of the corresponding physical phenomena.[8] In real materials, due to disorder, Landau levels are enlarged and overlap to form Landau bands but extended states still persist at the center of each Landau band, as revealed, for instance, by the divergence of the localization length near these critical energies.[9] The studies of the associated eigenstates inferred a complicated nature described by multifractality.[10,11] Here, a real-space algorithm to evaluate Hall conductivity is proposed for investigating universalities in the quantum Hall effect. After discussing briefly the spectrum of the pure systems with magnetic field, we detail how the method may bring complementary results for studying the transition regions when σ_{xy} goes from one quantized plateau to the next, while σ_{xx} goes through a peaked value and decrease again. Besides, it also enables a study of the phase diagram of the integer quantum Hall effect (QHE) through the calculation of the transport coefficients as a function of disorder and magnetic strengths.

The concept of multifractal states, proposed by Kohmoto[12] for quasiperiodic systems, is an important related issue. Indeed, anomalous quantum diffusion in quantum Hall systems[13] (QHS's) and in quasicrystals[4,14] may have some direct relations with the observed physical properties. The possibility of an experimental observation of multifractal exponents in the QHS has been proposed recently by Brandes and co-workers.[15] To understand properly the effects of these complicated eigenstates, one has to develop suitable methods. By a similar approach, calculation of Rudermann-Kittel-Kasuya-Yosida (RKKY) interaction in two-dimensional (2D) quasiperiodic systems is shown to produce original patterns related to critical states. Finally, applications to large-scale computational methods are suggested in the context of electronic properties of nanostructures.

II. NONINTERACTING ELECTRONS IN 2D SYSTEMS WITH MAGNETIC FIELD

A. Spectral properties for pure systems

The density of states on 2D disordered systems with magnetic field is a well-established result which can also be investigated by recursion method.[16] In the zero-disorder limit, one gets a Landau-level-type spectrum where the number of gaps are defined by the dimensionless measure (magnetic strength) $\alpha = eBa^2/2\pi c$ (a is the lattice unit, B the magnetic field). To investigate spectral and transport properties by recursion method, let us consider the tight-binding representation of the Hamiltonian,

$$\mathcal{H} = \sum_{n_x,n_y} \varepsilon_n |n_x,n_y\rangle\langle n_x,n_y| + \sum_{n_x,n_y} t(|n_x+1,n_y\rangle + |n_x-1,n_y\rangle + e^{2i\pi\alpha n_x}|n_x,n_y+1\rangle \times e^{-2i\pi\alpha n_x}|n_x,n_y-1\rangle)\langle|n_x,n_y|.$$

A recursive construction of an orthogonal basis $|\Psi_n\rangle$ such that

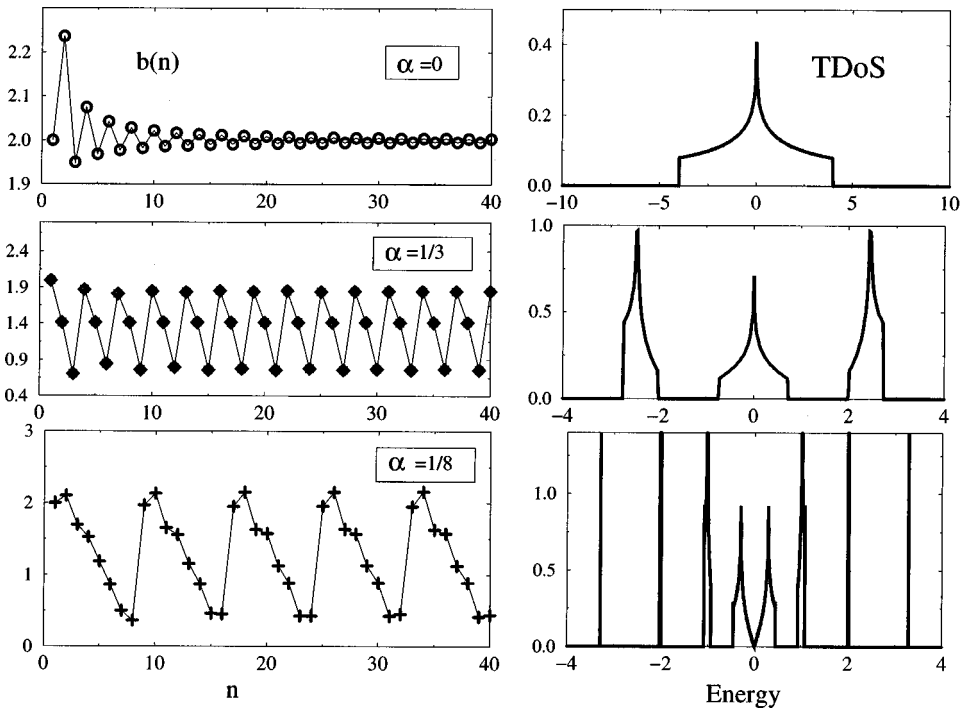

FIG. 1. Recursion coefficients b_n and corresponding total density of states for three different strengths of the magnetic field.

