A tutorial on the polaron transformed Redfield equation

Huo Chen

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0.1 Correlation function in the polaron frame

This tutorial demonstrates how to use the polaron transformed Redfield equation (PTRE) in HOQST. For more details on the PTRE, see [1] Non-canonical distribution and non-equilibrium transport beyond weak system-bath coupling regime: A polaron transformation approach.

We solve both the Redfield equation and the PTRE for a single qubit Hamiltonian

$$H_{\mathrm{S}} = \epsilon\sigma_z + \Delta\sigma_x$$

coupled to an Ohmic bath via σ_z interaction:

$$H = H_{\mathrm{S}} + \sigma_z \otimes B + H_{\mathrm{B}} \ .$$

Loosely, the main difference between the Redfield equation and PTRE is that they have different bath correlation functions. For the Redfield equation, the bath correlation function is

$$C(t_1, t_2) = \langle B(t_1)B(t_2)\rangle \ .$$

In the polaron frame, however, the bath correlation function becomes

$$K(t_1, t_2) = \exp\Big\{ -4\int_0^t \int_{-\infty}^0 C(t_1, t_2)\mathrm{d}t_1\mathrm{d}t_2 \Big\} \ .$$

Interested readers can refer to [2] Macroscopic Resonant Tunneling in the Presence of Low Frequency Noise and [3] Dynamics of the dissipative two-state system for more details.

0.1.1 Error bound on the second-order master equation

The most straightforward analysis is to compare the error bounds given in [4] Completely positive master equation for arbitrary driving and small level spacing between the Redfield equation and PTRE. We define the error scaling parameter as

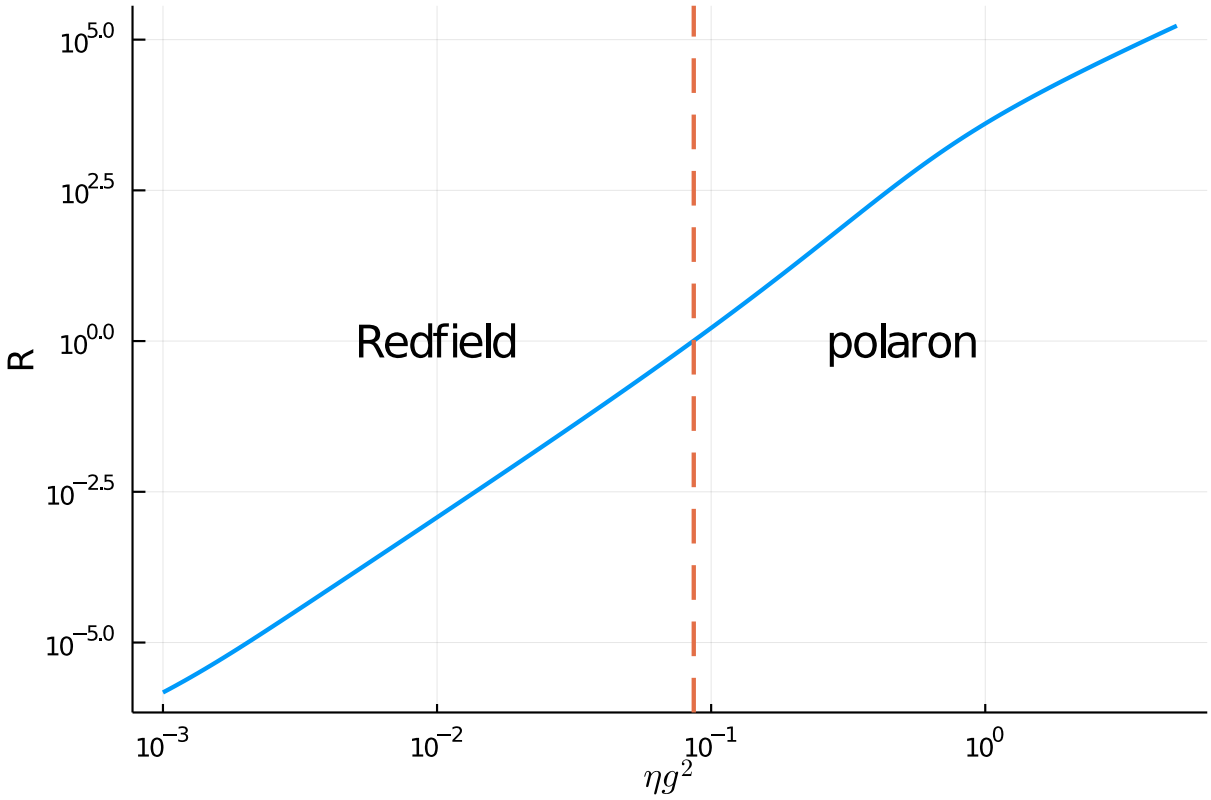
$$error = \frac{\tau_{\mathrm{B}}}{\tau_{\mathrm{SB}}} \ .$$

