Numerical calculation of the Landauer conductance through an interacting electron system in the Hartree-Fock approximation

Yoichi Asada

Department of Physics, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8551, Japan

We develop a new numerical method to calculate the Landauer conductance through an interacting electron system in the first order perturbation or in the self-consistent Hartree-Fock approximation. It is applied to one and two dimensional systems with nearest-neighbor electron-electron interaction.

KEYWORDS: Landauer conductance, electron-electron interaction, Hartree-Fock approximation

1. Introduction

The interplay between disorder and electron-electron interaction in quantum electron transport phenomena is one of the most challenging problems. Although the non-interacting approximation successfully explains many aspects of experiments, we may need to take into account the electron-electron interaction to understand some phenomena, such as the metallic behavior in two dimensional (2D) systems in Si-MOS and heterostructures, and the critical phenomena of the 3D metal-insulator transitions. In theoretical works, important corrections due to electron-electron interaction in disordered electron systems were found. Furthermore, the study of the nonlinear \( \sigma \) model suggested new universality classes.

The Hartree-Fock (HF) approximation was employed in some numerical works to study interacting disordered electron systems. It enables us to simulate relatively large systems. Even at the level of the HF approximation, however, our understanding is not yet complete. One of the reasons is the lack of numerical simulations of the Landauer conductance. As used in the scaling theory of Anderson localization (See Refs. 20–22 for more detailed discussions on the scaling hypothesis of the Landauer conductance.), the conductance is one of the most important physical quantities to characterize a disordered electron system. We expect that numerical simulation of the Landauer conductance would improve our understanding on the interplay between disorder and electron-electron interaction.

Motivated by this, we have decided to perform a numerical calculation of the Landauer conductance in interacting disordered electron systems in the HF approximation. As a first step toward it we have developed a numerical method, which we report here. The generalization of the Landauer approach to interacting electron systems is a very active topic not only to study interacting disordered electron systems but also to study transport phenomena through low dimensional electron systems. Although much progress has been made in the generalization of the Landauer approach, the calculation method is still being improved.

This paper is organized as follows: In § 2 the model considered is described and in § 3 the Landauer formula is described. The HF approximation is described in § 4. In § 5, we explain a new numerical method, which we call wide band method. In § 6 and § 7, we apply the wide band method to 1D and 2D systems of interacting electrons. The last section is devoted to summary and discussion.

2. Model

We consider spinless electrons on a 2D square lattice. As illustrated in Fig. 1, the system considered consists of a sample region with size \( L_x \times L_y \) (denoted by \( \mathcal{S} \)) and two semi-infinite leads with width \( L_y \) (denoted by \( \mathcal{L} \)). We impose fixed boundary conditions in the transverse direction. We suppose that electrons are interacting in the sample region, while non-interacting in the lead region. In the present paper we do not consider random potential for simplicity. We take the \( x \) direction as the current direction and the \( y \) direction as the transverse direction.

The tight binding Hamiltonian is given by

\[
\mathcal{H} = \mathcal{H}_s + \mathcal{H}_\ell + \mathcal{H}_{\ell s} + \mathcal{H}_u, \tag{1}
\]

where \( \mathcal{H}_s \) is the non-interacting part for the sample region \( \mathcal{S} \), \( \mathcal{H}_\ell \) the Hamiltonian for the perfect leads at the left and right, \( \mathcal{H}_{\ell s} \) the coupling between the sample and leads, and \( \mathcal{H}_u \) electron-electron interaction in the sample region. They are given by

\[
\mathcal{H}_s = -t_s \sum_{(i,j) \in \mathcal{S}} c_{i}^{\dagger} c_{j}, \tag{2}
\]

\[
\mathcal{H}_\ell = -t_\ell \sum_{(i,j) \in \mathcal{L}} c_{i}^{\dagger} c_{j}, \tag{3}
\]

\[
\mathcal{H}_{\ell s} = -t_{\ell s} \sum_{y=1}^{L_y} \left( c_{0,y}^{\dagger} c_{1,y} + c_{1,y}^{\dagger} c_{0,y} \right) + t_{\ell s} \sum_{y=1}^{L_y} \left( c_{L_s,y}^{\dagger} c_{L_s+1,y} + c_{L_s+1,y}^{\dagger} c_{L_s,y} \right), \tag{4}
\]

\[
\mathcal{H}_u = \frac{1}{2} \sum_{i,j \in \mathcal{S}, i \neq j} \left( c_{i}^{\dagger} c_{i} - K \right) U_{i,j} \left( c_{j}^{\dagger} c_{j} - K \right). \tag{5}
\]

Here \( c_i^{\dagger} \) denotes the creation (annihilation) operator of an electron at the site \( i \), \( U_{i,j} \) is the interaction between
Here $G$ and $\Sigma^{(HF)}$ obtained by expanding the time ordered Green’s function change contributions: only in the sample region. It consists of Hartree and exchange in the HF approximation, which is non-zero

\begin{equation}
\end{equation}

3. Landauer conductance

The Landauer conductance $g$ at zero temperature in the linear response regime is expressed using Green’s functions as

\begin{equation}
g = \frac{e^2}{h} \text{tr} \left[ \Gamma^{(L)}(\mu) G_{r,s}^{\alpha}(\mu) \Gamma^{(R)}(\mu) G_{s,r}^{\alpha}(\mu) \right].
\end{equation}

Here $\mu$ is the chemical potential of the system, $G_{r,s}^{\alpha}$ and $G_{s,r}^{\alpha}$ the submatrices of the retarded and advanced Green’s functions in equilibrium, and $\Gamma^{(L,R)}$ the matrices determined by the attached leads.\textsuperscript{23} The matrices $\Gamma^{(L,R)}$ are explicitly shown in Appendix.

