Alternative Approach to Computing Transport Coefficients: Application to Conductivity and Hall Coefficient of Hydrogenated Amorphous Silicon

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We introduce a theoretical framework for computing transport coefficients for complex materials with extended states, and defect or band-tail states originating from static topological disorder. As a first example, we resolve long-standing inconsistencies between experiment and theory pertaining to the conductivity and Hall mobility for amorphous silicon and show that the Hall sign anomaly is a consequence of localized states. Next, we compute the ac conductivity of amorphous polyaniline. The method may be readily integrated with current *ab initio* methods.

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The atomistic understanding of electrical conductivity [1,2] and the Hall coefficient [3–7] is a key unsolved problem in the physics of amorphous semiconductors [8]. The challenge is due to two factors: (1) the existence of localized states of varying physical origin; and (2) at moderate temperature, both localized states and extended states are accessible excited states [9,10]. Previous work on the conductivity [11,12] and Hall coefficient [13–17] of amorphous semiconductors has involved either Miller-Abrahams theory or small polaron models [9]. Neither approach is ideal for amorphous semiconductors, with their complex menagerie of localized states due to defects, and tail states due to topological [18] or chemical disorder [8] and electron-phonon couplings strongly dependent upon carrier localization [19].

In this Letter, we first develop a novel formalism for estimating the linear response to a mechanical perturbation [20]. The method properly includes the four possible transitions between extended or localized initial and final states. The full results and many intermediate details are provided in Ref. [21]; here we require only transitions between localized states. Our work resolves the puzzle of the sign anomaly of the Hall mobility in *a*-Si:H:, provides the temperature dependence of the transport coefficients, and accurately predicts the ac conductivity of polyaniline. The new formalism is expected to be applicable well beyond the examples of this Letter and lends itself to inclusion in current *ab initio* schemes.

In the small polaron hopping regime, the Kubo linear response formula [20] has been used to compute conductivity and Hall mobility [12,15–17]. The key mathematical obstacle to computing the current-current correlation function is the imaginary time integral [12,15–17], which results from the commutator between the microscopic current and density matrix [20]. For a "mechanical perturbation" (for which an external disturbance may be expressed with additional terms in the Hamiltonian [20]), the local density operator $\hat{\rho}$ of a quantity (charge, energy, etc.) can be easily constructed [22]. We can avoid this troublesome commutator.

We first average $\hat{\rho}$ over a state $\Psi'(t)$ of the system with the mechanical perturbation, from which the *microscopic* local density $\rho(\mathbf{r},t)=\langle\Psi'(t)|\hat{\rho}|\Psi'(t)\rangle$ is obtained. Next we calculate $\partial\rho(\mathbf{r},t)/\partial t$ by means of the time-dependent Schrödinger equation $i\hbar\partial\Psi'(t)/\partial t=H'(t)\Psi'(t)$, where $H'(t)$ is the total Hamiltonian of [system + mechanical perturbation]. The third step is to apply the local density (charge density, energy density) continuity equation: $\partial\rho(\mathbf{r},t)/\partial t+\nabla\cdot\ \mathbf{j}_m(\mathbf{r},t)=0$; the *microscopic* response $\mathbf{j}_m$ (current density, energy flux, etc.) is then expressed in terms of $\Psi'(t)$. Practically speaking, $\Psi'(t)$ may be computed to the required order with perturbation theory. By substituting $\Psi'(t)$ into the expression for $\mathbf{j}_m(\mathbf{r},t)$, one can obtain the *microscopic* response to the required order of mechanical disturbance. Spatial and ensemble average are taken at the final stage. The desired transport coefficients can then be extracted from the ensemble average of the spatially averaged flux $\mathbf{j}$.

Since the state of the system is determined from the initial conditions, averaging over the initial state can be delayed until the final stage. Thus we can avoid the commutator between flux and density matrix, i.e., the integral over imaginary time.