Then we plot the error ratio between the Redfield equation and the PTRE

$$R = \frac{error_{\text{Redfield}}}{error_{\text{PTRE}}} ,$$

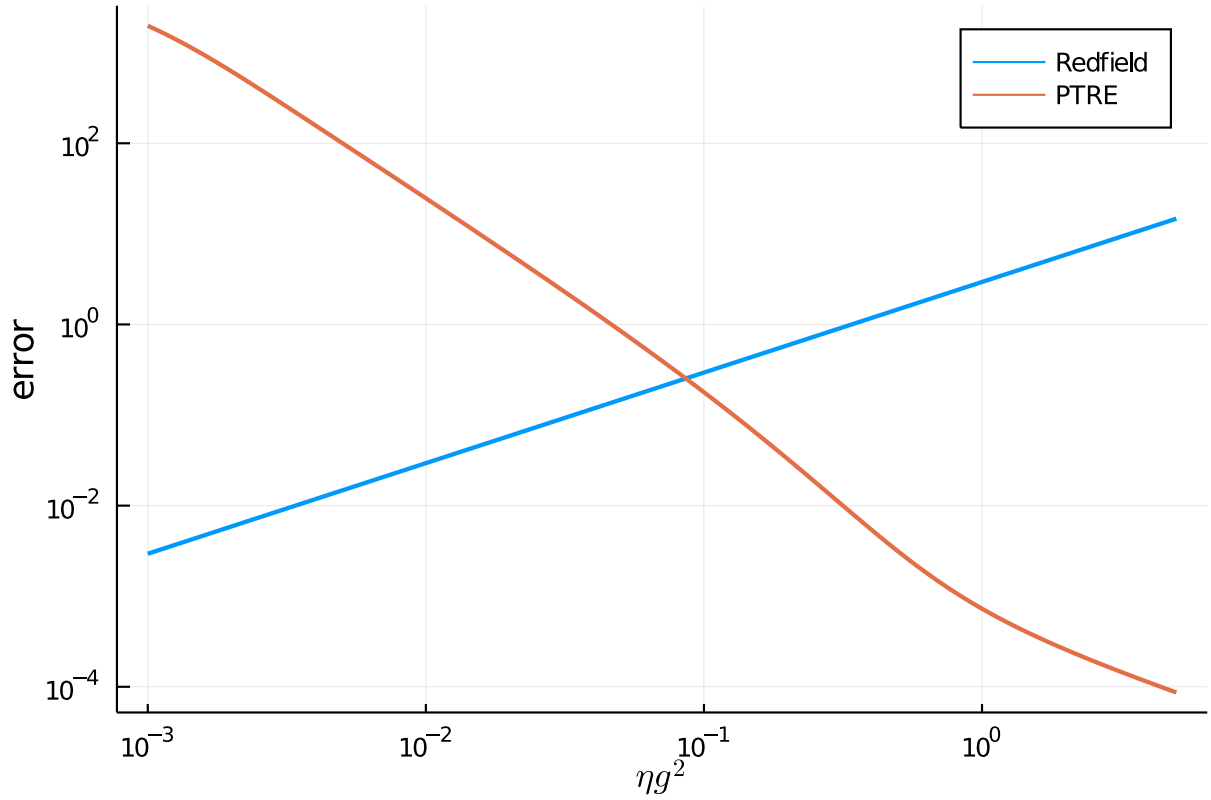
vs. the system bath coupling strength ηg^2 while fixing other parameters in the Ohmic bath.

```
using OrdinaryDiffEq, OpenQuantumTools, Plots
using LaTeXStrings

function err_bound(tf, cfun)
    tsb, esb = τ_SB(cfun)
    tb, eb = τ_B(cfun, tf, tsb)
    tb / tsb
end

fc = 4; T =12; tf = 1000;
ηlist = log_uniform(1e-3, 5, 1000)
err_ratio = []
err_clist = []
err_klist = []
for η in ηlist
    bath = Ohmic(η, fc, T)
    cfun = (x)->correlation(x, bath)
    pfun = (x)->polaron_correlation(x, bath)
    err_c = err_bound(tf, cfun)
    err_k = err_bound(tf, pfun)
    push!(err_clist, err_c)
    push!(err_klist, err_k)
    push!(err_ratio, err_c/err_k)
end
idx = findfirst((x)->x>=1, err_ratio)
plot(ηlist, err_ratio, xscale=:log10, yscale=:log10, label="", linewidth=2)
vline!([ηlist[idx]], label="", linestyle=:dash, linewidth=2)
annotate!([(0.5, 1.0, Plots.text("polaron")), (0.01, 1.0, Plots.text("Redfield"))])
xlabel!(L"\eta g^2")
ylabel!("R")
```