It has been shown in Refs. 29 and 31 that the expression (6) can also be justified based on the Keldysh Green’s function method.\textsuperscript{23}

In the following sections, we only consider the retarded Green’s function $G^r$ since the advanced Green’s function $G^a$ is simply Hermitian conjugate of the retarded Green’s function.

4. Hartree-Fock approximation

We describe the HF approximation in the Green’s function formalism\textsuperscript{37} for the system (1).

The Dyson equation for $G^r$ in the HF approximation is obtained by expanding the time ordered Green’s function in $H_u$ and by performing an analytic continuation. We have

\begin{equation}
G^r(\epsilon) = G^0_r(\epsilon) + G^0_r(\epsilon) \Sigma^{(HF)} G^r(\epsilon).
\end{equation}

Here $G^0_r$ is the retarded Green’s function for the non-interacting part of the Hamiltonian $H_0 = H_u + H_s + H_{ts}$, and $\Sigma^{(HF)}$ is the self-energy due to electron-electron interaction in the HF approximation, which is non-zero only in the sample region. It consists of Hartree and exchange contributions:

\begin{equation}
\Sigma^{(HF)}_{i,j} = \sum_{j(j\neq i)} U_{i,j} \left[ -\frac{1}{\pi} \int_0^{\mu} \text{d} \text{Im} G^r_{j,i}(\epsilon) - K \right],
\end{equation}

\begin{equation}
\Sigma^{(HF)}_{i,j,(i\neq j)} = \frac{U_{i,j}}{\pi} \int_0^{\mu} \text{d} \text{Im} G^r_{i,j}(\epsilon),
\end{equation}

where $i,j \in S$. (In more general expression, Im$G^r(\epsilon)$ is replaced with $(-i/2) [G^r(\epsilon) - G^a(\epsilon)]$. For our model, they are the same.) From (7), we have

\begin{equation}
G^r(\epsilon) = \left[ \epsilon - H_0 - \Sigma^{(HF)} + i\eta \right]^{-1}.
\end{equation}

Here $H_0$ is the single particle Hamiltonian in the matrix form corresponding to the non-interacting part $H_0$ and $\eta$ is an infinitesimal positive number. The HF self-energy $\Sigma^{(HF)}$ is a solution of the self-consistent equations (8)–(10).

In practice there are two difficulties we need to solve:

- Since the Landauer geometry corresponds to an open system, the size of the matrix $H_0$ is infinite. We need to make the matrix size finite to perform numerical simulations.
- To calculate the HF self-energy $\Sigma^{(HF)}$, we need to perform an integral over $\epsilon$.

The first problem can be solved by taking account of the effects of the semi-infinite leads in terms of a self-energy.\textsuperscript{23,38–40} For example, if we expand the Green’s function in $H_{ts}$ in addition to $H_u$, we obtain the Dyson equation for the retarded Green’s function $G^r_{i,j}$ ($i, j \in S$) in the HF approximation in a finite size matrix form that is closed in the sample region $S$. The Green’s function $G^r_{i,j}$, with $i,j \in S$, is written as

\begin{equation}
G^r(\epsilon) = \left[ \epsilon - H_s - \Sigma^{(r)}(\epsilon) - \Sigma^{(HF)} + i\eta \right]^{-1}.
\end{equation}

Here $H_s$ is the single particle Hamiltonian in the matrix form corresponding to $H_s$, $\Sigma^{(HF)}$ is the HF self-energy which is given by Eqs. (8) and (9), and $\Sigma^{(r)}$ is the retarded self-energy due to the attached semi-infinite leads. An element of the self-energy $\Sigma^{(r)}_{xy,x'y'}$ is non-zero only when $x = x' = 1$ or $x = x' = L_s$. The non-zero elements are written as (see Appendix)

\begin{equation}
\Sigma^{(r)}_{X,y,X,y'}(\epsilon) = \frac{t_2}{t_1} \sum_n \chi_n(y) \chi_n(y') \left( \frac{\epsilon}{t_1} - \lambda_n \right),
\end{equation}

where $X = 1$ or $L_s$. The Green’s function $G^r_{i,j}$ ($i, j \in S$) of (11) is exactly the same as that of (10) since we have taken into account all orders in $H_{ts}$. Now in (11) the size of the matrices is finite, $L_s L_y \times L_s L_y$, so it is possible to perform numerical calculations in principle.