Consider then, a system with N_e electrons and $\mathcal{N}$ nuclei in the presence of an electromagnetic field with potentials $(\mathbf{A},\ \phi)$, the charge density of state Ψ' at $\mathbf{r}$ $\rho'(\mathbf{r},t)=\int d\tau\Psi'^{*}\hat{\rho}(\mathbf{r})\Psi'$, where the arguments of wave function Ψ' are $(\mathbf{r}_1\cdots\mathbf{r}_{N_e};\mathbf{W}_1\cdots\mathbf{W}_{\mathcal{N}};t)$, $\mathbf{W}_1$ is the position of the first nucleus, etc. $\hat{\rho}(\mathbf{r})=\sum_j e\delta(\mathbf{r}-\mathbf{r}_j)-\sum_L Z_L e\delta(\mathbf{r}-\mathbf{W}_L)$ is the charge density operator. $d\tau=d\mathbf{r}_1\cdots d\mathbf{r}_{N_e}d\mathbf{W}_1\cdots d\mathbf{W}_{\mathcal{N}}$ is the volume element in configuration space. The evolution of the state is determined by the time-dependent Schrödinger equation for which the total Hamiltonian includes the interaction between system and external field. The contribution from the electrons is:

$$\mathbf{j}_m(\mathbf{r},t)=\frac{i\hbar eN_e}{2m}\int d\tau'(\Psi'\nabla_{\mathbf{r}}\Psi'^{*}-\Psi'^{*}\nabla_{\mathbf{r}}\Psi')-\frac{e^2N_e}{m}\mathbf{A}(\mathbf{r},t)\int d\tau'\Psi'^{*}\Psi', \qquad (1)$$

where the arguments of Ψ' are $(\mathbf{r},\mathbf{r}_2,\cdots,\mathbf{r}_{N_e};\mathbf{W}_1,\mathbf{W}_2,\cdots,\mathbf{W}_{\mathcal{N}};t;)$, $d\tau'=d\mathbf{r}_2\cdots d\mathbf{r}_{N_e}d\mathbf{W}_1d\mathbf{W}_2\cdots d\mathbf{W}_{N_n}$. In Eq. (1), the antisymmetry of Ψ' under exchange of particles was used, and the Coulomb gauge $\nabla\cdot\mathbf{A}(\mathbf{r},t)=0$ was adopted to simplify the expression. $\mathbf{j}_m(\mathbf{r},t)$ is gauge invariant[14,23]. Without the nuclear coordinates, Eq. (1) is identical to the form used by BCS to compute paramagnetic and diamagnetic currents for superconductors in which Bloch states are not radically modified by the electron-phonon (e-ph) interaction [23]. Equation (1) is a generalization to arbitrary strength of e-ph interaction, and may be used for the localized carriers in amorphous semiconductors or the polarons in ionic and molecular crystals. The ratio of the second term to the first term is eA/p (p is electron momentum), so that the contribution from the 2nd term may be neglected.

We now apply Eq. (1) to compute the conductivity and Hall mobility of an amorphous semiconductor. Since the carrier concentration is low in lightly-doped amorphous semiconductors, one can invoke the single-electron approximation, and $\Psi'(t)$ for $\mathbf{j}_m$ may be replaced by the single-electron wave function $\psi'(\mathbf{r};x_1,x_2,\cdots,x_{3\mathcal{N}};t)$, where $\mathbf{r}$ is the coordinate of the carrier, $x_1,x_2,\cdots,x_{3\mathcal{N}}$ are the displacements of $3\mathcal{N}$ vibrational degrees of freedom. Using perturbation theory, one can expand $\psi'(t)$ to the required order of external field [10,21]. We use A with subscripts to label localized states, and denote the coupling between two localized states ϕ_A and ϕ_{A_1} caused by external field as $J^{\text{field}}_{A_1A}=\int d\mathbf{r}\phi^*_{A_1}h_{\text{fm}}\phi_A$, where $h_{\text{fm}}=(i\hbar e/m)\mathbf{A}(\mathbf{r})\cdot\nabla_{\mathbf{r}}+e^2\mathbf{A}^2(\mathbf{r})/(2m)+e\phi(\mathbf{r})$. The spatially averaged *microscopic* current density to second order of J^{field} is

$$\mathbf{j}(\mathbf{s},t)=-\frac{N_e\hbar e}{m\Omega_{\mathbf{s}}}\int_{\Omega_{\mathbf{s}}}d\mathbf{r}\int\Big[\prod_{j=1}^{3\mathcal{N}}dx_j\Big]\{\mathrm{Im}(\psi^{(0)}\nabla_{\mathbf{r}}\psi^{(1)*}-\psi^{(1)*}\nabla_{\mathbf{r}}\psi^{(0)})+\mathrm{Im}(\psi^{(0)}\nabla\psi^{(2)*}-\psi^{(2)*}\nabla\psi^{(0)}+\psi^{(1)}\nabla\psi^{(1)*})\}, \qquad (2)$$

