

# Qutip-lattice: A python package for quantum information, measurement, and dynamics problems defined on lattice

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## I. INTRODUCTION

Lattice models are of fundamental interest in physics. From gauge theories defined on lattices to tight-binding models embodying effective theories, the reach and manifestation of lattice models are all-pervasive. QuTiP is an open source python software package especially for simulating open system dynamics problems in quantum optics [1]. The versatility of the capabilities of QuTiP with open system dynamics are amenable to integration with widely used lattice models with legacies of their own. The single particle physics, while numerically less demanding suffice for the explanation of a vast treasure trove of physics encompassing problems of topological phases of matter, excitation spectra and transport properties. Many particle models, on the other hand, are numerically burdensome and require clever techniques of symmetry transformations for making computations feasible. Qutip-lattice package offers the famous many-particle physics Hubbard models implementations in bases of symmetry with manageable computational load. A few fermionic and bosonic models and interesting transformation properties are included. Some well known transformations useful for diagonalization calculations, the calculation of the ground state and excitation spectra are offered. Some Non-Hermitian Hamiltonian(NHH) models which are driving new avenues of research can also be

investigated. Many-body physics of atoms and light [2] and models embodying gain and loss mechanism [3] are of special interest.

Notable among existing open source packages for lattice dynamics problems is QuSpin [4, 5], which is exact diagonalization based. quutip-lattice offers some of the functionalities covered in QuSpin and more on topology and non-Hermitian models. The ALPS project is a distant fore-runner for strongly correlated physics [6], with support for modern approximate methods of Matrix Product States(MPS) and Density Matrix Renormalization Group (DMRG)[7]. Among python based DMRG softwares for lattice models Quimb is noteworthy [8].

## II. DYNAMICS PROBLEMS ON QUTIP

QuTiP's functionality include Schrödinger evolution, Markovian open system master equation dynamics, Bloch-Redfield equation, non-Markovian hierarchical equation of motion[15] etc.

### A. Closed system/unitary evolution

Dynamics in quantum mechanics is deterministic. A specification of the Hamiltonian and the initial state completely specifies the evolution of a closed system. In QuTiP, the coherent evolution is completely specified by the Hamiltonians (possibly with time dependence). The explicit time dependence can be conveniently input through time dependent coefficients of the Hamiltonian

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terms.

$$H(t) = \sum_i c_i(t) H_i(t) \quad (1)$$

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle$$

QuTiP has the functionality to calculate the evolution of the state as well as any observable desired with the `mesolve()` function as well as the `mesolve()` function.

### III. OPEN SYSTEM/NON-UNITARY EVOLUTION

Quantum systems we study are not isolated completely from the rest of the universe. The usual approach of resolving the universe into ‘system and environment’ enables a focused view on the dynamics of system where environment has a dissipative influence. The two most useful dynamics calculation QuTiP offers is the Lindblad master equation approach and Monte Carlo simulation of quantum trajectories.

#### A. Deterministic master equation

One of QuTiP’s most useful function, `qutip.mesolve()` solves the evolution of the system density matrix,  $\rho$  under the action of the superoperator  $\mathcal{L}$  called the Liouvillian defined by the following ‘master equation’.

$$\frac{\partial}{\partial t} \rho(t) = \mathcal{L} \rho(t) \quad (2)$$

The Liouvillian is split into a coherent dynamics part dictated by the system Hamiltonian  $H$  and an incoherent dynamics part dictated by a set of collapse/jump operators both of which can be time-dependent. A plethora of physical processes can be simulated with the formalism including coherent evolution, pump/drive and loss. Non-markovian physics can also be probed with time dependence in the collapse operators. For the fundamentally and quantum computing application wise important example of the evolution of multiple (N) qubits, we can enumerate the relevant terms embodying coherent evolution, pure dephasing, decoherence and pumping in the Born Markov Secular (BMS) approximation.

$$\begin{aligned} \frac{\partial}{\partial t} \rho(t) = & -i [H(t), \rho] + \sum_{j=0}^{N-1} \gamma_j \mathcal{D} [\sigma_j^-] \rho(t) \\ & + \sum_{j=0}^{N-1} \frac{\gamma_j^D}{2} \mathcal{D} [\sigma_j^z] \rho(t) + \sum_{j=0}^{N-1} 2\Gamma \mathcal{D} [\sigma_j^+] \rho(t), \end{aligned} \quad (3)$$

with  $\gamma_j$  the relaxation rate of qubit  $j$ ,  $\gamma_j^D$  pure dephasing and  $\Gamma$  a pump rate.  $H(t)$  is responsible for the coherent part of the evolution.  $\mathcal{D}[X]\rho = X\rho X^\dagger - \frac{1}{2}X^\dagger X\rho -$