$$\mathcal{H}|\Psi_n\rangle = a_n|\Psi_n\rangle + b_n|\Psi_{n+1}\rangle + b_{n-1}|\Psi_{n-1}\rangle,$$

$$a_n = \langle\Psi_n|\mathcal{H}|\Psi_n\rangle,$$

$$b_n = \langle\Psi_{n+1}|\mathcal{H}|\Psi_n\rangle,$$

tridiagonalizes the Hamiltonian and enables to evaluate the spectral properties quickly and accurately.[1] In the one-band case, the series a_n, b_n usually converge after about 20 recursion steps, and the limit a_∞, b_∞ give the final form of the Jacobi matrix, e.g., the convergence of the continuous fraction development of the Green's function is achieved:

$$\mathcal{J} = \begin{pmatrix} a_0 & b_1 & 0 & \dots & \dots & 0 \\ b_1 & a_1 & b_2 & 0 & \dots & 0 \\ 0 & b_2 & a_2 & \ddots & 0 & \dots \\ \vdots & 0 & \ddots & \ddots & b_\infty & \dots \\ \vdots & \dots & 0 & b_\infty & a_\infty & b_\infty \\ 0 & & \dots & 0 & b_\infty & a_\infty \end{pmatrix}. \qquad (1)$$

Introducing a magnetic field with rational flux $\alpha = P/Q$ leads to Q bands, separated by gaps. The asymptotic regime is given by q distincts values b_q, $q = 1...,Q$, moreover the terminator of the continuous fraction expansion can be evaluated exactly:

$$\mathcal{T}(z) = \cfrac{1}{z - \cfrac{b_0^2}{z - \cfrac{b_1^2}{z - \cfrac{\ddots}{z - b_q^2 \mathcal{T}(z)}}}} \quad \mathcal{T}(z) = \frac{\alpha_q + \beta_q \mathcal{T}(z)}{\gamma_q + \delta_q \mathcal{T}(z)}$$

with

$$\gamma_n \equiv z\gamma_{n-1} - b_{q-n+1}\alpha_{n-1}, \alpha_n = \gamma_{n-1},$$

$$\delta_n = z\gamma_{n+1} - b_{q-n+1}\beta_{n-1}, \beta_n = \delta_{n-1}.$$

For $n = 2,\dots,q$ and initial values $\alpha_1 = 1$, $\beta_1 = 0$, $\gamma_1 = z$, $\delta_1 = -b_q^2$. The explicit form of the terminator and Green's function $G(z) = (z - \mathcal{H})^{-1}$ are thus given by

$$\mathcal{T}(z) = \frac{1}{2\delta_q}[\beta_q - \gamma_q \pm \sqrt{(\beta_q - \gamma_q)^2 + 4\delta_q\alpha_q}],$$

$$\langle\psi_0|G(z)|\psi_0\rangle = \cfrac{1}{z - \cfrac{b_0^2}{z - \cfrac{b_1^2}{z - \cfrac{b_2^2}{z - \dots \cfrac{b_{q-1}^2}{z - b_q^2 \mathcal{T}(z)}}}}}$$

so that the exact density of states can be determined.[17] In Fig. 1, the recursion coefficients b_n and the corresponding total density of states (TDOS) for $\alpha = 0,1/3,1/8$ are presented. The relation between the number of bands and the asymptotic behavior of recursion coefficients becomes obvious.

We now introduce the disorder through the site energies, which are chosen randomly (with uniform probability) within the interval $[-W/2, W/2]$. The presence of disorder will smear out the gaps. This allows us to simplify the termination of the continuous fraction.

In the following, after discussing current open problems of the integer quantum Hall effect (IQHE), the method we used to investigate Kubo formula,[18] different from the usual Landauer method,[19,20] is presented and extended to the calculation of the nondissipative conductivity. It was initially

proposed by Mayou[3] for studying frequency dependent conductivity $\sigma(\omega)$ in disordered systems. An investigation of Kubo conductivity and anomalous quantum diffusion in 3D quasiperiodic systems has been carried out by developing a similar algorithm for static conductivity at zero temperature.[4]

B. Effect of disorder on quantum transport in magnetic fields

In the presence of disorder, extended states exist only at energies for which localization length diverges as $\xi \sim (E-E_c)^{-\nu}$, $\nu = 2.4 \pm 0.1$.[8] At the critical value E_c, some controversies about the universality of the absolute value for the diagonal conductivity still remain. Experimentally $\sigma_{xx}^c \sim 0.2-0.5$, which is in agreement with some numerical scaling analysis of $\sigma_{xx}^L(E,\eta)$.[21–23]

The question of the disappearance of these extended states is important. In a study by Yang and Bhatt,[23] a critical strength of randomness W_c by which all the extended states vanish was found to be independent of magnetic field and finite $W_c \sim 6.t$ in units of t (the constant hopping term). The driven mechanism of the metal-insulator transition was concluded to be consistent with the floating up picture of extended states, as proposed theoretically by Khmel'nitzkii and Laughlin (KL) for the continuous model.[24,25] On the other hand, Sheng and Weng[16] argued for a continuous disappearance of IQHE for the lattice model, in contradiction with the abovementioned floating up scenario. Recent work[26] shows, however, that the discussion of the floating argument turns out to be more subtle and needs careful analysis when interpolating numerical results from lattice models to the continuum limit.

