An tutorial on polaron transformed Redfield equation

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August 18, 2020

0.1 Correlation function in polaron frame

This is an tutorial for using polaron transformed Redfield equation (PTRE) in OSQAT. For more details on PTRE, Xu and Cao is a good reference.

In this example, we solve both Redfield equation and PTRE for a single qubit model with system Hamiltonian

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

coupling to an Ohmic bath via σ_z interaction

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

Loosely speaking, the main difference between these two approaches is, they have different types of correlation functions. For Redfield equation, we have the normal bath correlation function

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

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

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

Again, interesting reader can refer to [Amin and Averin] and Leggett et al for more details.

0.1.1 Error bound on the second order master equation

The simplest thing we can do is to compare the error bounds given in Mozgunov and Lidar between Redfield and PTRE. We define the error scaling parameter as

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

then we compare the error ration between Redfield and PTRE

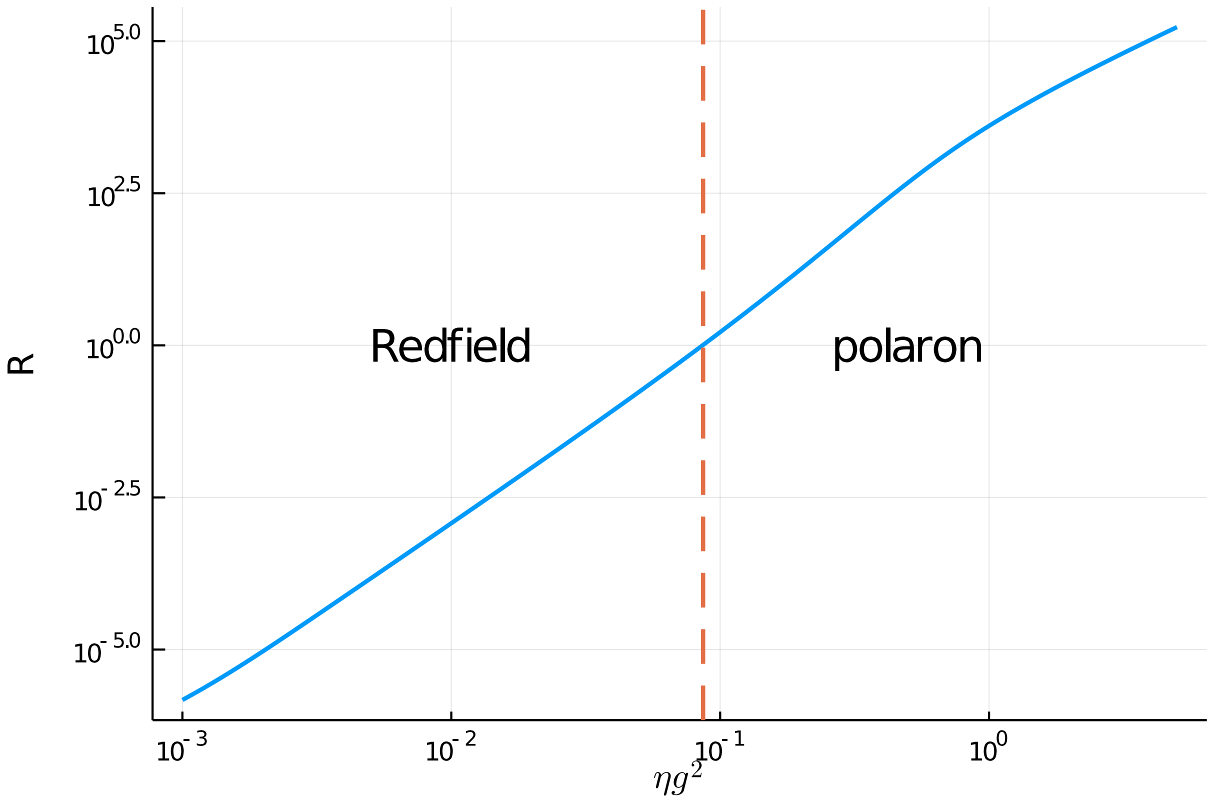
$$R = \frac{error_{\mathrm{Redfield}}}{error_{\mathrm{PTRE}}} \ ,$$