$\frac{1}{2}\rho X^\dagger X$  is a Lindblad dissipator for a jump/collapse operator  $X$ . The decay constants of the collapse operators are modified according to the nature of the bath (vacuum, thermal or squeezed among the common types). Mathematically, Liouvillian superoperator is a Completely Positive Trace Preserving (CPTP) map [16]. A general quantum map can be written as a sum of Kraus operators ( $\rho(t+dt) = \sum_\nu K_\nu \rho K_\nu^\dagger$ ) and the CPTP requirement restricts them to the preconditioned form below,

$$K_0 = 1 - iHdt - \sum_\mu \frac{\gamma_\mu}{2} J_\mu^\dagger J_\mu dt = 1 - iH_{\text{eff}} dt$$

$$H_{\text{eff}} = H(t) - i \sum_\mu \frac{\gamma_\mu}{2} J_\mu^\dagger J_\mu \quad (4)$$

$$K_\nu = \sqrt{\gamma_\nu dt} J_\nu$$

#### B. Monte-Carlo quantum trajectories

Each Kraus operator correspond to a possible outcome of the measurement process, whose backaction on the system is codified by the Kraus operator. Whenever any  $\nu \neq 0$  outcome is obtained (a ‘click’ in the detector device) at time  $t$ , and the system undergoes a quantum jump/collapse according to  $K_\nu$ . In the absence of all  $\nu \neq 0$ , the system evolves according to  $K_0$ . What is striking about  $K_0$  is that it entails an evolution under the Non Hermitian Hamiltonian (NHH),  $H_{\text{eff}}$  (in eq. 10).

For an observable  $X$ , measurement outcomes may be distributed around the average in a normal distribution. Ito calculus takes  $\Delta W$  to be a zero-mean (stochastic mean, average over many measurement outcomes), Gaussian random variable with variance  $\Delta t$  [17],

$$dy = \langle X \rangle dt + \frac{dW}{(8k)^{\frac{1}{2}}}$$

$$\Delta t \rightarrow 0, (\Delta W)^2 \rightarrow (dW)^2 = dt$$

##### 1. Stochastic Schrödinger Equation (SSE)

In quantum measurement theory, given the measurement result  $dy$ , the evolution of the quantum state of a system in a time interval  $dt$  obeys the stochastic differential equation,

$$d|\psi\rangle = \left\{ -k(X - \langle X \rangle)^2 dt + (2k)^{\frac{1}{2}} (X - \langle X \rangle) dW \right\} |\psi(t)\rangle \quad (5)$$

Eq. 5 is referred to as Stochastic Schrödinger Equation (SSE). QuTiP’s `qutip.stochastic.ssesolve()` function facilitates solving SSEs.

## 2. Stochastic Master Equation (SME)

Eq. 5 is a stochastic differential equation for the quantum state. An equivalent equation for the density matrix conditioned upon a stream of measurement outcome is also defined.

$$d\rho = -k[X[X, \rho]]dt + \sqrt{2k}(X\rho + \rho X - 2\langle X \rangle \rho)dW \quad (6)$$

QuTiP's `qutip.stochastic.smesolve()` function facilitates solving SMEs.

## 3. Unravelling the master equation

The function `qutip.mesolve()` calculates dynamics as an ensemble average approach, averaging dynamics over many identically prepared system average. It can be thought of as the system evolving under continuous measurement where all baths (decay channels) are monitored continually and evolution is ceaselessly dictated by the simultaneous actions of all  $K_\nu$  terms but  $K_0$ , so system evolution is always normalized. Now, there are several kinds of measurements that observe the intensity or the phase quadratures of a bosonic mode, for example. So, for specific decay channel(s) where “click”s are registering stochastically, single trajectories may take different form, each Monte Carlo trajectory observed as discrete jumps separated by decaying evolutions in between. For a particular method of measurement (photocurrent/homodyne/heterodyne), `qutip.mcsolve()` evolves an initial state under the specified NHH  $H_{eff}$  (in eq. 10) and keep track of the norm of the unnormalized wavefunction. Whenever a random number sampled from a uniform distribution greater than the evolving norm, a quantum jump is applied and state is renormalized (norm is restored to 1),

$$|\psi(t + \delta t)\rangle = \frac{\Gamma_n |\psi(t + \delta t)\rangle}{\sqrt{\langle \psi(t) | \Gamma_n^\dagger \Gamma_n | \psi(t) \rangle}}$$

Since the density matrix is evolved in accordance with measurement records, the evolution is also referred to as measurement induced post selected evolution.