According to the KL argument, the energies of extended states within a given energy range in the vicinity of the center of a Landau band $E_n = (n+1/2)\hbar\omega_c\{[1+(\omega_c\tau)^2]/[(\omega_c\tau)^2]\}$ tend to infinity if the magnetic field is vanishingly small (as expected by Anderson theory of localization). This scenario is believed to be crucial for understanding the global phase diagram as proposed by Kivelson, Lee, and Zhang (KLZ).[27] Indeed, the KLZ approach leads to a physical relation between different quantum Hall liquids, known as the law of corresponding states. Accordingly, transitions from a quantum Hall states to insulators are allowed for certain values of $\nu = 1,1/3,\ldots,$ and forbidden for others ($\nu = 2,3,4\ldots,\ \nu = 2/5,\ldots$).

However, this picture has been recently contradicted by recent experiments by Song *et al.*[28] where transitions from a $\nu = 2$ state to an insulator were observed. In addition, an unprecedented universal relation was found between dissipative and nondissipative components of conductivity $\sigma_{xx}(E_c, W_c) = \sigma_{xy}(E_c, W_c)$. The physical explanation of this phenomenon still remains unclear since different components of transport stem from quite different physical mechanisms.

1. Kubo formula by recursion: diagonal conductivity

The real-space calculation of the diagonal Kubo formula of the electronic conductivity may be considered as an alternative for usual Landauer conductance calculations, or diagonalization methods. The use of the Landauer formula for investigating quantum zero-temperature transport is usually associated with free escape boundary conditions. One direction of the system is periodic whereas the other, of size L, is connected to metallic leads with different chemical potentials. Scaling analysis is performed through L. By the recursion method, we avoid exact diagonalization of the Hamiltonian, so that we can treat, in principle, larger and more complex systems. To reduce the possible numerical instability at boundary conditions induced by the velocity operator (periodic boundary conditions will indeed generate a short-circuit across the sample), we transform the Kubo formula in the following way [$\hat{\mathcal{X}}(t) = e^{i\mathcal{H}t/\hbar}\hat{\mathcal{X}}e^{-i\mathcal{H}t/\hbar}$ and $\hat{\mathcal{X}}$ is the component along direction x of the position operator, Ω the volume of the system]:

$$\sigma_{xx}(E_F) = \frac{2\hbar e^2\pi}{\Omega} \lim_{t\to\infty} \mathrm{Tr}\left(\delta(E_F - H)\frac{[\hat{\mathcal{X}}(t) - \hat{\mathcal{X}}(0)]^2}{t} \right)$$

and we keep control of the asymptotic behavior of the quantum diffusion of the wave packets.[4] The conductivity reads

$$\frac{2\hbar e^2\pi}{\Omega} \sum_{j_x, j_y} \mathcal{D}_j(t) \times \mathrm{Im}_{\eta\to 0} \langle \tilde{\Phi}_j(t) | G(E_F + i\eta) | \tilde{\Phi}_j(t) \rangle,$$

where

$$\mathcal{D}_j(t) = \frac{\langle \Psi_j(t) | \hat{\mathcal{X}}^2 | \Psi_j(t) \rangle}{t}$$

and with $|\Psi_j(t)\rangle = e^{-i\mathcal{H}t/\hbar}|j_x, j_y\rangle$, $|\Phi_j(t)\rangle = \hat{\mathcal{X}}|\Psi_j(t)\rangle$ and $|\tilde{\Phi}_j(t)\rangle$, its normalized counterpart. The summation should be done over the total basis of states $|j_x, j_y\rangle$, but it turns out that a limited number of initial sites is sufficient to achieve convergence of the calculation. The time-dependent evolution of a wave packet initially localized at $|j_x, j_y\rangle$ is also evaluated by polynomial expansion of the evolution operator $e^{-i\mathcal{H}t/\hbar} = \Sigma_n (\int dE \mathcal{P}_n e^{-iEt/\hbar}) \mathcal{P}_n(\mathcal{H})$, where we choose Chebyshev polynomials of the first kind (see Appendix).[4]

