

8 / Level Broadening

8.1. Open systems

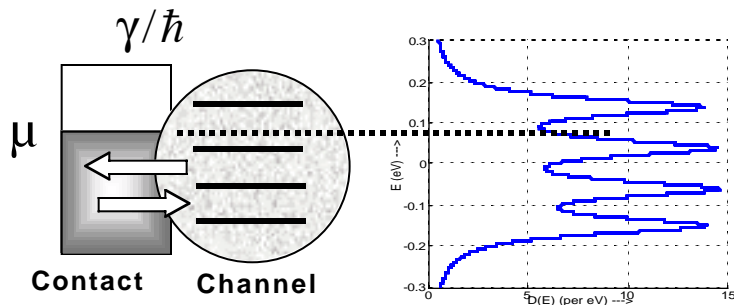
8.2. Local density of states

8.3. Lifetime

8.4. Irreversibility

In the introductory Chapter, we saw that current flow typically involves a channel connected to two contacts which are out of equilibrium with each other, having two distinct electrochemical potentials. One contact keeps filling up the channel while the other keeps emptying it causing a net current to flow from one contact to the other. In the next Chapter we will take up a quantum treatment of this problem. My purpose in this Chapter is to set the stage by introducing a few key concepts using a simpler example: *a channel connected to just one contact* as shown below.

Fig.8.1. A channel connected to one contact. The set of discrete levels broaden into a continuous density of states as shown.



Since there is only one contact, the channel simply comes to equilibrium with it and there is no current flow under steady state conditions. As such this problem does not involve the additional complexities associated with multiple contacts and non-equilibrium conditions. This allows us to concentrate on a different physics that arises simply from connecting the channel with a large contact: The set of discrete levels broadens into a continuous density of states as shown on the right.

In the introductory chapter I introduced this broadening without any formal justification pointing out the need to include it in order to get the correct value for the conductance. My objective in this Chapter is to provide a quantum mechanical treatment

whereby the broadening will arise naturally along with the “uncertainty” relation $\gamma = \hbar/\tau$ connecting it to the escape rate $1/\tau$ for an electron from the channel into the contact. Moreover, we will see that in general the broadening is not just a number γ as we assumed, but a matrix $[\Gamma]$ of the same size as the Hamiltonian matrix $[H]$, which can be energy dependent (unlike $[H]$).

I will start in Section 8.1 from a Schrodinger equation describing the entire channel + contact system (see Fig.8.2):

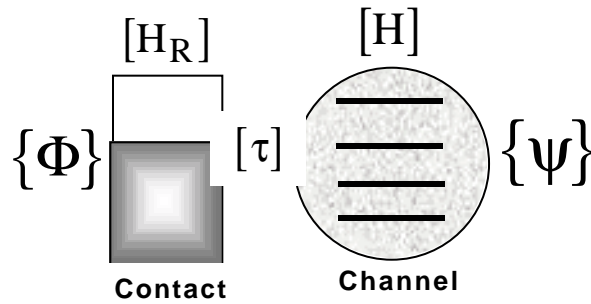
$$E \begin{Bmatrix} \Psi \\ \Phi \end{Bmatrix} = \begin{bmatrix} H & \tau \\ \tau^\dagger & H_R \end{bmatrix} \begin{Bmatrix} \Psi \\ \Phi \end{Bmatrix} \quad (8.1)$$

and show that the contact (denoted by ‘R’ for reservoir) can be eliminated to obtain an equation for the channel only that has the form

$$E \{\Psi\} = [H + \Sigma] \{\Psi\} + \{S\} \quad (8.2)$$

This is the central result that we will use as a starting point in Chapter 8 when we discuss current flow between two contacts. Here $\{S\}$ is a “source” term representing the excitation of the channel by electron waves from the contact, while the *self-energy matrix* $[\Sigma]$ could be viewed as a modification of the Hamiltonian $[H]$ so as to incorporate the “boundary conditions”, somewhat the same way that we added a couple of terms to $[H]$ to account for the periodic boundary conditions (see Eq.(1.3.3)).

Fig.8.2. A channel described by $[H]$ is connected through $[\tau]$ to a contact described by $[H_R]$. We can write an equation for the channel alone that has the form shown in Eq.(8.2).



However, there are two factors that make $[\Sigma]$ much more than a minor modification to $[H]$. Firstly it is energy dependent, which requires a change in our viewpoint from previous chapters where we viewed the system as having resonant energies given by the eigenvalues of

[H]. Since $[\Sigma]$ is energy dependent, we would need to find each of the eigenvalues ϵ_n iteratively, so that it is an eigenvalue of $[H + \Sigma(E = \epsilon_n)]$. It is more convenient to think of the energy E as an *independent variable* and look for the response of the device to incident electrons with different energies and that is the viewpoint we will adopt from hereon.

The second distinguishing feature of the self-energy Σ is that, unlike $[H]$ it is NOT Hermitian and so the eigenvalues of $H + \Sigma$ are complex. Indeed the anti-Hermitian part of Σ

$$\Gamma = -i[\Sigma - \Sigma^\dagger] \quad (8.3)$$

can be viewed as the matrix version of the broadening γ introduced earlier for a one-level device and in Section 8.2 we will relate it to the broadened density of states in the channel. In Section 8.3, we will relate the broadening to the finite lifetime of the electronic states, reflecting the fact that an electron introduced into a state does not stay there forever, but leaks away into the contact.

You might wonder how we managed to obtain a non-Hermitian matrix $[H + \Sigma]$ out of the Hermitian matrix in Eq.(8.1). Actually we do not really start from a Hermitian matrix: we add a infinitesimal quantity $i0^+$ to the reservoir Hamiltonian H_R making it a “tiny bit” non-Hermitian. This little infinitesimal for the reservoir gives rise to a finite broadening Γ for the channel whose magnitude is independent of the precise value of 0^+ . But this seemingly innocuous step merits a more careful discussion, for it essentially converts a reversible system into an irreversible one. As we will explain in Section 8.4, it also raises deeper questions about how large a system needs to be in order to function as a reservoir that leads to irreversible behavior.

In this chapter we are using the concept of self-energy to account for the contacts (like the source and drain) to the channel. However, the concept of self-energy is far more general and can be used to describe all kinds of interactions (reversible and irreversible) with the surroundings and not just the contacts. Indeed this is one of the seminal concepts of many-body physics that is commonly used to describe complicated interactions, compared to which our problem of contacts is a relatively trivial one that could be treated with more elementary methods, though not quite so “elegantly”. My objective, however, is not so much to provide an elegant treatment of a simple problem, as to introduce a deep and profound concept in a simple context. In Chapter 9 we will extend this concept to describe less trivial “contacts”, like the interaction with photons and phonons.

8.1. Open systems

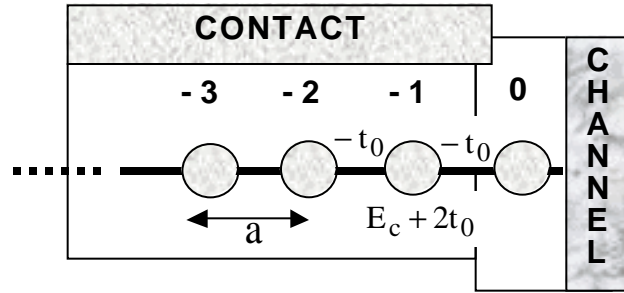
Our objective in this Section is to obtain an equation of the form (see Eq.(8.2))

$$E \{ \psi \} = [H + \Sigma] \{ \psi \} + \{ S \} \quad (8.1.1)$$

describing an open system, unlike the equation $E \{ \psi \} = [H] \{ \psi \}$ that we have been using for closed systems so far. The basic idea is easy to see using a simple toy example.

Toy example: Consider a semi-infinite 1-D wire described by a one-band effective mass Hamiltonian of the form shown in Fig.8.1.1. Let us treat the first point of the wire labeled '0' as our channel and the rest of the wire labeled 'n', $n < 0$ as the contact.

Fig.8.1.1. Toy example: A semi-infinite wire described by a one-band effective mass Hamiltonian. The first point '0' is treated as the channel and the rest as the contact.