when fixing other parameters in the Ohmic bath.

```julia
using OrdinaryDiffEq, QuantumAnnealingTools, 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 = []
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_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 above figure we can see that, as the system-bath coupling strength is bigger than 10^{-1}, PTRE should have better error scaling than the usual form of Redfield equation.

0.1.2 Solving PTRE

Since PTRE and the Redfield equation have identical forms, `solve_redfield` can also be used for 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

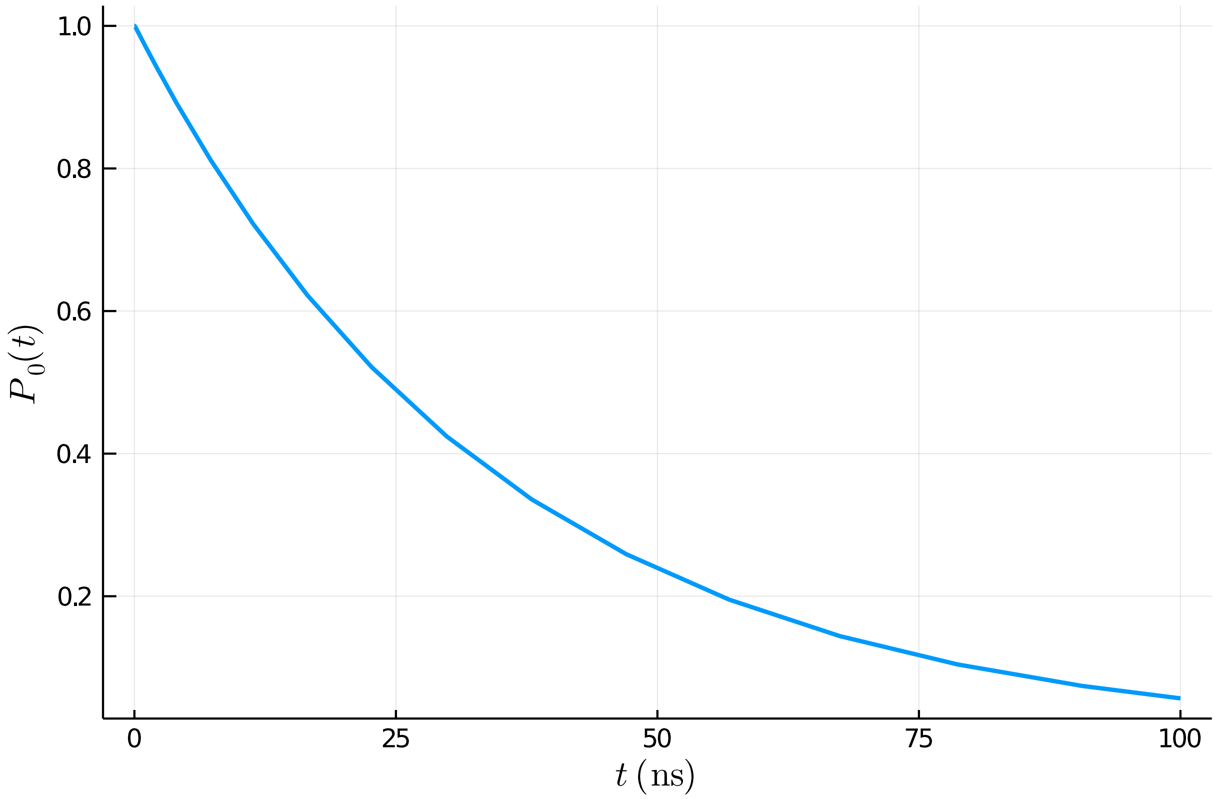
$$\Lambda_i(t) = \Delta^2 \int_0^t K(t-\tau)U(t,\tau)\sigma_j U^\dagger(t,\tau)\mathrm{d}\tau \ .$$

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

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

The following code block illustrates how these can be done in OSQAT