Finally, one could also define a scaling parameter from the construction of the recursion basis. Indeed, after computing N recursion steps, the energy resolution is roughly $\Gamma \sim (W/N)$ where W is the total bandwidth of the DOS. Starting from a localized state in $|\Psi_0\rangle = |j_x, j_y\rangle$ the time corresponding to the ''propagation'' of the N states $|\Psi_N\rangle = \mathcal{P}_N|\Psi_0\rangle$ is $\tau \sim \hbar N/W$. Accordingly, a scaling analysis as a function of N may be done. Besides, the use of Kubo formula implicitly requires taking the limit of an infinite system, as the spectrum of any finite system is discrete. By retaining a finite η imaginary part in the Green's function, one replaces the δ function by a peaked smooth function of width η, which must be greater than the level spacing in the finite system. The thermodynamic limit is achieved with increasing system size $L \to \infty$, and $\eta \to 0$ in order to retain all the contributions from the spectrum. In our calculation, we find that the thermodynamic limit is achieved for a finite number of initial states $|j_x, j_y\rangle$ and typically our systems contain approximately 10^6 sites. Concerning the transition regions mentioned earlier, one notes that the effect of finite temperature or frequency is to smear the QH-metal-QH phase transitions.

In Fig. 2, the diagonal conductivities obtained for a disorder and magnetic strength $W = 2,5$, $\alpha = 1/3$, and $\eta = 0.15$, are similar to those from Ref. 23. The increasing of disor-

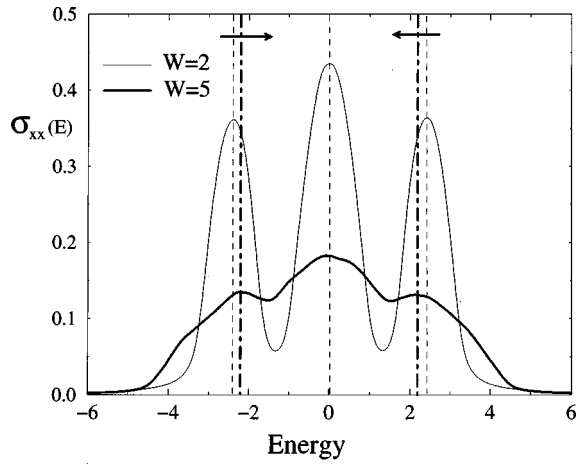

FIG. 2. Diagonal conductivity for quantum Hall systems with different disorder strengths ($\alpha=1/3$, $\eta=0.15$) in e^2/h unit.

dered strength leads to a reduction of the conductivity, as well as a shift of extended states towards the center of the band (as indicated by the arrows in Fig. 2). Ando first described numerically this effect by studying the density of states and Thouless numbers.[29,30] A physical interpretation of this levitation mechanism associated with Landau-level mixing has been proposed for high magnetic field.[31]

The question of universality of the diagonal conductance at critical energies is also addressed in Fig. 3. As the finite imaginary part of the Green's function tends to zero, one clearly sees that the $e^2/2h$ limit is approached with our method. One notes that the figures ($\eta=0.15,0.09,0.05$), in the inset, are obtained for only one initial state $|j_x,j_y\rangle$, so that the fluctuations of the exact shape are artificials. The central figure is an average result over ten different sites.

We also discuss the numerical results obtained in Ref. 22 for $\alpha=1/16$ and different values of the disorder strength. To study the universal relation between the transport coefficients, the authors have computed $\sigma_{xx}(W_c,E_F)$ and $\sigma_{xy}(W_c,E_F)$ for $E_F=-2.75$ in proper units. In Fig. 4, $\sigma_{xx}(W,E_F=-2.75)$ for different disorder strengths is shown. The Fermi energy $E_F=-2.75$ considered in Ref. 22

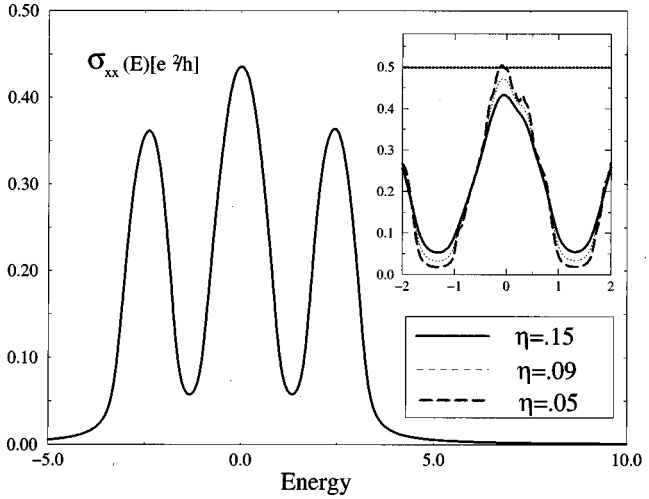

FIG. 3. Diagonal conductivity vs Fermi energy and (inset) the finite imaginary part of the Green's function η.

