Chapter 8: Transport (Mainly, Boltzmann transport equation)

- Boltzmann transport equation Relaxation time approximation
- 3. Conductivity

- 1. Impuirty scaltering
 5. Electron phonon scaltering
 6. Electron-electron scattering

- Refs: 1. hecture notes by Brown. (Sec 22)
 - 2. J. Selom (Vola) Chapter 29
 - 3. P. Phillips chapter 11-5.

Generally, every thermodynamically extensive quantity or order parameter that we study, such as number denisty, charge denisty, magnetization, energy durity, heat durity, enhopy durity, etc, has an associated current density, which is defined by the density times reloatly. (of course, some of the durnities one related to each other, such as charge density and current density are related to each other by charge e' and entropy durity is related to heat denity by the forofortionality constant Teta). Generally, what does that mean in that time decirative of the dentity of the quantity in hard is defined by the spatial gradient of the corresponsiting current density, is, the continuity equation. The continuity equation is a manifestation of the conservation of energy and monuntum. But as the electron undergoes scattering with external perturbation (such as impurity, phonon) they loose I gain momentum and for energy and hence the continuity equation is modified to the Boltzmann countries that me want to duive hue.

In conducted matter we measure current durity and the corresponding response furctions (such as electrical conductivity.) Itermal conductivity) to the corresponding external perturbations in a linear response theory. The conductivity of present interest is related to the current-current (retarded) communitator which we have computed already in a fermiomic system and axise from the energy absorption due to particle hale continuum.

But this calculation does not include the impurity scattering and abdront phonon scattering which does not conserve the every and momentum of clictons.

A full quantum nuchamical formulation of from post in which we compute the evolution of an eletronic state with a Hamiltonian that incorporates energy, momentum nonconservation is difficult and requires non-Hermitian Hamiltonian formulism. The Drude model is a fully classical one in which one studies the evolution of the elictron's coordinates (7) urder a "dissipative force" which models scattering to impurity, nucleus etc. A dissipative force, by difinition, in proportional to the relouty of the electron as defined by $\vec{F} \propto -\vec{v} = -2\vec{v}$, where \vec{r} is like the friction, arising due to collision of elictrons with impurity, nucleus etc. Here it is customery to express of in terms of "relaxation time" & Cor mean free path 1 = 42) between the two collisions (on average). This can be defined using dimensional analysis (since force = m i) to be n= m/x, where m is the electron's mass. For an applied electric field, the electric force F=- & E equates to the dissipative force, in a steady state, which gives

$$-e\vec{E} = -\frac{m}{2}\vec{v} = -\frac{m}{nez}\vec{J} \qquad [\vec{J} = ne\vec{v}]$$

Then using Coulomb's law I = 0 E, we get

To or mean free path in the only parameter in this theory. In the Fermi liquid theory and in the electron-phonon coupling chapter, we argued that if the relaxation time is governed by the electron's life time in a momentum (Bloch) state. This is captured

by the imaginary found of the self-energy. Alternatively, & can be calculated by using the Fermi Golden rule, evaluating the matrix element of scattering of a state to omother state under a given potential. At finite temperature, the thermal energy kgT also contribute to the relaxation time as $X = T_i(k_BT)$.

The Drude model, dispite being a fully classical model, is quite successful in the case where the mean-free falts l=2 2 is much larger than their de-Oroglie wavelength such that quantum effect i nigligible. Do improve the Drude model, we have to divelop a quantum theory of the evolution of the want furchion *(r) under a dissipative force. Shi is very hard and is under active current research. Here we will consider an intermediate route - the semiclassical route - in with me will study the evolution of the occupation density n(F) of chetrons under a dissipative force. Occupation denvity itself is a quantum operator and can be written in terms of the field operator Y(x) as n(x) = 4 (x) Y(x). We are however going to thudy its evolution as a "classical" protectivity for occupying a ringle boutide state, but we will enforce the quantum statistics by restricting to single occupancy for electring. Hence it a semi-classical trentment.

