

Photosynthesis Course Note

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July 8, 2016

Contents

1	8th, July	1
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1 8th, July

pp.2 of PPT In the last lecture, the *master equation* for density matrix ¹ could lead to problematic result. As the density matrix propagates as described by the master equation, the eigenvalues for it might involved into negative values. This is because the added terms are not rigorously derived, but just an approximation.

Digression: PRE 65 056120, something about entanglement between oscillators.

pp.3 of PPT Lindblad equations This equation ensures that the density matrix $\rho \geq 0$ (i.e. having all positive eigenvalues). However, this operator sometimes breaks down the symmetries of the system. That is, a system started with translation symmetry at t_0 might not have translation symmetry at $t > t_0$.

An Example for Lindblad equation:

Considering the case of a harmonic oscillator.

$$H = w_0 a^\dagger a$$

If we add interaction of oscillator and other excitons:

$$A^\dagger A(a^\dagger + a) = \text{extra} + \text{bath}$$

Then $A^\dagger A$ is V_m in ppt.

Digression Two Spin system. One way to judge whether the two particles are entangled or not, is to do partial transpose: transposing only part of the density matrix corresponding to only one particle of the system.

¹Reference not found.

Energy Transfer **Note:** This section's material could be found in *Excitonic energy transfer in light-harvesting complexes in purple bacteria*. *JChemPhys_136_245104.pdf*

pp.5 of PPT Exciton transport process. External influence to the system includes trapping, decaying and dissipation.

The k_t characterizes the trapping rate. And k_d characterizes the decay rate.

pp.6 of PPT Life time $\tau_n = \int_0^\infty \rho(t)_n dt$, where $\rho_n \equiv \rho_{nn}$. We hope the $\langle t \rangle = \sum \tau_n$ to be small, because the shorter an exciton is fixed on a state, the more random the system is and the more likely that the exciton is trapped.

Quantum yield $q = \text{On PPT} = \frac{\text{trapped}}{\text{trapped} + \text{died}}$.

pp.8 of PPT Showcase of calculating the $\rho(t)$ using the Haken-Strobl model A simple Ring.

pp.9 of PPT Complex models with more and more elements in the ring.

pp.10 of PPT ² The 16 sites ring shows that there is always a peak in the opposite site (See upper-left plot). This is because there is always two channels of equal length for it to get to the opposite side.

pp.11 of PPT A two ring case, with 8 sites on each ring. The initial configuration is evenly excited in the left ring. The right ring comprised of trapping sites.

pp.12 of PPT Another two ring case, with a change in the right ring's number of trapping sites. It shows that an asymmetric design would somehow improve the efficiency, since the right side plot has a maximum region.

pp.15 of PPT Start with a reduced single-electron density matrix. Consider an external interruption caused by Laser, and apply the *Principle of the near-sightedness of equilibrium systems* to reduce the computation difficulties. This principle is related R.P.A. in condensed matter physics.

Caution: I am quite confused by the following content, from pp.16 to the end of PPT. Ergo the following notes are not well organized. It is advised that one should look at the original paper

pp.16 of PPT ³ instead.

Calculating the absorption spectrum, with the result that only one level is acceptable. $A \propto \text{amplitude}$ characterizes the behavior of laser input. M_{mn} : the angle between oscillation angles.

² Could be found on *Efficient energy transfer in light-harvesting systems*. Cao and Silbey et al *New J Phys* (2010)

³ <http://journals.aps.org/pre/pdf/10.1103/PhysRevE.69.032902>

pp.17 of PPT Changing the behavior of lasers could result (in generally) more different acceptable levels. However, the laser configuration is not practical.

pp.19 of PPT Using Frankel-Exciton Model and find very good fit, balabala.