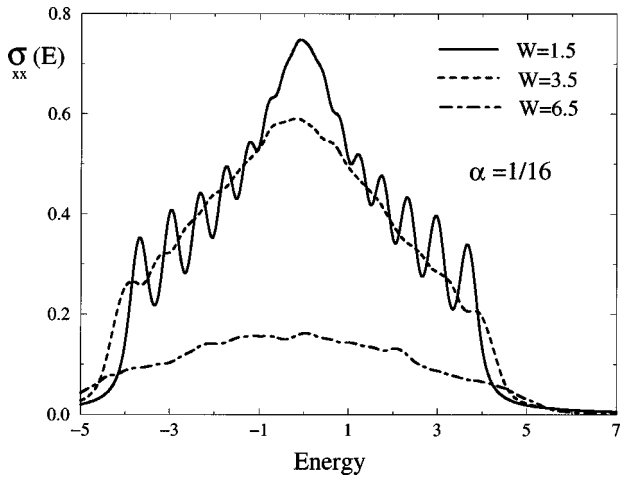

FIG. 4. Diagonal conductivity vs Fermi energy and disorder strength for $\alpha=1/16$.

turns out to lie within a gap of the spectrum. The results from Ref. 22 are then inconsistent with the physics of the problem. Indeed, if the Fermi energy is located within a gap of the pure system, by increasing disorder, a consequent enhancement of the conductivity may be induced for a finite system, as is illustrated in Fig. 5. However, if the Fermi level lies within the center of a Landau band, such behavior is not seen in our results for the Fermi energy in the center of a Landau band. The authors of Ref. 22 may have not considered the correct location of the Fermi energy (remember that the position of the extended state will be affected by the disorder) and, accordingly, their statement is at least numerically questionable.

In Fig. 6, we show the $\sigma_{xx}(E_F)$ for two different values of disorder. The normal-line curves are the results obtained for one site $\mathcal{D}_j(t)\mathrm{Im}_{\eta\to 0}\langle\tilde{\Phi}_j(t)|G(E_F+i\eta)|\tilde{\Phi}_j(t)\rangle$, whereas the bold one is the averaged result. Fluctuations for different site components (entering in the sum of the Kubo expression in real space) can be seen but is not critical, so that a finite number of sites is sufficient to achieve convergence.

2. Hall-Kubo conductivity

The most spectacular result for 2D electrons in magnetic field is given by the quantization of the Hall conductance in

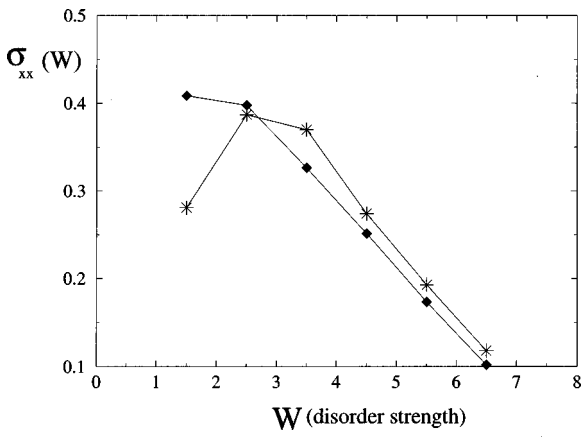

FIG. 5. Dissipative conductivity as a function of disorder strength. Stars are associated with a Fermi level in the gap of the pure system (no disorder) whereas the Fermi level lies within the middle of a Landau band for diamonds.

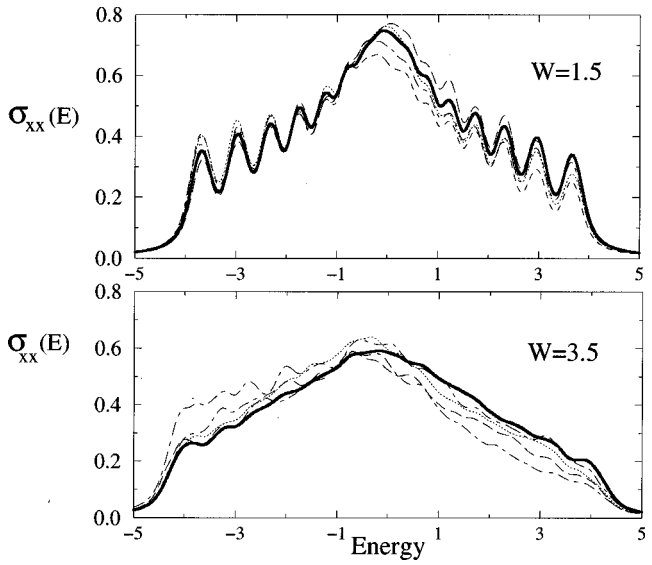

FIG. 6. Components of the dissipative conductivity as a function of disorder strength and Fermi energy (dot, dashed, and dot-dashed curves), and averaged result (black curve).

