Research Update: Non-Markovian Quantum Walk, Finite Size, Finite Coupling Strength

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18.01.2023

Starting Point

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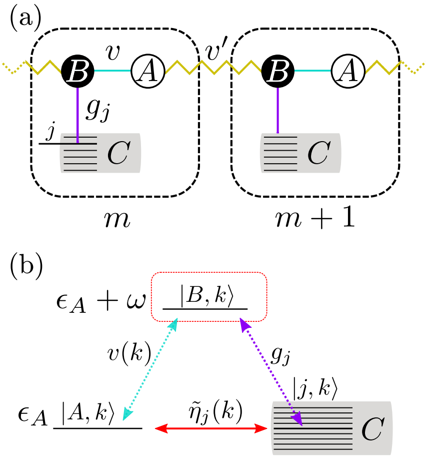
Model[1]



- consider an SSH chain lattice with extra levels in each unit cell

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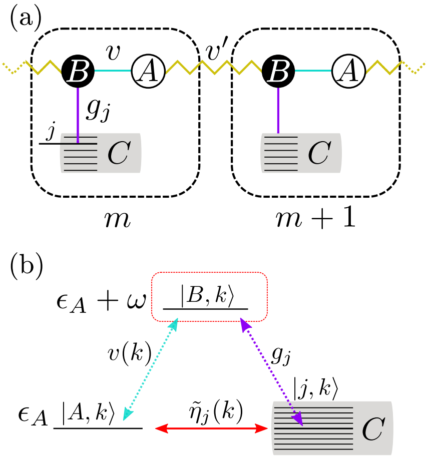
Model[1]

- consider an SSH chain lattice with extra levels in each unit cell

$$H_A = \sum_m \omega_A |A,m\rangle\langle A,m|$$
$$H_{\bar{A}} = \Sigma_m (\omega_A + \omega) |B,m\rangle\langle B,m| + \sum_j \left[\omega_j |j,k\rangle\langle j,k| + g_j(|j,m\rangle\langle B,m| + \text{h.c.})\right]$$
$$V = \sum_m v(|A,m\rangle\langle B,m| + u |A,m\rangle\langle B,m+1| + \text{h.c.})$$



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Model[1]

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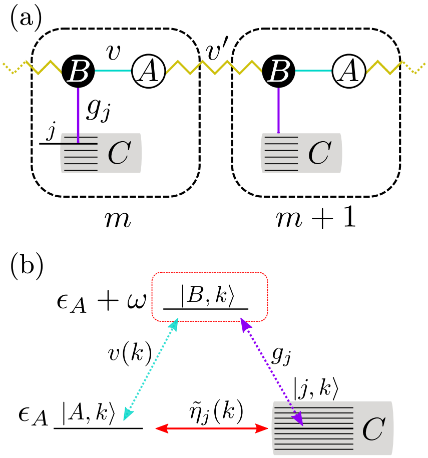
$$
\begin{aligned}
H_A(k) &= \omega_A \,|A,k\rangle\langle A,k| \\
H_{\bar{A}}(k) &= \ (\omega_A+\omega)\,|B,k\rangle\langle B,k| \\
&\quad + \sum_j \left[\omega_j\,|j,k\rangle\langle j,k| + g_j(|j,k\rangle\langle B,k| + \mathrm{h.c.})\right] \\
V(k) &= |v(k)|\big(\mathrm{e}^{i\phi(k)}\,|A,k\rangle\langle B,k| + \mathrm{h.c.}\big)
\end{aligned}
$$



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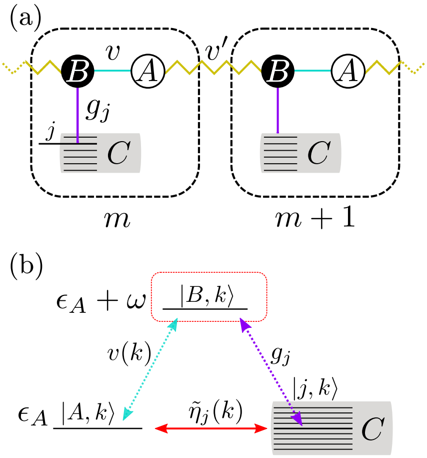
Model[1]