As for the second problem, a numerical integration was employed in similar approaches.\textsuperscript{39,40} The numerical integration of the Green’s function is not very difficult if a simple system is considered. However the numerical integration is troublesome in general, so we have developed a method to avoid it. The method is explained in the next section.

5. Wide band method

We have developed a new method, which we call wide band method, to avoid the numerical integration as follows.

We change the system considered from the original Landauer system, illustrated in Fig. 1, to another system as illustrated in Fig. 2. We call it wide band system. The lead region is divided into two parts: the region $C$ up to
a length \( L_c \) on both sides of the sample, and the region \( \mathcal{W} \) consisting of two semi-infinite regions. The wide band system is described by the following Hamiltonian,

\[
\hat{H} = \hat{H}_s + \hat{H}_t + \hat{H}_w + \hat{H}_{cw},
\]

which are given by

\[
\hat{H}_t = \hat{H}_c + \hat{H}_w + \hat{H}_{cw},
\]

with \( X_L = -L_c + 1 \) and \( X_R = L_s + L_c \). Here \( \hat{H}_s \) is the Hamiltonian for the finite regions \( \mathcal{C} \) on the sample, \( \hat{H}_w \) the Hamiltonian for the semi-infinite regions \( \mathcal{W} \), and \( \hat{H}_{cw} \) the coupling between the regions \( \mathcal{C} \) and \( \mathcal{W} \). Two hopping parameters \( t_w, t_{cw} \) and one parameter for uniform potential \( \epsilon_w \) are introduced for the wide band system. If \( t_w = t_{cw} = t_t \) and \( \epsilon_w = 0 \), the Hamiltonian (13) is exactly the same as the original Hamiltonian (1), which is the system we want to solve. However, as we explain below, we take a limit \( t_w, t_{cw}, \epsilon_w \rightarrow \infty \) under certain conditions (conditions (24) and (25)). We call this limit wide band limit since the band width in the region \( \mathcal{W} \) becomes infinity in the limit \( t_w \rightarrow \infty \).

We expand the Green’s functions in \( \hat{H}_{cw} \) and \( \hat{H}_w \). The retarded Green’s function for the wide band system (13) in the HF approximation is written as,

\[
\tilde{G}_r^{(w)}(\epsilon) = \left[ -\hat{H}_t - \tilde{\Sigma}^{(w)r}(\epsilon) - \tilde{\Sigma}^{(HF)} + i\eta \right]^{-1}.
\]

Here \( \hat{H}_t \) is the Hamiltonian in a matrix form corresponding to \( \hat{H}_t = \hat{H}_c + \hat{H}_w + \hat{H}_{cw} \), \( \tilde{\Sigma}^{(HF)} \) the self-energy in the HF approximation for the system (13)

\[
\tilde{\Sigma}_{i,i}^{(HF)} = \sum_{j(j \neq i)} U_{i,j} \int_{-\infty}^{\mu} \text{dIm} \tilde{G}_r^{(w)}(\epsilon) - K, \quad (19)
\]

where \( i, j \in \mathcal{S} \), and \( \tilde{\Sigma}^{(w)r} \) the retarded self-energy due to the semi-infinite region \( \mathcal{W} \). An element \( \tilde{\Sigma}_{i,j}^{(x,y,x',y',r)} \) is non-zero only when \( x = x' = X_L \) or \( x = x' = X_R \). The non-zero elements are given by

\[
\tilde{\Sigma}_{X,y,X,y'}^{(w)r}(\epsilon) = \frac{t^2}{t_w} \sum_n \chi_n(y)\chi_n(y') \zeta \left( \frac{\epsilon - \epsilon_w - \lambda_n}{t_w} \right), \quad (21)
\]

where \( X = X_L \) or \( X_R \). The size of matrices in (18) is finite, \( (L_s + 2L_c)L_y \times (L_s + 2L_c)L_y \). We use the tilde to denote that they are the Green’s function and the self-energy not for the original system but for the wide band system.

In the semi-infinite regions \( \mathcal{W} \) we take the wide band limit. In this limit the self-energy \( \tilde{\Sigma}^{(w)r} \) becomes independent of \( \epsilon \) and the non-zero elements of \( \tilde{\Sigma}^{(w)r} \) are equal to

\[
\tilde{\Sigma}_{X,y,X,y'}^{(w)r} = t_t \sum_n \chi_n(y)\chi_n(y') \zeta \left( \frac{\mu}{t_t} - \lambda_n \right). \quad (22)
\]

This limit is obtained by taking the limit,

\[
t_w, t_{cw}, \epsilon_w \rightarrow \infty, \quad (23)
\]

while keeping

\[
t^2_{cw}/t_w = t_t, \quad (24)
\]

\[
\epsilon_w/t_w = -\mu/t_t. \quad (25)
\]

(When \( \mu = 0 \), we do not need to introduce \( \epsilon_w \)).