units of e^2/h, when the Fermi level lies within a gap. This result has been well established and related to topological invariants known as the Chern numbers, which count the exact number of extended states up to the Fermi energy. The contribution to electronic conductivity of a given eigenstate $|k\rangle$ can be calculated from

$$\sigma_{xy}^{k}=\frac{ie^2\hbar}{\Omega}\sum_{q\neq k}\frac{\langle k|\hat{V}_y|q\rangle\langle q|\hat{V}_x|k\rangle-\langle k|\hat{V}_x|q\rangle\langle q|\hat{V}_y|k\rangle}{(\varepsilon_q-\varepsilon_k)^2},$$

$$\langle\sigma_{xy}^{k}\rangle=\frac{1}{4\pi^2}\int d\varphi_1 d\varphi_2\sigma_{xy}^{k}(\varphi_1,\varphi_2)=\frac{e^2}{h}\mathcal{N}_k.$$

In finite-size systems, Hall conductance (boundary condition average) enables us to identify whether $\langle\sigma_{xy}^{k}\rangle$ is a nonzero Chern number $\mathcal{N}_k$ or not, thus whether the corresponding $|k\rangle$ is an extended state or localized state (formulation is due to Thouless and co-workers[33,34]).

As we are interested, in particular, in computing the nondissipative conductivity for energies in the transition regions, (where σ_{xy} is not quantized), one has to adopt a different strategy. To that end, we propose a real-space approach of Hall conductivity. Starting from the general off-diagonal form of the Kubo conductivity, one shows that the proper algorithm allowing the expansion of the Hall conductance in a real-space basis is given by

$$\sigma_{xy}=-\frac{ie^2\hbar}{2\Omega}\int_{\substack{E_2>E_F\\E_1<E_F}}dE_1dE_2\frac{f(E_1)-f(E_2)}{E_1-E_2}$$

$$\times\mathrm{Tr}[\,\delta(E_1-\mathcal{H})\dot{\mathcal{Y}}\delta(E_2-\mathcal{H})\dot{\mathcal{X}}],$$

which enables us to expand the spectral measure on the basis of Chebyshev polynomials. Note that $\dot{\mathcal{X}}$ and $\dot{\mathcal{Y}}$ are the time-dependent position operators in both respective directions of the plane. Some simple algebra yields two parts to be evaluated separately:

$$\sigma_{xy}=-\frac{ie^2\hbar}{2\Omega}\sum_{m,n,i}I_{mn}\langle i_x,i_y|\mathcal{P}_n(\mathcal{H})\dot{\mathcal{Y}}\mathcal{P}_m(\mathcal{H})\dot{\mathcal{X}}|i_x,i_y\rangle,$$

where I_{mn} is analytical and depends on the choice of the polynomial basis. In our case, it corresponds to $\{A_F=\mathrm{Arcos}[(E_F-a)/2b]$, with a and b associated with the weight function of Chebyshev polynomials$\}$:

$$I_{mn}=\frac{1}{\pi b}\left\{\frac{\sin(m+n+3)A_F}{(m+n+3)}-\frac{\sin(m+n+1)A_F}{(m+n+1)}\right\}.$$

The other part implies the calculation of the coefficients $\langle j_x,j_y|\mathcal{P}_n(\mathcal{H})\dot{\mathcal{Y}}\mathcal{P}_m(\mathcal{H})\dot{\mathcal{X}}|j_x,j_y\rangle$. A reasonable number of initial sites $|j_x,j_y\rangle$ should be considered. The sum over m and n indices is, given the form of the I_{mn} factors, limited by some appropriate cutoff. One notes that the computational time is, however, much larger compared to the σ_{xx} calculation.[32]

III. RKKY MAGNETIC INTERACTION IN NONPERIODIC SYSTEMS

Among the interesting phenomena related to electronic propagation, RKKY (Ref. 35) between magnetic sites in disordered systems has been the subject of great attention. In particular, it has been shown to be very important for understanding the spin-glass transition or, more recently, giant magnetoresistance effects in magnetic multilayers.

The RKKY interaction is generically given by $\mathcal{I}_{RKKY}(r_i,r_j,E_F)=J^2\chi(r_i,r_j,E_F)\mathbf{S}_{r_i}\cdot\mathbf{S}_{r_j}$, where J is the interaction between the localized moment $\mathbf{S}_{r_i}$ and the spin of the itinerant electrons, and $\chi(r_i,r_j,E_F)$ contains the sum of all of the electron-hole propagation paths from $|r_i\rangle$ to $|r_j\rangle$. The susceptibility can be written as

$$\chi(r_i,r_j,E_F)=2\,\mathrm{Re}\int_{\substack{E>E_F\\E'<E_F}}dEdE'\times\frac{\langle r_i|\,\delta(E-\mathcal{H})|r_j\rangle\langle r_j|\,\delta(E'-\mathcal{H})|r_i\rangle}{E-E'}$$

and by development of the spectral measure on Chebyshev polynomials one gets[5]

$$\chi_{ij}=2\,\mathrm{Re}\sum_{m,n}I_{mn}\langle r_i|P_n(\mathcal{H})|r_j\rangle\langle r_j|P_m(\mathcal{H})|r_i\rangle,$$

$$I_{mn}=\int_{\substack{E>E_F\\E'<E_F}}N(E)N(E')\frac{P_m(E)P_n(E')}{E-E'}dEdE',$$

where the coefficients I_{mn} have been previously defined for the Hall conductance.