If the 'channel' were decoupled from the 'contact' it would be described by the equation:

$$E \psi = \underbrace{(E_c + 2t_0)}_{H \psi} \psi$$

Once we couple it to the 'contact' this equation is modified to

$$E \psi = (E_c + 2t_0) \psi - t_0 \Phi_{-1} \quad (8.1.2)$$

where the contact wavefunctions Φ_n satisfy an infinite series of equations ($n < 0$)

$$E \Phi_n = -t_0 \Phi_{n-1} + (E_c + 2t_0) \Phi_n - t_0 \Phi_{n+1} \quad (8.1.3)$$

Now, since this infinite set of equations all have the same structure we can use the basic principle of bandstructure calculation (see Eq.(4.2.4)) to write the solutions in the form of plane waves, labeled by 'k'. Assuming the solution to have the form of an incident wave from the left and a reflected wave we can write

$$\Phi_n = B \exp(+ikna) + C \exp(-ikna) \quad (8.1.4)$$

$$\text{where } E = E_c + 2t_0 (1 - \cos ka) \quad (8.1.5)$$

Using Eq.(8.1.4) we can write

$$\psi \equiv \Phi_0 = B + C$$

$$\text{and } \Phi_{-1} = B \exp(-ika) + C \exp(+ika)$$

$$\text{so that } \Phi_{-1} = \psi \exp(+ika) + B (\exp(-ika) - \exp(+ika))$$

Substituting back into Eq.(8.1.1) we obtain

$$E \psi = \underbrace{(E_c + 2t_0)\psi}_{H \psi} - \underbrace{t_0 \exp(+ika)\psi}_{\Sigma \psi} + \underbrace{t_0 B (\exp(+ika) - \exp(-ika))}_S \quad (8.1.6)$$

which has exactly the form we are looking for with

$$\Sigma = -t_0 \exp(+ika) \quad (8.1.7a)$$

$$\text{and } S = i t_0 2B \sin(ka) \quad (8.1.7b)$$

Note that the self-energy Σ is non-Hermitian and is independent of the amplitudes B,C of the contact wavefunction. It represents the fact that the channel wavefunction can leak out into the contact. The source term S on the other hand represents the excitation of the channel by the contact and is proportional to B. Let us now go onto a general treatment with an arbitrary channel connected to an arbitrary contact.

General formulation: Consider first a channel with no electrons and is disconnected from the contacts as shown in Fig.8.1.2a. The electrons in the contact have wavefunctions $\{\Phi_R\}$ that obey the Schrodinger equations for the isolated contact

$$[E I_R - H_R + i\eta] \{\Phi_R\} = \{0\} \quad (8.1.8a)$$

where $[H_R]$ is the Hamiltonian for the contact and $[I_R]$ is an identity matrix of the same size as $[H_R]$. I have added a small positive infinitesimal times an identity matrix, $[\eta] = 0^+ [I_R]$ whose significance we will discuss later in Section 8.4.

Fig. 8.1.2. (a) Channel contains no electrons and is disconnected from the contact where the electrons occupy the states described by $\{\Phi_R\}$.

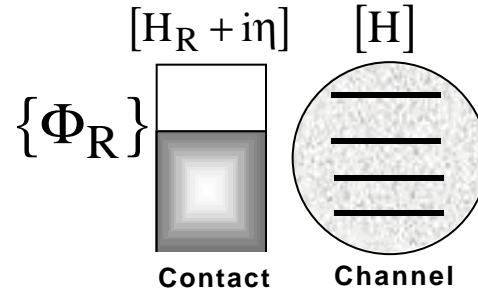
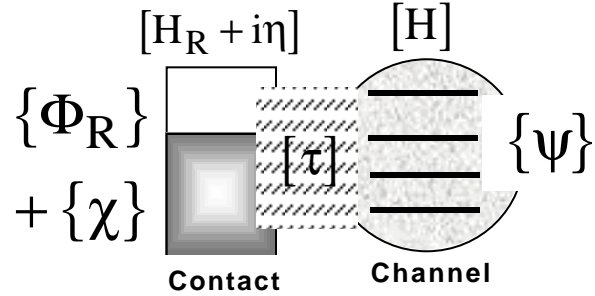


Fig.8.1.2.b. On connecting to the contact, the contact wavefunctions $\{\Phi_R\}$ “spill over” into the device giving rise to a wavefunction $\{\psi\}$ in the channel which in turn generates a scattered wave $\{\chi\}$ in the contact.



Now if we couple the channel to the contact as shown in Fig.8.1.2b, the contact wavefunctions will “spill over” giving rise to a wavefunction $\{\psi\}$ inside the device which in turn will excite scattered waves $\{\chi\}$. The overall wavefunction will satisfy the composite Schrodinger equation for the composite contact – device system which we can write in two blocks:

$$\begin{array}{cc} \text{contact} & \text{device} \\ \text{contact} & \begin{pmatrix} E I_R - H_R + i\eta & -\tau^+ \\ -\tau & EI - H \end{pmatrix} \begin{Bmatrix} \Phi_R + \chi \\ \psi \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \end{array} \quad (8.1.8b)$$

where $[H]$ is the device Hamiltonian. Note that the different quantities appearing in this equation are not numbers (except for the energy E). They are matrices of different sizes

size of the reservoir (R) is often infinite. However, we note that although the matrix $[\tau]$ is formally of size $(d \times R)$, in “real space” it only couples the ‘r’ surface elements of the reservoir next to the channel. So we could truncate it to a $(d \times r)$ matrix and write

$$\Sigma \equiv \begin{matrix} \tau & g_R & \tau^+ \\ (d \times d) & (d \times r) & (r \times r) & (r \times d) \end{matrix} \quad (8.1.12a)$$

$$\text{and} \quad S \equiv \begin{matrix} \tau & \phi_R \\ (d \times 1) & (d \times r) & (r \times 1) \end{matrix} \quad (8.1.12b)$$

where the surface Green’s function g_R represents a $(r \times r)$ subset of the full Green’s function G_R involving just the ‘r’ points at the surface, and $\{\phi_R\}$ represents a $(r \times 1)$ subset of the contact wavefunction $\{\Phi_R\}$. For example for the toy example that we discussed at the beginning of this section, we can show that

$$\tau = -t_0 \quad \phi_R = -i 2B \sin ka \quad (8.1.13a)$$

$$\text{and} \quad g_R = -(1/t_0) \exp(ika) \quad (8.1.13b)$$

which when substituted into Eqs.(8.1.12a,b)) yields the same results that we obtained earlier (cf. Eqs.(8.1.7a,b)). The expression for ϕ_R is obtained by noting that it is equal to the wavefunction Φ_{-1} that we would have in the contact (at the point that is connected to the channel) if it were decoupled from the channel. This decoupling would impose the boundary condition that $\Phi_0 = 0$, making $C = -B$, and the corresponding Φ_{-1} is equal to $(-i 2B \sin ka)$ as stated above. The expression for g_R takes a little more algebra to work out which we will delegate to exercise E.8.1 at the end of the Chapter.

Another way to evaluate Σ and S is to work in the *eigenstate representation* of the contact, so that the contact Hamiltonian H_R is diagonal and the Green's function G_R is easily written down in terms of the eigenvalues ϵ_n of H_R :

$$[G_R(E)] = \begin{bmatrix} \frac{1}{E - \epsilon_1 + i0^+} & 0 & \dots \\ 0 & \frac{1}{E - \epsilon_2 + i0^+} & \dots \\ \dots & \dots & \dots \end{bmatrix} \quad (8.1.14)$$

In this representation, the coupling matrix $[\tau]$ cannot be truncated to a smaller size and we have to evaluate an infinite summation over the eigenstates of the reservoir:

$$\Sigma(E) = \sum_n \frac{[\tau_n][\tau_n]^+}{E - \epsilon_n + i0^+} \quad (8.1.15a)$$

$$S(E) \equiv \sum_n [\tau_n]\{\Phi_R\}_n \quad (8.1.15b)$$

However, this summation can often be carried out analytically after converting to a summation. As an example, Exercise E.8.2 shows how we can obtain our old results (Eqs.(8.1.7a,b)) for the toy problem starting from Eq.(8.1.15).

Before moving on let me briefly summarize what we have accomplished. A channel described by a Hamiltonian $[H]$ of size $(d \times d)$ is coupled to a contact described by a $(R \times R)$ matrix $[H_R]$, where R is typically much larger than d ($R \gg d$). We have shown that the effect of the reservoir on the device can be described through a self-energy matrix $\Sigma(E)$ of size $(d \times d)$ and a source term $S(E)$ of size $(d \times 1)$.

8.2. Local density of states

We have just seen that a channel coupled to a contact can be described by a modified Schrodinger equation of the form $E\{\psi\} = [H + \Sigma]\{\psi\} + \{S\}$ where $\{S\}$ represents the excitation from the contact and the self-energy Σ represents the modification of the channel by the coupling. Unlike $[H]$, $[H + \Sigma]$ has complex eigenvalues and the imaginary part of the eigenvalues (a) broadens the density of states and (b) gives the eigenstates a finite lifetime. In this Section we will talk about the first effect and explain how we can calculate the density of states in an open system. In the next section we will talk about the second effect.