- consider an SSH chain lattice with extra levels in each unit cell
- to make calculations simpler: eliminate B sites

$$H(k) = \sum_j \left[\tilde{\omega}_j \left|j,k\right\rangle\!\left\langle j,k\right| + \left(\tilde{\eta}_j \left|A,k\right\rangle\!\left\langle j,k\right| + \mathrm{h.c.}\right)\right]$$
$$\tilde{\omega}_A \left|j,k\right\rangle\!\left\langle j,k\right| \qquad (1)$$



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Observable

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- in momentum space $\phi(k) = \arg[v(k)] = \arg\left[v\left(1 + ue^{ik}\right)\right]$, $u = \frac{v'}{v}$

$$\langle m \rangle = \int_0^{2\pi} (1 - \rho_A) \frac{\partial \phi(k)}{\partial k} \frac{\mathrm{d}k}{2\pi} \tag{4}$$

with

$$\rho_A(k) = \lim_{T\to\infty} \frac{1}{T} \int_0^T \rho_A(t,k) \, \mathrm{d}t = \lim_{T\to\infty} \frac{1}{T} \int_0^T |\langle A, k|\psi(t)\rangle|^2 \, \mathrm{d}t \,. \tag{5}$$

Spectral Densities

- we need some values for the η_j
- in the continuum limit $\sum_j |\eta_j|^2 \delta(\omega - \omega_j) = J(\omega)$

$$J(\omega) = g_0^2 \frac{\alpha + 1}{\omega_c^{\alpha+1}} \begin{cases} \omega^\alpha & \text{if } \omega \leq \omega_c, \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

- we need the inverse choose η_j such that

$$\int_0^\infty f(\omega) \sum_j |\eta_j|^2 \delta(\omega - \omega_j)^2 \, \mathrm{d}\omega = \int_0^\infty J(\omega) f(\omega) \tag{7}$$

- can be done more intricately, but for present purposes

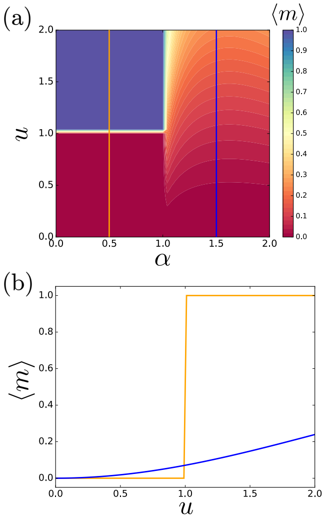
$$\omega_j = \frac{j\omega_c}{N} \quad \eta_j^2 = J(\omega_j) \frac{\omega_c}{N} \tag{8}$$

Behavior in Weak-Coupling Limit

- for $\alpha < 1$ $\rho_A \to 0$, for $\alpha > 0$ persistent oscillations

$$\langle m \rangle = \int_0^{2\pi} (1 - \rho_A) \frac{\partial \phi(k)}{\partial k} \frac{\mathrm{d}k}{2\pi} \tag{9}$$

  - $\rho_A = 0 \to \langle m \rangle$ is winding number $\to$ universal behavior
  - otherwise: any value of $\langle m \rangle$ is possible



Solution in Weak Coupling Limit

- can construct Master equation to second order in coupling

$$\dot{\rho}_A(k,t) = \int_0^t \Sigma(k,t-t')\rho_A(k,t') \tag{10}$$

- solvable by Laplace transform, we only need long time limit though

$$\rho_A(k) = \lim_{T\to\infty} \frac{1}{T}\int_0^\infty \mathrm{e}^{-\frac{t}{T}}\,\rho_A(k,t)\,\mathrm{d}t = \lim_{s\to 0} s\tilde{\rho}_A(k,s) = \left[\frac{\mathrm{d}}{\mathrm{d}s}\frac{1}{\tilde{\rho}_A(k,s)}\right]^{-1}\Bigg|_{s=0} \tag{11}$$