It we are in some single particle sixurstate and that the system is in some thermal equilibrium, then the occupation durity is simply the Fermi-Dirac distribution function $n = f(k) = [\exp((E_R - \mu)/k_BT + 1)]$. But so we apply an electrostatic

potential difference $\vec{E} = -\vec{\nabla} \vec{\varphi}$, it gives a spatial variation of the chemical potential M(r) or as a temperature gradient in applied, we have T(r). To the first approximation, we incorporate the r-observance in $\mu \not\in T$ in the same occupation durity

n(r, k) = f(r, k) = [exp(&_-min)/kBT(r)+1] --- (2).

This is actually a crude approximation in which we assume the energy cipenvalue En remains the dame. We will see below that this approximation is valid for slow vorceation of μ + T in space. In fact, the occupation durity can also be time deferredult, in general, for mon-equilibrium case. Then such a distribution functions of (5, k, t) is called the non-equilibrium distribution function. It looks strange to define the distribution function to be a function of both possition and momentum. Because, in cord melter, we often define the states in the momentum space only by the usage of Bloch states. This definition is justified when we use a wave fachel form of the wave function, not just the Bloch state.

Therefore, f(r,k,t) is like a prosphility distribution obligance of in the Phase space (r,k). The time evolution of a number durity in the phase space was derived by Bollzmann in 1873 or so when the quantum mechanics was not formulated. This is severally called the Boltzmann transport equation, we once going during this Boltzmann transport equation for the fermion distribution function have in the phase space for elichostatic potential as well as with

a te	mperature gradien Conductivity du dissipatron.	t, and there	by compute elu etering mechanis	trical m whi
causes	dissipation.		U	

Boltzmann Transport Equation:

In the phase space, $f(\bar{r}, \bar{k}, t)$ is like the ensemble density of defining the number of electrons present at time t in a phase space volume element $d^3 \delta d^3 k$ around a point (\bar{r}, \bar{k}) .

(r, k) at t

In the Bolkmann transport formalism, the total Re number of particle (N) is conserved, which

is given by

 $2 \int f(r, k, t) \frac{d^3r d^3k}{\sqrt{(2R)^3}} = N$

V in the real space volume and (25)3/v is the

momentum space volume. The freter 2° is introduced for spin.

We assume that the measure of the integral d3r d3k remain
in varioust in time. This is the Lionville theorem. Lionville 10

theorem is generally applicable in "flat" phone space, and is only riolated by the phone space is curved which happens if we

apply a magnetic field, or if the phase space is topologically

non-fried or in general theory of relativity when the meanne

is despired with a space-fine defendant metric. There the meane also evolves in time. Here we will assume "flat" phone space.

Thun, instead of Atadying how the particles a coordinate (T. k) evolves in time, we can simply focus locally " at (T. k), and ask how the density f (T, k, t) evolves in time. The total fine-docivative of f in them obtained to be

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial t} = 2issipation / --(4)$$

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial t} = 2issipation / --(4)$$

This is the Boltzmann equation.

In equilibrium, there is no net loss of occupation density and hence the Dissipation / Diffusion like term on the A.H.S is sero. This gives the continuity equation. But when collisions are included the occupations denvits changes with in the volume element and the change in the occupation during is denoted by st collection. cleanly, results from the net inward flow from the ontward flow of electrons in the volume element in the time internal de

Returning back to eq (3), i and is are obtained from the Hamiltonian equation of motion = 84/8 and = - 24/8 = (4=1)

and indistituting them we have

$$= \frac{\delta f}{\delta t} = \left\{ H, f \right\} + \frac{\delta f}{\delta t} \left| coll \right| - (5)$$

This time evolution of a function in phase space $f(\tau, k, t)$ giverned by the Poisson brockel in classical mechanics is replaced with The commutator for operator in quantum mechanics. Do quantum nuchanics we work with density matrix 3 = 14>2+1 instead, of the occupation durity.

