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A Real-Space Approach to Electronic Transport

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Abstract. — Using orthogonal polynomials, a novel approach for studying DC and AC conductivity and velocity-velocity correlation function has been developed. The method works in direct space and can treat order or disordered, finite or infinite, and pure or alloy systems with equal ease. Further, it is not computer intensive and allows conductivity calculations as a function of frequency or the location of the Fermi energy in an efficient manner.

Although electrical conductivity is a widely experimentally studied electronic property, realistic calculations of the conductivity are feasible only in limiting cases. For weak scattering, the Boltzmann equation provides a fairly good description of the conductivity problem. However, as the scattering becomes important, the Boltzmann approach becomes inadequate and one needs a better description. One-electron Kubo formulae [1] relate the conductivity to an average of the product of Green's functions and thus provide a viable alternative. However, it is difficult to calculate the average of the product of Green's functions and one of the approaches has been to approximate the average of the product by the product of the average of a single Green's function. Such a simplification ignores the so-called vertex corrections known to be important, and attempts have been made to find ways in which one could avoid the above simplification. Indeed, by modelling the system within effective medium theories such as Coherent Potential Approximation [2, 3] using numerical techniques based on the equation of motion method [4, 5] or recursion method [6, 7] conductivity calculations including vertex correction have been reported.

In this paper we propose a different approach to the electronic transport. It is based on a generalization of the modified moments approach [8] which has been successfully applied to study the electronic structure of ordered and disordered systems. The new scheme works in both the weak and the strong scattering regime. For the case of weak scattering, the new approach gives conductivity in agreement with Boltzmann equation. However, it becomes more efficient as the scattering is increased and it is here that its true application lies. Another feature of the present approach is that conductivity calculations as a function of frequency or as a function of the location of the Fermi energy can be made in a single calculation. The new approach also permits an effective way to study correlation functions such as velocity-velocity

correlation function. As we show, variations in the mean relaxation time of electrons and transitions to localized regime are most transparent in this correlation function.

In the framework of linear response theory and the one electron approximation, the conductivity can be studied via the Kubo-Greenwood formula [1]

$$\text{Re}(\sigma(\omega)) = 2\pi e^2 \hbar / \Omega \int dE \left[\frac{f(E) - f(E + \hbar\omega)}{\hbar\omega} \right] F(E, E + \hbar\omega) \quad (1)$$

with

$$F(E, E') = \text{Tr} [V_x \delta(E - H) V_x \delta(E' - H)] \quad (2)$$

Here H is the Hamiltonian of the system, V_x is the velocity operator, and $f(E)$ is the Fermi Dirac distribution function. The central problem is the calculation of $F(E, E')$.

In this work we propose an expansion of $\delta(E - H)$ in polynomials $P_n(H)$ of the Hamiltonian. Consider any function $N(E)$ finite in a region of real axes. The theory of orthogonal polynomials [9] lets one define a set of polynomials $P_n(E)$ of degree n which are orthogonal in the sense

$$\delta_{n,m} = \int N(E) P_n(E) P_m(E) dE \quad (3)$$

It can be shown that polynomials $P_n(E)$ satisfy the recurrence relation

$$EP_n(E) = a_n P_n(E) + b_n P_{n+1}(E) + b_{n-1} P_{n-1}(E) \quad (4)$$

where a_n and b_n depend on the density $N(E)$ via its moments and $b_{-1} = 0$. The crucial point is that $P_n(E)$ form the basis for expansion of any function and in particular one can express $\delta(E - H)$ as [8]

$$\delta(E - H) = N(E) \sum_{n=0}^{\infty} P_n(E) P_n(H), \quad (5)$$

provided $N(E)$ is non zero on the spectrum of H . Using this expansion, the function $F(E, E')$ can be expressed as

$$F(E, E') = \sum_{n,m} C_{n,m} P_n(E) P_m(E') N(E) N(E') \quad (6)$$

with

$$C_{n,m} = \text{Tr} [V_x P_n(H) V_x P_m(H)]. \quad (7)$$

All the physics of the conductivity is contained in $C_{n,m}$.

The convergence of the expansion depends on the choice of the density $N(E)$. We expect a faster convergence when $N(E)$ is not too different from the mean density of electronic states [8]. Indeed, in the present work, we have used the mean density of electronic states determined using the recursion method for $N(E)$. With this choice, the random phase approximation (RPA) used by Mott *et al.* [4], in the case of mean free path shorter than the interatomic distance is equivalent to keeping only $C_{0,0}$ in expansion (6). The remaining terms, therefore, represent a systematic development beyond the RPA.