- we find

$$\rho_A(k) = \frac{1}{1+2\sum_j \frac{|\eta_j|^2}{\omega_j^2}} = \frac{1}{1+2U_A}. \tag{12}$$

- U_A blows up for $\alpha < 1$, $N\to\infty$

The Conundrum

- we would like to realize this model in a finite system
- coupling not necessarily vanishing (don't have infinite time)
- naive idea: just implement it numerically for a finite system and see what happens

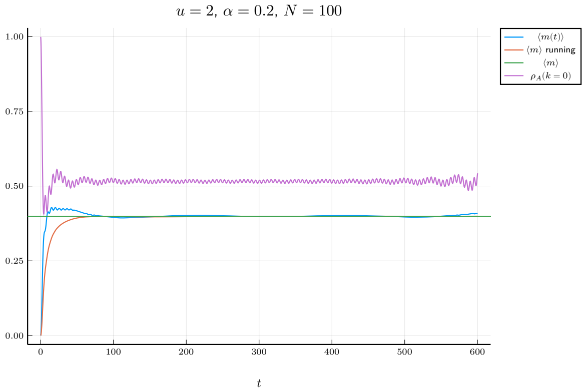
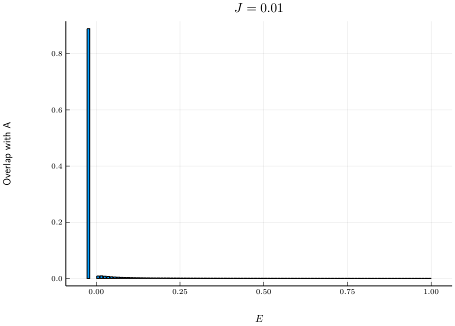
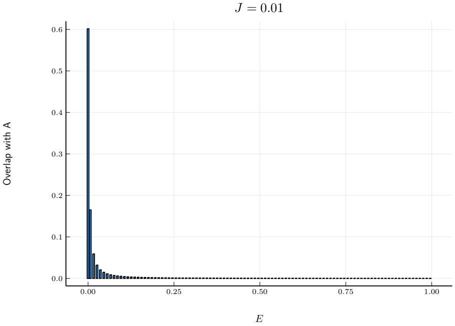


Figure: A numerical simulation for $g_0 = 10^{-2}$.

Problems

- $\rho_A \not\to 0 \implies$ no universality
- finite $N \implies$ recurrences
- played around with numerics: found that shifting ω_A can make $\rho_A \to 0$
- at finite strength: level repulsion shifts energy of the state that used to be $|A\rangle$
- destroys sensitivity for $J(\omega \to 0)$
- shifting ω_A to compensate that Lamb shift can close the gap





Failed Idea: Brute-Forcing the Shift

- a priori not clear how far to shift
- first approach: optimize ω_A to make gap in spectrum as small as possible
- leads to $\rho_A \to 0$ regardless of α
- heuristic: first $\omega_1 = \omega_c/N \implies$ closing the gap $\omega_1 \to 0 \implies J(0) \neq 0 \implies \rho_A \to 0$

Exact Solution

- Hamiltonian is very simple $\implies$ exact solution actually exists
- define $|\psi\rangle = \alpha |A\rangle + \sum_j \beta_j |j\rangle$

$$\dot{\alpha} = -i\omega_A \alpha - \int_0^t \mathrm{K}(t-\tau)\alpha(\tau)\,\mathrm{d}\tau \tag{13}$$

with $\mathrm{K}(t-\tau) = \sum_j |\eta_j|^2 \,\mathrm{e}^{-i\omega_i(t-\tau)}$

- Solution: Laplace-Transform

$$\tilde{\alpha}(s) = \frac{\alpha(0)}{s + i\omega_A + \tilde{\mathrm{K}}(s)} \qquad \tilde{\mathrm{K}}(s) = \sum_j \frac{|\eta_j|^2}{s + i\omega_j}, \tag{14}$$

