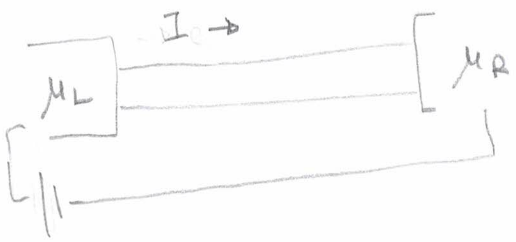
2.1 What are electric currents?

Electric currents describe the motion of charged particles.

We shall mostly consider the motion of "free charges".

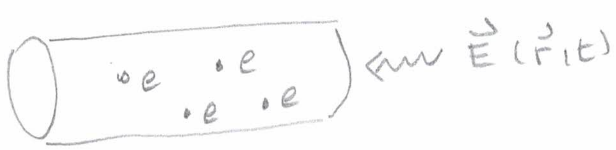
Besides free charges, which are able to move across a conductor, there might be bound charges and localized currents.

Free charges. In a conductor they can arise due to a potential difference between electrodes (e.g. connected to a battery)



$\mu_L - \mu_R = eV$

Alternatively, charged particles can be set in motion by an external electromagnetic field

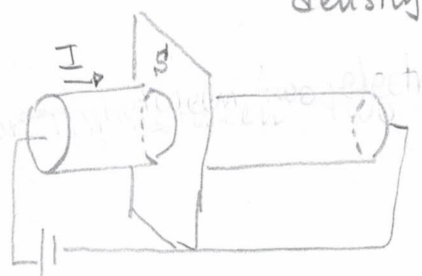


e.g. from battery or electrom. radiation

Current:

$$\boxed{I(t) = \int_S d\vec{S} \cdot \vec{J}(\vec{r},t)} \quad (2.1)$$

$\vec{J}(\vec{r},t)$ current density



with S an arbitrary surface cutting a conductor in between two electrodes

Classical derivation of (2.1) and significance of $j(\vec{r},t)$

Currents describe a contribution of an ensemble of charged particles

↳ given N charges in a conductor, one does not follow the trajectory $(\vec{r}_j(t), \dot{\vec{r}}_j(t))$ of each particle j;

rather ensemble (statistical) averages are considered

$\langle N \rangle$, $\langle \vec{v} \rangle$

↳ $\begin{cases} n(\vec{r},t) & \text{particle density at } \vec{r} \text{ at time } t \\ \vec{v}(\vec{r},t) & \text{average velocity of particles at } \vec{r} \text{ at time } t \text{ (ensemble average)} \end{cases}$

↳ infinitesimal charge crossing surface $d\vec{S} = dS\,\vec{\ell}$ in time dt

$$dQ = e\, n\, \vec{v} \cdot \vec{\ell}\, dS\, dt$$

↳ current across dS

$$dI = \frac{dQ}{dt} = e\, n\, \vec{v} \cdot \vec{\ell}\, dS \equiv \vec{j} \cdot d\vec{S}$$

with the current density vector

$$\boxed{\vec{j}(\vec{r},t) = e\, n(\vec{r},t)\, \vec{v}(\vec{r},t)} \qquad (2.2)$$

Upon integrating over the whole surface Eq. (2.1) follows.

- Finally, charge conservation implies the continuity eq

$$\boxed{e\, \frac{\partial n(\vec{r},t)}{\partial t} = -\vec{\nabla} \cdot \vec{j}(\vec{r},t)} \qquad (2.3)$$

2.2 One current and different viewpoints

- How can we calculate currents?

Electrical currents describe the motion of charged particles. In practice, there are different viewpoints on how to view and thus calculate them.