Consider a system described by a tight-binding Hamiltonian

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{ij} V_{ij} |i\rangle\langle j| \quad (8)$$

where ϵ_i are the site energies and V_{ij} are the hopping matrix elements assumed to be $V_{ij} = V$ between near neighbors and zero otherwise. To evaluate the trace in (7), we calculate the diagonal element on randomly chosen initial vectors as follows [7]. Consider a vector $|\alpha\rangle$

$$|\alpha\rangle = \sum_i a_i |i\rangle \quad \bar{a}_i = 0 \quad \overline{a_i^* a_j} = 1/N \delta_{ij} \quad (9)$$

where a_i are independent random variables for site i and the bar indicates an average over the probability distribution of a_i . N is the total number of sites in the system. For any operator A , one has

$$\text{Tr } A = N \overline{\langle \alpha | A | \alpha \rangle} \quad (10)$$

the bar indicating an average over all $|\alpha\rangle$. Thus,

$$C_{n,m} = \overline{C_{n,m}(\alpha)} \quad (11)$$

with

$$C_{n,m}(\alpha) = \langle \beta_n | V_x | \gamma_m \rangle \quad (12)$$

where

$$|\beta_n\rangle = P_n(H) V_x | \alpha \rangle \quad \text{and} \quad |\gamma_m\rangle = P_m(H) | \alpha \rangle$$

Knowing the density $N(E)$, sets $|\beta_n\rangle$ and $|\gamma_n\rangle$ can be easily calculated by the recurrence relation similar to equation (4) for $P_n(E)$, i.e., using the expression

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

where $\Psi = \beta$ or γ with

$$\begin{aligned} |\beta_0\rangle &= V_x | \alpha \rangle & |\beta_{-1}\rangle &= 0 \\ |\gamma_0\rangle &= | \alpha \rangle & |\gamma_{-1}\rangle &= 0 \end{aligned}$$

Knowing $C_{n,m}$, the conductivity can be calculated using equations (1) and (6). The details are given in Appendix A. The effect of the magnetic field can also be easily included. In fact, it can be shown [10] that the effect of a magnetic field, \mathbf{B} , is to change the hopping matrix elements in equation (8) by the complex elements

$$V(c)_{ij} = V(0)_{ij} \exp \left[-(e/\hbar c) \mathbf{B} \left(\mathbf{R}_i \times \frac{1}{2} \mathbf{R}_j \right) \right] \quad (13)$$

where $V(0)_{ij}$ are the matrix elements in the absence of the field and R_i are the positions of the ions. The conductivity calculation then proceeds as before, the only difference being that $V(c)_{ij}$ are complex and depend on the position of sites i and j . We refer the reader to our previous article [11] for details.

As we pointed out in the beginning, the expansion outlined in equations (5) and (6) can also be used to calculate correlation functions such as velocity-velocity correlation function $C(E, t)$ given by

$$C(E, t) = \langle V(0) V(t) \delta(E - H) \rangle \quad (14)$$

Using equation (5) for $\delta(E - H)$, $C(E, t)$ can be expressed as

$$C(E, t) = \int \exp [iE't/\hbar] F(E, E') \exp [-iEt/\hbar] dE' \quad (15)$$

where $F(E, E')$ is given by equation (6) which can be easily calculated using the present approach. The details are given in Appendix B.

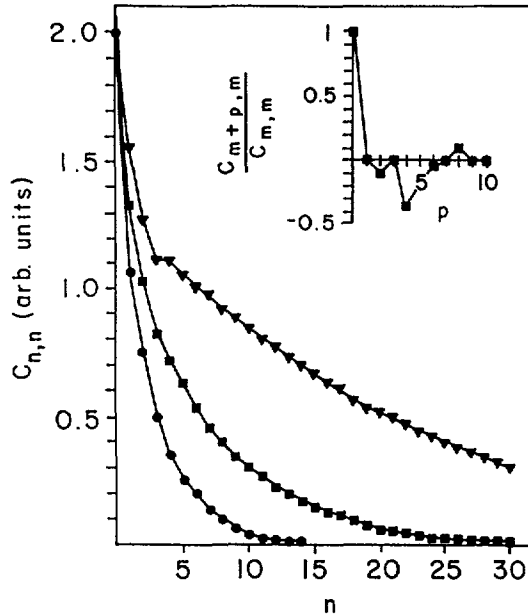


Fig. 1. — Coefficients $C_{n,n}$ for $\frac{W}{V} = 2(\blacktriangle)$; $\frac{W}{V} = 4(\blacksquare)$ and $\frac{W}{V} = 6(\bullet)$. The inset shows $\frac{C_{m+p,m}}{C_{m,m}}$ for $\frac{W}{V} = 6$ and $m = 14$.