- inversion: find poles ε_i ($=$ finding the roots of the characteristic polynomial), calculate residues

$$\alpha_i = i \lim_{\varepsilon \to \varepsilon_i} (\varepsilon - \varepsilon_i)\tilde{\alpha}(-i\varepsilon) = \left[\frac{\mathrm{d}}{\mathrm{d}s}\frac{1}{\tilde{\alpha}(-is)}\right]^{-1}\Bigg|_{s=\varepsilon_i} = \frac{\alpha(0)}{1 + \tilde{\mathrm{K}}'(-i\varepsilon_i)} = \frac{\alpha(0)}{1 + U_i} \tag{15}$$

Mean Displacement

- $\rho_A(t) = |\alpha(t)|^2 = \sum_{jk} \alpha_j \alpha_k^* \, \mathrm{e}^{-i(\varepsilon_j - \varepsilon_k)t}$ $\rightarrow$ Laplace transform inversion does not commute $\rightarrow$ need all poles, residues
- perturbation theory: have one state with great overlap with $|A\rangle$ $\rightarrow$ gives main contribution to $|\alpha(t)|^2$
- by choosing ω_A we can tune energy of this state
- let's set it to 0

$$0 = i\omega_A + \tilde{\mathrm{K}}(0) \implies \omega_A = \sum_j \frac{|\eta_j|^2}{\varepsilon_j} \tag{16}$$

$$U_A = \sum_j \frac{|\eta_j|^2}{\omega_j^2} \implies \rho_A \geq |\alpha_A|^2 = \frac{\alpha(0)}{(1+U_A)^2}, \tag{17}$$

Comparison with Born

- same expression for $U_A \implies$ inherit behavior
- but ρ_A only compatible if $U_A \ll 1 \implies (1+U_A)^2 \approx (1+2U_A)$
- also compatibility if $U_A \to \infty$ in both cases and $\omega_A \to 0$
- in continuum limit
$$\omega_A = \int_0^{\omega_c} \frac{J(\omega)}{\omega} = J_\alpha \frac{\omega_c^\alpha}{\alpha}. \tag{18}$$
- using this in
$$\rho_A(k) = \frac{1}{1 + 2\sum_j \frac{|\eta_j|^2}{(\omega_j - \omega_A)^2}} \tag{19}$$
  leads to $\rho_A \to 1 \, \forall \alpha$
- limits $N \to \infty$ and $g_0^2 \to 0$ do not commute
- have to choose g_0 for each N such that $\omega_A \to 0$, then limit works

Formula for other Eigenvalues

Let us assume that eq. (14) has a pole at $-i(\omega_j + \delta\omega_j) = -i\varepsilon_j$ with $\delta\omega_j \ll \omega_j$ so that

$$0 \overset{!}{=} \omega_j + \delta\omega_j + \omega_A - \sum_l \frac{|\eta_l|^2}{\omega_l - \omega_j - \delta\omega_j} \approx \sum_{l\neq j} \frac{|\eta_l|^2}{\omega_l - \omega_j} + \delta\omega_j \sum_{l\neq j} \frac{|\eta_l|^2}{(\omega_l - \omega_j)^2} - \frac{|\eta_j|^2}{\delta\omega_j}, \tag{20}$$

which can be solved for $\delta\omega_j$

$$\delta\omega_j = \frac{\operatorname{sgn} A_j}{2(1+B_j)}\left[|A_j| - \sqrt{A_j^2 + 4(B_j+1)|\eta_j|^2}\right] \tag{21}$$

with

$$A_j = \sum_{l\neq j} \frac{|\eta_l|^2}{\omega_l - \omega_j} + \omega_j - \omega_A \quad B_j = \sum_{l\neq j} \frac{|\eta_l|^2}{(\omega_l - \omega_j)^2}. \tag{22}$$

Strong Coupling Limit

For $\sum_j |\eta_j|^2 \gg \omega_c^2$ we can find an effective two-level system.