where $\psi^{(1)}$ is change in state to order J^{field}, and $\psi^{(2)}$ is change in state to order $[J^{\text{field}}]^2$, where $\psi^{(0)}(t)$ is the state of a carrier at time t *without* external field. $\Omega_{\mathbf{s}}$ is the "physical infinitesimal" volume of Kubo [24]. Because the initial state of the phonon-dressed carrier is unknown, we need to average j_k ($k=x,y,z$) over the initial phonon distribution and single-electron states. To compute the conductivity, we only require the order J^{field} term of Eq. (2). If one applies a voltage drop across the material, the potentials are $\mathbf{A}=0$ and $\phi=-2\mathbf{E}_0\cdot\mathbf{r}\cos\omega t$. Using perturbation theory, one can compute $\psi^{(0)}$ and $\psi^{(1)}$ to order J^1. By substituting $\psi^{(0)}$ and $\psi^{(1)}$ into the first term of Eq. (2), one can use $j_x=\sum_k\sigma_{xk}E_{0k}$ etc. to find the conductivity tensor. The conductivity from the LL transitions is [21]:

$$\left.\begin{matrix}\mathrm{Re}\sigma_{jk}(\omega)\\ \mathrm{Im}\sigma_{jk}(\omega)\end{matrix}\right\}=-\frac{N_ee^2}{\Omega_{\mathbf{s}}}\mathrm{Im}i\sum_{AA_1}[I_{A_1A+}\pm I_{A_1A-}]\times f(E^0_A)[1-f(E^0_{A_1})]v^{k*}_{A_1A}(E^0_A-E^0_{A_1})^{-1}(v^T-v)^j_{A_1A}$$
$$-\frac{N_ee^2}{\Omega_{\mathbf{s}}}\mathrm{Im}\sum_{AA_1A_3}f(E^0_A)[1-f(E^0_{A_1})][1-f(E^0_{A_3})](v^T-v)^j_{A_1A_3}(E^0_A-E^0_{A_1})^{-1}\hbar^{-1}v^{k*}_{A_1A}J_{A_3A}[I_{A_3A_1A+}\pm I_{A_3A_1A-}] \qquad (3)$$
$$+\frac{N_ee^2}{2\hbar\Omega_s}\sum_{A_2A_1A}f(E_A)[1-f(E_{A_2})]\mathrm{Im}(v^T-v)^j_{A_2A}\{(E^0_{A_1}-E^0_{A_2})^{-1}(v^k_{A_2A_1})^*J^*_{A_1A}(Q_{1A_2A_1A+}\pm Q_{1A_2A_1A-})$$
$$+J^*_{A_2A_1}(E^0_A-E^0_{A_1})^{-1}(v^k_{A_1A})^*(Q_{2A_2A_1A_+}\pm Q_{2A_2A_1A_-})\}.$$