Three is a longer divivation of the i and k term, which can be found in the book of hirrin and Yang. We only une the semiclassical result given by: $\dot{\vec{r}} = v_R = \frac{1}{\pi} \frac{\partial \varepsilon_R}{\partial L}$

$$\vec{r} = v_R = \frac{1}{\pi} \frac{\partial \mathcal{E}_R}{\partial h}$$
 [Group reloats of -- (6a) a wave packet]

and
$$t\bar{k} = Lorentz$$
 Fince $F = -2 \left[E(\bar{r}, t) + \frac{1}{c} \bar{v}_{k} \times \bar{B}(\bar{r}, t) \right]$

$$--(6b)$$

(we are actually not going to work with magnetic field term which gives stall effect. However we will picked it for the fime-being).

substituting eq (60) and (65) in up (5) we have

$$\frac{\partial f}{\partial t} = -\vec{v}_{k} \cdot \vec{v}_{f} - \frac{1}{k} \vec{F} \cdot \vec{v}_{k} f + \frac{\partial f}{\partial t} |_{coll}, \quad -(\vec{f}_{a})$$

Densitz variation Densitz variation in real space in movement space.

This is the semi classical Boltzmann fransport formula for electrone in a metal.

- For only electrical conductivity (of the durity is uniform in real space and hence $\nabla r f = 0$. There is also no explicit timedefendance in f and hence $\partial f [\partial f = 0]$. So, we are left with $F \cdot \overline{\nabla}_{b} f = -f \frac{\partial f}{\partial t}|_{coll}$.
 - For thermal conductivity (k), f has a spatial vorcention due to spatial vorciation of temperature $T(\cdot)$ and we have $\overline{\nabla} f = \frac{\partial f}{\partial T} \overline{\nabla} T$.

$$\hbar \vec{v}_{k} \cdot \vec{\nabla} \vec{\tau} \left(\frac{\partial f}{\partial \tau} \right) = \frac{\partial f}{\partial \tau} |_{\text{coll}}$$

* The linearized Boltzmann Equation

In the next step, we assume that on average f(r,k,t) is a stoody varying function in the phase space. Before, the external potential is applied, the system is in thermal equilibrium as f(r,k,t) = f(k) = Fermi-Dirac distribution function.(The thermal equilibrium is admirved via including all the collision (scaltering process present in the system). With the external potential (characterist potential and/or temperature gradient), the occupation density deviates slowly wirth its equilibrium value. So, we diffine:

$$f(\tau, k, t) = f_0(x, k) + \delta f(\tau, k, t) - - (8)$$

$$[A \tau - dip can be kept for the thermal cone T(v)]$$
By the definition of equilibrium, the system reached to the

thermal equilibrium due to collision | scattering, and hence

$$\frac{\partial f_0}{\partial t}\Big|_{coll} = 0$$

Then from eq (7a), ignoring the explicit time defendance, we get

$$\frac{\partial (8f)}{\partial t} = \frac{\partial}{\partial k} \cdot \frac{\partial f_0(t)}{\partial k} + \frac{1}{k} \stackrel{?}{=} \frac{\partial f_0(t)}{\partial k} - (9)$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t} \cdot \frac{\partial}{\partial k} \cdot \frac{\partial}{\partial k} + \frac{1}{k} \stackrel{?}{=} \frac{\partial}{\partial k} \cdot \frac{\partial}{\partial k} - (9)$$

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$$\frac{\partial}{\partial k} = \frac$$

$$= \vec{v}_{k} \cdot \left(\vec{v}_{r} + \frac{\partial f_{0}}{\partial T} \right) + \vec{F} \cdot \left(\vec{v}_{k} \cdot \frac{\partial f_{0}}{\partial S_{k}} \right)$$

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$$= \vec{v}_{k} \cdot \left(\vec{v}_{r} + \frac{\partial f_{0}}{\partial T} \right) + \vec{v}_{r} \cdot \left(\vec{v}_{r} - \frac{\partial f_{0}}{\partial S_{k}} \right)$$

$$= \vec{v}_{k} \cdot \left(\vec{v}_{r} - \frac{\partial f_{0}}{\partial T} \right) + \vec{v}_{r} \cdot \left(\vec{v}_{r} - \frac{\partial f_{0}}{\partial S_{k}} \right)$$

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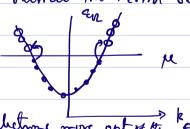
$$= \vec{v}_{k} \cdot \left(\vec{v}_{r} - \frac{\partial f_{0}}{\partial S_{k}} \right) + \vec{v}_{r} \cdot \left(\vec{v}_{r} - \frac{\partial f_{0}}{\partial S_{k}} \right)$$

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$$\frac{\partial (85)}{\partial t}\Big|_{coll} = v_k \cdot \left[\frac{\varepsilon - \mu}{\tau} \vec{\nabla} \tau + e \vec{\varepsilon} \right] \delta(\varepsilon - \mu) - 00$$

- · Let us look into how the Fermi surface response to the two perturbation on R. H. S (also discussed in the Fermi liquid Chapter)
 - -> Temperature gradient: It excites electrons from the formisea to outside the Fermi sea.



electrons more out of the FS.