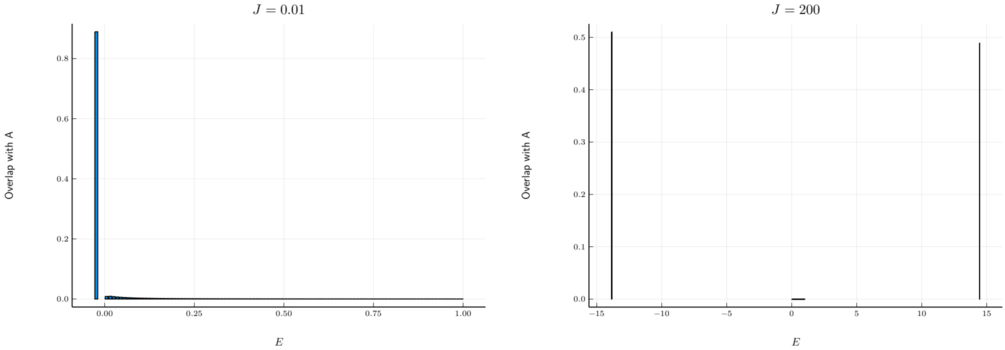
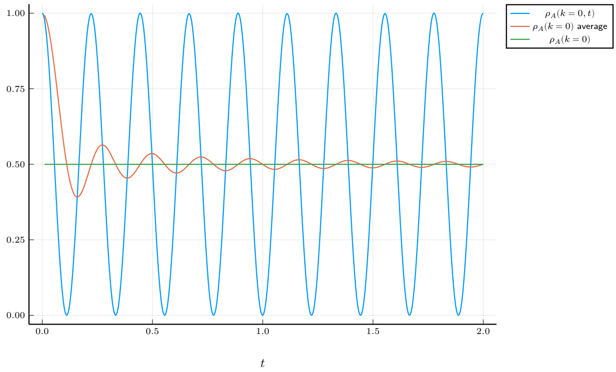


Figure: The spectrum of the model in fig. 1 for two different coupling strengths. The bars show the overlap $|\langle A|E\rangle|^2$ of the eigenstate $|E\rangle$ at energy E with the $|A\rangle$ state.

Trivial Behavior of ρ_A

- two eigenstates are complete basis of subspace that has overlap with $|A\rangle$ level
- perfect oscillations between $|A\rangle$ and some state support only in the bath $\rho_A = 1/2$



$$\langle m \rangle = \begin{cases} \frac{1}{2} & \text{if } u > 1, \\ 0 & \text{if } u < 1. \end{cases} \tag{23}$$

Bath Size Requirements

- assume $N \sim 100$ and constant DOS $\eta_j^2 = J_\alpha \omega_j^\alpha$ and $\omega_j = j\omega_c/N$
-

$$U_A = \sum_j \frac{\eta_j^2}{\omega_j^2} = J_\alpha \frac{\omega_C}{N} \sum_j \omega_j^{\alpha-2} = g_0^2 \frac{\alpha+1}{\omega_c^2} N^{1-\alpha} \sum_j j^{\alpha-2}. \tag{24}$$

For $1/N$ sufficiently smaller than 1 we can approximate the sum in eq. (24) as

$$N^{1-\alpha} \sum_j j^{\alpha-2} \approx \frac{g_0^2(\alpha+1)}{\omega_c^2} \left(N^{1-\alpha} \zeta(2-\alpha) + \frac{1}{\alpha-1} \right). \tag{25}$$

Demanding that $\rho_A \approx |\alpha_A|^2$ takes on a particular value for a given α yields

$$N = \left[\left(\frac{\omega_c^2}{g_0^2} \frac{\left(|\alpha_A|^{-1} - 1\right)}{(\alpha+1)} + \frac{1}{1-\alpha} \right) \frac{1}{\zeta(2-\alpha)} \right]^{\frac{1}{1-\alpha}}. \tag{26}$$

How far away is the continuum limit?