To demonstrate the strength of our approach we have carried out calculations of the conductivity as a function of frequency and Fermi energy, and $C(E, t)$ for a cubic lattice with nearest neighbor interaction V and diagonal disorder. The site energies ϵ_i are randomly distributed uniformly from $-W/2$ to $W/2$. The disorder can also be characterized by the mean free path ℓ calculated with a Boltzmann approach. An average value over the whole band is

$$\frac{\ell}{a} = 14 \left(\frac{2V}{W} \right)^2 \quad (16)$$

where a is the lattice spacing. The model has been previously studied by various authors [5] and it is fairly accepted that all the electronic states become localized at $W/V \approx 15$. In this work we primarily focus on the conducting region $W/V \leq 10$. To carry out the configurational average, all calculations were carried out on five random configurations. This was found to be sufficient to converge to average values. We would like to point out that the same $N(E)$ is used for all configurations.

In Figure 1 we show the coefficients $C_{n,n}$ for different strengths of disorder. In all cases, the coefficients decrease with increasing n . However, the rate of decrease depends on the strength of disorder. We found that $C_{n,n}$ for $n \geq 2$ decrease exponentially with n if the disorder is not too strong ($\frac{W}{V} \leq 6$ in our calculation which corresponds to $\frac{\ell}{a} \sim 1.5$). We further observed that the variation of $C_{n,n}$ in this regime is well represented by the expression

$$C_{n,n} = 1.3 \exp \left[-\frac{1}{6} \left(\frac{W}{4V} \right)^2 (n-1) \right] \quad n \geq 2.$$

As is easily shown using equations (1), (3) and (6), the $\sum_{n=0}^{\infty} C_{n,n}$ is related to the integral of the diffusivity, $\frac{\sigma(E)}{N(E)}$, over all energies. Using the above expression, and the fact that $n = 0$ and $n = 1$ give only a small contribution, we find that

$$\sum_n C_{n,n} \alpha \int \frac{\sigma(E)}{N(E)} dE \alpha \left(\frac{V}{W} \right)^2$$

This dependence of the integral of diffusivity is in agreement with the prediction of the Boltzmann equation where the conductivity $\sigma(E)$ varies as $\left(\frac{V}{W} \right)^2$

As the disorder becomes stronger, the localization becomes important and the coefficients $C_{n,n}$ become negative for larger n ($W/V \sim 10$, not shown in Fig. 1). This is a consequence of backscattering [9]. It may appear from the figure that only $C_{0,0}$ will be non-zero in the limit of strong scattering. This is not the case and the entire set of coefficients are needed to calculate the conductivity. The inset in Figure 1 shows $C_{m+p,m}/C_{m,m}$. We found that this ratio is independent of m for large m values, which means that $C_{m,m+p}$ can be expressed as $C_{m,m}f(p)$ where $f(p)$ only depends on p . Furthermore, when localization effects are not too important, the function $f(p)$ decreases rapidly with p , indicating that only the elements close to the diagonal in the matrix $C_{n,m}$ contribute to conductivity. This regular behavior of the coefficients $C_{n,m}$ can be used to give confidence in the convergence of the series used to calculate conductivity. It is of interest to point out that one can invert relation (6) to obtain

$$C_{n,m} = \int F(E, E') P_n(E) P_m(E') dE dE'.$$

Thus information on $F(E, E')$ could be used to understand the behavior of $C_{n,m}$. This will be discussed in a forthcoming paper. To give an estimate of the computational efforts, we calculated $C_{n,m}$ on a cubic lattice consisting of 68921 sites with periodic boundary conditions. Calculation of all $C_{n,m}$ up to $n, m = 30$ took 30 minutes on a VAX 8650 computer. We would like to emphasize that the bulk of the numerical effort is involved in the calculation of $C_{n,m}$. Once $C_{n,m}$ are determined, conductivity as a function of Fermi energy or frequency can be calculated extremely rapidly. We refer the reader to Appendix A for details.