$\mathrm{Re}\sigma_{jk}(\omega)$ takes the positive sign and $\mathrm{Im}\sigma_{jk}(\omega)$ takes the negative sign. Equation (3) is a special case of the general conductivity formula (Eq. (42) of Ref. [21]) for LL transition (between localized states). Unlike previous theories [9], the dc conductivity may be directly extracted from Eq. (3) without a limiting process. Here, $v^k_{A_1A}=\int d\mathbf{r}\phi^*_{A_1}v^k\phi_A$, $v^k=-i\hbar m^{-1}\partial/\partial x_k$, $\mathbf{v}^T$ is the transpose operator of $\mathbf{v}$. E^0_A is the eigenvalue of state ϕ_A, $f(E^0_A)$ is the Fermi distribution. $J_{A_1A}=\int d\mathbf{r}\phi^*_{A_1}\sum_{p\notin D_A}U(r-\mathcal{R}_p)\phi_A$ is transfer integral from ϕ_A to ϕ_{A_1}, D_A is the spatial region in which ϕ_A is nonzero, $p\notin D_A$ indicates the atoms not in D_A [10]. In Eq. (3), the first term is the order J^0 contribution, the remaining terms are order J^1 contributions. Here I_s and Q_s are vibrational contributions. $I_{A_1A\pm}(\omega,T)$ has dimension of time (denote its order as $t^{\pm}_{A_1A}$). $t^{\pm}_{A_1A}$ may be interpreted as the mean free carrier time, indicating the time evolution of $\psi'(t)$ in a field-driven 2-site transition, cf. Eq. (C1) in Ref. [21]. Similarly the twofold time integrals $I_{A_3A_1A\pm}$, $Q_{1A_2A_1A\pm}$, and $Q_{1A_2A_1A\pm}$, have dimension of $[\text{time}]^2$, reflect the time evolution of $\psi'(t)$ in 3-site transitions induced by transfer integral J, they have same order of magnitude $[t^{\pm}_{A_3A_1A}]^2$, cf. Eqs. (C3, C7-C9) in Ref. [21]. $\hbar^{-1}J_{A_3A}[t^{\pm}_{A_3A_1A}]^2$ may be explained as the mean-free time in a 3-site process. The interference between J^{field} and J is displayed in the interference between two components (reached through different paths) of the final state [21]. The interference between different paths in real space [14] is a special case of the present ansatz. At high temperature $k_BT>\hbar\bar{\omega}$ ($\bar{\omega}$ is first peak in phonon spectrum), I_s and Q_s can be approximately computed using the method of steepest descent (see Appendix D in Ref. [21]). For example:

$$I_{A_1A\pm} = e^{-\beta\hbar(\omega'_{A_1A}\mp\omega)/2-\beta\lambda_{A_1A}/4}\left\{C^{-1/2}\sum_{n=0}^{\infty}\frac{(-i)^n(\omega-\omega'_{A_1A})^n}{n!C^{n/2}}\Gamma\left(\frac{n+1}{2}\right)-i\left[\sum_{\alpha}\frac{1}{2}(\theta_\alpha^{A_1}-\theta_\alpha^{A})^2\omega_\alpha\cosh\frac{\beta\hbar\omega_\alpha}{2}\right]^{-1}\right\}, \quad (4)$$

where $\theta_\alpha^{A_1}$ is the shift in origin of the α^{th} normal mode caused by a carrier in state ϕ_{A_1}, $\lambda_{A_1A} = \frac{1}{2}\sum_\alpha \hbar\omega_\alpha(\theta_\alpha^{A_1}-\theta_\alpha^{A})^2$ is the reorganization energy for a LL transition[10]. $C = \hbar^{-2}k_BT\lambda_{A_1A}$[10,21]. The mean-free time decreases with increasing λ_{A_1A} and energy difference: $t^{\pm}_{A_1A} \sim \hbar(k_BT\lambda_{A_1A})^{-1/2}e^{-\beta\hbar(\omega'_{A_1A}\mp\omega)/2-\beta\lambda_{A_1A}/4}$. The average mobility μ is defined by $\sigma_{xx} = e^2(N_e/\Omega_{\mathbf{s}})\mu$. From Eq. (3), one can see that μ depends on the energy distribution and spatial distribution of localized states. A typical value of μ can be estimated: $\mu \sim v^2_{A_1A}t_{A_1A}(E^0_A - E^0_{A_1})^{-1} + v_{A_1A}v_{A_3A_1}(t^2_{A_3A_1A}\hbar^{-1}J_{A_3A}) \times (E^0_A - E^0_{A_1})^{-1}$. As a test, we apply Eqs. (3) and (4) to the frequency dependence of the ac conductivity in polyaniline at $T = 300$ K [25]. The Austin-Mott $\omega^{0.8}$ law [9] derived from dipole loss does not accurately fit experiments [26]. In Fig. 1, we fit the data [25] with the first three terms (a quadratic polynomial in ω) in Eq. (4). Because the highest frequency of external field 10^6 Hz $\ll T = 300$ K, factors $e^{\pm\beta\hbar\omega} \approx 1$ do not play a role in the low frequency regime $\hbar\omega \ll k_BT$.