Viewpoint 1 : The electrical current is a consequence of an applied electric field inside the conductor

drive: $\vec{E}(\vec{r},t)$ electric field

observable: $\vec{J}(\vec{r},t)$ current density

example: linear response

↳ to first order in $\vec{E}(\vec{r},t)$ (linear response)

$$\boxed{J_\alpha(\vec{r},t) = \int_{-\infty}^{t} dt' \int d\vec{r}\,' \sum_\beta \sigma_{\alpha\beta}(\vec{r}t, \vec{r}\,'t')\, E_\beta(\vec{r}\,'t')} \quad (2.4)$$

with $\sigma_{\alpha\beta}$ the conductivity tensor being a microscopic property of the sample, due to the linear response assumption is an equilibrium property ⇒ a function of time difference: $\sigma_{\alpha\beta}(\vec{r},\vec{r}\,'; t-t')$

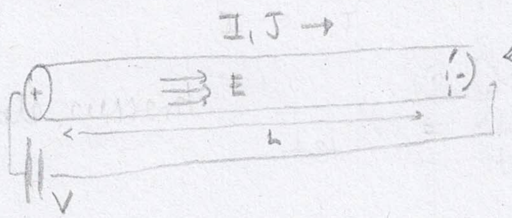
Current: $\boxed{I(t) = \int_S d\vec{S}\cdot\vec{J}(\vec{r},t)}$ (2.1)

↳ wanted: $\vec{J}(\vec{r},t) = \langle \hat{J}(\vec{r},t)\rangle$

with $\hat{J}(\vec{r},t)$ current operator ; $\langle\dots\rangle$ q.m. statistical average

↳ needed: conductivity tensor $\bar{\bar{\sigma}}(\vec{r},\vec{r}\,'; t-t')$

Example: steady-state DC-current of a classical wire



← uniform cross-section A

$d\vec{s} = ds\,\hat{e}_x$

- potential V generates (after a transient) a uniform, static electric field

$$\vec{E} = E\hat{e}_x = \frac{V}{L}\hat{e}_x$$

- In turn the electric field generates according to (2.4) a current density J_x along x:

$$J_x(\vec{r},t) = \int d\vec{r}\,' \int_{-\infty}^{t} dt'\, \sigma_{xx}(\vec{r},\vec{r}\,', t-t')\, E_x(\vec{r}\,',t') \quad \leftarrow E_x(\vec{r},t') \neq 0 \text{ for } t' \geq t_0$$

(battery switched on at t_0=

because the problem is uniform in space $\Rightarrow \sigma_{xx}(\vec{r}-\vec{r}\,')$

$$J_x(t) = \int_{-\infty}^{t} dt'\, \sigma_{xx}(\vec{k}=0, t-t')\, E_x(t') \quad , \quad \sigma_{xx}(\vec{k}) = \int d\vec{r}\,'\, \sigma(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}$$

steady state:

It is convenient to use the final value theorem

$$\lim_{t\to\infty} A(t) = \lim_{\lambda\to 0} \lambda \tilde{A}(\lambda) \quad \leftarrow \quad \tilde{A}(\lambda) = \int_0^\infty dt\, e^{-\lambda t} A(t) \quad \text{Laplace transform}$$

$$\hookrightarrow \quad J_{st} = \lim_{t\to\infty} J_x(t) = \lim_{\lambda\to 0} \tilde{\sigma}_{xx}(\vec{k}=0, \lambda)\, \lambda \tilde{E}_x(\lambda) = \tilde{\sigma}_{xx}(\vec{k}=0, \lambda=0)\, E_{st}$$

E_{st}: stationary electric field

↳ Ohm's law recovered

$$\hookrightarrow \begin{cases} J_{st} = \sigma E \\ \sigma = \lim_{\lambda\to 0} \int_0^\infty dt\, e^{-\lambda t} \left[\int d\vec{r}\,'\, \sigma_{xx}(\vec{r}\,', t) \right] \quad \text{dc-conductivity} \end{cases}$$

$\uparrow$ $k=0$ component of $\sigma_{xx}(\vec{k},t)$

$$\hookrightarrow \quad J_{st} \equiv J = \frac{I}{A} = \sigma E = \sigma \frac{V}{L} \quad \Rightarrow \quad \boxed{I = \frac{V}{R} \quad , \quad R = \frac{L}{\sigma A}} \quad \text{Ohm's law}$$