On the other hand, electric field boost the electrone and hence 121 fot&f Fermi surface shifts formands the eletre feld: E 181

@ The relaxation time Approximation

Finally me introduce another important approximation, called the Relaxation-time Approximation. Here we assume that the distribution function relaxes to equilibrium one to after a charafestic time.

E. This means $\frac{\partial f}{\partial t}|_{coll} \rightarrow -\frac{\partial f}{2}$ - - (100)

(More generally, the relaxation time should be position and momentum dependent 2(r,k) which we will consider later).

Clearly, how long does the system takes to relax to equilibrium defends on the scattling mechanism (collision process that the system has (a) impurity, evelon-phonon confling, electron-electron interaction). For an integrable model, where fockstalls are the cisenstales of the Hamiltonian, is, IH, ffpg =0 too the classical case, there is no scallering mechanism and have the system does not relax at all . Here $z \to \infty$.

So, owr job below in to comforte & due to impuiling, electronphonon and due to electron-electron interaction. For the two later
cases, it is tempting to assume the relaxation time & in the dame
as the electron's lifetime that we derived from the imaginary
food of the self-energy or from the Fermi holden rule. They are
often the same, but there can be some difference.

By substituting, eq (109) in eq (96), we obtain the change in the distribution function due to the enternal perturbation, in terms of the relevation time & oo:

(This is amby to the linear response theory in that the induced occupation durinty fluctuation is brearly proportional to the external perturbation.)

Once we know &, we can evalue the induced devily and obtain the conductivity. & is a parameterizethoris of all the inferraction, scattering with impurity, chetrom school compling term in a single parameter. In fact, in terms of this parameter &, eq (106) recovers the Drude formalism. In the reminder of that chapter, we want to discurs from lism/approximation to compute &.

€ Low-temperature (T→0) conductivity: Recovery of Drade model.

By kuping the relaxation fine & on a parameter and going to $T \rightarrow 0$ limit in eq. (90), we can recover the Drule model's result for the electric and thermal wordechivities or, k, respective and the Wiedemann - Franz land

> The electrical carrent is defined as

$$\overline{J} = -e \sum \langle \overline{V}_{k} \rangle f_{k}$$

$$= -e \sum \langle \overline{V}_{k} \rangle (f_{0} + \delta f)$$

$$= -e \sum \langle \overline{V}_{n} \rangle \delta f_{k} \qquad As \langle V_{n} \rangle = 0 \text{ in equilibrium}$$

$$--(110)$$

For electrical conductivity, we set \$7 =0 in eq (90). Then substituting eq (10), we get from ear (90)

$$\delta f_{\mathbf{k}} = \gamma \vec{v}_{\mathbf{k}} \cdot (\mathbf{e} \vec{\mathbf{e}}) \delta(\mathbf{u} \cdot \mathbf{p})$$

substituting this in eq (11) we get

Because of the 8-function, the states near the fermi level contributes. So, we replace LV_k with an isotropic fermi relointy V_f . We also focus on longitudinal conductivity in $J = \sigma \vec{E}$, so, we have

$$J_{\chi} = e^{\gamma} \mathcal{E}_{\chi} v_{f}^{2} \sum_{k} \delta(s_{k} - \mu)$$

$$d(0) = \text{density of stalin}$$

$$\sigma_{1}$$
, J_{2} = $e^{x} \varepsilon_{x} v_{x}^{2} dv_{y}$

 $\frac{2 + d(0)}{m} = \frac{n}{m} \text{ as } d(0) = \frac{n}{2 + n}$ (For 30, multiply by 3 in dw) and for or do
devide by 3 for energy $r = \frac{n}{2 + n} + \frac{n}{2 + n}$.
(The factor of 2 for spin also drops out)

Thurson, the electrical coordinativity is $\sigma_{xx} = \frac{me^{x}}{m} z$, nehich is the Drude coorductivity.