Consider the composite system consisting of the channel and the contact. Earlier in Chapter 5 we agreed that a system with a set of eigenvalues ϵ_α has a density of states given by

$$D(E) = \sum_{\alpha} \delta(E - \epsilon_{\alpha}) \quad (8.2.1)$$

How can different energy levels have different weights as implied in the broadened lineshape on the right of Fig.8.1? Doesn't Eq.(8.2.1) tell us that each energy level gives rise to a delta function whose weight is one? The problem is that the density of states in Eq.(8.2.1) does not take into account the spatial distribution of the states. If we want to know the local density of states in the channel we need to weight each state by the fraction of its squared wavefunction that resides in the channel denoted by 'd':

$$D(d;E) = \sum_{\alpha} |\phi_{\alpha}(d)|^2 \delta(E - \epsilon_{\alpha})$$

For example, suppose the device with one energy level ϵ were decoupled from the reservoir with a dense set of energy levels $\{\epsilon_R\}$. The total density of states would then be given by

$$D(E) = \sum_{\alpha} \delta(E - \epsilon_{\alpha}) = \delta(E - \epsilon) + \sum_n \delta(E - \epsilon_n)$$

while the local density of states on the channel would simply be given by

$$D(d;E) = \sum_{\alpha} |\phi_{\alpha}(d)|^2 \delta(E - \epsilon_{\alpha}) = \delta(E - \epsilon)$$

since the reservoir states have wavefunctions that have no amplitude in the channel at all. Once we couple the channel to the reservoir, things will not be so clear cut any more. There will be one level with its wavefunction largely on the channel, but there will be many other neighboring states with their wavefunctions residing partially on the channel. If we look at the local density of states in the channel we see a series of energy levels with varying heights reflecting the fraction of the squared wavefunction residing in the channel.

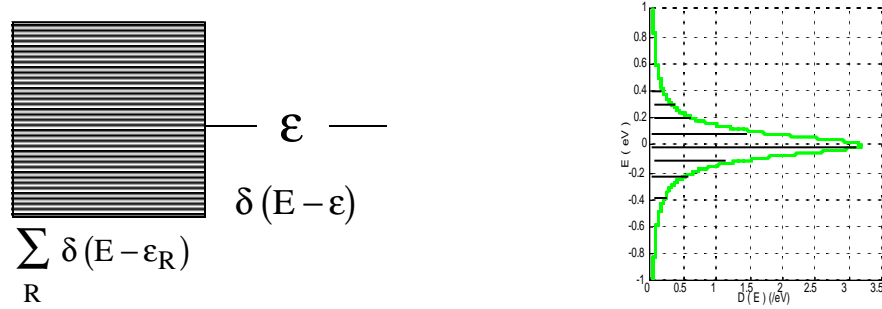


Fig.8.1.1. A channel with a single energy level ε coupled to a reservoir with a dense set of energy levels $\{\varepsilon_n\}$. The local density of states on the channel shows a single sharp level, before being coupled to the reservoir. But on being coupled, it shows a series of levels of varying heights reflecting the fraction of their squared wavefunction that reside in the channel.

In general we can define a local density of states (LDOS) $D(\vec{r};E)$ that weights each level by the square of its wavefunction at the location \vec{r} :

$$D(\vec{r};E) = \sum_{\alpha} |\phi_{\alpha}(\vec{r})|^2 \delta(E - \varepsilon_{\alpha}) \quad (8.2.2)$$

which can be viewed as the diagonal element (divided by 2π) of a more general concept called the spectral function, $[A(E)]$:

$$A(\vec{r}, \vec{r}'; E) = 2\pi \sum_{\alpha} \phi_{\alpha}(\vec{r}) \delta(E - \varepsilon_{\alpha}) \phi_{\alpha}^*(\vec{r}') \quad (8.2.3)$$

$$\text{just as the electron density} \quad n(\vec{r}) = \sum_{\alpha} |\phi_{\alpha}(\vec{r})|^2 f_0(\varepsilon_{\alpha} - \mu) \quad (8.2.4)$$

can be viewed as the diagonal element of the density matrix:

$$\rho(\vec{r}, \vec{r}') = \sum_{\alpha} \phi_{\alpha}(\vec{r}) f_0(\epsilon_{\alpha} - \mu) \phi_{\alpha}^*(\vec{r}') \quad (8.2.5)$$

We have argued earlier in Section 3.3 that Eq.(8.2.5) is just the real space representation of the matrix relation:

$$[\rho] = f_0 ([H] - \mu [I]) \quad (8.2.6)$$

Using the same argument we could write the spectral function as

$$[A(E)] = 2\pi \delta(E [I] - [H]) \quad (8.2.7)$$

and view Eq.(8.2.3) as its real space representation. If we use the eigenstates of H as our basis

then [H] is diagonal : $[H] = \begin{bmatrix} \epsilon_1 & 0 & 0 & \dots \\ 0 & \epsilon_2 & 0 & \dots \\ 0 & 0 & \epsilon_3 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}$

and so is [A(E)] :

$$[A(E)] = 2\pi \begin{bmatrix} \delta(E - \epsilon_1) & 0 & 0 & \dots \\ 0 & \delta(E - \epsilon_2) & 0 & \dots \\ 0 & 0 & \delta(E - \epsilon_3) & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \quad (8.2.8)$$

Eq.(8.2.3) transforms this matrix to a real space representation. In principle we could write the spectral function in any representation and its diagonal elements will tell us the LDOS (times 2π) at energy E in that representation, just as the diagonal elements of the density matrix tell us the local electron density in that representation. The total number of electrons, N is given by the sum of all the diagonal elements of $[\rho]$ or the trace of $[\rho]$ which is independent of representation:

$$N = \text{Trace} [\rho] = \sum_{\alpha} f_0(\epsilon_{\alpha} - \mu)$$

Similarly, the total density of states given by the trace of the spectral function $[A]$ divided by 2π is independent of representation and is readily written down from the eigenstate representation:

$$D(E) = \frac{1}{2\pi} \text{Trace} [A(E)] = \sum_{\alpha} \delta(E - \epsilon_{\alpha}) \quad (8.2.9)$$

Sum rule: An important point to note is that if we look at the total number of states at any point integrated over all energy, the answer is one. If we start with a device having one level and couple it to reservoir, it will broaden into a series of levels (Fig.8.1.1) of varying strengths representing the fact that wavefunction for each level contributes to different extents to the device. But if we add up the strengths of all the levels the answer is the same as that of the original level. What the device loses from its one level due to hybridization, it gains back from the other levels so that the broadened level in the device can accommodate exactly the same number of electrons that the one discrete level could accommodate before it got coupled to the reservoir. This sum rule could be stated as follows:

$$\int_{-\infty}^{+\infty} dE D(\vec{r}; E) = 1$$

and can be proved by noting that

$$\int_{-\infty}^{+\infty} dE D(\vec{r}; E)$$

is basically the diagonal element of the matrix

$$\int_{-\infty}^{+\infty} dE [A(E)]/2\pi$$

evaluated in the real space representation. It is easy to see from Eq.(8.1.8) that in the eigenstate representation

$$\int_{-\infty}^{+\infty} \frac{dE}{2\pi} [A(E)] = \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \quad \text{since} \quad \int_{-\infty}^{+\infty} dE \delta(E - \epsilon) = 1$$

The point is that this quantity will look the same in *any representation* since the identity matrix remains unchanged by a change in basis.

Green's function: In evaluating the spectral function it is convenient to make use of the identity

$$\begin{aligned} 2\pi \delta(E - \epsilon_\alpha) &= \left[\frac{2\eta}{(E - \epsilon_\alpha)^2 + \eta^2} \right]_{\eta \rightarrow 0^+} \\ &= i \left[\frac{1}{E - \epsilon_\alpha + i0^+} - \frac{1}{E - \epsilon_\alpha - i0^+} \right] \end{aligned} \quad (8.2.10a)$$

to write
$$2\pi \delta(EI - H) = i \left(\left[(E + i0^+)I - H \right]^{-1} - \left[(E - i0^+)I - H \right]^{-1} \right) \quad (8.2.10b)$$

where 0^+ denotes a positive infinitesimal (whose physical significance we will discuss at length in the Section 8.4). Eqs.(8.2.10b) would be a simple extension of (8.2.10a) if the argument $(EI - H)$ were an ordinary number. But since $(EI - H)$ is a matrix, Eq.(8.2.10b) may seem like a big jump from Eq.(8.2.10a). However, we can justify it by going to a representation that diagonalizes $[H]$, so that both sides of Eq.(8.2.10b) are diagonal matrices and the equality of each diagonal element is ensured by Eq.(8.2.10a). We can thus establish the matrix equality, Eq.(8.2.10b) in the eigenstate representation, which should ensure its validity in any other representation.

Using Eqs.(8.2.7) and (8.2.10b) we can write

$$A(E) = i [G(E) - G^+(E)] \quad (8.2.11)$$

where the retarded Green's function is defined as

$$G(E) = \left[(E + i0^+)I - H \right]^{-1} \quad (8.2.12a)$$

and the advanced Green's function is defined as

$$G^+(E) = \left[(E - i0^+)I - H \right]^{-1} \quad (8.2.12b)$$

In the next section we will see how the Green's function (and hence the spectral function) can be evaluated for open systems.