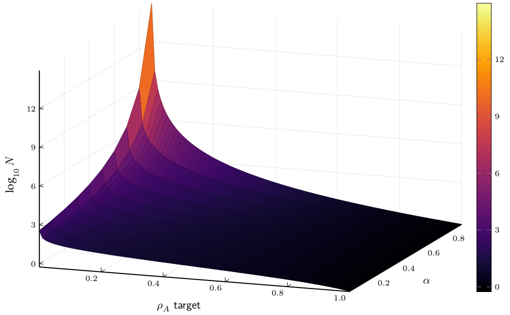


Figure: Equation (26) evaluated for $g_0^2 = 0.05$ and $\omega_c = 1$. For $\alpha \lesssim 4$ we can expect relatively good results for $\langle m \rangle$ for $\mathcal{O}(100)$ bath levels.

- $\alpha \approx 1$ gives limit

$$N \approx \left(\frac{\omega_c^2}{g_0^2} \left(|\alpha_A|^{-1} - 1 \right) \cdot \frac{1-\alpha}{1+\alpha} + 1 \right)^{\frac{1}{1-\alpha}} \xrightarrow{\alpha \to 1} e^{\frac{\omega_c^2}{2g_0^2}\left(|\alpha_A|^{-1} - 1\right)} \tag{27}$$

Mean Displacement with ω_A shift

- k dependence $\implies$ calculate ω_A for $k = 0$
  - as $\omega_A(k) \geq \omega_A(0)$ we will have $\rho_A \to 0$ generically
  - not the whole picture though $\implies$ for u large variations in coupling strength
  - note also: should normalize $v(1+u) = v + v'$ remains constant