To describe the Hall effect, one needs $\psi'(t)$ to second order of J^{field}: one J^{field} includes electric field E_x, and another includes magnetic field B_z. After substituting $\psi^{(0)}$, $\psi^{(1)}$ and $\psi^{(2)}$ into the second term in Eq. (2), and averaging over various initial conditions, σ_{yx} is determined from j_y, see Eq. (49) in Ref. [21]. The primary temperature dependence of σ_{yz} is included in the time integrals which are obtained from integrating out vibrational states. There are two types of 3-site processes (Fig. 10 of Ref. [21]). The twofold time integrals result from electron-phonon interaction and have dimension $[\text{time}]^2$ and the same order of magnitude $s^2_{AA_2A_1}$, where $s_{AA_2A_1}$ is the characteristic time for the 3-site processes. Similarly there are 8 types of 4-site processes (Figs. 11 and 12 of Ref. [21]), they lead to threefold time integrals, the order of magnitudes are $s^3_{AA_3A_2A_1}$, where $s_{AA_3A_2A_1}$ is the characteristic time for the 4-site processes. $s_{AA_2A_1}$ (3-site processes) and $[\hbar^{-1}Js^3_{AA_3A_2A_1}]^{1/2}$ (4-site processes) may be explained as the mean-free times in presence of magnetic field. The order J^1 contributions of σ_{yx} come from various 4-site processes, their order is $n_ee^2(\hbar^{-1}J_{A_3A}s^3_{AA_3A_2A_1})\hbar^{-2}[B_zeL_z^{A_2A_1}/m]x_{A_1A}v_{A_3A_2}$, where x and v are the matrix elements of coordinate and velocity, $L_z^{A_2A_1} = \int d\mathbf{r}\phi^*_{A_2}L_z\phi_{A_1}$ is the matrix element of the z component of electronic orbital angular momentum. The widely used 3-site process in the literature[4,7,14–16] is a special case of Fig. (11) of Ref. [21] when $A_2 = A_3$. The order J^0 contributions of σ_{yx} comes from 3-site processes. Their order is $n_ee^2s^2_{AA_2A_1}\hbar^{-2}(B_zeL_z/m)xv$. It roughly corresponds to the "interference" contribution (involving two sites)[16]. They are neglected in some other calculations[14,17]. The ratio of the order J^1 terms to J^0 terms is $(\hbar^{-1}J_{A_3A}s^3_{AA_3A_2A_1})s^{-2}_{AA_2A_1} \sim 1$. For a more quantitative comparison with experiment, one needs to apply Eq. (49) in Ref. [21].

Amorphous semiconductors are isotropic, so that one may estimate the Hall mobility as: $\mu_H = B_z^{-1}\sigma_{xy}/\sigma_{xx} \sim \frac{e}{\hbar}xvs^2_{AA_2A_1}t^{-1}_{A_1A}$, where $x_{A_3A} = i\hbar v_{A_3A}(E^0_A - E^0_{A_3})^{-1}$. For a-Si:H [8], ξ and $R_{A_1A} \sim 5$–10 Å, $J \sim 0.02$ eV, one has $\mu_H \sim 0.1$–0.2 cm^2 V^{-1} sec^{-1}. The temperature dependence of μ_H may be obtained from those of σ_{xy} and σ_{xx}:

$$\mu_H \sim \frac{e}{\hbar}xvs^2_{AA_2A_1}t^{-1}_{A_1A}\exp\left\{-\frac{E^a_{A_1A}}{2k_BT}-\frac{3}{2}k_BT \times \sum_\alpha(\hbar\omega_\alpha)^{-1}(\theta_\alpha^{A_1}-\theta_\alpha^{A})^2\right\}. \quad (5)$$

At low frequency, the phonon spectral density $\propto \omega^2$, so that the sum in Eq. (5) converges. Figure 2 gives the Hall mobility vs temperature for n-type a-Si:H. Both Eq. (5) and the Friedman-Holstein result [14], are roughly consistent with experimental data[8]. $E^a_{A_1A} = \lambda_{A_1A}(1 + \Delta G_{A_1A}/\lambda_{A_1A})^2/4$ is estimated from typical parameters $\Delta G_{A_1A} = 0.05$ eV and $\lambda_{A_1A} = 0.2$ eV for a-Si [10].

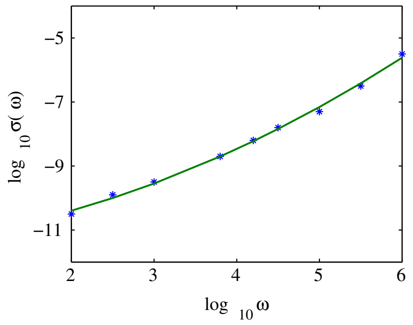

FIG. 1 (color online). ac conductivity of polyaniline as a function of frequency at $T = 300$ K: star symbols denote experimental data [25], solid line is from the first three terms in Eq. (4).