Note:

For time-space varying E-field it is convenient to work in $(\vec{k},\omega)$ space

$$J_\alpha(\vec{k},\omega) = \sum_\beta \sum_{\vec{k}'} \sigma_{\alpha\beta}(\vec{k},\vec{k}',\omega)\, E_\beta(\vec{k}',\omega)$$

The current operator

For a system of N electrons interacting with an arbitrary electromagnetic field with vector potential $\vec{A}(\vec{r},t)$ the current density operator is

$$\hat{\vec{J}}(\vec{r},t) = \frac{e}{2} \sum_{i=1}^{N} \{ \delta(\vec{r}-\hat{\vec{r}}_i), \hat{\vec{v}}_i \} \qquad (2.5)$$

with $\hat{\vec{v}}_i$ the velocity operator

$$\hat{\vec{v}}_i = \frac{\hat{\vec{P}}_i - e A(\hat{\vec{r}}_i, t)/c}{m} \qquad (2.6)$$

with $\{\hat{A},\hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ anticommutator

Further, by introducing the number density operator

$$\hat{n}(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r}-\hat{\vec{r}}_i) \qquad (2.7)$$

$$\Rightarrow \boxed{\hat{\vec{J}}(\vec{r},t) = \hat{\vec{J}}_p(\vec{r}) - \frac{e^2}{mc} \hat{n}(\vec{r}) \vec{A}(\vec{r},t)} \qquad (2.8)$$

where

$$\hat{\vec{J}}_p(\vec{r}) = \frac{e}{2m} \sum_i \{ \delta(\vec{r}-\hat{\vec{r}}_i), \hat{\vec{P}}_i \} \qquad (2.9)$$

paramagnetic current density operator

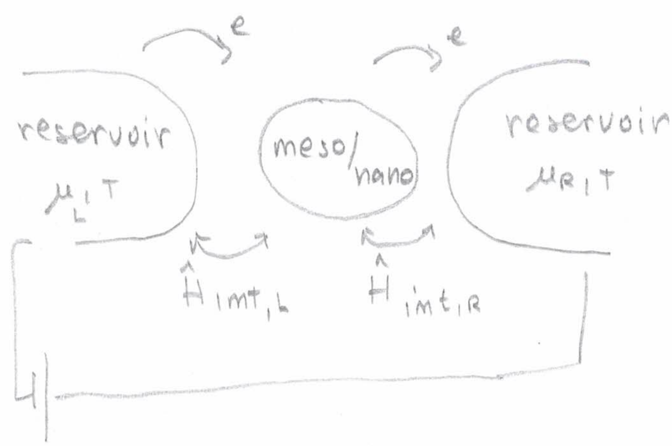
$$-\frac{e^2}{c} \hat{n}(\vec{r}) \vec{A}(\vec{r},t)$$

diamagnetic current density operator

↳ How do we calculate $\langle \hat{\vec{J}}(\vec{r},t) \rangle$ quantum mechanically?

Viewpoint 2:

The current flux is determined by boundary conditions at the conductor's boundaries; A potential difference at the boundaries generates flow of charge (and hence an electric field).



$\mu_L - \mu_R = eV$

The current is defined as the variation of particle nr. per unit time at reservoir α:

$$I_\alpha(t) = e\frac{d}{dt} N_\alpha(t) = e\frac{d}{dt}\langle \hat{N}_\alpha(t)\rangle \qquad (2.10)$$

with $\hat{N}_\alpha(t)$ particle nr. operator

$\langle \ldots \rangle$ q.m. statistical average

$\Rightarrow$ wanted $\frac{d}{dt}\langle \hat{N}_\alpha(t)\rangle$

Schematically

current implies a net flow of charge into (out) of L

$I_L < 0$ if net flux of particle out ($\dot{N}_L > 0$)

