Two level system
coupled to an oscillator

a density matrix approach

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The model

\[ H = \omega_0 a^\dagger a - J(c_1^\dagger c_2 + c_2^\dagger c_1) - g (c_1^\dagger c_1 - c_2^\dagger c_2)(a^\dagger + a) \]

- Electron, moving between two sites, interacting with molecular vibrations (phonons)
- Electron interacting with an electromagnetic field inside an optical cavity

- Adiabatic parameter \( \gamma = \omega_0/J \): ratio between the oscillator energy and the electron’s kinetic energy
  - Adiabatic regime \( \omega_0/J < 1 \)
  - Antiadiabatic regime \( \omega_0/J > 1 \)

- Coupling (adiabatic) \( \lambda = 2g^2/\omega_0 J \): ratio between the “polaronic” energy \( (E_p = g^2/\omega_0) \) and kinetic energy

- Coupling (antiadiabatic) \( \alpha^2 = g^2/\omega_0^2 \): ratio between the “polaronic” energy and the oscillator’s energy
polaron state

If $J = 0$

$$H = \omega_0 a^\dagger a - g(c_1^\dagger c_1 - c_2^\dagger c_2)(a^\dagger + a)$$

can be diagonalized by Lang-Firsov (LF) transformation

$$D = e^{\alpha(c_1^\dagger c_1 - c_2^\dagger c_2)(a^\dagger - a)}$$

$$\tilde{H}_0 = D^\dagger H_0 D = \omega_0 a^\dagger a + E_p/2$$

with eigenvalues:

$$|\psi^j_n, j\rangle = D|n, j\rangle = \tilde{c}_j^\dagger |n\rangle$$

corresponding to a localized electron with a displaced oscillator. It is possible to define a quasiparticle (fermionic) called Polaron:

$$\tilde{c}_j^\dagger = Dc_j^\dagger D^\dagger = c_j^\dagger e^{(-1)^j \alpha(a^\dagger - a)}$$

consisting in a charge dressed by an oscillator cloud.
Phase diagram

\[ \gamma = \frac{\omega_0}{J} \text{  adiabatic ratio} \]

\[ \lambda = \frac{2g^2}{\omega_0 J} \text{  coupling} \]

**Figure 1.** Lines separating monomodality (on the left) from bimodality (right). Arrows indicate the \( T = 0 \) crossover point.
Spectral function

adiabatic regime
Density matrix

We want to focus on the dynamics in the strong coupling regime. The charge dynamics is not trivial because electron and oscillator are entangled. We must first consider the total density matrix.

Initial preparation:

- charge localized on the site $|1\rangle$
- oscillator (unperturbed or displaced) in a thermal distribution of states
- the oscillator (or the displaced oscillator) plays the rule of an environment for the fermion

$$\rho(t) = \sum_n e^{-\beta \omega_0 n} \frac{1}{Z} e^{-iHt} |\phi_n, 1\rangle \langle \phi_n, 1| e^{iHt}$$

Two different preparations:

1. starting from the free Hamiltonian and switching on the interaction $g$. Here $|\phi_n\rangle = |n\rangle$
2. starting from the atomic Hamiltonian and switching on the hopping $J$. Here $|\phi_n\rangle$ becomes a state of a displaced oscillator.
We are interested in the charge dynamics. We can consider both the electron and the polaron

\[
\rho_{el}(t) = \sum_n \frac{e^{-\beta \omega_0 n}}{Z} e^{-iHt} |n, 1\rangle \langle n, 1| e^{iHt} \quad \text{Electron}
\]

\[
\rho_{pol}(t) = \sum_n \frac{e^{-\beta \omega_0 n}}{Z} D^\dagger e^{-iHt} |\psi^1_n, 1\rangle \langle \psi^1_n, 1| e^{iHt} D \quad \text{Polaron}
\]

Reduced density matrix

\[
\bar{\rho}_{el/pol}(t) = \sum_m \langle m | \rho_{el/pol}(t) | m \rangle
\]

- \(\bar{\rho}_{2,2}\) transition probability
- \(\bar{\rho}_{2,1}\) coherence, quantum interference term
- \(\text{Tr}[\bar{\rho}^2]\) purity, indicates how much the state is pure
Initial preparation

(1)
polaron

(2)
electron
Three time scales

- Tunneling between 2 electron states
- Oscillator period
- Tunneling between 2 polaron states

\[ \tau_J = \frac{2\pi}{J} \]
\[ \tau_{\omega_0} = \frac{4\pi}{\omega_0} \]
\[ \tau_Q = \frac{4\pi}{\Delta E} \]
(Antia)diabatic

Figure 2. (pol)(top) and (el)(bottom) populations and purity. Left panels antiadiabatic and strong coupling regime: $\gamma = 10 \lambda = 40$. Right panels antiadiabatic and weak coupling regime $\gamma = 10 \lambda = 10$. Curves are for $T/\omega_0 = 0.0$ (magenta), $T/\omega_0 = 0.5$ (blue), $T/\omega_0 = 2.0$ (green), $T/\omega_0 = 10.0$ (red). Vertical lines markes from left to right the timescales $\tau_{\omega_0}, \tau_J, \tau_Q$. 
(Antia)diabatic average

Figure 3. (el)(top) and (pol)(bottom) time-averaged populations and purity. Parameters and labels are the same of Fig. 2.
**Figure 4.** (el)(top) and (pol)(bottom) populations and purity. Left panels Adiabatic and strong coupling regime: $\gamma = 0.1 \lambda = 2$. Right panels adiabatic and weak coupling regime $\gamma = 0.1 \lambda = 0.5$. Curves are for $T/\omega_0 = 0.0$ (magenta), $T/\omega_0 = 0.5$ (blue), $T/\omega_0 = 2.0$ (green), $T/\omega_0 = 10.0$ (red). Vertical lines markes from left to right the timescales $T_J, T_{\omega_0}, T_Q$. 

Adiabatic
**Figure 5.** (el)(top) and (pol)(bottom) time-averaged populations and purity. Parameters and labels are the same of Fig. 4
Figure 6. Time averaged transition probability for $\lambda = 2.0, \gamma = 0.1$, temperatures are from bottom to upper curves $T/\omega_0 = 0.1, 0.5, 1.0, 2.0, 10.0, 20.0$. Vertical lines mark from left to right timescales $\tau_J, \tau_{\omega_0}$ and $\tau_Q$ respectively. Inset: levels reached at time $\tau_{\omega_0}$ (arrows in the main panel) as a function of the inverse temperature.
Figure 7. Polaron (top) and electron (bottom) populations and purity in the adiabatic strong coupling regime $\gamma = 0.1 \lambda = 2$. Left panels low temperature $T/\omega_0 = 0.1$. Right panels high temperatures $T/\omega_0 = 10.0$. Curves refers to ED (black), QC (blue), SA (green) approximations. Vertical lines marks from left to right the timescales $\tau_J, \tau_{\omega_0}, \tau_Q$. 
Conclusions

- **non dissipative** evolution of a tunneling system strongly coupled to a single oscillator can give rise to decoherence phenomena when the initial distribution of the oscillator is thermal and when the oscillator distribution is not initially equilibrated in the presence of the charge (el preparation).

- Temperature modifies level of coherence and transition probability but not timescales, recoherence occurs at low temperature on a very long time-scale

- System simple enough to allow exact solution for large times and to check different schemes of quasi-classical evolution

- In a non equilibrium experiment in which a charge is introduced in a molecular system and interacts strongly with a particular mode of the molecular system, decoherence effects can be triggered alone by this coupling and by the initial non equilibrium distribution of the molecule.