Density matrix: Starting from $[\rho] = f_0 ([H] - \mu [I])$ (same as Eq.(8.2.6))

we can write

$$\begin{aligned}
 [\rho] &= \int_{-\infty}^{+\infty} dE f_0(E - \mu) \delta([E] - [H]) \\
 &= \int_{-\infty}^{+\infty} \frac{dE}{2\pi} f_0(E - \mu) [A(E)]
 \end{aligned}
 \tag{8.2.13}$$

which makes good sense if we note that $[A(E)] / 2\pi$ is the matrix version of the density of states $D(E)$, the same way that the density matrix $[\rho]$ is the matrix version of the total number of electrons, N . We could view Eq.(8.2.10) as the matrix version of the common sense relation

$$N = \int_{-\infty}^{+\infty} dE f_0(E - \mu) D(E)$$

which simply states that the number of electrons is obtained by multiplying the number of states $D(E) dE$ by the probability $f_0(E)$ that they are occupied and adding up the contributions from all energies.

Why should we want to use Eq.(8.2.13) rather than Eq.(8.2.6)? In previous chapters we have evaluated the density matrix using Eq.(8.2.6) and it may not be clear why we might want to use Eq.(8.2.10) since it involves an extra integration over energy. Indeed if we are dealing with the entire system described by a matrix $[H]$ then there is no reason to do so. But if we are dealing with an open system described by a matrix of the form (see Fig.8.2)

$$\bar{H} = \begin{bmatrix} H & \tau \\ \tau^+ & H_R \end{bmatrix}$$

then Eq.(8.2.6) requires us to deal with the entire matrix which could be huge compared to $[H]$ since the reservoir matrix $[H_R]$ is typically huge – that is why we call it a reservoir! The spectral function appearing in Eq.(8.2.10) or the Green's function too is technically just as large

$$\bar{A} = \begin{bmatrix} A & A_{dR} \\ A_{Rd} & A_{RR} \end{bmatrix}, \quad \bar{G} = \begin{bmatrix} G & G_{dR} \\ G_{Rd} & G_{RR} \end{bmatrix}$$

but we only care about the top (dxd) subsection of this matrix and the great advantage of the Green's function approach is that this subsection of $[G(E)]$, and hence $[A(E)]$, can be calculated without the need to deal with the full matrix. This is what we will show next, where we will encounter the same self-energy matrix Σ that we encountered in the last Section.

Self-energy matrix - all over again: The overall Green's function can be written from Eq.(8.2.12a) as

$$\bar{G} \equiv \begin{bmatrix} G & G_{dR} \\ G_{Rd} & G_{RR} \end{bmatrix} = \begin{bmatrix} (E + i0^+)I - H & -\tau \\ -\tau^\dagger & (E + i0^+)I - H_R \end{bmatrix}^{-1} \quad (8.2.14)$$

The power of the Green's function method comes from the fact that we can evaluate the (dxd) subsection $[G]$ that we care about *exactly* from the relation

$$G = [(E + i0^+)I - H - \Sigma(E)]^{-1} \quad (8.2.15)$$

where $\Sigma(E)$ is the self-energy matrix given in Eq.(8.1.11).

Eq.(8.2.15) follows from Eq.(8.2.14) using straightforward matrix algebra. The basic result we make use of is the following.

$$\text{If } \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} \quad (8.2.16a)$$

$$\text{then } \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}$$

$$\text{so that } Aa + Bc = I \text{ and } Ca + Dc = 0 \rightarrow c = -D^{-1}Ca$$

$$\text{Hence } a = (A - BD^{-1}C)^{-1} \quad (8.2.16b)$$

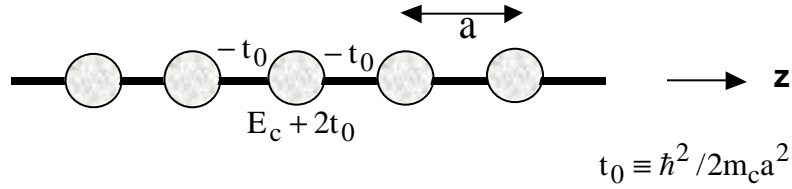
Comparing Eq.(8.2.16a) with Eq.(8.2.14) and making the obvious replacements we obtain from Eq.(8.2.16b)

$$G = \left[(E + i0^+)I - H - \tau G_R \tau^+ \right]^{-1} \quad \text{where} \quad G_R = \left[(E + i0^+)I - H_R \right]^{-1}$$

which yields the result stated above in Eq.(8.2.15).

Eq.(8.2.16b) is a well-known result that is often used to find the inverse of large matrices by *partitioning* them into smaller ones. Typically in such cases we are interested in finding all the component matrices a, b, c and d and they are all approximately equal in size. In our problem, however, the matrices a, A are much smaller than the matrices d, D and we only want to find ‘a’. Eq.(8.2.15) allows us to evaluate [G] by inverting a matrix of size (dxd) rather than the full (d+R) x (d+R) matrix in Eq.(8.2.14). This can be a major practical advantage since R is typically much larger than d. But the idea of describing the effect of the surroundings on a device through a self-energy function [Σ] is not just a convenient numerical tool. It represents a major conceptual step and we will try to convey some of the implications in the next Section. For the moment, let us look at a couple of examples, one analytical and one numerical.

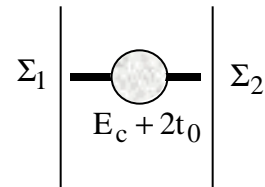
Analytical example: Consider a uniform infinite 1-D wire modeled with a one-band effective mass Hamiltonian of the form



Since this is a uniform wire the eigenstates can be catalogued in terms of ‘k’ obeying a dispersion relation and we can use our results from Chapter 5 to write the DOS per unit cell as

$$D(E) = a / \pi \hbar v(E) \quad \text{where} \quad v = (1/\hbar) dE / dk$$

Now let us obtain this same result using the Green’s function method developed in this section. We replace the infinite 1-D wire with a *single* unit cell and add self-energy terms to account for the two semi-infinite wires on either side.



The Green's function for this single cell is a (1x1) matrix or a number

$$G(E) = \frac{1}{E - (E_c + 2t_0 - t_0 \exp[ika] - t_0 \exp[-ika])}$$

which is simplified making use of the dispersion relation $E = E_c + 2t_0 (1 - \cos ka)$ to obtain

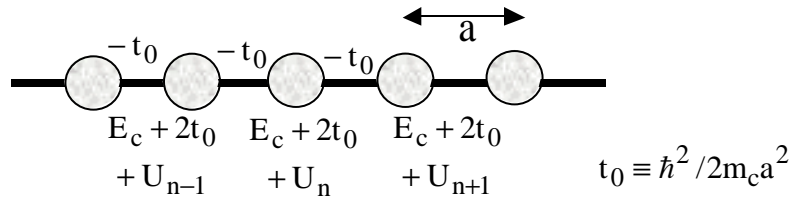
$$G(E) = \frac{1}{t_0 \exp[ika] - t_0 \exp[-ika]} = \frac{1}{2i t_0 \sin ka}$$

from which the DOS is obtained:

$$\begin{aligned} D(E) &= i[G - G^+]/2\pi \\ &= 1/2\pi t_0 \sin ka = a/\pi \hbar v \quad \rightarrow \quad \text{same as previous result} \end{aligned}$$

since $\hbar v = dE/dk = 2at_0 \sin ka$

Numerical example: To get a feeling for the self-energy method, it is instructive to redo the problem of finding the equilibrium electron density in a 1-D box that we discussed in Chapter 3 (see Fig.3.3.1). We consider a similar problem, namely, a 1-D box with a potential $U(x)$ that changes linearly from -0.1 eV at one end to $+0.1$ eV at the other end. We model it using a one-band Hamiltonian with a lattice of 50 points spaced by $a = 2\text{\AA}$ and with the effective mass m_c equal to 0.25 times the free electron mass m :



We wish to evaluate the electron density $n(z)$ in the box assuming that it is in equilibrium with an electrochemical potential $\mu = E_c + 0.25$ eV and $k_B T = 0.025$ eV. The electron density is

given by the diagonal elements of the density matrix ρ which we can evaluate in one of two ways:

1. We could assume periodic boundary conditions: $H(1,100) = H(100,1) = -t_0$ and then evaluate ρ from Eq.(8.1.6).
2. We could add self-energy terms (Eqs.(8.2.14), (8.2.15)) which have non-zero values of $-t_0 \exp[ika]$ only on the end points (1,1) or (100,100), evaluate the Green's function from Eq.(8.2.3)

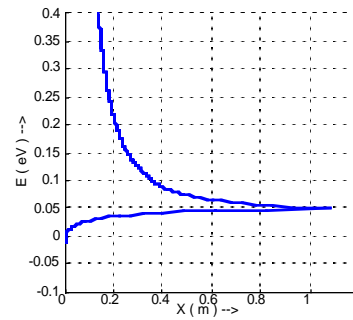
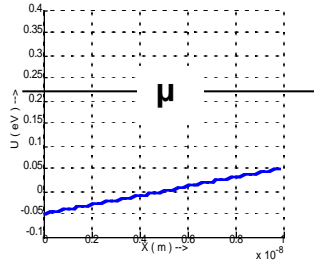
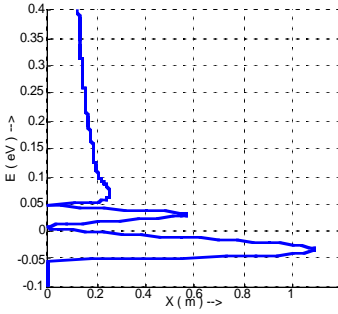
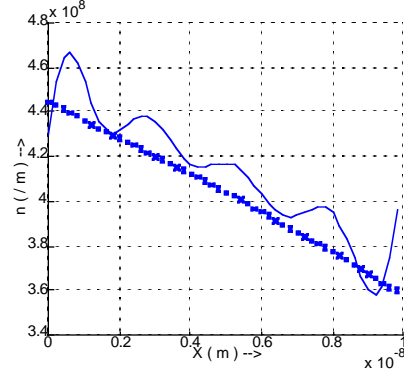
$$G = [(E + i0^+)I - H - \Sigma_1 - \Sigma_2]^{-1}$$

obtain the spectral function from Eq.(8.2.11)) and then calculate the equilibrium density matrix from Eq.(8.2.10).