A similar idea to use an energy independent self-energy can be seen in many papers, for example, Refs. 31 and 41. Two important differences from previous works are:

- We keep non-interacting regions up to a length \( L_c \) on both sides of the sample to reduce artifacts of taking the wide band limit.
- The self-energy for the wide band region is chosen so that electrons at \( \epsilon = \mu \) are not scattered at the boundaries between the regions \( \mathcal{C} \) and \( \mathcal{W} \). This makes it easier to reduce the artifacts.

The self-energy (22) in the wide band limit is equal to the self-energy at \( \epsilon = \mu \) for the original system, i.e., the self-energy (21) with \( t_w = t_{cw} = t_t \) and \( \epsilon_w = 0 \). This means that electrons at the Fermi energy \( \epsilon = \mu \) are not scattered at the boundaries between the regions \( \mathcal{C} \) and \( \mathcal{W} \). When electron-electron interaction is neglected, the Landauer conductance for the wide band system is exactly the same as that for the original Landauer system since the self-energy only at \( \epsilon = \mu \) is relevant for the conductance in non-interacting systems. When we take account of the electron-electron interaction, the conductances for the wide band system and for the original system are no longer the same, because electrons below the Fermi energy affect the motion of electrons at the Fermi energy through the HF self-energy. To reduce such artifacts of taking the wide band limit on the calculated conductance, we keep non-interacting regions up to a length \( L_c \) on both sides of the sample. We expect that the artifacts of taking the wide band limit decrease as \( L_c \) increases, and they are finally removed in the limit \( L_c \rightarrow \infty \).
The absence of boundary scattering for electrons at \( \epsilon = \mu \) is important for the efficiency in removing the artifacts. If electrons near \( \epsilon = \mu \) are scattered strongly at the two boundaries, resonant states due to the boundary scattering can be formed near \( \epsilon = \mu \). In this case, the Green’s function \( \tilde{G}(\mu) \) at the Fermi energy shows larger fluctuation as a function of \( L_c \), and we need to simulate systems with longer \( L_c \) to remove the artifacts. On the other hand, our choice minimize the boundary scattering of electrons near the Fermi energy, that makes it easier to reduce the artifacts of taking the wide band limit.

By taking the wide band limit, the self-energy \( \Sigma^{(w)} \) becomes independent of \( \epsilon \). We define an effective Hamiltonian by

\[
\tilde{H}^{(\text{eff})r} = H_r + \Sigma^{(w)}r + \Sigma^{(\text{HF})}. \tag{26}
\]

Then the Green’s function (18) is written as

\[
\tilde{G}^{r}(\epsilon) = \left[ \epsilon - \tilde{H}^{(\text{eff})r} + i\eta \right]^{-1}. \tag{27}
\]

Note that \( \tilde{H}^{(\text{eff})r} \) is not a Hermitian matrix but is a complex symmetric matrix since \( H_r \) and \( \Sigma^{(\text{HF})} \) are real symmetric matrices and \( \Sigma^{(w)}r \) is a complex symmetric matrix. The effective Hamiltonian has right and left eigenvectors

\[
\langle l_n | \tilde{H}^{(\text{eff})r} | r_n \rangle = q_n | r_n \rangle, \tag{28}
\]

\[
\langle l_n | \tilde{H}^{(\text{eff})r} | q_n \rangle = \langle l_n | q_n \rangle. \tag{29}
\]

Here \( q_n \) is an eigenvalue, which is complex in general. Since the effective Hamiltonian is a complex symmetric matrix, the transpose of the corresponding right eigenvector is the left eigenvector,

\[
\langle l_n | = | r_n \rangle^\top. \tag{30}
\]

For convenience, we impose the following normalization conditions.

\[
\langle l_n | r_m \rangle = \delta_{n,m}. \tag{31}
\]

Then they satisfies the completeness relation,

\[
\sum_n | r_n \rangle \langle l_n | = 1. \tag{32}
\]

By using eigenvalues \( q_n \) and right eigenvectors \( | r_n \rangle \), the retarded Green’s function is expressed as

\[
\tilde{G}^{r}_{i,j}(\epsilon) = \sum_n \frac{\delta_{n,i} \phi_n(j)}{\epsilon - a_n + ib_n + i\eta}. \tag{33}
\]

Here \( a_n \) and \( b_n \) are the real part and the imaginary part of the eigenvalue, \( q_n = a_n - ib_n \), and \( \phi_n(j) = \langle j | r_n \rangle \).

To calculate the self-energy \( \Sigma^{(\text{HF})} \), we need to perform the integral of the imaginary part of the retarded Green’s function

\[
J_{i,j}(\mu, -\epsilon_c) = -\int_{-\epsilon_c}^\mu d\epsilon \text{Im} \tilde{G}^{r}_{i,j}(\epsilon). \tag{34}
\]

For a moment, we introduce a cutoff parameter \( \epsilon_c \). We will take the limit \( \epsilon_c \to \infty \) later. By using the expression

\[
J_{i,j}(\mu, -\epsilon_c) = \sum_n \left\{ \text{Re} \left[ \phi_n(i) \phi_n(j) \right] \left[ \theta_n(\mu) - \theta_n(-\epsilon_c) \right] + \text{Im} \left[ \phi_n(i) \phi_n(j) \right] \ln \left[ \frac{\cos \theta_n(\mu)}{\cos \theta_n(-\epsilon_c)} \right] \right\}, \tag{35}
\]

where \( \theta_n(\epsilon) \in [-\pi/2, \pi/2] \) is defined by

\[
\theta_n(\epsilon) = \tan^{-1} \left( \frac{\epsilon - a_n}{b_n + \eta} \right). \tag{36}
\]