In Figure 2a we show the DC conductivity $\sigma(0, E)$, diffusivity $D(E)$, and the density of states $N(E)$ as a function of energy. Notice that, while the diffusivity is marked by two shoulders, the conductivity is maximum in the middle of the band and decreases to zero at the band edges. In Figure 2b we show the corresponding quantities in the Boltzmann limit. Notice that $N(E)$ in Figure 2b is the density of states of the cubic lattice without disorder as opposed to $N(E)$ in Figure 2a which includes effect of disorder. The Boltzmann limit is probably less valid around the band edges because of the importance of fluctuations which will first localize states in this region. Also, the mean free path is shorter in the center of the band and the Boltzmann equation has limited validity. Except for these limitations, we find that the Boltzmann approach lead to the same conductivity variation as obtained by us, namely that the conductivity increases as one goes towards the middle of the band. Also it is interesting to note that the diffusivity, which has a pronounced shoulder in the Boltzmann limit retains this feature in the more exact calculation shown in Figure 2a.

In Figure 3 we show the frequency dependent conductivity as a function of frequency for various values of the Fermi energy. The results correspond to $W/V = 6$. It is seen that $\sigma(\omega)$

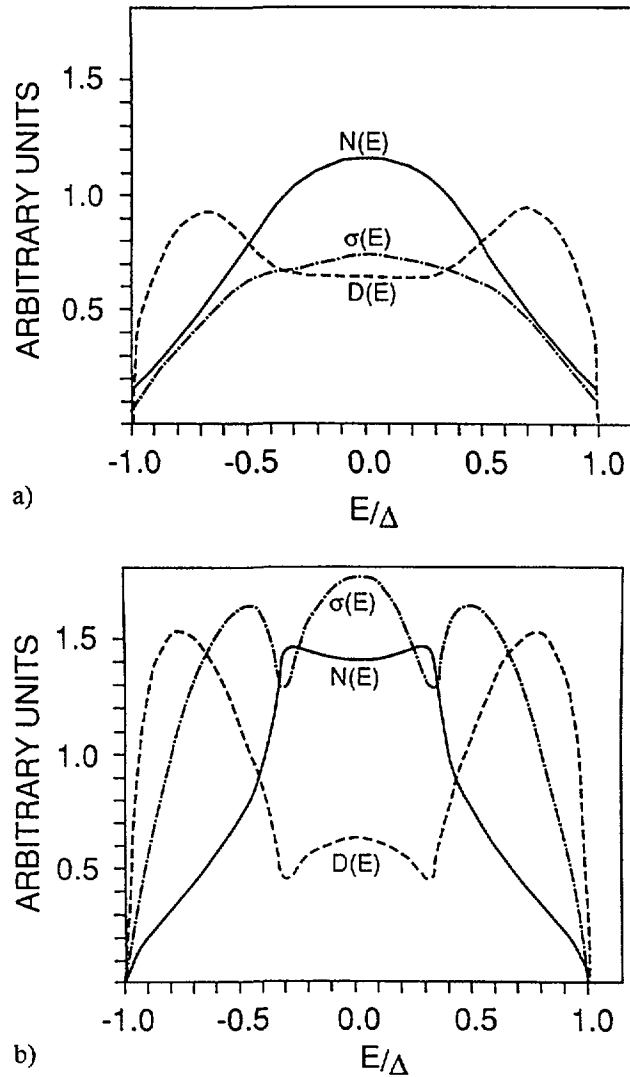


Fig. 2. — a) DC conductivity $\sigma(E)$, diffusivity $D(E)$ and the density of states $N(E)$ as a function of energy; b) DC conductivity $\sigma(E)$, diffusivity $D(E)$ and the density of states $N(E)$ based on the Boltzmann limit.

is maximum at $\omega = 0$ and decreases to zero as analogous to a Lorentzian form obtained in the weak scattering Boltzmann limit. It is interesting to compare the full width at half maximum (FWHM) obtained in this work with those based on Boltzmann equation where one obtains

$$\frac{\text{Re } \sigma(\omega, E_F)}{\sigma(0, E_F)} = \frac{4\Gamma^2}{(\hbar\omega)^2 + 4\Gamma^2}$$

where $\frac{\Gamma}{\Delta} = \frac{1}{6} \frac{\Pi}{3} \left[\frac{W}{2V} \right]^2 \left(\frac{\Delta}{6} \right) n_T(E_F)$.