Fig.8.2.3 shows that the two results agree well. Indeed some discrepancy is likely due to errors introduced by the discreteness of the energy grid used for the integration in the last step of method. We have used a grid having 250 points in the energy range $E_c - 0.1 \text{ eV} < E < E_c + 0.4 \text{ eV}$. However, the oscillations in the first method arise from the standing waves in a closed ring (resulting from the use of periodic boundary conditions) which are absent in the open system modeled by the self-energy method. These oscillations in method 1 will be less pronounced for longer devices (or larger effective mass), because the energy levels will get closer together.

As we know the effect of the self-energy is to broaden the energy level, but its integrated strength is unchanged because of the sum rule mentioned earlier. Consequently the distinction between the two methods is somewhat obscured when we look at the electron density since it involves an integration over energy. The self-energy method allows us to investigate in detail the local density of states in different parts of the device (see Fig.8.2.4).

Fig.8.2.3. Plot of electron density, $n(z)$ calculated for a 1-D wire with a linear potential $U(z)$ (see Fig.8.2.4) using periodic boundary conditions (solid line) and using the self-energy method to enforce open boundary conditions (x's).



(a) LDOS at left end of device (b) Potential $U(x)$ across device (c) LDOS at right end of device

Fig. 8.2.4. Local density of states (LDOS) at two ends of a 1-D wire with a linear potential $U(x)$ impressed across it. The corresponding electron density is shown in Fig.8.2.3. with $\mu = E_c + 0.25$ eV and $k_B T = 0.025$ eV.

8.3. Lifetime

In Section 8.2 we introduced the concept of Green's function, $G(E)$ as a convenient way to evaluate the spectral function, $A(E)$ based on the mathematical identity:

$$2\pi\delta(EI-H) = i \left(\left[(E + i0^+)I - H \right]^{-1} - \left[(E - i0^+)I - H \right]^{-1} \right)$$

$$[A(E)] = i ([G(E)] - [G^+(E)])$$

However, as we will explain in this Section, the Green's function has a physical significance of its own as the *impulse response* of the Schrodinger equation and this will help us understand the “uncertainty” relation between the broadening of a level and the finite lifetime, both of which result from the coupling to the reservoir. To understand the meaning of the Green's function let us use the eigenstates of H as our basis so that the Green's function is diagonal :

$$[G(E)] = \begin{bmatrix} \frac{1}{E - \epsilon_1 + i0^+} & 0 & 0 & \dots \\ 0 & \frac{1}{E - \epsilon_2 + i0^+} & 0 & \dots \\ 0 & 0 & \frac{1}{E - \epsilon_3 + i0^+} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \quad (8.3.1)$$

Consider the Fourier transform of $G(E)$ defined by

$$[\tilde{G}^R(t)] = \int_{-\infty}^{+\infty} \frac{dE}{2\pi\hbar} e^{+iEt/\hbar} [G(E)]$$

which is also diagonal and looks like this :

$$[\tilde{G}^R(t)] = \frac{-i}{\hbar} \vartheta(t) e^{-0^+ t} \begin{bmatrix} \exp(-i\epsilon_1 t/\hbar) & 0 & 0 & \dots \\ 0 & \exp(-i\epsilon_2 t/\hbar) & 0 & \dots \\ 0 & 0 & \exp(-i\epsilon_3 t/\hbar) & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \quad (8.3.2)$$

It takes a little work (involving contour integration on a complex plane) to get from Eq.(8.3.1) to Eq.(8.3.2). But it is quite straightforward to go the other way from Eq.(8.3.2) to Eq.(8.3.1)

using the inverse transform relation: $[G(E)] = \int_{-\infty}^{+\infty} dt e^{+iEt/\hbar} [\tilde{G}^R(t)]$

$$\begin{aligned} \frac{-i}{\hbar} \int_{-\infty}^{+\infty} dt e^{iEt/\hbar} \vartheta(t) e^{-i\epsilon t/\hbar} e^{-0^+ t} \\ = \frac{-i}{\hbar} \int_0^{+\infty} dt e^{i(E-\epsilon)t/\hbar} e^{-0^+ t} = \frac{1}{E - \epsilon + i0^+} \end{aligned}$$

I should mention that here I am not using the superscript ‘R’ to denote reservoir. I am using it to denote ‘retarded’ which refers to the fact that the function $\tilde{G}^R(t)$ is zero at all times $t < 0$. It is easy to see that the diagonal elements of this function satisfies the differential equation

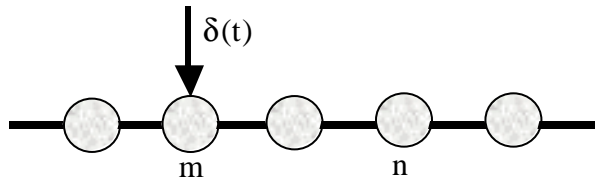
$$\left(i\hbar \frac{\partial}{\partial t} - \epsilon_\alpha \right) \tilde{G}_{\alpha\alpha}^R(t) = \delta(t)$$

$$\text{so that we can write } \left(i\hbar \frac{\partial}{\partial t} - [H] \right) [\tilde{G}^R(t)] = [I] \delta(t) \quad (8.3.3)$$

suggesting the interpretation of $\tilde{G}^R(t)$ as the impulse response of the Schrodinger equation

$$\left(i\hbar \frac{\partial}{\partial t} - [H] \right) \{\Psi(t)\} = 0 \quad (8.3.4)$$

The (n,m) element of this matrix $\tilde{G}_{nm}^R(t)$ tells us the n th component of the wavefunction if the system is given an impulse excitation at its m th component:



From this point of view it seems natural to expect that the Green's function should be “retarded”, since we cannot have a response before the impulse is applied (which is at $t = 0$). Mathematically, however, this is not the only solution to Eq.(8.3.3). It is straightforward to show that the “advanced” Green's function

$$[\tilde{G}^A(t)] = [\tilde{G}^R(-t)]^* \quad (8.3.5)$$

satisfies the same equation,
$$\left(i\hbar \frac{\partial}{\partial t} - [H] \right) [\tilde{G}^A(t)] = [I] \delta(t) \quad (8.3.6)$$

but it is zero at all times *after* $t = 0$. In the eigenstate representation we can write from Eqs.(8.3.2) and (8.3.5):

$$[\tilde{G}^A(t)] = \frac{i}{\hbar} \vartheta(-t) e^{+0^+ t} \begin{bmatrix} \exp(-i\varepsilon_1 t/\hbar) & 0 & 0 & \dots \\ 0 & \exp(-i\varepsilon_2 t/\hbar) & 0 & \dots \\ 0 & 0 & \exp(-i\varepsilon_3 t/\hbar) & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \quad (8.3.7)$$

This is actually the Fourier transform of $G^+(E)$ (once again it is easier to do the inverse transform). The difference between the retarded and advanced Green's function in the energy domain

$$\begin{array}{cc} \textit{Retarded} & \textit{Advanced} \\ G(E) = [(E + i0^+)I - H]^{-1} & G^+(E) = [(E - i0^+)I - H]^{-1} \end{array}$$

looks very minor: The two only differ in the sign of an infinitesimally small quantity 0^+ - one is tempted to conclude wrongly that they differ only in some insignificant sense. In the time domain, however, their difference is hard to miss. One is zero for $t < 0$ (causal) and the other is zero for $t > 0$ (non-causal). One is interpreted as the response to an impulse excitation at $t = 0$; the other has no physical interpretation but is a mathematically valid solution of the same equation with a different unphysical initial condition. In Fig. 8.3.1 we have sketched the magnitude of one of the diagonal elements of $\tilde{G}_{\alpha\alpha}^R(t)$ and $\tilde{G}_{\alpha\alpha}^A(t)$. Note that the spectral function is proportional to the difference between the retarded and advanced Green's functions (see Eq.(8.1.11)) :

$$\tilde{A}_{\alpha\alpha}^R(t) = i [\tilde{G}_{\alpha\alpha}^R(t) - \tilde{G}_{\alpha\alpha}^A(t)]$$

Since both Green's functions satisfy the same differential equation, the spectral function, $[a(t)]$ satisfies the homogeneous differential equation without the impulse excitation :

$$\left(i\hbar \frac{\partial}{\partial t} - [H] \right) [\tilde{A}(t)] = [0]$$

and hence has no discontinuity at $t = 0$ unlike $\tilde{G}^R(t)$ and $\tilde{G}^A(t)$ as shown in Fig.8.3.1.