For the second term in (35), we should not take the limit \( \epsilon_c \to \infty \) before taking the summation over \( n \) because of the logarithmic divergence

\[
\ln \left[ \cos \theta_n(-\epsilon_c) \right] = -\ln \epsilon_c + \ln(b_n + \eta) + O(\epsilon_c^{-1}). \tag{37}
\]

The logarithmic divergence disappears when we take the summation over \( n \) because (32) implies

\[
\sum_n \text{Im} \left[ \phi_n(i) \phi_n(j) \right] = 0. \tag{38}
\]

Therefore, in the limit \( \epsilon_c \to \infty \) we have

\[
J_{i,j}(\mu, -\infty) = \sum_n \left\{ \text{Re} \left[ \phi_n(i) \phi_n(j) \right] \left[ \theta_n(\mu + \frac{\pi}{2}) \right] + \text{Im} \left[ \phi_n(i) \phi_n(j) \right] \ln \left[ \frac{\cos \theta_n(\mu)}{b_n + \eta} \right] \right\}. \tag{39}
\]

Thus we calculate the self-energy from the eigenvalues and the right eigenvectors of \( \tilde{H}^{(\text{eff})} \) without performing numerical integration.

Finally the numerical implementation of the wide band method is summarized. First we prepare an initial matrix for \( \Sigma^{(\text{HF})} \). Then we calculate the eigenvalues and eigenvectors by diagonalizing the effective Hamiltonian \( \tilde{H}^{(\text{eff})r} \). From the eigenvalues and right eigenvectors, we calculate the self-energy \( \tilde{\Sigma}^{(\text{HF})} \), (19) and (20), by using (39). We continue this self-consistent iteration until \( \Sigma^{(\text{HF})} \) converges with enough precision. (To ensure convergence, we have used “the method of potential mixing”.) After convergence, we calculate the conductance \( \tilde{g}(L_c) \) for the wide band system by using the expression (6), where \( \tilde{G}^{r,s}(\mu) \) is substituted for \( \tilde{G}^{r,s}(\mu) \). We expect that the conductance \( \tilde{g}(L_c) \) for the wide band system approaches to the conductance \( g \) for the original system in the limit \( L_c \to \infty \),

\[
g = \lim_{L_c \to \infty} \tilde{g}(L_c). \tag{40}
\]

In the case of 1D system (56) we extrapolate \( \tilde{g}(L_c) \) by using an empirical fitting function. In the case of 2D system (57) we make \( L_c \) large enough so that the artifacts of the wide band limit can be negligible to a good approximation.
Hamiltonian $H_0$. The first order Hartree term is zero because the uniform negative charge of the electrons cancels with the uniform positive charge in the background. The first order exchange term at $\mu = 0$ is given by

$$\Sigma_{x,x+1}^{(1st)} = -\frac{U}{\pi} \quad (1 \leq x \leq L_s - 1).$$  \hspace{1cm} (42)

From this self-energy, we obtain the conductance in the first order perturbation. When $L_s$ is odd, we have a perfect transmission,

$$g = \frac{e^2}{h} \quad (L_s : \text{odd}).$$  \hspace{1cm} (43)

For even $L_s$ we have

$$g = \frac{e^2}{h} \left[ \frac{2(1 + U/\pi)}{(1 + U/\pi)^2 + 1} \right]^2 \quad (L_s : \text{even}).$$  \hspace{1cm} (44)

When $U = 0.5$ and $L_s$ is even, we find $g \approx 0.9785e^2/h$.

We have also calculated the conductance in the first order perturbation by using the wide band method. The numerical result in the first order perturbation has been obtained by stopping the self-consistent iteration after just one iteration. When $L_s$ is odd, the conductance is always $e^2/h$ independent of $L_c$ and $L_s$. When $L_s$ is even, the conductance is reduced from $e^2/h$. As shown in Fig. 3, $\tilde{g}(L_c)$ oscillates as a function of $L_c$ when $L_s$ is even.

To remove the artifacts of taking the wide band limit, we need to extrapolate the conductance $\tilde{g}(L_c)$ to $L_c \to \infty$. The extrapolation has been done by using an empirical fitting function of the form,

$$\tilde{g}(L_c) = g + a \cos(\pi L_c/L_s^2).$$  \hspace{1cm} (45)

Here $g$, $a$, and $y$ are fitting parameters. We expect that the asymptotic value $g$ is equal to the conductance for the original system. By fitting numerical data with $L_c = [11, 30]$, we have found $g \approx 0.9785e^2/h$ for any even $L_s$ in the range $L_s = [2, 16]$. The estimates of $a$ and $y$ weakly depend on the range of $L_c$ used for the fit. On the other hand, the estimate of the asymptotic value $g$ is stable against the change of the range of $L_c$.