Here, Δ is half the band width, and $n_T(E_F)$ is the normalized density of states, i.e.,

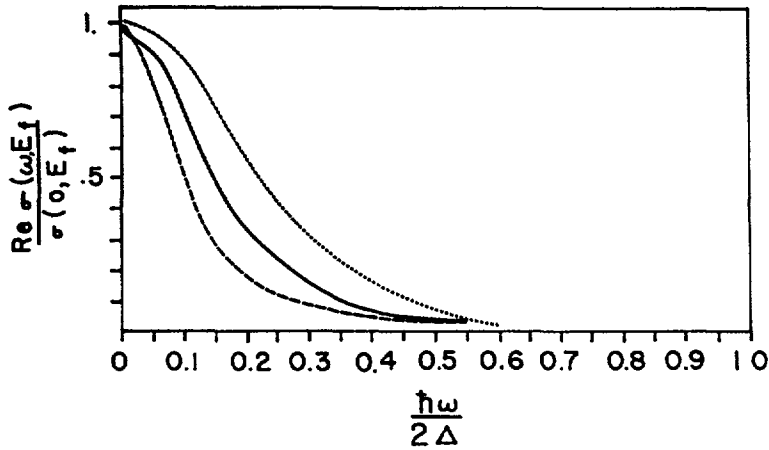


Fig. 3. — $\frac{\text{Re}\sigma(\omega, E_F)}{\sigma(0, E_F)}$ for Fermi energies at $-\frac{3}{4}\Delta$ (- - -), $-\frac{1}{2}\Delta$ (—) and 0 (...), where Δ is half the band width.

$\int n_T(E)dE = 1$. For the three cases namely $E_F = -3\frac{\Delta}{4}$, $-\frac{\Delta}{2}$ and 0 considered in our work, we obtain FWHM of 0.2Δ , 0.3Δ and 0.44Δ . The Boltzmann approximation, using the density of states of the disordered system yields FWHM of 0.14Δ , 0.27Δ and 0.36Δ , showing that the Boltzmann limit already includes most of the effect. It is also interesting to compare the present results with the corresponding results in binary alloy chains obtained by Hwang *et al.* [2], within the coherent-potential approximation. The density of states for the binary alloy contains a minimum in the density of states in the middle of the band which leads to zero conductivity at $\omega = 0$ for the Fermi energy in the middle of the band. In the present case, the density of states has no such feature and the conductivity decreases to zero as ω is increased.

In Figure 4 we show our results on the velocity-velocity correlation function. The correlation function decreases to zero for longer times. In the Boltzmann picture, this correlation function decreases exponentially with time, i.e.,

$$C(E, t)/C(E, 0) = \exp(-2\Gamma|t|/\hbar)$$

We have also shown in Figure 4, $C(E, t)/C(E, 0)$ calculated using this expression for the case of $\frac{W}{V} = 6$. As seen from this figure, the Boltzmann approach is quantitatively inaccurate. A comparison of $C(E, t)$ for $W/V = 6$ and $W/V = 10$ shows that the correlation function starts to develop negative components as the disorder increases. This is a result of backscattering. As one approaches the localization limit, the correlation function develops more and more of the negative region until the time average becomes zero and the states become localized. To our knowledge, our studies represent the first realistic calculations of this function.

To summarise, we have proposed a new approach to electronic transport which is computationally efficient, allows studies of a variety of transport coefficients, and can be applied to a wide range of systems. The present approach is numerically ideal for the cases where the mean free path is less than a few interatomic distances. It is in this region that the Boltzmann approximation becomes less accurate, as also shown by us, and therefore our approach is complementary to the Boltzmann equation. The other merits of our approach are that (i) the conductivity as a function of frequency and energy can be easily determined, (ii) the con-