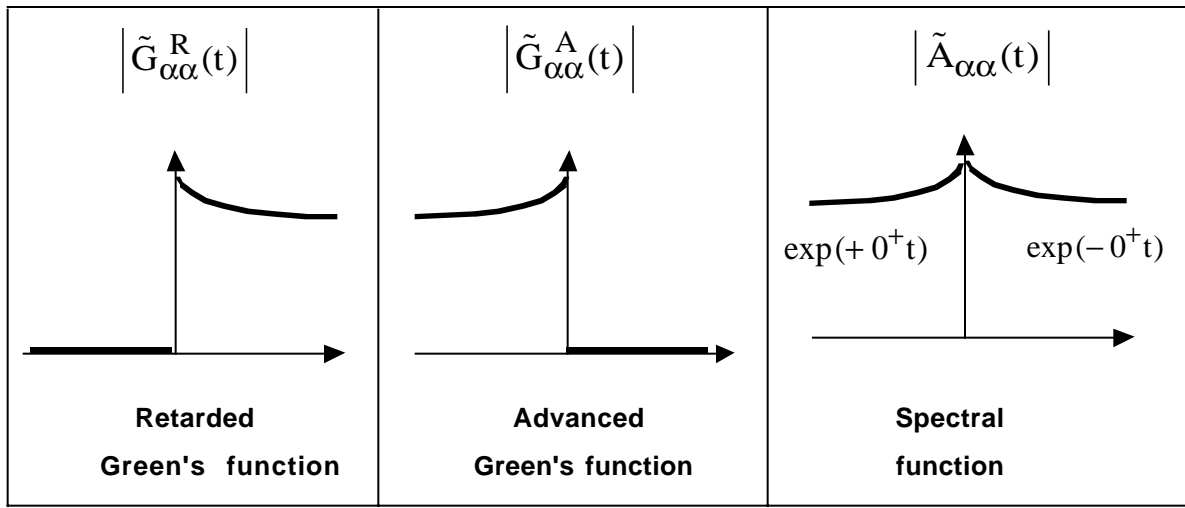


Fig.8.3.1. Sketch of the magnitude of any diagonal element (in the eigenstate representation) of the retarded and advanced Green's functions and the spectral function in the time domain.

Physical meaning of the self-energy: We have seen in Section 8.2 that we can calculate the device subsection of the full Green's function

$$\bar{G} \equiv \begin{bmatrix} G & G_{dR} \\ G_{Rd} & G_{RR} \end{bmatrix} = \begin{bmatrix} (E + i0^+)I - H & -\tau \\ -\tau^+ & (E + i0^+)I - H_R \end{bmatrix}^{-1} \quad (\text{same as Eq.(8.2.2)})$$

exactly from the relation $G = [(E + i0^+)I - H - \Sigma(E)]^{-1}$ (same as Eq.(8.2.3))

where the self-energy $\Sigma(E) = \tau g_R(E) \tau^+$ (same as Eq.(8.2.7))

can be calculated from a knowledge of the surface property of the reservoir (g_R) and the device-reservoir coupling (τ).

Now that we have interpreted the time domain Green's function as the impulse response of the Schrodinger equation (see Eq.(8.3.3)), we could write a similar equation for the device subset of the Green's function by Fourier transforming Eq.(8.2.3). This would be straightforward if the self-energy Σ were independent of the energy E :

$$\left(i\hbar \frac{\partial}{\partial t} - [H] - [\Sigma] \right) [\tilde{G}^R(t)] = [I] \delta(t) \quad (8.3.8a)$$

If we take the energy dependence into account then the Fourier transform looks more complicated. The product of $\Sigma(E)$ and $G(E)$ when transformed becomes a convolution in time domain.

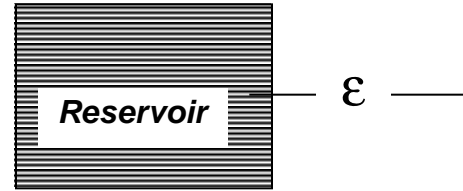
$$\left(i\hbar \frac{\partial}{\partial t} - [H] \right) [\tilde{G}^R(t)] - \int dt' [\tilde{\Sigma}(t-t')] [\tilde{G}^R(t')] = [I] \delta(t) \quad (8.3.8b)$$

To get some insight into the physical meaning of Σ let us ignore this “detail”. In fact, let us make the problem real simple by considering a small device with just a single energy level ϵ so that $[H]$ and $[\Sigma]$ are both simple numbers rather than matrices:

$$\left(i\hbar \frac{\partial}{\partial t} - \epsilon - \Sigma \right) \tilde{G}^R(t) = \delta(t)$$

The solution to this equation

$$\tilde{G}^R(t) = -\frac{i}{\hbar} e^{-i(\epsilon+\Sigma)t/\hbar} \vartheta(t)$$



tells us the wavefunction in response to an impulse excitation of the device at $t = 0$. we can write

$$\tilde{G}^R(t) = -\frac{i}{\hbar} e^{-i\epsilon't/\hbar} e^{-\gamma t/2\hbar} \vartheta(t) \quad (8.3.9)$$

$$\text{where } \epsilon' = \epsilon + \text{Re } \Sigma \quad \text{and} \quad \gamma = -2 \text{Im } \Sigma \quad (8.3.10)$$

The real part of the self-energy causes a shift in the device energy level from ϵ to ϵ' , while the imaginary part has the effect of giving the eigenstates a finite lifetime. This is evident from the squared magnitude of this wavefunction which tells us how the probability decays with time after the initial excitation:

$$\left| \tilde{G}^R(t) \right|^2 = \frac{1}{\hbar^2} \vartheta(t) \exp(-\gamma t / \hbar)$$

Clearly we can relate the lifetime of the state to the imaginary part of the self-energy:

$$\frac{1}{\tau} = \frac{\gamma}{\hbar} = -\frac{2\text{Im}\Sigma}{\hbar} \quad (8.3.11)$$

We can identify this as the “uncertainty” relation between lifetime and broadening if we note that the imaginary part of the self-energy is equal to the broadening of the density of states. To see this we note that the Fourier transform of the simple version of the Green’s function in Eq.(8.3.9) is given by

$$G(E) = \frac{1}{E - \epsilon' + i\gamma/2}$$

$$\begin{aligned} \text{so that} \quad \frac{A(E)}{2\pi} \equiv D(E) &= i \left(\frac{1}{E - \epsilon' + i\gamma/2} - \frac{1}{E - \epsilon' - i\gamma/2} \right) \\ &= \frac{\gamma}{(E - \epsilon')^2 + (\gamma/2)^2} \end{aligned}$$

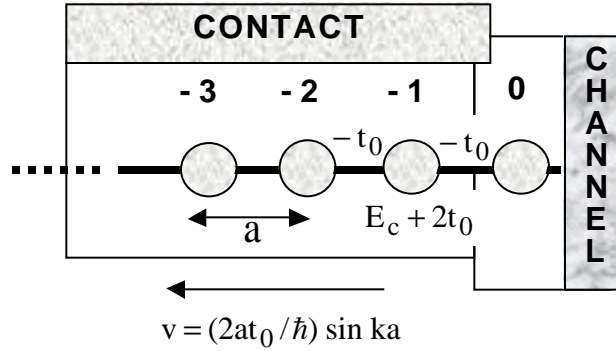
showing that the LDOS on the device is broadened into a Lorentzian of width γ equal to twice the imaginary part of the self-energy. Of course, the lineshape in general need not be Lorentzian. We have obtained this result because in this discussion we ignored the energy dependence of the self-energy (in the time domain one would call it the memory effect of the reservoir) and used Eq.(8.3.8a) instead of (8.3.8b) for the purpose of clarity in this physical discussion.

We have seen in Section 8.1 that the self-energy for a one-dimensional contact is diagonal with two non-zero entries:

$$\Sigma(1,1) = -t_0 \exp(ika) = -t_0 \cos(ka) - it_0 \sin(ka)$$

From Eq.(8.3.11) we could write the corresponding lifetime for the site '1' as

$$\frac{1}{\tau} = \frac{\gamma}{\hbar} = \frac{2t_0 \sin ka}{\hbar}$$



It is interesting to note that the velocity associated with a particular 'k' in the wire is given by

$$v = \frac{1}{\hbar} \frac{\partial E}{\partial k} = \frac{1}{\hbar} \frac{\partial}{\partial k} [2t_0(1 - \cos ka)] = \frac{2at_0}{\hbar} \sin(ka)$$

so that we can write $\frac{1}{\tau} = \frac{\gamma}{\hbar} = \frac{v}{a}$

which is intuitively satisfying since we expect the escape rate from a given cell to equal the escape velocity divided by the size of a cell. Indeed one could use this principle to write down the imaginary part of the self-energy approximately for more complicated geometries where an exact calculation of the surface Green's function may not be easy:

$$\text{Im } \Sigma(E) \approx \hbar v(E) / R \quad (8.3.12)$$

Here 'R' is a linear dimension of the unit cell, the precise arithmetic factor depending on the specific geometry.