<u>Current conservation</u> in steady state $\Leftrightarrow$ $\begin{cases} I_L = -I_R & \text{(what exits L enters R)} \\ I_S = I_L + I_R = 0 \end{cases}$

2.3. Electrical current as quantum statistical average

For both viewpoints 1 and 2:

I(t) is a macroscopic quantity obtained upon quantum statistical average

$$I(t) = \langle \hat{I} \rangle_t \equiv \mathrm{Tr}\{\hat{\varrho}_{tot}(t)\,\hat{I}\} = \mathrm{Tr}\{\hat{\varrho}_{tot}(t_0)\,\hat{I}_H(t)\} \quad (2.4)$$

quantum statistical average

current operator in Schrödinger picture

trace (basis indep.)

density operator of total system capturing the statistical character of the measurement

current operator in Heisenberg picture

recall: quantum mechanical expectation values are independent of representation (Schrödinger, Heisenberg, Interaction)

recall: Heisenberg representation operators evolve in time but states do not

$$\hat{I}_H(t) = \hat{U}^+(t,t_0)\,\hat{I}\,\hat{U}(t,t_0) \quad (2.11)$$

with $\hat{U}(t,t_0)$ the time evolution operator associated to the Hamilton operator $\hat{\mathcal{H}}_{tot}$ of the total system:

$$i\hbar \frac{\partial \hat{U}(t,t_0)}{\partial t} = \hat{H}_{tot}(t)\,\hat{U}(t,t_0) \quad (2.12)$$

This equation follows from the time-dependent Schrödinger equation for the many-body states of our total system

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}_{tot}(t)|\psi(t)\rangle \quad , \quad |\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle \quad (2.13)$$

Statistical operator $\hat{\rho}_{tot}$: it reflects the many degrees of freedom of the total system (meso conductor + reservoirs) which only allow for a statistical treatment of the transport problem.

Given a set of orthonormal state vectors $\{|\psi_i(t)\rangle\}$ occurring with probability p_i, the statistical operator is

$$\hat{\rho}_{tot}(t) \equiv \sum_i p_i |\psi_i(t)\rangle\langle\psi_i(t)| \quad , \quad \sum_i p_i = 1 \quad , \qquad (2.14)$$

where the latter condition ensures conservation of probability

- Mixed state: $p_i \neq 0$ for more than one i
- Pure state: $p_i = 1$ if $i=j$, $p_i = 0 \quad \forall i \neq j \Rightarrow \hat{\rho}_{tot} = |\psi_j\rangle\langle\psi_j|$

From (2.7) $\Rightarrow$ $$\boxed{\hat{\rho}_{tot}(t) = \hat{U}(t,t_0)\, \hat{\rho}_{tot}(t_0)\, U^{+}(t,t_0)} \qquad (2.15)$$

And also from (2.3) it follows

$$\hookrightarrow \boxed{\frac{\partial}{\partial t}\hat{\rho}_{tot}(t) = -\frac{i}{\hbar}[\hat{H}_{tot}, \hat{\rho}_{tot}]} \quad (2.16) \qquad \text{Liouville-von Neumann equation}$$

which describes the time evolution of the statistical operator in the Hilbert space

Note: Exercise: $\hat{\rho}_{tot} = \hat{\rho}^{+}_{tot}$, $\underbrace{\langle\psi|\hat{\rho}_{tot}|\psi\rangle \geq 0 \;\forall |\psi\rangle}_{\text{positiveness of } \hat{\rho}_{tot}}$

Fazit: The transport problem involves evaluation of quantum st. averages. Evaluation of $\hat{\rho}_{tot}(t)$ or related quantities to it is typically a non trivial ta

.4 Quantum correlations

What is the meaning of the matrix elements of the statistical operator in a given basis set?