Sufficient number of trial runs, elucidates a mean path of the system in the single excitation subspace with measures of statistical fluctuations/deviations. For a detailed review, see [18–22]. For further information on the algorithms and simulations, see [23]. While bosonic modes are most widely studied both theoretically and experimentally with ever improving homodyne and heterodyne techniques, proposals have been made for quantum trajectory simulation of fermions as well[24] (non-interacting fermions).

## IV. NON HERMITIAN LATTICE MODELS

NHH are a partial description, it is necessarily part of a larger system where the probability conserving properties of quantum evolution holds. From NHH, we want to find larger systems with probability conserving physics (not uniquely). When incoherent pump and/or loss is present, the general description eq. by generalizing 3 [3],

$$\frac{\partial}{\partial t} \hat{\rho}(t) = -i [\hat{H}(t), \hat{\rho}] + \sum_{\mu=1}^{M_{loss}} \mathcal{D}[\hat{L}_\mu] \hat{\rho}(t) + \sum_{\mu=1}^{M_{gain}} \mathcal{D}[\hat{G}_\mu] \hat{\rho}(t), \quad (7)$$

$$\hat{L}_\mu = \sum_{j=1}^N l_{\mu j} \hat{c}_j, \quad \hat{G}_\mu = \sum_{j=1}^N g_{\mu j}^* \hat{c}_j^\dagger \quad (8)$$

The incoherent loss/gain operators are linear in creation/annihilation operators and the Hamiltonian is that of a lattice.  $\frac{\gamma_j^D}{2} 2\Gamma$  The Hamiltonian for a no-jump evolution or post-conditioned evolution (repeating an experiment many times till a run is found with no quantum jumps),

$$\hat{H}_{cond} = \sum_{n,m} \hat{c}_n^\dagger \hat{c}_m - \frac{i}{2} \sum_{\gamma} L_{\gamma} \hat{l}_{\gamma}^\dagger \hat{l}_{\gamma} - \frac{i}{2} \sum_{\delta} G_{\delta} (1 \mp \hat{g}_{\delta}^\dagger \hat{g}_{\delta}),$$

- and + are for fermionic and bosonic operators respectively. Also,  $\hat{l}_{\gamma} = \sum_m \langle l_{\gamma} | m \rangle \hat{c}_m$  and  $\hat{g}_{\delta}^\dagger = \sum_n \langle n | g_{\delta} \rangle \hat{c}_n^\dagger$ .  $|\hat{l}_{\gamma}\rangle$  and  $|g_{\delta}\rangle$  are eigenvectors of the Hermitian positive definite matrices  $L_{nm} = (\hat{l}^\dagger \hat{l})_{nm}$  and  $G_{nm} = (\hat{g}^\dagger \hat{g})_{nm}$  respectively. In the evolution of  $\hat{\rho}$  dictated by eq. 8, is it possible to find a part of ‘drift’ dynamics defined by some Hamiltonian?

As done in [3], an evolution equation can be calculated for the normal ordered covariance matrix,

$$i\partial_t \langle \hat{c}_n^\dagger \hat{c}_m \rangle = \sum_a \left( \left( \hat{H}_{eff} \right)_{ma} \langle \hat{c}_n^\dagger \hat{c}_a \rangle - \left( \hat{H}_{eff}^\dagger \right)_{an} \langle \hat{c}_a^\dagger \hat{c}_m \rangle \right) \quad (9)$$

And we observe the dynamics generated by NHH,

$$\hat{H}_{eff} = \hat{H} - \frac{i}{2} (\hat{L} \pm \hat{G}) \quad (10)$$

For both fermions and bosons, The Hamiltonian  $\hat{H}_{eff}$  is similar to  $\hat{H}_{cond}$ , with signs of the generator operators alternating.

$$\hat{H}_{cond} = \hat{H} - \frac{i}{2} (\hat{L} \mp \hat{G}) \quad (11)$$

### A. Atom-field models

Collective decay/ many body signature [34] [35]

Localized emitters arranged on a lattice are amenable to engineered atom-photon interactions and high fidelity long range interactions between them [34–36]. Qutip-lattice package includes code functionality in the single excitation limit. The model was used to investigate atomic emission properties under dipole-dipole interaction coupled interstitial impurities in the array in [36]. With a regular periodic arrangement, translational symmetry aids in the computational challenge as the dynamics problem at each quasi-momentum decouple.