Knowing the imaginary part, one can calculate the real part too from a general principle independent of the specific details. The principle is that the real and imaginary part must be Hilbert transforms of each other (\otimes denotes convolution)

$$\text{Re } \Sigma(E) = \int dE' \frac{\text{Im } \Sigma(E')}{E - E'} = \text{Im } \Sigma(E) \otimes \frac{1}{E} \quad (8.3.13)$$

so that the self-energy can be written in the form

$$\Sigma(E) = [\text{Re } \Sigma(E)] - i [\text{Im } \Sigma(E)] = -i \text{Im } \Sigma(E) \otimes \left(\delta(E) + \frac{i}{E} \right) \quad (8.3.14)$$

This principle is obeyed by any function whose Fourier transform is causal (that is, the Fourier transform is zero for $t < 0$). The self-energy function is causal because it is proportional to the surface Green's function of the reservoir (see Eq.(8.2.7)) which is causal as we discussed earlier. To see why causal functions obey this principle, we note that $\delta(E) + (i/E)$ is the Fourier transform of the unit step function: $\vartheta(t)$. This means that any time domain function of the form $\vartheta(t) f(t)$ has a Fourier transform that can be written as (product in the time domain becomes a convolution in the transform domain)

$$F(E) \otimes \left(\delta(E) + \frac{i}{E} \right)$$

where $F(E)$ is the transform of $f(t)$ and is real if $f(t)$ is a symmetric function.

Broadening matrix: In the simple case of a one-level device we have seen that the imaginary part of the self-energy gives us the broadening or inverse lifetime of the level (see Eq.(8.3.11)). More generally, the self-energy is a matrix and one can define a broadening matrix $\Gamma(E)$ equal to its anti-Hermitian component:

$$\Gamma(E) = i [\Sigma(E) - \Sigma^\dagger(E)] \quad (8.3.15)$$

This component of the self-energy is responsible for the broadening of the level, while the Hermitian component

$$\Sigma_H(E) = \frac{1}{2} [\Sigma(E) + \Sigma^+(E)]$$

can conceptually be viewed as a correction to the Hamiltonian $[H]$. Overall we could write

$$H + \Sigma(E) = [H + \Sigma_H(E)] - \frac{i\Gamma(E)}{2}$$

We have often made use of the fact that we can simplify our description of a problem by using the eigenstates of the Hamiltonian $[H]$ as our basis. For open systems we would want to use a representation that diagonalizes $[H + \Sigma_H]$ in our energy range of interest. If the same representation also diagonalizes $[\Gamma]$, then the problem could be viewed simply in terms of many one-level devices in parallel. But in general this may not be the case. The representation that diagonalizes $[H + \Sigma_H]$ may not diagonalize $[\Gamma]$ and vice versa. We can then diagonalize one or the other but not both and interesting new physics beyond the one-level example can result.

8.4. Irreversibility

One might wonder how a non-Hermitian operator Σ could emerge from a system consisting of two parts each of which is described by a Hermitian operator (H and H_R in Fig.8.2)! Mathematically, this results from the “infinitesimal” $i0^+$ (see Eq.(8.3.1)) that converts the retarded Green’s function (see Fig.8.3.1) from the non-decaying function on the left to a weakly decaying function on the right:



This is often justified mathematically as an artifice used to ensure the convergence of the Fourier transform. However, this seemingly innocuous step essentially converts a reversible system into an irreversible one by adding an imaginary (non-Hermitian) component $i0^+$ [I] into an otherwise Hermitian matrix [H]. Surely something this profound cannot be the result of a minor mathematical artifice designed to ensure convergence! It is thus reasonable to ask what this infinitesimal $i0^+$ physically represents.

To understand this, let us consider a device with a single state with $\varepsilon = 0$, and a reservoir that consists of numerous closely spaced energy levels: $\{\varepsilon_r, r = 1, 2, \dots\}$ as shown in Fig.8.4.1. The point I want to make is that the infinitesimal $i0^+$ represents the rate at which the electron is extracted from the reservoir levels by external devices (like a battery terminal for instance) and the system will behave irreversibly as long as this quantity exceeds the spacing between the energy levels in the reservoir. Typically with large reservoirs, the energy levels are extremely closely spaced (perhaps by pico eV!) and only an infinitesimal external influence (expressed by the infinitesimal $i0^+$, whose precise value is unimportant) is needed to induce irreversible behavior. But if the level spacing were larger, say meV (and this is not unlikely with “nanostructured contacts”) then the behavior of the system will depend on the precise value of $i0^+$ reflecting the actual broadening of “reservoir” levels by external influences. In this case the contact is really not functioning like a reservoir.

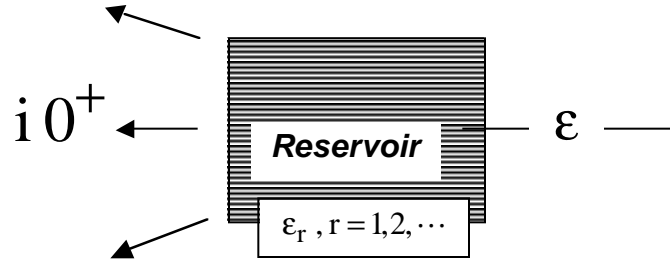


Fig.8.4.1. A device with a single state with $\varepsilon = 0$ is coupled to a reservoir that consists of numerous closely spaced energy levels: $\{\varepsilon_r, r = 1, 2, \dots\}$. The infinitesimal $i0^+$ represents the rate at which the electron is extracted from the reservoir levels by external devices (like a battery terminal for instance) and the system will behave irreversibly as long as this quantity exceeds the spacing between the energy levels in the reservoir.

Let me explain my point a little further with a numerical example. The overall system in Fig.8.4.1 is described by a large Hamiltonian matrix of the form

$$\begin{bmatrix} \varepsilon & \tau_1 & \tau_2 & \tau_3 & \dots \\ \tau_1^* & \varepsilon_1 & 0 & 0 & \dots \\ \tau_2^* & 0 & \varepsilon_2 & 0 & \dots \\ \tau_3^* & 0 & 0 & \varepsilon_3 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}$$

We have seen that we can eliminate the reservoir degrees of freedom and describe the device with a (1x1) “matrix” $[\varepsilon + \Sigma]$ where (see Eq.(8.2.4))

$$\Sigma = \left[\sum_r \frac{|\tau_r|^2}{E - \varepsilon_r + i\eta} \right]_{\eta \rightarrow 0^+}$$

so that

$$\text{Re } \Sigma = \left[\sum_r \frac{|\tau_r|^2 (E - \varepsilon_r)}{(E - \varepsilon_r)^2 + \eta^2} \right]_{\eta \rightarrow 0^+} \quad (8.4.1)$$

$$-\text{Im } \Sigma = \left[\sum_r \frac{|\tau_r|^2 \eta}{(E - \epsilon_r)^2 + \eta^2} \right]_{\eta \rightarrow 0^+} \quad (8.4.2a)$$

$$\longrightarrow \pi \sum_r |\tau_r|^2 \delta(E - \epsilon_r) \quad (8.4.2b)$$

We have seen that the broadening and the inverse lifetime are related to the imaginary part of the self-energy and can be written as (see Eq.(8.3.11))

$$\frac{1}{\tau} = \frac{\gamma}{\hbar} = -\frac{2\text{Im}\Sigma}{\hbar} = \frac{2\pi}{\hbar} \sum_r |\tau_r|^2 \delta(E - \epsilon_r) \quad (8.4.3a)$$

If the coupling elements τ_r are all approximately equal, then we can take it outside the summation and simplify Eq.(8.4.3) to

$$\frac{1}{\tau} = \frac{\gamma}{\hbar} \approx \frac{2\pi}{\hbar} |\tau_r|^2 \sum_r \delta(E - \epsilon_r) = \frac{2\pi}{\hbar} |\tau_r|^2 D_R(E) \quad (8.4.3b)$$

where $D_R(E)$ is the reservoir density of states. This is a standard result, often referred to as Fermi's golden rule.