From the above figure we observe that when the system-bath coupling strength is larger than 10^{-1}, the PTRE should have better error scaling than the standard form of the Redfield equation. We also plot the corresponding error values for both the Redfield equation and the PTRE:

```
plot(ηlist, err_clist, xscale=:log10, yscale=:log10, label="Redfield", linewidth=2)
plot!(ηlist, err_klist, xscale=:log10, yscale=:log10, label="PTRE", linewidth=2)
xlabel!(L"\eta g^2")
ylabel!("error")
```



The above figure confirms that the Redfield equation applies to the weak-coupling regime while the PTRE applies to the strong coupling regime.

0.1.2 Solving PTRE

Since the Redfield equation and the PTRE have identical forms, `solve_redfield` can also be used for the PTRE. To see this, let's first write down the PTRE for our example.

$$\dot{\rho}_{\mathrm{S}} = \epsilon\sigma_z + [\sigma_i, \Lambda_i(t)\rho_{\mathrm{S}}(t)] + h.c.$$

where $i, j \in [+, -]$, $i \neq j$ and

$$\Lambda_i(t) = \Delta^2 \int_0^t K(t-\tau)U(t,\tau)\sigma_j U^\dagger(t,\tau)\mathrm{d}\tau \ .$$

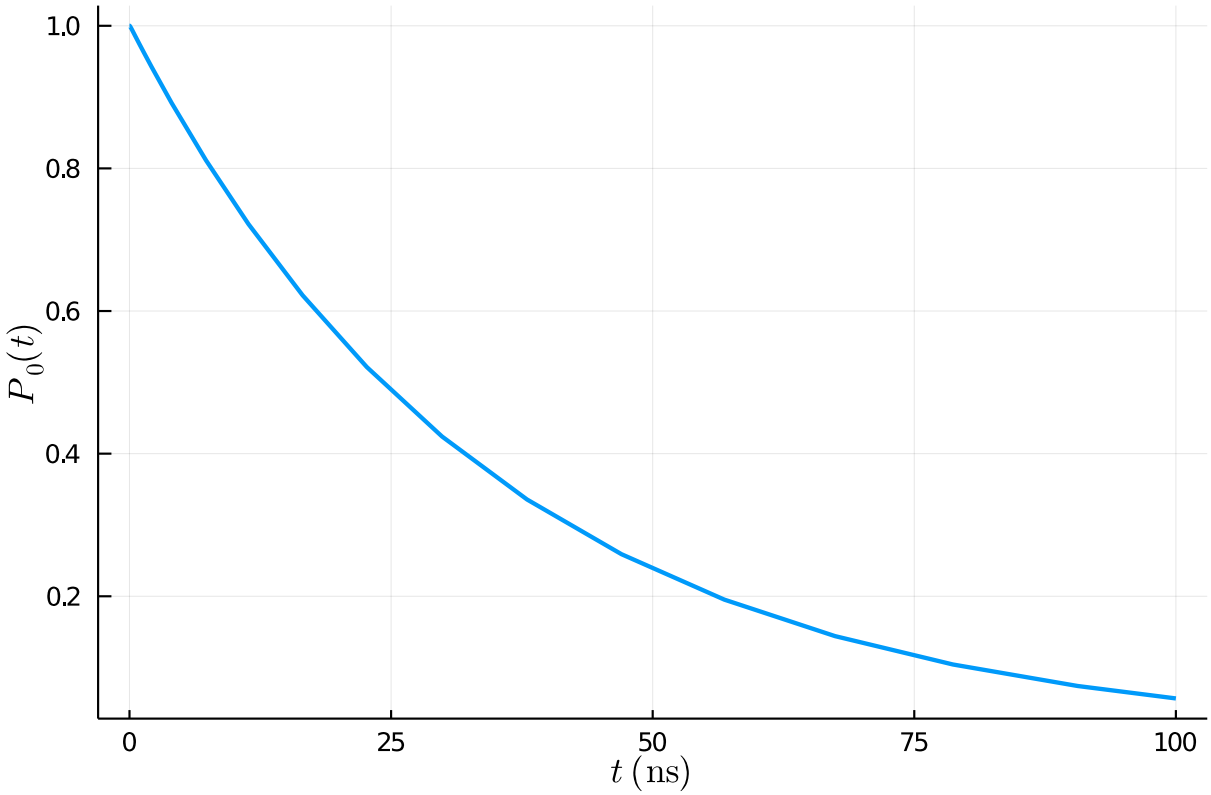
From the above equations, it is clear that the following steps are needed to define an evolution in the polaron frame:

1. define a new Hamiltonian $H = \epsilon\sigma_z$;
2. define new coupling operators σ_- and σ_+;
3. define a new correlated bath with two-point correlation $K_{i,j}(t_1, t_2)$;

The following code block illustrates how this can be done in HOQST:

```
# assume ϵ = 1
    const Δ = 0.1
    # define the Ohmic bath in the polaron transformed frame
```

```
    η = 0.5; bath = Ohmic(η, fc, T)
    K(t1, t2) = Δ^2 * polaron_correlation(t1-t2, bath)
    cfun = [nothing K; K nothing]
    pbath = CorrelatedBath(((1,2),(2,1)), correlation=cfun)
    # define coupling as σ+ and σ- operators
    σp = [0 1;0 0.0im]; σm = [0 0;1 0.0im]
    coupling = ConstantCouplings([σp, σm])
    # manually define the unitary operator
    U(t) = exp(-2.0im * π * σz * t)
    H = DenseHamiltonian([(s)->1.0], [σz])
    u0 = PauliVec[3][1]
    annealing = Annealing(H, u0, coupling = coupling, bath = pbath)
    tf = 100
    sol_ptre = solve_redfield(annealing, tf, U, alg=Tsit5(), Ta=2, reltol=1e-5)
    pop_e = [real(s[1,1]) for s in sol_ptre.u]
    plot(sol_ptre.t, pop_e, xlabel=L"t\ (\mathrm{ns})", ylabel=L"P_0(t)", label="",
linewidth = 2)
```