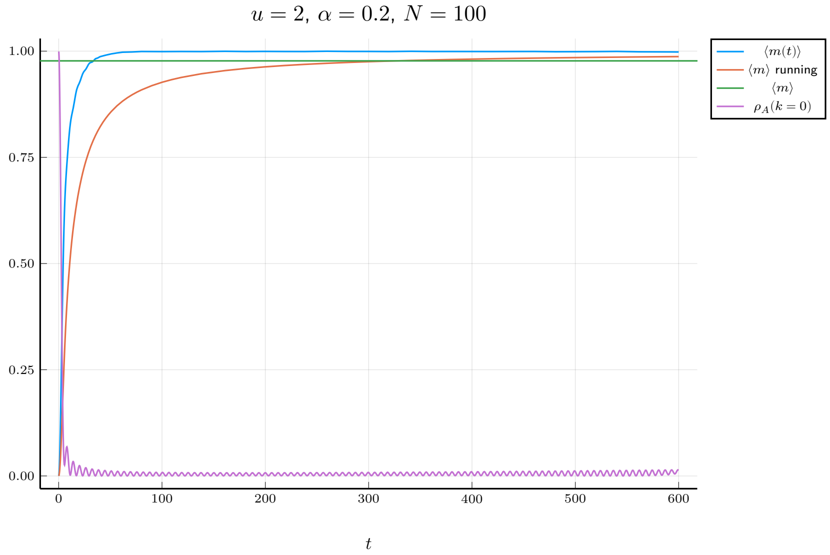
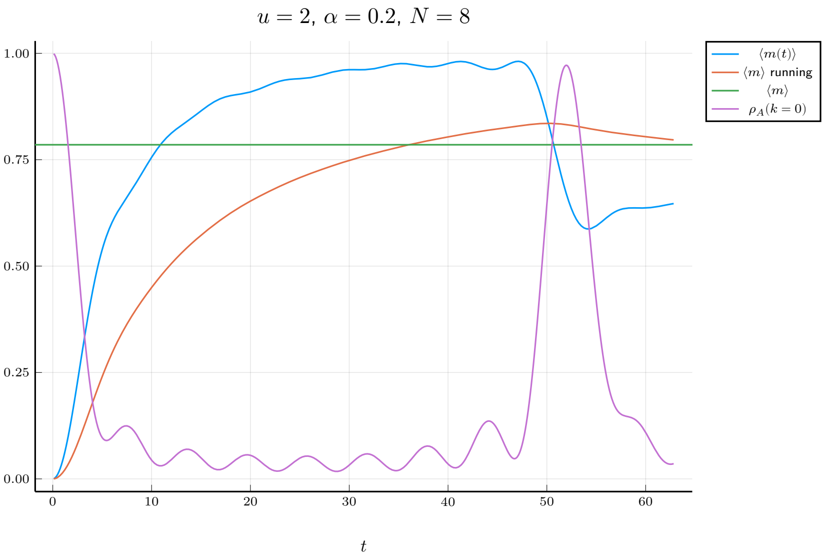
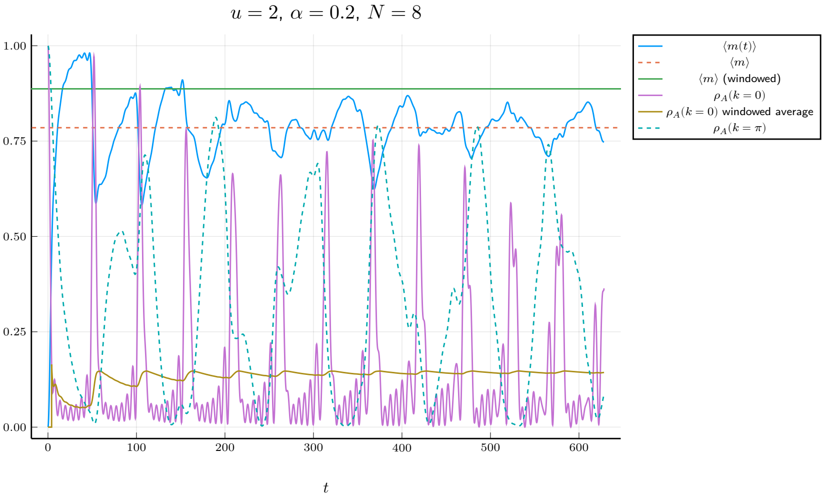


Figure: With $N = 100$ bath levels and $g_0^2 = 0.1$. The mean displacement approaches the universal value for finite times and the infinite time limit is not too far off.



$u = 2,\ \alpha = 0.2,\ N = 8$
1.00
0.75
0.50
0.25
0.00
0
10
20
30
40
50
60
t
$\langle m(t) \rangle$
$\langle m \rangle$ running
$\langle m \rangle$
$\rho_A(k=0)$


$u = 2,\ \alpha = 0.2,\ N = 8$
$\langle m(t) \rangle$
$\langle m \rangle$
$\langle m \rangle$ (windowed)
$\rho_A(k = 0)$
$\rho_A(k = 0)$ windowed average
$\rho_A(k = \pi)$
1.00
0.75
0.50
0.25
0.00
0
100
200
300
400
500
600
t