The asymptotic value $g \approx 0.9785e^2/h$ for even $L_s$ estimated with the wide band method is in good agreement with the analytical result (44) for the original Landauer geometry. The difference of the conductance is of order $10^{-8}$ to $10^{-6}$ in units of $e^2/h$. The good agreement indicates that the wide band method works well to estimate the conductance $g$ by extrapolating the conductance $\tilde{g}(L_c)$ for the wide band system to $L_c \to \infty$.

6.3 In the self-consistent Hartree-Fock approximation

We have then calculated the conductance in 1D in the HF approximation with the wide band method. When $L_s$ is odd, we have found $\tilde{g}(L_c) = e^2/h$ for any $L_c$. When $L_s$ is even, the conductance is reduced from $e^2/h$. We extrapolated the conductance for each even $L_s$ to $L_c \to \infty$ by using the fitting function (45), as in the case of the first order perturbation. Some numerical data and the corresponding fits are shown in Fig. 4. From the fit, we have obtained the asymptotic value $g$ for each even $L_s$. 

Fig. 3. The conductance $\tilde{g}(L_c)$ for the wide band system calculated with the wide band method in 1D in the first order perturbation is shown as a function of $L_c$. We set $K = 0.5$, $\mu = 0.0$, and $U = 0.5$. The dotted lines are the fit of (45) to the data with $L_c = [11, 30]$. The fit deviates from the numerical data when $L_c$ is much smaller than this range. The solid line indicates the conductance for the original system, $g \approx 0.9785e^2/h$, obtained from (44).
Even in the HF approximation it is not impossible to calculate the conductance \( g \) for the original system without using the wide band method. So far we have calculated \( g \) only for \( L_s = 2 \). The Hartree term \( \Sigma_{1,2}^{(HF)} \) is zero when \( \mu = 0 \) because of the particle-hole symmetry. The exchange self-energy \( \Sigma_{1,2}^{(HF)} \) for \( L_s = 2 \) is a solution of

\[
1 - v = -U \left\{ \frac{v^2 - 1}{2v^2} \left[ 1 - \frac{1}{\pi} \tan^{-1} \left( \frac{2v}{v^2 - 1} \right) \right] + \frac{1}{\pi v} \right\},
\]

with \( v = 1 - \Sigma_{1,2}^{(HF)} \). From this equation we find \( \Sigma_{1,2}^{(HF)} \approx -0.1733 \) for \( U = 0.5 \). By using a formula for the conductance

\[
g = \frac{e^2}{h} \left[ \frac{2(1 - \Sigma_{1,2}^{(HF)})}{(1 - \Sigma_{1,2}^{(HF)})^2 + 1} \right]^2,
\]

we find \( g \approx 0.9749e^2/h \) for \( L_s = 2 \) and \( U = 0.5 \). This value of the conductance is indicated with a solid line in Fig. 4. The difference between this value and that estimated from the numerical data when \( L_s \) is much smaller than this range. The solid line indicates the conductance for the original system with \( L_s = 16 \) since it is too difficult for us to calculate the conductance for the original system with \( L_s = 16 \) in the HF approximation.

6.4 Length dependence of the conductance – comparison of numerical results

Figure 5 shows the \( L_s \) dependence of the conductance within the first order perturbation and within the HF approximation. For a reference, the conductance calculated with the embedding method by R. A. Molina and J.-L. Pichard is also shown. In the embedding method, the electron-electron interaction is treated exactly, hence it is thought that the calculated conductance is also exact.

In all three cases, the perfect conductance \( g = e^2/h \) is obtained when \( L_s \) is odd, and the conductance is reduced from it when \( L_s \) is even. This even-odd oscillation was found in Ref. 43. A similar parity oscillation in the Hubbard chain was reported in Ref. 30.

Within the first order perturbation, the conductance is independent of \( L_s \) for all even \( L_s \). However, the result of the embedding method, which is thought to be exact, indicates that the conductance for even \( L_s \) decreases when \( L_s \) increases. The conductance for even \( L_s \) in the HF approximation also shows that the conductance decreases with increasing \( L_s \). So we find a qualitative agreement between the behavior of the conductance in the HF approximation and that of the embedding method. Furthermore, the results indicate that the HF approximation is more accurate than the first order perturbation quantitatively.

7. Application to a 2D system

7.1 System

The application of the wide band method is not restricted to 1D systems. Here we apply it to a 2D system, i.e., a square system \( (L_s = L_w) \). The hopping parameter is supposed to be uniform and set it unity as a unit of energy, \( t_s = t_t = t_{ss} = 1 \). We consider the nearest neighbor electron-electron interaction in the sample region,

\[
U_{i,j} = \begin{cases} 
U & \text{(if } (i,j) \text{ is a n.n pair)} \\
0 & \text{(otherwise).}
\end{cases}
\]

In our simulation, we set the strength of electron-electron interaction \( U = 0.5 \). We set the chemical potential \( \mu = 0 \) and the positive charge \( K = 0.5 \), which corresponds to half-filling.
7.2 In the first order perturbation

First we have calculated the conductance within the first order perturbation to test the wide band method in 2D as it has been tested in 1D in §6.