The inverse lifetime in Eq.(8.4.3) is interpreted as the rate at which an electron initially located in the device escapes into the reservoir. But this interpretation is appropriate only if the infinitesimal η appearing in Eq.(8.4.2) is larger than the spacing between the energy levels of the reservoir. For example, if we assume that the reservoir has 2000 equally spaced energy levels between -1 and 1 eV, then $D_R(E) = 1000/\text{eV}$ (since we have 2000 levels evenly distributed over 2 eV). Fig.8.4.1a shows the device LDOS calculated from

$$D(E) = \frac{A(E)}{2\pi} = -\frac{1}{\pi} \text{Im } G(E) = -\frac{1}{\pi} \text{Im} \left(\frac{1}{E - \epsilon - \Sigma(E)} \right)$$

using the expression for the self-energy $\Sigma(E)$ from Eq.(8.4.2a) with each of the coupling matrix elements τ_r set to .005 eV and the infinitesimal 0^+ set to .001eV.

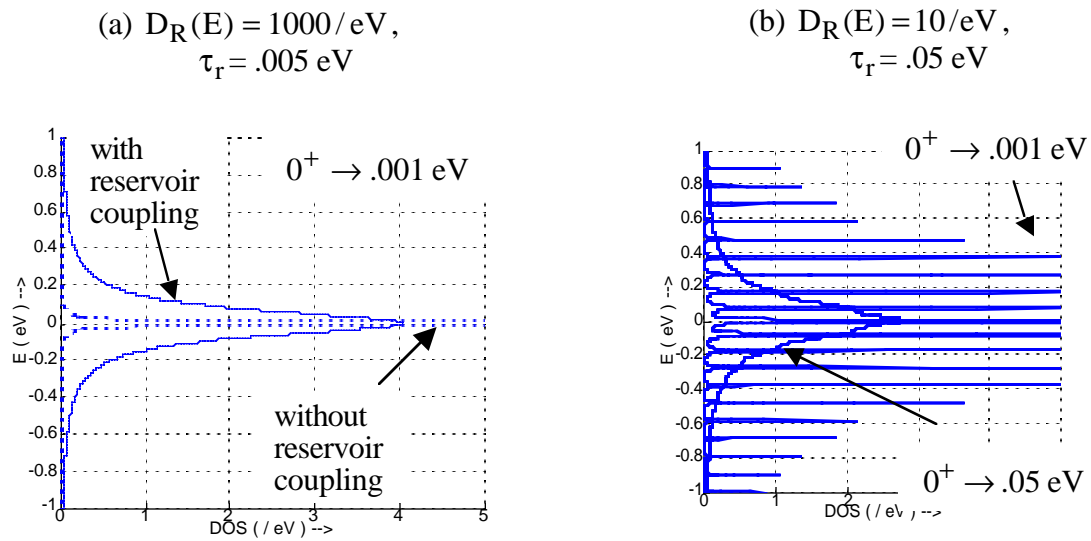


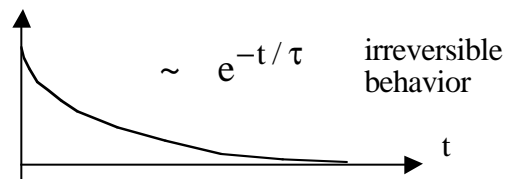
Fig.8.4.1. LDOS for a one-level device connected to a reservoir: (a) $D_R(E) = 1000/\text{eV}$, $\tau_r = .005 \text{ eV}$ and $0^+ \rightarrow .001 \text{ eV}$. (b) $D_R(E) = 10/\text{eV}$, $\tau_r = .05 \text{ eV}$ and two values of 0^+ .

The resulting lineshape is well described by a Lorentzian

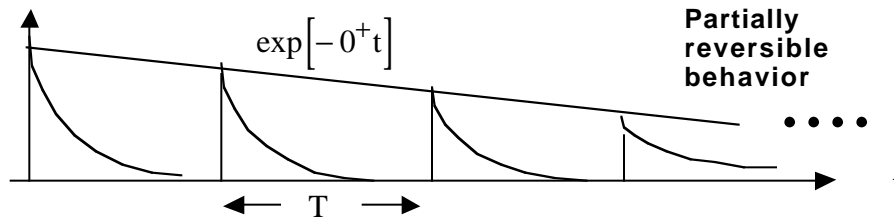
$$D(E) = \frac{\gamma/2\pi}{E^2 + (\gamma/2)^2} \quad (8.4.4)$$

with a width γ given by Eq.(8.4.3b): $\gamma = 2\pi [0.005 \text{ eV}]^2 [1000/\text{eV}] \approx 0.0785 \text{ eV}$.

Now consider what happens if we choose a reservoir with states that are 100 times less dense but with the coupling elements τ_r that are 10 times as strong. The corresponding broadening γ is unchanged. But the LDOS now looks distinctly different, depending on whether we use $0^+ \rightarrow .05 \text{ eV}$ or $0^+ \rightarrow .001 \text{ eV}$ (see Fig.8.4.1b). With $0^+ \rightarrow .05 \text{ eV}$, we have a single broadened line whose Fourier transform looks like a decaying exponential



indicating that an electron placed in the device will escape into the reservoir with a lifetime of τ . By contrast, with $0^+ \rightarrow .001$ eV, we have a line consisting of multiple spikes whose Fourier transform looks periodic with a period $T = h/\Delta E$ (ΔE : spacing between energy levels in the reservoir) which is known as the recurrence time



indicating that an electron placed in the device will oscillate back and forth between the device and reservoir if the infinitesimal " 0^+ " is smaller than ΔE .

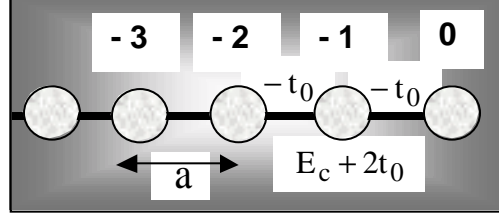
This is really an old problem in physics that is not unique to quantum mechanics. For example we know that if we turn off a car it will slow down and lose its energy to the surface of the road which will get heated. But if we tried to use Newton's law to model this by coupling the car to a finite number of "molecules" on the surface of the road, we would end up with reversible behavior. The car would slow down initially, but after some time would gain back all the energy from the road – a result completely at odds with our everyday experience where the energy flows away for ever and never comes back. To include this in a theoretical model we would either have to add a damping term to the molecules (equivalent to adding $i0^+$) or use a system so large that the recurrence time is larger than our time of simulation.

The same is true of electrons escaping into any "contact". Occasionally experiments do show "echoes" but this happens seldom enough that people write papers when they see it. And so to describe the observed behavior in the real world it is necessary to assume that the reservoir states have a broadening 0^+ from their interaction with the surroundings that exceeds their level spacing, making the reservoir density of states essentially a continuous function of energy, rather than a set of discrete impulses. But it is important to remember that a "nanocontact" may not function like a traditional reservoir if it has an energy level spacing that exceeds its broadening " 0^+ " due to external influences.

Exercises

E.8.1. Assume a 1-D one band effective mass model for a 1-D lead

$$t_0 \equiv \hbar^2 / 2m_c a^2$$

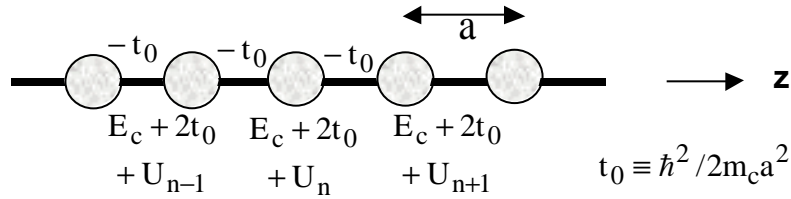


Starting from Eq.(8.1.9) $G_R = \left[(E + i0^+)I - H_R \right]^{-1}$

Show that $G_R(0,0) \equiv g_R = -\exp(ika) / t_0$ (8.1.13b)

E.8.2. Starting from Eqs.(8.1.15a), evaluate the self-energy for a semi-infinite lead by carrying out the summation analytically after converting to an integral and compare with Eq.(8.1.15).

E.8.3. Consider a 1-D wire with a potential $U(x)$ that changes linearly from -0.1 eV at one end to $+0.1$ eV at the other end and model it using a one-band Hamiltonian with a lattice of 50 points spaced by $a = 2\text{\AA}$ and with the effective mass m_c equal to 0.25 times the free electron mass m :



Calculate the electron density $n(z)$ in the wire assuming that it is in equilibrium with an electrochemical potential $\mu = E_c + 0.25$ eV and $k_B T = 0.025$ eV, using (a) periodic boundary conditions and (b) the self-energy method. Compare with Fig.8.2.3.

Calculate the LDOS at the two ends of the box from the self-energy method and compare with Fig.8.2.4.

E.8.4. Consider a device with a single state with $\varepsilon = 0$, connected to a reservoir such that the overall system is described by a Hamiltonian $[H]$ of the form

$$\begin{bmatrix} \varepsilon & \tau_1 & \tau_2 & \tau_3 & \cdots \\ \tau_1^* & \varepsilon_1 & 0 & 0 & \cdots \\ \tau_2^* & 0 & \varepsilon_2 & 0 & \cdots \\ \tau_3^* & 0 & 0 & \varepsilon_3 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}$$

Calculate the LDOS in the device as a function of the energy E using the parameters indicated in **Fig.8.4.1**.