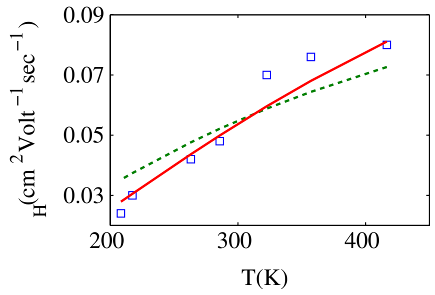

FIG. 2 (color online). Hall mobility vs temperature: square symbols for n-type a-Si:H [8], dashed line from best fit of Friedman-Holstein formula [14], solid line is from Eq. (5).

We may demonstrate the sign of Hall voltage from Ehrenfest's theorem. The expected value for the acceleration on a carrier is:

$$\frac{d}{dt}\int d\tau\,\psi'^{*}(t)\Big(\frac{d\mathbf{r}}{dt}\Big)\psi'(t) = -\frac{qi\hbar}{2m^2}\int d\tau\,\psi'^{*}\psi'\nabla\times\mathbf{B} + \frac{1}{m}\int d\tau\,\psi'^{*}(t)[q\mathbf{E} - \nabla_{\mathbf{r}}V(\mathbf{r},\{\mathbf{W}_{\mathbf{n}}\})]\psi'(t)$$
$$- \frac{q}{m^2}\int d\tau\,\psi'^{*}\mathbf{B}\times(-i\hbar\nabla_{\mathbf{r}}\psi') + \int d\tau\,\psi'^{*}\frac{q^2}{m^2}(\mathbf{B}\times\mathbf{A})\psi', \qquad (6)$$

where q is the charge of the carrier. If a system has only extended states, because the mean-free time of a carrier is much larger than the effective interaction time with phonons and defects, the drift velocity is along the direction of $q\mathbf{E}$ for a nearly free carrier. The direction of the average magnetic force in an extended state (diagonal element) is the same as the classical one $q\mathbf{E}\times\mathbf{B}$, the sign of the Hall voltage is as expected. Because the force exerted on a carrier by the external $\mathbf{E}$ field is much weaker than the binding force of disorder potential, the time average of $m^{-1}\int\phi^{*}_{A_1}(-i\hbar\nabla_{\mathbf{r}} - q\mathbf{A})\phi_{A_1}$ in a localized state ϕ_{A_1} is zero: no net magnetic force acts on a localized carrier. The mean trapping time that a localized carrier spends in a localized state before making a transition to other states is $\sim\hbar J^{-2}(\lambda k_B T)^{1/2}e^{E_a/k_B T}$ (high temperature) or $\sim\hbar J^{-2}(\Delta G)$ (low temperature), where ΔG is the typical energy difference between the final and the initial states [10]. The mean transition time needed for a transition event is $\sim mdR/\hbar$, where d is a typical bond length, R is the distance between two localized states for a LL transition, R is localization length for a LE transition. The mean transition time is much shorter than the mean trapping time in a typical localized state. Comparing with the transition speed $\hbar/(md)$, the speed $qEdR/\hbar$ obtained from external electric field $\mathbf{E}$ during the transition time is negligible. The magnetic force suffered by a carrier during a transition is along the direction of $q\mathbf{v}\times\mathbf{B}$, where $\mathbf{v}$ is the transition velocity of the carrier. However, $\mathbf{v}$ does not have any relation to the direction of $\mathbf{E}$. If one applies an E field along the x axis and B field along the z axis, a direction dependent Hall voltage should be detectable along any direction in the yz plane, not only along the y axis. Checking this prediction would be a crucial test for this work. A recent experiment [27] shows that the signs of Hall voltage in several a-Si:H films are not always reverse to those expected from $q\mathbf{E}\times\mathbf{B}$, the present analysis seems to agree with this observation.

We have devised an accurate and practical method for computing transport coefficients, with applications to amorphous semiconductors and potential application to many other systems. The localized states make the anomalous sign of Hall voltage possible. The method has the potential to be implemented with current single-particle *ab initio* simulations, and requires only the eigenvalues and eigenvectors of the single-electron Hamiltonian, dynamical matrix, and quantities easily derived from these.

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