Within the first order perturbation, we can calculate the conductance without using the wide band method since the self-energy $\Sigma^{(1st)}$ in the first order perturbation for the original Landauer system is obtained as follows. The Hartree contribution is zero since the positive background charge compensates the negative charge of electrons. The exchange contribution is given by

$$\Sigma^{(1st)}_{x,y;x+1,y} = -\frac{2U}{(L_y + 1)\pi} \sum_{n=1}^{L_x} \sin k_y^{(n)} \sin^2 (k_y^{(n)} y), \quad (49)$$

$$\Sigma^{(1st)}_{x,y;x,y+1} = \frac{2U}{(L_y + 1)\pi} \sum_{n=1}^{L_y} k_y^{(n)} \sin (k_y^{(n)} y) \times \sin \left[ k_y^{(n)} (y + 1) \right], \quad (50)$$

where $k_y^{(n)} = \pi n / (L_y + 1)$. We have calculated $\Sigma^{(1st)}$ by taking the summation over $n$ in (49) and (50) numerically, and then have calculated the corresponding conductance $g$.

We have also calculated the conductance making use of the wide band method in the first order perturbation. Figure 6 shows the $L_c$ dependence of the conductance $\tilde{g}(L_c)$ for the wide band systems with sample size $L_s = 8$ and $L_s = 16$. For a reference, the conductance $g$ calculated from (49) and (50) is also shown with the solid line. The figure indicates that $\tilde{g}(L_c)$ fluctuates around the value $g$ and the fluctuation becomes smaller when $L_c$ increases. It is reasonable to assume that the influence of the wide band limit is, to a good approximation, negligible when $L_c = 30$.

$$g \approx \tilde{g}(L_c = 30). \quad (51)$$

We have found that the differences between the value $g$ obtained from (49) and (50) and $\tilde{g}(L_c = 30)$ are of order $10^{-3}$ to $10^{-5}$ in units of $e^2/h$ for $L_s = [2, 16]$. This indicates that the wide band method also works well in 2D.

7.3 In the self-consistent Hartree-Fock approximation

We have then calculated the conductance in 2D with the wide band method in the HF approximation. Figure 7 shows the $L_c$ dependence of the conductance $\tilde{g}(L_c)$ for the wide band systems with sample size $L_s = 8$ and $L_s = 16$. The $L_c$ dependence of $\tilde{g}(L_c)$ is qualitatively similar to that in the first order perturbation. We again assume that the influence of the wide band limit is negligible when $L_c = 30$.

In the range $L_c = [21, 30]$, the fluctuation of $\tilde{g}(L_c)$ is of order $10^{-3}$ in units of $e^2/h$. Assuming that $\tilde{g}(L_c)$ is fluctuating around the asymptotic value $g$, we can consider the amplitude of the fluctuation as a precision of $g$ in the wide band method.

7.4 $L_s$ dependence of the conductance

Figure 8 shows $L_s$ dependence of the conductance in the first order perturbation and in the HF approximation in 2D. For a reference, the value $N_c e^2/h$ corresponding...
Fig. 8. $L_s$ dependence of the conductance $g$ in 2D in the first-order perturbation and in the HF approximations. We set $K = 0.5$, $\mu = 0.0$, and $U = 0.5$. For a reference, the conductance corresponding to the perfect transmission $N_c e^2/h$ is also shown. (At $\mu = 0$, $N_c = L_s$ in the 2D strip imposed fixed boundary conditions in the transverse direction.) The dotted and dashed lines are a guide to the eye only.

to a perfect transmission, with $N_c$ being the number of propagating channels, is also shown. The conductance in the HF approximation tends to be smaller than that in the first order perturbation as it is in 1D.

8. Summary and Discussion

We have developed a new numerical method to calculate the Landauer conductance through an interacting electron system at zero temperature in the first order perturbation or in the self-consistent HF approximation. A troublesome numerical integration is avoided by taking a wide band limit. We can remove the artifacts of taking the wide band limit by increasing the length of non-interacting region $L_c$ kept on both sides of the sample. We have applied it to 1D and 2D interacting systems.

The method does not require much CPU time, so it permits us to accumulate many samples in studying interacting disordered systems. Simulation in the presence of disorder is left for future.

The wide band method has an advantage that the dimensionality is not restricted to one. This method can be useful when studying various quantum transport phenomena not only in interacting disordered systems but also in quantum dots, quantum point contacts, quantum nanowires, atomic chains, and so on. It is possible to consider spin degree of freedom. It is also possible to take account of other effects, such as spin-orbit coupling and a magnetic field, by generalizing the wide band method. In the presence of such effects, the effective Hamiltonian might be no longer a complex symmetric matrix. When it is not a complex symmetric matrix, we need to calculate not only the right eigenvectors but also the left eigenvectors.