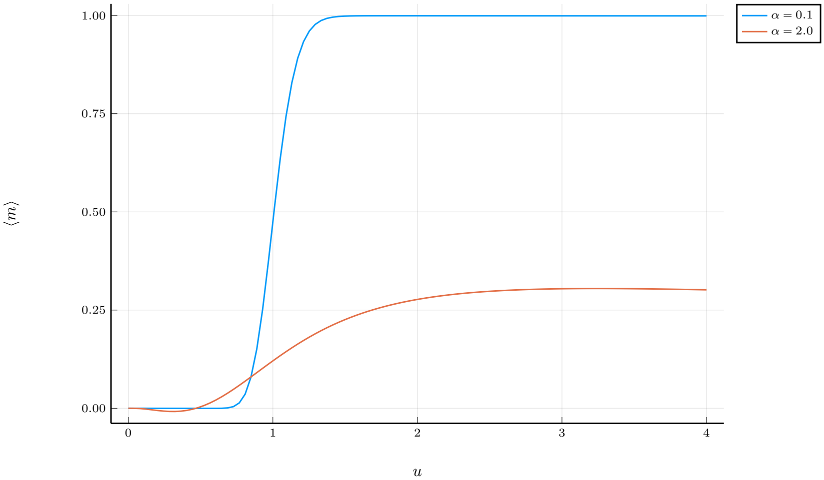
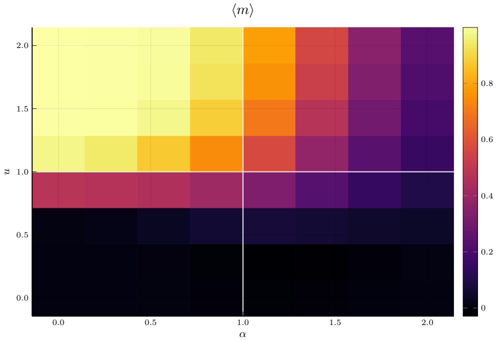
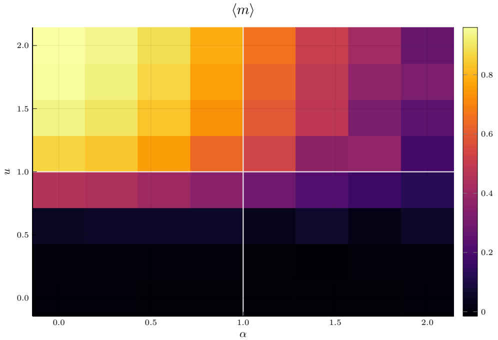


Figure: $\langle m(t) \rangle$ averaged over an interval $[0.5\tau, 0.95\tau]$ where τ is the recurrence time. The coupling strength was $g_0^2 = .05$ and $N = 100$ bath levels were used. This is on the same order of magnitude of what eq. (26) would suggest, but windowing improves the result.

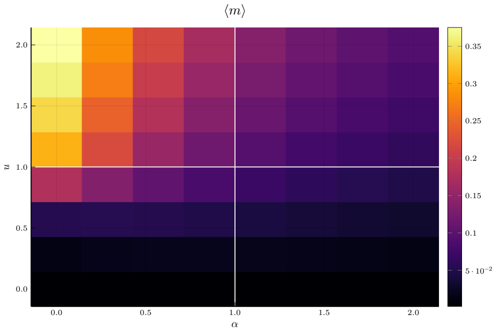


a) With windowing.

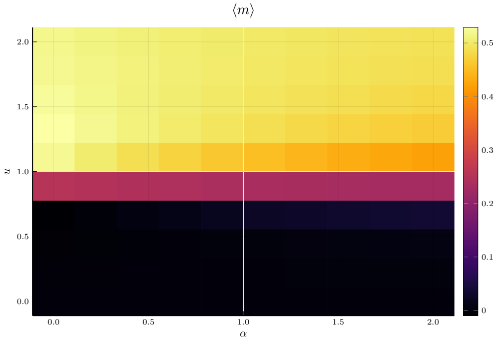


b) Without windowing. The phase diagram is slightly less crisp, but still acceptable.

Figure: Full phase diagrams with the same parameters as fig. 6.



a) Without Lamb-Shift compensation. No universal values of $\langle m \rangle$ are being reached.



b) Without Lamb-Shift compensation in the strong coupling limit.

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