-) Similarly, the thermal current is defined as

$$= -\frac{\varepsilon}{\tau} \sum_{k} \vec{v}_{k} (\vec{v}_{k} \cdot \vec{\nabla} \tau) (\varepsilon_{\vec{k}} \mu)^{2} \frac{\partial f^{\circ}}{\partial \varepsilon_{k}}$$

= - K. ∇ T when k is the thermal conduction to - (11c) tensor.

The function $(E_k - \mu)^2 \frac{\partial f_0}{\partial E_k}$ has a double perhet structure about μ : for $\int_{0}^{\infty} \frac{\partial f_0}{\partial E_k}$

M EN DEN

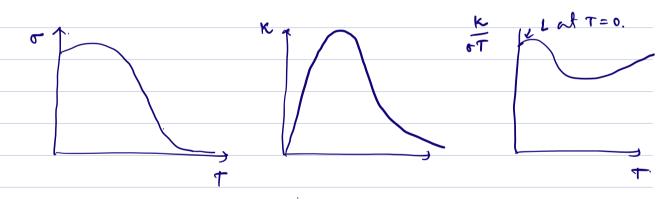
to do this integral we can use the sommerfeld uppossion

and the final result is

$$K_{xx} = \frac{n2}{m} \left(\frac{x^2}{3} b_{\beta}^2 \right) T \qquad - (11d)$$

$$\frac{K}{\sigma r} = \frac{\pi^2 k s^2}{3 e^{\nu}} = Lorentz ratio(L)$$

-> In a metal



From the above discussion, an intriguing physical interpretation of the transport phenomena emerges - which is analogous to the Fluctuation - Dissipation Theory. With external perturbation (E or ∇T) we have excited finduced "St" density at a given k station to thermal requilibrium, and then arbaing, with collisions, it relaxes back to equilibrium value (St=0) after a time scale "2".

So, Z' measures how long an electron esperolo in the state k, of, Z' in the lafe time of the electron in the k-state. Z in finite because the electron scatters from their state k to some other state k' due to information I electron-shown I impurity scallering, we have computed the lafe-time of electrons for the former two process as the imaginary fact of the self energy I've

We can also evaluate & using the ferm-holden rule.

Depending on the scattering potential, there will be difference between the relaxation time and the lifetime of electrons in a system, but we will not look into those cases here. The relaxation time & in often called the transport time, in which an external perturbation is applied, compared to electron's infinisic lifetime.

At in often useful to express De coll in terms of scattering amplitudes for some over through potential. There are two scattering process: one which scatter our electron from the wave packed Yplv to some other work packed Yplv - resulting in a decrese in the occupancy at the (k, v) point in the phase space. This is the loss terms. For this scattering to occur the initial state Yplv must be filled while Yplv's must be filled while Yplv's must be filled while Yplv's then we have

Luss:
$$\frac{\partial f}{\partial t}$$
 $(\tau, \mathbf{k}) = \int \frac{d^3k'}{(2\pi)^3} d^3k' W_{\mathbf{k},\mathbf{k}'} f(\tau, \mathbf{k}, t) \left(1 - f(\tau, \mathbf{k}, t)\right)$

$$--(2\pi)$$

Similarly, the probability durity incremes (sair) for a reverse process

hain =
$$\frac{\partial f}{\partial t}$$
 | $(r, k) = \int \frac{d^3k'd^3r'}{(ar)^3}$ White $(1-f(r, k, t))f(r, k, t)$

The scattering is assumed to be instatement, and no memory effect of the frevious scattering is included. We olso assume the scattering is only happoening in the momentum space, ii, $\bar{\tau}' = \bar{\tau}$. Then we have

$$\frac{\partial f}{\partial t}\Big|_{Coll}(Y, k) = \frac{\partial f}{\partial t}\Big|_{gain} - \frac{\partial f}{\partial t}\Big|_{coss} - -(12c)$$