Example: 2 dimensional Hilbert space spanned by $\{|\uparrow\rangle, |\downarrow\rangle\}$

Assume system in a pure state $|\psi\rangle$

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle, \qquad |\alpha|^2 + |\beta|^2 = 1 \qquad (2.17)$$

↳ statistical operator

$$\hat{\rho} = |\psi\rangle\langle\psi| = |\alpha|^2 |\uparrow\rangle\langle\uparrow| + \alpha\beta^* |\uparrow\rangle\langle\downarrow| + \alpha^*\beta |\downarrow\rangle\langle\uparrow| + |\beta|^2 |\downarrow\rangle\langle\downarrow|$$

↳ matrix form in $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis

$$\rho = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \beta^*\alpha & |\beta|^2 \end{pmatrix} \qquad (2.18)$$

diagonal elements : probability of finding the system in $|\uparrow\rangle$, $|\downarrow\rangle$

off diagonal elements (coherences): originate from the coherent superposition of quantum mechanical states (expressed by Eq. (2.17))

Note: Coherences do not have a classical counterpart

Note: The evolution of $\hat{\rho}$ is determined by the Liouville-von Neumann eq. (2.10) according to the system Hamiltonian $\hat{H}$

↳ the evolution is deterministic (unitary)

Example: Evolution of a two-level system

$$\hat{\rho}(t_0) = |\uparrow\rangle\langle\uparrow|$$

e.g. transverse magnetic field

$$\hat{\mathcal{H}}_{TLS} = -\frac{\hbar}{2}\Delta\sigma_x \quad , \quad \sigma_x = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\uparrow| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\hookrightarrow \hat{\mathcal{U}}(t,t_0) = e^{-it\hat{H}_{tot}(t-t_0)/\hbar}$$

$$\hookrightarrow \quad \hat{\rho}(t) = \hat{U}(t,t_0)\,\hat{\rho}(t_0)\,\hat{U}^{+}(t,t_0)$$

In particular,

$$\rho_{\uparrow\uparrow}(t) = \langle\uparrow|\hat{\rho}(t)|\uparrow\rangle = |\langle\uparrow|\hat{U}(t,t_0)|\uparrow\rangle|^2$$

$$= |\langle\uparrow| e^{-i\frac{\Delta t}{2}\sigma_x}|\uparrow\rangle|^2 =$$

$$= |\langle\uparrow| \cos\frac{\Delta t}{2} - i\sin\frac{\Delta t}{2}\sigma_x|\uparrow\rangle|^2 = \cos^2\frac{\Delta t}{2}$$

similarly, $\rho_{\downarrow\downarrow} = 1-\cos^2\frac{\Delta t}{2} = \sin^2\frac{\Delta t}{2}$

$$\rho_{\uparrow\downarrow}(t) = \langle\uparrow|\hat{U}(t,t_0)|\uparrow\rangle\langle\uparrow|\hat{U}^{+}(t,t_0)|\downarrow\rangle$$

$$= \cos\frac{\Delta t}{2}\cdot i\sin\frac{\Delta t}{2} = \frac{i}{2}\sin\Delta t$$

$$\hookrightarrow \hat{\rho}(t) = \begin{pmatrix} \cos^2\frac{\Delta t}{2} & \frac{i}{2}\sin\Delta t \\ -\frac{i}{2}\sin\Delta t & \sin^2\frac{\Delta t}{2} \end{pmatrix}$$ in $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis

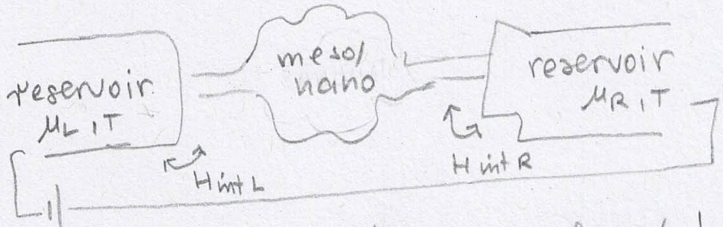
$\hookrightarrow$ oscillatory, coherent dynamics

__Note__: Reason is that eigenstates are $\begin{cases} |g\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \\ |e\rangle = 1/\sqrt{2}\,(|\uparrow\rangle - |\downarrow\rangle) \end{cases}$ $\Rightarrow |\uparrow\rangle$ coherent superposition of $|g\rangle, |e\rangle$

.5 Open quantum systems

What is the density operator of our transport problem?