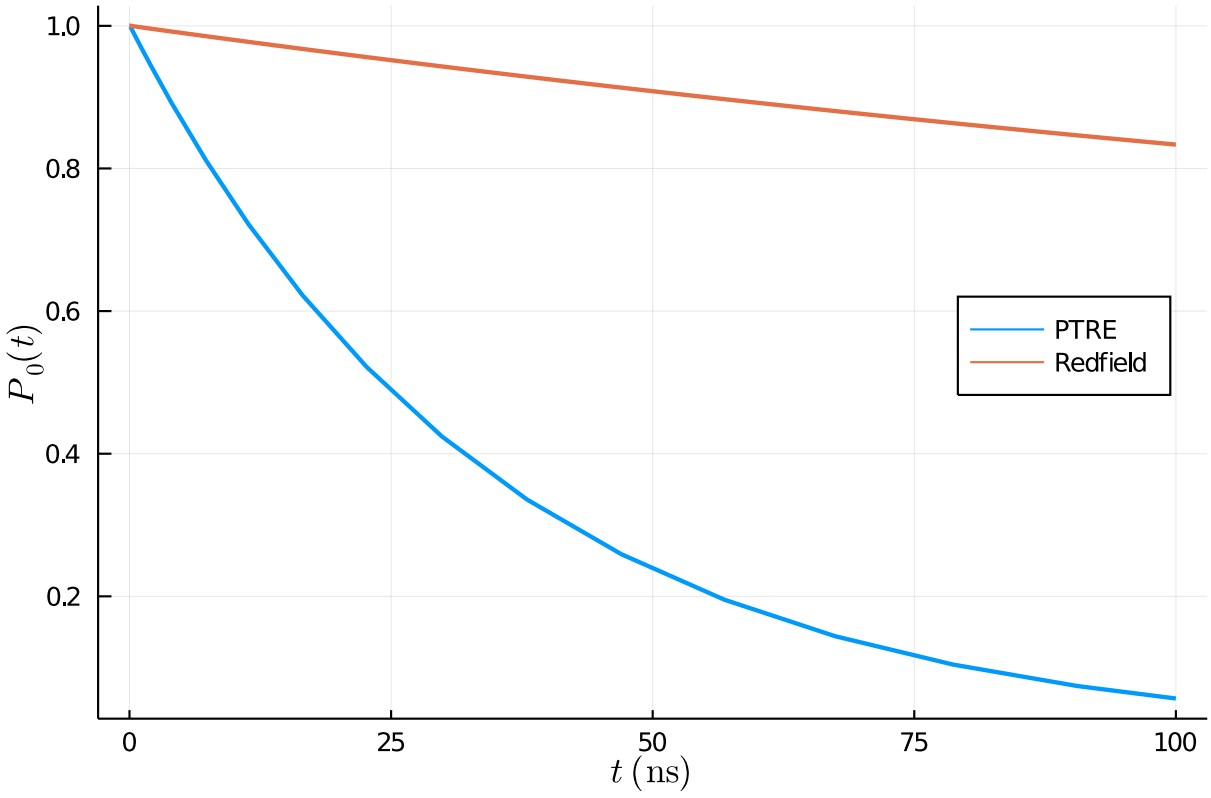
For historical reasons, this is known as an example of "incoherent tunneling". The off-diagonal elements of the density matrix in the computational basis (the Z-basis) vanish during the entire evolution (shown in the next section).

0.1.3 Redfield equation

What happens to the Redfield equation in this regime? We can also try:

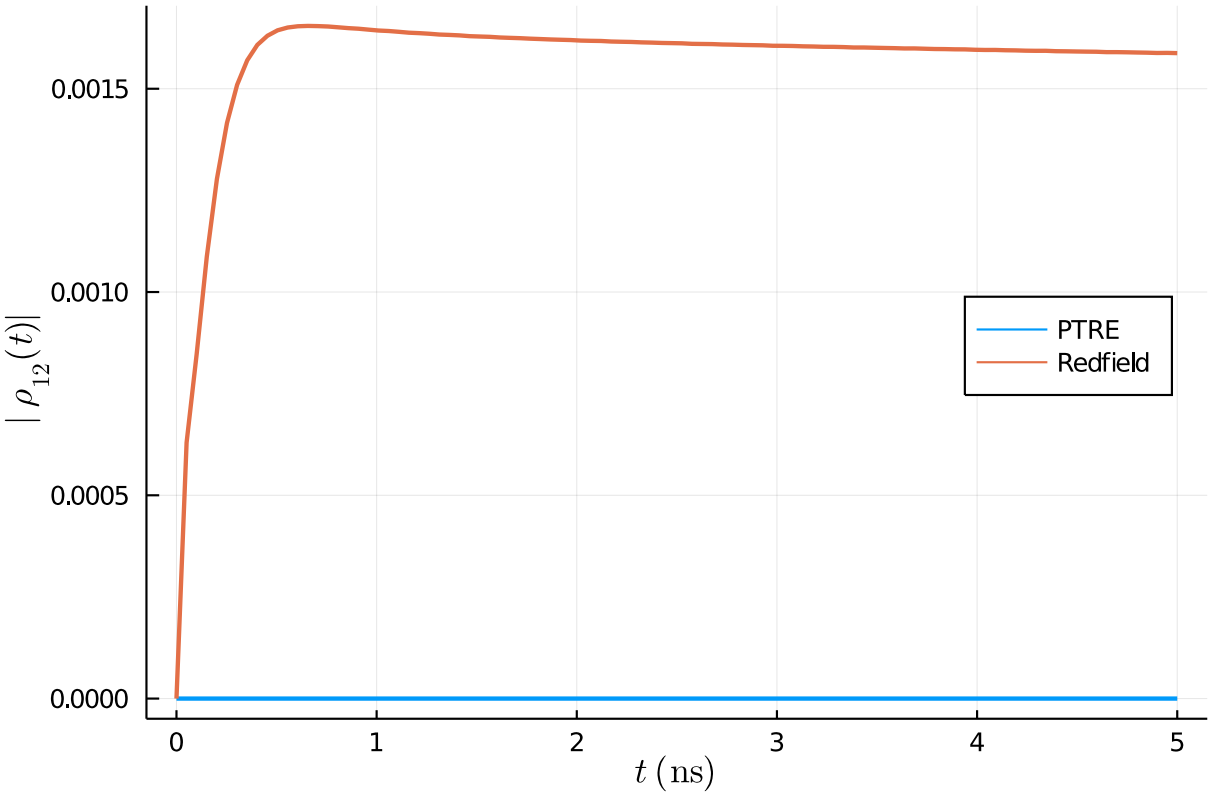
```
H = DenseHamiltonian([(s)->1.0], [σz+0.1*σx])
coupling = ConstantCouplings(["Z"])
annealing = Annealing(H, u0, coupling = coupling, bath = bath)
tf = 100
```

```
sol_redfield = solve_redfield(annealing, tf, U, alg=Tsit5(), Ta=40, reltol=1e-5,
callback=PositivityCheckCallback())
pop_e_redfield = [real(s[1,1]) for s in sol_redfield.u]
plot(sol_ptre.t, pop_e, xlabel=L"t\ (\mathrm{ns})", ylabel=L"P_0(t)", label="PTRE",
linewidth = 2, legend = :right)
plot!(sol_redfield.t, pop_e_redfield, xlabel=L"t\ (\mathrm{ns})", ylabel=L"P_0(t)",
label="Redfield", linewidth = 2)
```



The PTRE gives a much stronger decay than the Redfield equation for the parameters chosen in this example. One can also verify the amplitude of the off-diagonal elements during the evolution. Unlike the PTRE, the solution of the Redfield equation has non-vanishing off-diagonal elements of the density matrix.

```
t_axis = range(0, 5, length=100)
off_diag_ptre = [abs(sol_ptre(t)[1,2]) for t in t_axis]
off_diag_redfield = [abs(sol_redfield(t)[1,2]) for t in t_axis]
plot(t_axis, off_diag_ptre, xlabel=L"t\ (\mathrm{ns})", ylabel=L"\lvert \rho_{12}
\rvert|(t)", label="PTRE", linewidth = 2, legend=:right)
plot!(t_axis, off_diag_redfield, xlabel=L"t\ (\mathrm{ns})", ylabel=L"|\rho_{12}(t)|",
label="Redfield", linewidth = 2)
```


0.0015
0.0010
0.0005
0.0000
$|\rho_{12}(t)|$
0
1
2
3
4
5
t (ns)
PTRE
Redfield