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Appendix: Green’s functions for semi-infinite leads and some related matrices

In this appendix, the retarded Green’s function for semi-infinite leads and some related matrices are shown explicitly. We suppose that the leads are described by the Hamiltonian (3) and coupled with a sample by (4).

First we calculate the retarded Green’s function $g^r(\epsilon)$ for the isolated lead at the left ($x \leq 0$). In particular, the important elements are those at the surface of the lead, i.e., the elements $g_{0y,0y'}^{r}(\epsilon)$. The eigenfunctions and eigenvalues of the lead are written as

$$\psi_{k_x,n}(x,y) = \frac{\sqrt{2}}{\pi} \sin[k_x(x-1)] \chi_n(y), \quad (A\cdot1)$$
$$E_{k_x,n} = -2t_\ell \cos k_x + t_\ell \lambda_n. \quad (A\cdot2)$$

where

$$\chi_n(y) = \frac{1}{\sqrt{2(L_y + 1)}} \sin \left( k^{(n)}_y y \right), \quad (A\cdot3)$$
$$\lambda_n = -2 \cos k^{(n)}_y. \quad (A\cdot4)$$

Here $k_x \in [0,\pi]$ is the wave number in the $x$-direction, and $k^{(n)}_y = \pi n / (L_y + 1)$. Using them we have

$$g_{0y,0y'}^{r}(\epsilon) = \frac{1}{t_\ell} \sum_{n=1}^{L_y} \chi_n(y) \chi_n(y') \zeta \left( \frac{\epsilon}{t_\ell} - \lambda_n \right). \quad (A\cdot5)$$

Here the function $\zeta(z_n)$ is given by

$$\zeta(z_n) = \begin{cases} \frac{z_n}{2} + \sqrt{\frac{z_n^2}{4} - 1} & (z_n < -2) \\ \frac{z_n}{2} - i \sqrt{1 - \frac{z_n^2}{4}} & (-2 \leq z_n \leq 2) \\ \frac{z_n}{2} - \sqrt{\frac{z_n^2}{4} - 1} & (z_n > 2). \end{cases} \quad (A\cdot6)$$

Similarly, the Green’s function for the other lead at the right ($x \geq L_s + 1$) is obtained as

$$g_{L_s+1y,L_s+1y'}^{r}(\epsilon) = \frac{1}{t_\ell} \sum_{n=1}^{L_y} \chi_n(y) \chi_n(y') \zeta \left( \frac{\epsilon}{t_\ell} - \lambda_n \right). \quad (A\cdot7)$$

A transverse mode $n$ is a propagating mode if $|\mu / t_\ell - \lambda_n| \leq 2$ and an evanescent mode otherwise. The Fermi wave number $k_F^{(n)} (0 \leq k_F^{(n)} \leq \pi)$ of the propagating mode $n$ in the $x$-direction is determined by

$$e^{-i k_F^{(n)}} = \frac{z_n}{2} - i \sqrt{1 - \frac{z_n^2}{4}}. \quad (A\cdot8)$$
with \( z_n = \mu/t - \lambda_n \).

When calculating the Landauer conductance the semi-infinite leads and the sample are coupled by (4). In the Green’s function method the effects of the lead are taken account in terms of the self-energy.\(^{23,38}\) The retarded self-energy \( \Sigma^{(r)}_{xy,x'y'} \) due to the leads becomes non-zero at the surfaces of the sample, i.e., when \( x = x' = 1 \) or \( x = x' = L_s \). The non-zero elements are defined by \( \Sigma^{(r)}_{1y,1'y'}(\epsilon) = t_{x,s}^2 g_{0y,0y'}(\epsilon) \) and \( \Sigma^{(r)}_{L_y,L_y',y,y'}(\epsilon) = t_{L_y,s}^2 g_{L_y'+1y,L_y+1y'}(\epsilon) \). Using the expression (A-5) we have

\[
\Sigma^{(r)}_{xy,x'y'}(\epsilon) = \frac{t_{x,s}^2}{\ell_s} \sum_{n=1}^{L_u} \chi_n(y)\chi_n(y') \zeta \left( \frac{\epsilon}{t_s} - \lambda_n \right),
\]

(A-9)

where \( X = 1 \) or \( L_s \).

The \( L_y \times L_y \) matrices \( \Gamma^{(L)} \) and \( \Gamma^{(R)} \), which appear in the Landauer formula (6), are defined by \( \Gamma^{(L)}(\epsilon) = i [\Sigma^{(r)}_{1y,1'y'}(\epsilon) - \Sigma^{(a)}_{1y,1'y'}(\epsilon)] \) and \( \Gamma^{(R)}(\epsilon) = i [\Sigma^{(r)}_{L_y,L_y',y,y'}(\epsilon) - \Sigma^{(a)}_{L_y,L_y',y,y'}(\epsilon)] \). At \( \epsilon = \mu \) we have

\[
\Gamma^{(L,R)}(\mu) = \frac{2t_{x,s}^2}{\ell_s} \sum_n \chi_n(y)\chi_n(y') \sin k_F^{(n)}. \quad \text{(A-10)}
\]

Here the summation is taken over propagating modes.

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