Let us consider viewpoint 2



The total system is closed!

$$\hat{H}_{tot} = \hat{H}_S + \underbrace{\hat{H}_L + \hat{H}_R}_{\text{Bath (reservoirs)}} + \underbrace{\hat{H}_{int\,L} + \hat{H}_{int\,R}}_{\hat{H}_{int}} \quad (2.19)$$

↳ Dynamics of $\hat{\rho}_{tot}(t)$ is deterministic and follows from (2.10):

$$\frac{\partial}{\partial t}\hat{\rho}_{tot}(t) = -\frac{i}{\hbar}[\hat{H}_{tot}, \hat{\rho}_{tot}(t)] \equiv \hat{\mathcal{L}}_{tot}\,\hat{\rho}_{tot}(t) \quad (2.20)$$

Liouvillian superoperator

However, the system described by (2.13) contains many degrees of freedom, such that the evolution of $\hat{\rho}_{tot}(t)$ is quite intricate.

Further, we are often interested in the effects of the environment on the small conductor.

These are captured by the reduced density operator

$$\hat{\rho}(t) \equiv \mathrm{Tr}_B\{\hat{\rho}_{tot}(t)\} \quad (2.21)$$

Correspondingly $\boxed{\frac{\partial}{\partial t}\hat{\rho}(t) = \mathrm{Tr}_B\{\mathcal{L}_{tot}\hat{\rho}_{tot}(t)\}}$ (2.22)

The effects of the partial trace are to induce

i) decoherence

ii) irreversibility

I.e., in contrast to (2.20), the evolution (2.12) is no longer unitary. If the interaction with the environment was switched on at time t_0 (e.g. battery connected), after waiting "long enough", the small conductor equilibrates with the environment and a steady state is reached.

$$\boxed{\lim_{t\to\infty} \underbrace{\frac{\partial}{\partial t}\hat{\rho}(t) = 0}_{\text{if } \hat{\rho}^{st} = \text{const}}} \qquad (2.23)$$

(if $\hat{H}_{tot}$ independent of t for $t > t_0$)

Example: Two-level system coupled to (dissipative) environment

$\boxed{S} \longleftrightarrow \boxed{\text{BATH}, T}$ (energy exchange)

$$\hat{H}_{tot} = \underset{\uparrow TLS}{\hat{H}_S} + \hat{H}_B + \hat{H}_{Int}, \quad \hat{H}_{TLS} = -\frac{\hbar}{2}\Delta\sigma_x$$

in $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis (no energy basis)

$$\hat{\rho}_{tot}(t_0) = \hat{\rho}_S(t_0) \otimes \hat{\rho}_B(t_0)$$

S and B uncorrelated at t_0

$$\hookrightarrow \hat{\rho}(t_0) = \mathrm{Tr}_B\{\hat{\rho}_{tot}(t_0)\} = \hat{\rho}_S(t_0), \quad \hat{\rho}_S(t_0) = |\uparrow\rangle\langle\uparrow|$$

with $|\uparrow\rangle = \frac{1}{\sqrt{2}}(|g\rangle + |e\rangle)$, $|g\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, $|e\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$

Energy basis

$$\hat{\rho}(t_0) = \begin{array}{cc} |g\rangle & |e\rangle \\ \end{array}\begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix} \xrightarrow[t\to\infty]{\text{environment}} \begin{array}{cc} |g\rangle & |e\rangle \\ \end{array}\begin{pmatrix} |\alpha'|^2 & 0 \\ 0 & |\beta'|^2 \end{pmatrix}$$