In metallic systems, the interaction is calculated exactly, $\mathcal{I}_{RKKY}(r,E_F)\sim A(\mathbf{r})\cos[2k_Fr+\delta(\mathbf{r})]/r^3$, in contrast to quasiperiodic or disorder systems where there are no simple analytical forms. However, in weakly disordered systems, one can evaluate the quantum fluctuations that arise in the higher moments of the interaction.[36] It is found that only even moments lead to significant contributions:

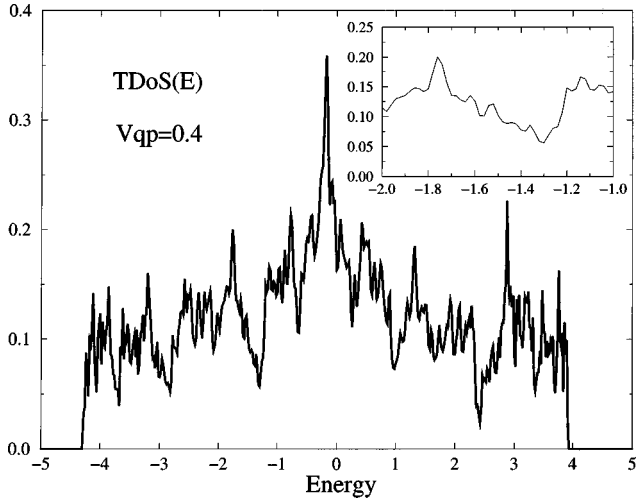

FIG. 7. Total density of states for a two-dimensional quasiperiodic lattice (V_{qp} is the strength of the Fibonacci quasiperiodic potential). In the inset is given the energy interval for which corresponding susceptibilities are calculated.

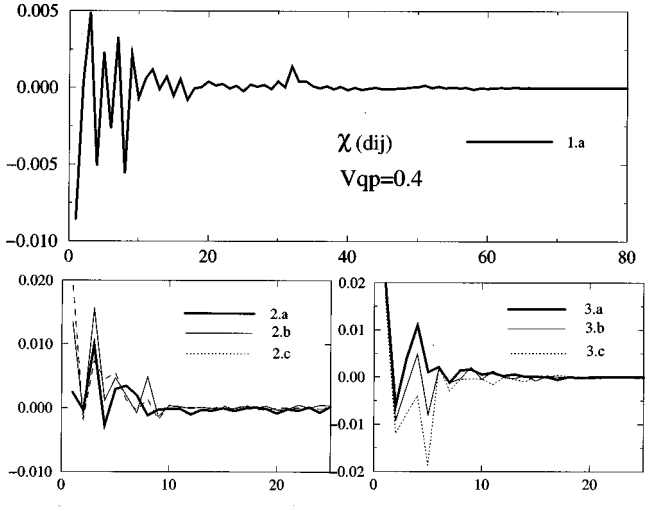

FIG. 8. Electronic susceptibility (in a units, a lattice parameter) as a function of Fermi energy with 1.a, 2.a, 2.b, 2.c, 3.a, 3.b, 3.c corresponding, respectively, to Fermi energy $-1.9+0.1\lambda$, $\lambda=0,1,2,3,4,5,6$.

$$\langle \chi^{2p}(|r_i-r_j|)\rangle \simeq \Omega_p \left(\frac{\rho^2(E_F)}{|r_i-r_j|^{2d}} \right)^p \sim [\langle \chi^2(|r_i-r_j|)\rangle]^p,$$

$$\langle \chi^{2p+1}(|r_i-r_j|)\rangle \simeq \exp\left(-\frac{|r_i-r_j|}{l_m} \right)$$

with $\rho(E_F)$ the density of states (DOS) at the Fermi level and l_m the mean free path, whereas Ω_p is a constant independent of the parameter of the Hamiltonian.