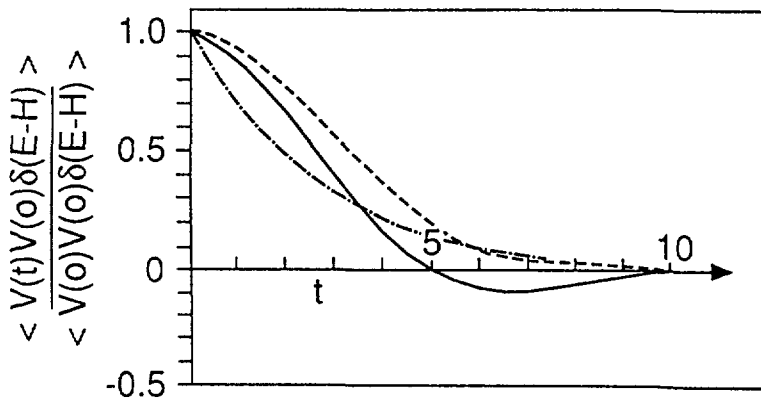


Fig. 4. — Velocity-velocity correlation function for $\frac{W}{V} = 6$ (- - -) and $\frac{W}{V} = 10$ (—) using the present approach and for $\frac{W}{V} = 6$ (- · - · -) using Boltzmann equation. Time is measured in units of $\frac{\hbar}{\Delta}$ where Δ is half the band width.

vergence can be tested by the behavior of the coefficients $C_{n,m}$ and (iii) systems of arbitrary complexity can be studied.

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Appendix A

A. Orthogonal Polynomials

A.1. DEFINITIONS AND BASIC RELATIONS. — It is known that given a positive function $N(E)$ which is zero for E outside the energy range $a \leq E \leq b$ and is such that

$$\int N(E)dE = 1$$

there exists a series of polynomials $P_n(E)$ of degree n such that

$$\int N(E)P_n(E)P_m(E)dE = \delta_{n,m} \quad (\text{A.1})$$

Further, these orthogonal polynomials obey a three term recurrence relation.

$$EP_n(E) = a_nP_n(E) + b_nP_{n+1}(E) + b_{n-1}P_{n-1}(E) \quad (\text{A.2})$$

with $b_{-1} = 0$ and $n \geq 0$.

The coefficients a_n and b_n are related to the moments of the density $N(E)$.

One can define a Hilbert transform $R(z)$ of $N(E)$

$$R(z) = \int \frac{N(E)}{Z - E} dE \quad (\text{A.3})$$

where Z is complex and outside the real axis. One has

$$N(E) = \lim_{\epsilon \rightarrow 0^+} \left[-\frac{1}{\pi} \text{Im} R(E + i\epsilon) \right] \quad (\text{A.4})$$

and $R(z)$ can be calculated from the continued fraction expansion

$$R(z) = \frac{1}{z - a_0 - \frac{b_0^2}{z - a_1 - \frac{b_1^2}{z - a_2}}} \quad (\text{A.5})$$

A.2. DECOMPOSITION OF A FUNCTION $f(E)$ IN THE BASIS OF ORTHOGONAL POLYNOMIALS

A function $f(E)$ can be expanded in the basis of orthogonal polynomials $P_n(E)$ provided that $N(E)$ is non zero, wherever $f(E)$ is non zero. One has

$$f(E) = \sum_{n=0}^{\infty} C_n P_n(E) \quad (\text{A.6})$$

and using (A.1) we get

$$C_n = \int N(E) f(E) P_n(E) dE \quad (\text{A.7})$$

A.3. ORTHOGONAL POLYNOMIALS AND RECURSION METHOD. — Given a normalized density of states $N(E)$, one can define an associate semi-infinite chain in the following manner.

Consider an orthonormal basis set composed of states $|\Psi_n\rangle$ with

$$\langle \Psi_n | \Psi_m \rangle = \delta_{n,m}, m \geq 0$$

and a Hamiltonian H defined by

$$H|\Psi_n\rangle = a_n|\Psi_n\rangle + b_n|\Psi_{n+1}\rangle + b_{n-1}|\Psi_{n-1}\rangle \quad (\text{A.8})$$

with $b_{-1} = 0$, $n \geq 0$, and with same coefficients a_n and b_n as in (A.2). For details on how to calculate a_n and b_n , the reader is referred to an earlier paper [12].

It is then easy to show that $N(E)$ is the partial density of states of state $|\Psi_0\rangle$ for the Hamiltonian H , namely

$$N(E) = \langle \Psi_0 | \delta(E - H) | \Psi_0 \rangle \quad (\text{A.9})$$

Notice that one can define orthogonal polynomials for the Hamiltonian H simply by replacing E by H in $P_n(E)$. They obey the same recurrence relations, namely

$$HP_n(H) = a_n P_n(H) + b_n P_{n+1}(H) + b_{n-1} P_{n-1}(H) \quad (\text{A.10})$$

with $b_{-1} = 0$ and $P_0(H) = 1$.