E.g. phonons:

$\hat{H}_{int} = \hat{X}(t)\hat{\sigma}_x$, $\hat{H}_B = \sum_j \hbar\omega_j (\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2})$

displacement field $\hat{X}(t) = \sum_j \gamma_j (\hat{a}_j^\dagger + \hat{a}_j)$

$\langle \hat{a}_j^\dagger \hat{a}_j \rangle = n_{BE}(\varepsilon)$ ← Bose-Einstein

$\hookrightarrow$ usually exponential decay in time at long times

coherences $\sim e^{-t/\tau_\varphi}$ $\hookrightarrow$ dephasing time

populations $\sim e^{-t/\tau_{rel}}$ $\hookrightarrow$ relaxation time

Example : Two-level system coupled to a dissipative environment

$$\boxed{S} \longleftrightarrow \boxed{\text{BATH}, T} \qquad S = \text{TLS}$$

$\hat{H}_{int}$ energy exchange

$$\hat{H}_{tot} = \hat{H}_S + \hat{H}_{int} + \hat{H}_B \quad ,$$

$$\hat{H}_S = \hat{H}_{TLS} = -\frac{\hbar}{2}\Delta\sigma_x \quad \text{in } \{|\uparrow\rangle, |\downarrow\rangle\} \text{ basis}$$

Initial state

$$\hat{\rho}_{tot}(t_0) = \hat{\rho}_S(t_0) \otimes \hat{\rho}_B(t_0) \qquad S \text{ and } B \text{ uncorrelated}$$

$$\hookrightarrow \hat{\rho}_{tot}(t_0) = \mathrm{Tr}_B\{\hat{\rho}_{tot}(t_0)\} = \hat{\rho}_S(t_0)$$

Assume e.g.

$$\hat{\rho}_S(t_0) = |\uparrow\rangle\langle\uparrow| \quad , \quad \hat{\rho}_B(t_0) = \frac{1}{Z} e^{-\beta \hat{H}_B} \quad , \quad \hat{H}_{int} = \hat{X}\sigma_x$$

$\Rightarrow$ In energy basis $\quad |\uparrow\rangle = \frac{1}{\sqrt{2}}(|g\rangle + |e\rangle) \quad , \quad |\downarrow\rangle = \frac{1}{\sqrt{2}}(|g\rangle - |e\rangle)$

$$\hat{\rho}_S(t_0) = \begin{array}{cc} |g\rangle & |e\rangle \\ \left(\begin{matrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{matrix}\right. & \left.\right) \end{array} \xrightarrow[t\to\infty]{} \begin{array}{cc} |g\rangle & |e\rangle \\ \end{array} \begin{pmatrix} \rho_{gg}^{st} & 0 \\ 0 & \rho_{ee}^{st} \end{pmatrix}$$

e.g. $\hat{H}_B = \sum_j \hbar\omega_j (\hat{a}_j^\dagger \hat{a}_j + 1/2)$, $\hat{X} = \sum_j \nu_j (\hat{a}_j^\dagger + \hat{a}_j)$ phonon bath

where: - ρ_{gg}, ρ_{ee} stationary populations

- coherences decay (exponentially) within time scale T_φ
- diagonal elements relax (exponentially) within " " T_{rel}

Note: Irreversibility requires a continuous spectrum of the environment

For the example of the phonon bath

$G(\omega) = \sum_j \nu_j^2 \, \delta(\omega - \omega_j)$ continuous function

Note: For weak coupling between system and reservoirs the dephasing and relaxation time of a TLS are

$$\tau_{rel} = \frac{\pi}{2} \, G(\Delta) \coth \beta \left(\frac{\Delta}{2}\right) \equiv T_1$$

$$\tau_\varphi = 2 \, \tau_{rel} \equiv T_2$$

- T_1, T_2 are the names given to such characteristic times in NMR experiments

- $\coth \beta \frac{\Delta}{2} = n_{BE}(\Delta) - n_{BE}(-\Delta)$

  gives the weight to processes where a phonon of energy Δ is emitted / absorbed from the environment

$$\coth \frac{x}{2} = \frac{e^{x/2} + e^{-x/2}}{e^{x/2} - e^{-x/2}} = \frac{1}{1 - e^{-x}} + \frac{1}{e^{x} - 1}$$