Quasiperiodic systems cannot be described by such an averaging process, so that the use of the recursion method gives here some interesting quantitative information, and further provides a framework for investigating mesoscopic interaction in inhomogeneously disordered systems.[5] In Figs. 7 and 8, the TDOS for a 2D quasiperiodic Fibonacci quasilattice, as well as typical signature of aperiodic long-range order are reported. The strength of the quasiperiodic potential is $V_{qp}=0.4t$ (with t the constant hopping integral between first neighbors) and the susceptibility is given as a function of the distance between interacting magnetic sites (in a units, with a the lattice spacing). In Fig. 8, typical features of the interaction are shown, and, in particular, due to the complicated nature of quasiperiodic potential, no Fermi wavelength can be properly defined and oscillations exhibit resurgences that are absent from the periodic potential.[5]

IV. POSSIBLE APPLICATIONS FOR LARGE-SCALE COMPUTATIONAL METHODS

The expansion of any operator on orthogonal polynomials can also be applied in the context of large-scale computational methods, which aim at reducing large memory and CPU time costs, for investigating more realistic models. For instance, spectral properties and optical spectra for a realistic model of silicon quantum dots have been evaluated and quantum confinement investigated.[37] One can also consider thermodynamical properties of quantum systems thanks to the development of the partition functions $\mathcal{Z}(\beta)=\mathrm{Tr}[e^{-\beta\mathcal{H}}]=\Sigma_n[\int dE\ e^{-\beta E}\mathcal{P}_n(E)]\mathcal{P}_n(\mathcal{H})$, with $\{\mathcal{P}_n\}$ a suitable basis of orthogonal polynomials. Indeed, one needs to consider average quantities as $\langle\hat{\mathcal{A}}\rangle=\mathrm{Tr}[\hat{\rho}\hat{\mathcal{A}}]/\mathrm{Tr}[\hat{\rho}]$ (where $\hat{\rho}$ is the density operator), but if the expansion of the partition function can be easily done in the case of a scalar argument, when applied to an operator (for large-scale systems), one may not be able to switch into the eigenrepresentation of the Hamiltonian since full diagonalization is practically impossible.[38–40] Consequently, polynomial expansions of operator are the only available alternative technique.

Finally, in order to perform realistic atomistic calculations of binding energies and interatomic forces, real-space methods turn out to be efficient and accurate $O(N)$ methods.[41,42]

V. CONCLUSION

Results regarding quantum transport by means of a real-space methods have been presented. The generality of the use of orthogonal polynomials for high-dimensional nonperiodic systems has been discussed. In two-dimensional disordered systems with magnetic field, a global phase diagram and new universalities of the quantum Hall effect may be studied by this method. One notes that, nowadays, considerable effort is devoted to improving the efficiency of available numerical algorithms. The well-known Car-Parinello method has opened new perspectives for *ab initio* electronic structure calculations, but the development of the so-called ''order-N scheme'' [43] is of major importance to investigating complex molecular systems. Quantum transport has also opened new challenges since the development of nanostructures (quantum dots, nanotubes,...) has become crucial in the field of electronic devices. In this context, further ''order-N'' schemes to investigate electronic propagation also need to be steadily improved.

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APPENDIX: ORTHOGONAL POLYNOMIALS

The principle of the real-space algorithms, used in this article, is based on expansion of spectral measures on orthogonal polynomials. Let us mention the requirements as well as the key points of this approach. For any $\rho(E)$ defined by $\int_a^b \rho(E)dE=1$, there exists a family of orthogonal polynomials $\mathcal{P}_n(E)$ of degree n, such that

$$\int_{-\infty}^{+\infty} \mathcal{P}(E)\mathcal{P}_n(E)\mathcal{P}_m(E)dE=\delta_{nm},$$

$$\rho(E)\sum_n \mathcal{P}_n(E)\mathcal{P}_n(E')=\delta(E-E')$$

for E,E' belonging to the spectral subset of $\rho(E)$ and $\rho(E)\neq\rho(E')$. These polynomials generally satisfy a three-term recursive relation $EP_n(E)=a_n\mathcal{P}_n(E)+b_n\mathcal{P}_{n+1}(E)+b_{n-1}\mathcal{P}_{n-1}(E)$ with $b_{-1}=0$, $n\geqslant 0$, a_n,b_n related to the moments of spectral function.[44,45] However, the expansion of spectral measure can be also done in a arbitrary basis of polynomials, for instance, on Chebyshev polynomials $\mathcal{Q}_n$:

$$\delta(E-\mathcal{H})=\tilde{\rho}(E)\sum_n \mathcal{Q}_n(E)\mathcal{Q}_n(\mathcal{H})=\rho(E)\sum_n \mathcal{P}_n(E)\mathcal{P}_n(\mathcal{H}),$$

where $\tilde{\rho}(E)=1/\pi\sqrt{4b^2-(E-a)^2}$ and $\rho(E)$ is the total density of states. Here, a and b define the band edges and bandwidth of the spectral function associated to Chebyshev polynomials.[6] The Green's functions can be obtained by Hilbert transformation of $\rho(E)$ (for the absolute continuous spectrum):

$$G(z)=\int dE\,\frac{\rho(E)}{(z-E)},$$

$$\rho(E)=\lim_{\eta\to 0^+} -\frac{1}{\pi}\,\mathrm{Im}\,G(E+i\eta),$$

and general analytic properties of the Green's function can be investigated through the properties of the considered polynomials.

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