Using (A.10) and comparing with (A.8) we get

$$|\Psi_n\rangle = P_n(H) |\Psi_0\rangle \quad (\text{A.11})$$

A.4. CALCULATION OF SCALAR PRODUCTS. — To decompose a function $f(E)$ in the basis of $P_n(E)$ one has to calculate the components C_n given by (A.7), i.e.,

$$C_n = \int N(E) f(E) P_n(E) dE.$$

The coefficient C_n is the scalar product of $f(E)$ and $P_n(E)$. Instead of performing this integral numerically, it can be more efficient and accurate to use the recursion method. In the space $\{|\Psi_n\rangle, n \geq 0\}$ and using equation (A.9) one has

$$C_n = \int \langle \Psi_0 | \delta(E - H) | \Psi_0 \rangle f(E) P_n(E) dE$$

and thus

$$C_n = \langle \Psi_0 | f(H) P_n(H) | \Psi_0 \rangle = \langle \Psi_0 | f(H) | \Psi_n \rangle \quad (\text{A.12})$$

We now show how these are calculated for the three forms of $f(E)$ appearing in this work

$$\text{a) } f(E) = P_q(E) P_r(E + \hbar\omega) \quad (\text{A.13})$$

In this case,

$$C_n = \langle \Psi_0 | P_q(H) P_r(H + \hbar\omega) | \Psi_n \rangle \quad (\text{A.14})$$

i.e.,

$$C_n = \langle \Psi_q | P_r(H + \hbar\omega) | \Psi_n \rangle \quad (\text{A.15})$$

In the basis $\{|\Psi_m\rangle\}$, the vector $P_r(H + \hbar\omega) |\Psi_n\rangle$ was calculated using the recurrence relation

$$H P_r(H + \hbar\omega) = (a_r - \hbar\omega) P_r(H + \hbar\omega) + b_r P_{r-1}(H + \hbar\omega) + b_{r-1} P_{r-1}(H + \hbar\omega) \quad (\text{A.16})$$

which can be obtained by replacing H by $H + \hbar\omega$ in (A.10). Note that $P_r(H + \hbar\omega) |\Psi_n\rangle$ obeys the same recurrence relation as $P_r(H + \hbar\omega)$ and can be easily obtained.

$$\text{b) } f(E) = e^{iEt} \quad (\text{A.17})$$

In this case

$$\begin{aligned} C_n &= \langle \Psi_0 | e^{iHt} | \Psi_n \rangle \\ &= \langle \Psi_0(t) | \Psi_n \rangle \end{aligned} \quad (\text{A.18})$$

$|\Psi_0(t)\rangle$ was calculated by solving the equation of motion for $|\Psi_0(t)\rangle$.

$$\text{c) } f(E) = \frac{1}{Z - E} \quad (\text{A.19})$$

In this case,

$$C_n = \int \frac{N(E)}{Z - E} P_n(E) dE = T_n(z) \quad (\text{A.20})$$

Also,

$$C_n = T_n(z) = \left\langle \Psi_0 \left| \frac{1}{Z - H} \right| \Psi_n \right\rangle \quad (\text{A.21})$$

Using the recursion relation (A.8) for $|\Psi_n\rangle$ one obtains the following recurrence relation for $T_n(z)$

$$Z T_n(Z) = a_n T_n(Z) + b_n T_{n+1}(Z) + b_{n-1} T_{n-1}(Z) + \delta_{n,0} \quad (\text{A.22})$$

with $b_{-1} = 0$ and $T_0(Z) = \int \frac{N(E) dE}{Z - E} = R(Z)$

$T_0(Z)$ is calculated from (A.5) and $T_n(Z)$ from (A.23).

Appendix B

B. Calculation of Frequency-Dependent Conductivity and Velocity Auto-Correlation Function from Coefficients $C_{n,m}$

B.1. GENERAL APPROACH. — If one calculates $F(E, E')$ using equation (6) and then $\text{Re}\sigma(\omega, E)$ or $C(E, t)$ using $C_{n,m}$ obtained in the recursion method, one finds oscillations in these functions as E is varied. These oscillations which have strengths going up to 10-20% of the value, are due to the finite number of $C_{n,m}$'s used in the summations, as well as the inaccuracies inherent in the calculation of $C_{n,m}$. Similar oscillations also appear in the calculation of density of states from the continued fraction in the recursion method.