```
# assume ϵ = 1
    const Δ = 0.1
    # define the Ohmic bath in 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)
```

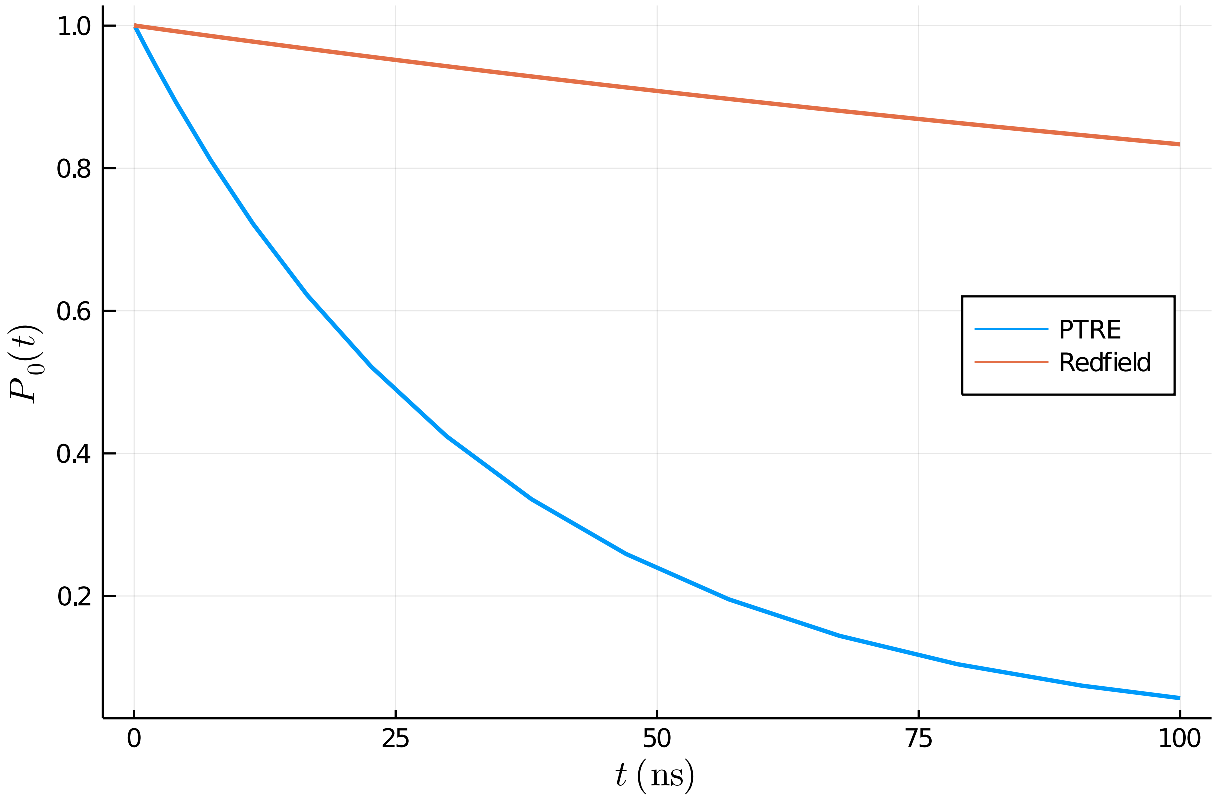


For historical reasons, this is know as an example of the ”incoherent tunneling”. The off-diagonal elements of the density matrix in computational bases(Z-bases) during the entire evolution is 0(, which is shown in next section).

0.1.3 Redfield equation

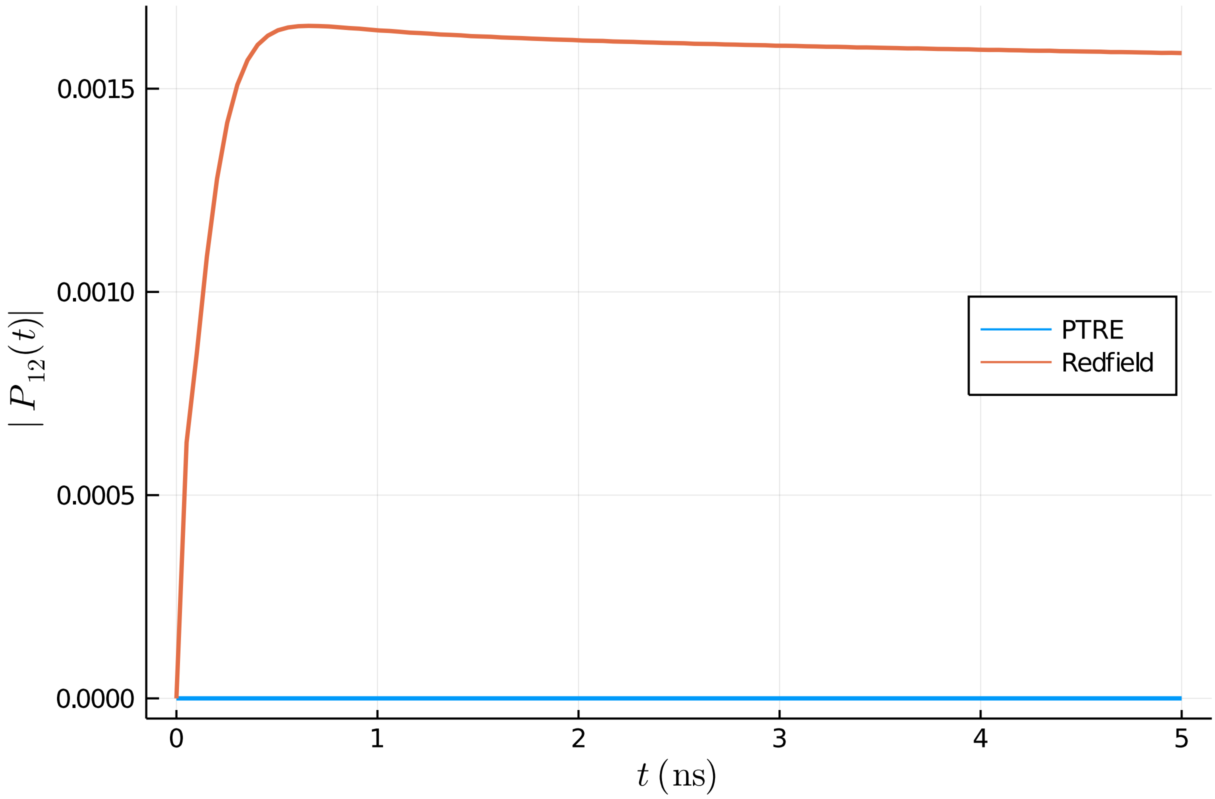
What would happend to normal Redfield equation in this regime? We can also try

```
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)
```



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 PTRE, the usual Redfield equation have 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 P_{12}
\rvert|(t)", label="PTRE", linewidth = 2, legend=:right)
plot!(t_axis, off_diag_redfield, xlabel=L"t\ (\mathrm{ns})", ylabel=L"|P_{12}(t)|",
label="Redfield", linewidth = 2)
```


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