With  $|g_i\rangle$  and  $|e_i\rangle$  being the emitter/atom's ground and excited states (resonance frequency of  $\omega_0$ ) respectively, the coherent interaction part of the dynamics is encoded in the Hamiltonian,

$$\mathcal{H} = \hbar \sum_{i=1}^N \omega_0 \hat{\sigma}_{ee}^i + \hbar \sum_{i,j=1}^N J^{ij} \hat{\sigma}_{eg}^i \hat{\sigma}_{ge}^j \quad (12)$$

The coherent  $J(r_i, r_j)$  and incoherent  $\Gamma(r_i, r_j)$  dipole-dipole interaction between two-atoms situated at  $r_i$  and  $r_j$ ,

$$J(r_i, r_j) - \frac{i}{2} \Gamma(r_i, r_j) = -\frac{3\pi\sqrt{\gamma_i\gamma_j}}{\omega_L} \hat{\mathbf{d}}_i^\dagger \cdot \mathbf{G}(r_i, r_j, \omega_L) \cdot \hat{\mathbf{d}}_j,$$

with the free-space Green's function (the propagator of the electromagnetic field between emitters at  $r_i$  and  $r_j$ )

$$G_{ij}(r) = \frac{e^{i\omega r}}{4\pi r} \left[ \left( 1 + \frac{i}{\omega r} - \frac{1}{\omega^2 r^2} \right) \delta_{ij} - \left( 1 + \frac{3i}{\omega r} - \frac{3}{\omega^2 r^2} \right) \frac{r_i r_j}{r^2} \right] - \frac{\delta(\mathbf{r})}{3\omega^2} \delta_{ij} \quad (13)$$

$\hat{\mathbf{d}}$  is the dipole matrix element of the atomic transition,  $\mathbf{r}=|\mathbf{r}_i - \mathbf{r}_j|$ . The dissipative interactions are codified in the jump operators  $\{\hat{O}_\nu\}$ ,  $\nu = 1, 2, \dots, N$ . Each individual jump operator  $\{\hat{O}_\nu\}$  is an eigenvector of the  $N \times N$  dimensional  $\Gamma$  matrix and the corresponding decay rates are the corresponding eigenvalue  $\Gamma_\nu$ . The  $\Gamma$  matrix is composed of the elements  $\Gamma_{ij}$ .

Each jump operator  $\hat{O}_\nu$  is a superposition of all the lowering operators,

$$\hat{O}_\nu = \sum_{i=1}^N \alpha_{\nu,i} \hat{\sigma}_{ge}^i = \sum_{i=1}^N \alpha_{\nu,i} |g_i\rangle \langle e_i| \quad (14)$$

subject to the normalization,

$$\sum_{i=1}^N \alpha_{\nu,i}^* \alpha_{\mu,i} = \delta_{\nu,\mu} \quad (15)$$

The spontaneous emission rate  $\Gamma_0$  of each atom is found in,

$$\sum_{i=1}^N \Gamma_\nu |\alpha_{\nu,i}|^2 = \Gamma_0 \quad (16)$$

The total emission rate  $R$  is calculated with,

$$R = -\frac{d}{dt} \sum_i \langle \sigma_{ee}^i \rangle = \sum_{i=1}^N \Gamma_\nu \langle \hat{O}_\nu^\dagger \hat{O}_\nu \rangle \quad (17)$$

In an infinite lattice, excitations are collective surface modes of in-plane quasimomentum  $\mathbf{k}$  with lowering operator  $\sigma_{\mathbf{k}}$ ,

$$J(\mathbf{k}) - \frac{i}{2} \Gamma(\mathbf{k}) = -\frac{3\pi\sqrt{\gamma_i\gamma_j}}{\omega_L} \hat{\mathbf{d}}_i^\dagger \cdot \mathbf{G}(\mathbf{k}, \omega_L) \cdot \hat{\mathbf{d}}_j, \quad (18)$$

$$J(\mathbf{k}) = \sum_i \mathbf{J}(\mathbf{r}_i - \mathbf{r}_s) e^{-i\mathbf{k} \cdot \mathbf{r}_i}$$

$$\Gamma(\mathbf{k}) = \sum_i \Gamma(\mathbf{r}_i - \mathbf{r}_s) e^{-i\mathbf{k} \cdot \mathbf{r}_i},$$

and  $G(\mathbf{k}, \omega_L)$  is the discrete Fourier Transformation of  $G(r_i, r_j, \omega_L)$  over the entire lattice. Interstitial impurities can give rise to new unit cell periodicities and coupled equation structures in the  $\mathbf{k}$ -space. The interaction picture Hamiltonian with dipole-dipole interaction between emitters and the impurity site is,

$$H_I^{(1)} = \sum_i \left( J(r_i, r_s) - \frac{i}{2} \Gamma(r_i, r_s) \right) \sigma_i^\dagger s + H.c.$$