To remove the above oscillations, one can try to make a convolution of $F(E, E')$ by Lorentzians $L(x)$ depending on E and E' , i.e.,

$$\tilde{F}(E, E') = \int F(t, t')L(t - E)L(t' - E')dt dt' \quad (\text{B.1})$$

Such a convolution suppresses oscillations as a function of E or E' and hence oscillations in $\text{Re}\sigma(\omega, E)$ or $C(E, t)$. Unfortunately, we found that the convolution also decreases the value of $F(E, E')$ by an appreciable amount. Indeed, it is clear from equation (2) that the convolution by a Lorentzian of width Γ is equivalent to introducing an inelastic scattering with relaxation time $\tau_{\text{in}} \sim \frac{\hbar}{\Gamma}$ which can appreciably decrease the conductivity.

We thus used an alternate procedure to calculate $\text{Re}\sigma(\omega, E)$ or $C(E, t)$. In each case we define an intermediate function $f(E)$ by

$$f(E) = N(E) \sum_{n=0}^{\infty} f_n P_n(E) \quad (\text{B.2})$$

where the coefficients f_n are calculated directly from $C_{n,m}$ (see below). $f(E)$ also presents oscillations as a function of E and these are eliminated by a convolution with a Lorentzian $L(x)$, i.e.,

$$\tilde{f}(E) = \int f(x)L(x - E)dx \quad (\text{B.3})$$

Using

$$L(x - E) = -\frac{1}{\pi} \text{Im} \left\{ E - \frac{1}{x} + i\Gamma \right\} \quad (\text{B.4})$$

where 2Γ is the full width at half maximum for the Lorentzian, we obtain

$$\tilde{f}(E) = -\frac{1}{\pi} \sum_{n=0}^{\infty} f_n I_n(T_n(E + i\Gamma)) \quad (\text{B.5})$$

where $T_n(Z)$ is defined in (A.20). For each value of E , $T_n(E + i\Gamma)$ is calculated via equation (A.22) which permits a precise and quick estimate of the convolution. We chose 2Γ to be around 5-10% of the total band width.

B.2. CALCULATION OF $\text{Re}\sigma(\omega, E)$. — In order to calculate $\text{Re}\sigma(\omega, E)$ we define

$$D(\hbar\omega, E) = N(E) \sum_{n,m} C_{n,m} P_n(E) P_m(E + \hbar\omega) \quad (\text{B.6})$$

Here, $D(\hbar\omega, E)$ corresponds to the function $f(E)$ defined in Section B.1. Using equation (1), one obtains

$$\operatorname{Re}\sigma(\omega, E) = \int_{E-\hbar\omega}^E N(E + \hbar\omega) D(E, \hbar\omega) \frac{dE}{\hbar\omega} \quad (\text{B.7})$$

As mentioned above, we develop $D(\hbar\omega, E)$ as

$$D(\hbar\omega, E) = N(E) \sum_{n=0}^{\infty} D_n(\hbar\omega) P_n(E), \quad (\text{B.8})$$

that is

$$\sum_n D_n(\hbar\omega) P_n(E) = \sum_{P,q} C_{P,q} P_P(E) P_q(E + \hbar\omega), \quad (\text{B.9})$$

and by inversion (see A.2) we get

$$D_n(\hbar\omega) = \sum_{P,q} N(E) P_P(E) P_q(E + \hbar\omega) P_n(E) dE, \quad (\text{B.10})$$

which can be calculated as explained in (A.4).

B.3. CALCULATION OF $C(E, t)$. — Using equation (2) we obtain for $C(E, t)$

$$C(E, t) = e^{-iEt} \tilde{C}(E, t), \quad (\text{B.11})$$

with $\tilde{C}(E, t)$ corresponding to $f(E)$ in B.1, i.e.,

$$\tilde{C}(E, t) = N(E) \sum_m \tilde{C}_m(t) P_m(E) \quad (\text{B.12})$$

and

$$\tilde{C}_m(t) = \sum_n C_{n,m} \left(\int N(E) P_n(E') e^{iE't} dE' \right) \quad (\text{B.13})$$

$\tilde{C}_m(t)$ is calculated as explained in A.4.

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