(In the language of gain & loss of brobability, the Boltzmann equation is also called the Master equation one encounters in brobability theory.) In the above formalism, the thermal equilibrium condition translates into the gain & loss terms componente each other at each k x k' states, is,

Wak' fo(k) (1-fo(k)) = Wa'k fo(k) (1-f(k)) -- (13a) where fo in the fermi-Dirac distribution function in thermal equilibrium. This equilibrium condition, which is called the condition of detailed balance, can now be written as

WER' e- PROT = WER e- PER' -- (136)

H.W. 1. For elastic scalturing Wek! = Wk'k. Then substitute eq (136) on the R.H.s of eq (12) with the assumption that $f = f_0 + Sf \approx f_0$ on the RH.s and in the d.H.s we substitute the relaxation time approximation $\partial f/\partial t |_{coll} \approx [f_0 - (f_0 + \delta f)]/2 \approx - Sf/2. Then, show that the relaxation time can be computed as$

The Start Wek

With the above form of the collision ferm, we now have to combine the scallwing amplitude Wen' for a given potential, say V (i). It is obvious that the scallwing cross section is obtained from V(1) via a and order perfurbation theory term, but here we are not interested in the perfurbation energy correction to the elichronis energy, but its scattering betime, ii, the imaginary fevril of the energy.

In this course, we are obtaining the imaginary back of the energy by introducing on imaginary fort of the self energy) by introducing on imaginary term in the denominator (the same we did for the correlation function and the response tunctions in the linear response theory).

(In a more regorase calculation, one goes to the complex blane and define propagator (areen's function and study its dynamics. Then by the real and imaginary foots one studied in equal footings).

The and order perforbation term is

$$\mathbf{F}_{\mathbf{k}}^{(2)} = \sum_{\mathbf{k}'} \frac{\left| \angle \mathbf{k} \mid \mathbf{H}_{in}\mathbf{t} \mid \mathbf{k}' \right|^{2}}{\left(\mathbf{F}_{\mathbf{k}} - \mathbf{F}_{\mathbf{k}'} \right)}, \text{ when } \mathbf{H}_{in}\mathbf{t} \sim \mathbf{V}(\mathbf{y})$$

Now we add an imaginary term in in the energy denominator and we the tormular

$$\lim_{N\to 0} \frac{1}{x-i\eta} = \mathcal{P}(\frac{1}{x}) - i\pi \mathcal{E}(x)$$
, to obtain the

imaginary part, which we denote here by Wkk' (without the k' summation:

• The scattering lifetime of a given state it is obtained by infegrating over all other k' states

Substituting the relaxation time in the drude formular we obtain the cooductivity co

$$\sigma = e^{2} \sum_{k} \frac{n_{k} \gamma_{k}}{m_{k}} = \sum_{k} \sigma_{k}$$
or for the revisionity:
$$\frac{1}{R} = \sum_{k} \frac{1}{R_{k}}.$$

Sheefor, in the independent eletron approximation, each b- eletron states near the fermi level proche ponallelly cornected resistor.

The mobility is defined by $\mu = \frac{er}{m}$ which charaferises the scattering process of the scattering.

We will not explicitly calculate ey (14) in this couse. Some of them can however be computed easily.

H.W.

(For dictron- 6 honor compliers core, we have already calculated The

Here. Hint = E gar cheq Ch (aq + qt), in the previous charloter.

In this case we alkanne, the phonon distribution function in in thermal equilibrium. In a better, and self-consistent scheme, we have to write a Boltzmann transport equation for phonon so well and compute the relaxation time for both chelven and phonon. (See Jeno Selom, and P. Phillips)

- For an impurity scatturing can, we have $V(\mathfrak{d}) = V \mathfrak{d}'(\mathfrak{f})$ with an impurity sitting at some fixed possition to. This calculation can be simply done by soing to the fourier space of $\mathfrak{S}^3(\mathfrak{d}) = \mathcal{I} \Sigma e^{i \tilde{\mathfrak{q}} \cdot \tilde{\mathfrak{r}}}$. Then I'm integration over \mathfrak{q} can be performed analytically.
- In the Anderson impuity model for mixed valence compound, we have such a Hermiltonian

H = I En Cho Cho + I Ne at a + I (Vicho a + h-c).

How the electron gets scatters to a localized electron state