Steady state

The steady state reduced density operator is defined as

$$\hat{\rho}^{st}(t) = \lim_{t\to\infty} \hat{\rho}(t) \quad (2.24) \qquad (\text{also sometimes } \hat{\rho}^{\infty})$$

If $\hat{H}_{tot}$ is time independent for $t>0$, it holds

- $\hat{\rho}^{st}(t) = \hat{\rho}^{st}$ time-independent $\Rightarrow \frac{\partial}{\partial t}\rho^{st} = 0$

- the form of $\hat{\rho}^{st}$ is independent of the initial preparation (ergodicity)

- if a situation of global equilibrium exists between system and environment (e.g. $\mu_L = \mu_R = \mu \rightarrow V=0$, $T_L = T_R = T$)

$$\hat{\rho}^{st} = \frac{1}{Z} e^{-\beta(\hat{H}_S - \mu \hat{N}_S)} \equiv \hat{\rho}^{eq} \quad (2.25) \qquad , \beta = \frac{1}{k_B T}$$

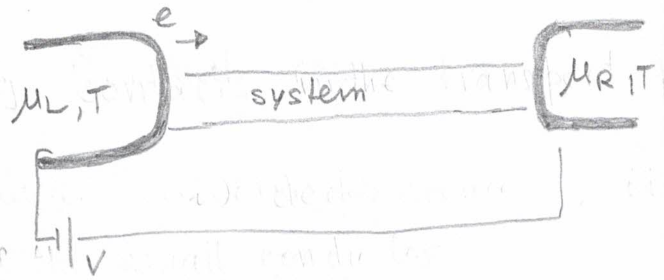
- If $\mu_L \neq \mu_R$ a situation of non equilibrium is established and it may occur that $\hat{\rho}^{st} \neq \hat{\rho}^{eq}$

- These properties of the steady state are independent of the details of the reservoir as long as the latter was in (grand) canonical equilibrium at time t_0,

$$\hat{\rho}_B = \frac{e^{-\beta(\hat{H}_B - \mu \hat{N}_B)}}{Z_B}$$

E.g. it also equally applies to equilibration to a bosonic environment e.g. (phonons)

⇒ One can describe in the same framework the impact of various different environments:



fermionic reservoirs

$\mu_L \neq \mu_R \Rightarrow$ exchange of particles (and energy)

(transport)

bosonic reservoir

exchange of energy

(inelastic processes)

note: phononic excitations are distributed according to the Bose-Einstein function ($\mu_{ph}=0$)

$$n_{BE}(\varepsilon) = \frac{1}{e^{\beta\varepsilon} - 1}$$

$$\varepsilon = \varepsilon_n = \hbar\omega_{ph}\left(n + \tfrac{1}{2}\right) ,$$

$$\Rightarrow n_{BE}(\varepsilon) \sim e^{-\beta\hbar\omega_{ph}} \quad \text{for} \quad kT \ll \hbar\omega_{ph} \Leftrightarrow \beta\hbar\omega_p \gg 1$$

↳ Impact of phonons is negligible at low temperatures (i.e. these inelastic processes are not relevant)

note: If $\hat{H}_{tot}(t)$ depend on time, is $\lim_{t\to\infty} \hat{\rho}(t) \neq$ constant

Outlook: In the next chapters we shall develop various schemes to determine $\langle \hat{I} \rangle$. We shall start first by considering a situation of global equilibrium at time t_0 and a <u>weak perturbation</u> at $t \geq t_0$. Then we shall proceed to include strong perturbations.