The effect of geometries was investigated in ref. [37]

## B. “No-jump” evolution

Defining the model,

```
1 nSites = 6
2 fermiHubbardLattice = LatticeId_f_Hubbard(
    num_sites=nSites, boundary="periodic", t=1,
    U=-4)
```

Listing 1. Python example

```
1 [Hamiltonian_Nk, basisReprUp, DownStatesPerRepr,
   normHubbardStates] = fermiHubbardLattice.
   Hamiltonian( fillingUp=4, fillingDown=4,
   kval=0)
```

Listing 2. Python example

## C. Scattering matrix of a regular tight binding chain

### D. Fermionic tight binding chain

For  $N$  fermionic sites each coupled to a reservoir(bath) of fermions, ( $c_\sigma, c_\sigma^\dagger$  being the fermionic annihilation and creation operators respectively, operators under  $\sim$  are the bath operators who are labelled with wavevectors). The coherent parts of the interactions between the fermionic system sites included in  $H_S$ , and the coupling to the baths described by,

$$\begin{aligned}
H_{Tot} &= H_0 + H_S + H_{int} \\
H_0 &= \sum_i \epsilon_i c_i^\dagger c_i + \sum_{k_j} \epsilon_{k_j} \tilde{c}_{k_j}^\dagger \tilde{c}_{k_j} \\
H_{int} &= \left( \sum_{i=1}^N V_i \sum_{k_j} c_i^\dagger \tilde{c}_{k_j} + H.c. \right) \quad (19)
\end{aligned}$$

The density matrix of the system+bath,  $\rho(t)$  follows the von Neumann equation,

$$\dot{\rho} = -i[H_{Tot}, \rho(t)] \quad (20)$$

Going into the interaction picture (all interaction picture terms are written with a  $\hat{\cdot}$ ), the interaction picture density operator,  $\hat{\rho}(t) = e^{iH_0 t} \rho(t) e^{-iH_0 t}$  [40],

$$\begin{aligned}
\dot{\hat{\rho}}(t) &= \mathcal{L}(t) \hat{\rho}_0 + \int_0^t dt_1 \mathcal{L}(t) \mathcal{L}(t_1) \hat{\rho}(t_1) \\
\mathcal{L}(t) \hat{\rho}(t_1) &= -i[\hat{V}(t), \hat{\rho}(t_1)]
\end{aligned}$$

The L reservoir has the injecting band of particles and R reservoir the transmottted bands. Using the Born approximation,  $\hat{\rho}(t) = \hat{\rho}_S(t) \otimes \hat{\rho}_L \otimes \hat{\rho}_R$ , we find for the system density operator,  $\hat{\rho}_S(t)$ , ( $\hat{\rho}_{L(R)}$  is the density operator of the L(R) reservoir)

$$\begin{aligned}
\dot{\hat{\rho}}_S(t) &= -i \int_0^t dt_1 \sum_{i,j} \left[ g_{ij}^>(t, t_1) \hat{d}_i^\dagger(t) \hat{d}_j(t_1) \hat{\rho}_S(t_1) \right. \\
&\quad \left. - g_{ji}^>(t_1, t) \hat{d}_i(t) \hat{\rho}_S(t_1) \hat{d}_j^\dagger(t_1) - g_{ji}^<(t_1, t) \hat{d}_i(t) \hat{d}_j^\dagger(t_1) \hat{\rho}_S(t_1) \right. \\
&\quad \left. + g_{ij}^<(t, t_1) \hat{d}_i^\dagger(t) \hat{\rho}_S(t_1) \hat{d}_j(t_1) \right] + H.c. \quad (21)
\end{aligned}$$

The first order correlation functions appearing in eq. 21 have the following definitions,

$$\begin{aligned}
g_{ij}^<(t, t') &= \delta_{ij} |V_i|^2 \sum_{k_i} i \langle \hat{c}_{k_i}^\dagger(t') \hat{c}_{k_i}(t) \rangle \\
g_{ij}^>(t, t') &= \delta_{ij} |V_i|^2 \sum_{k_i} (-i) \langle \hat{c}_{k_i}(t) \hat{c}_{k_i}^\dagger(t') \rangle
\end{aligned}$$

They can be approximated by the so-called wideband approximation.

$$\begin{aligned}
g_{ij}^<(t, t') &= i \delta_{ij} 2\pi \mathcal{D}_i |V_i|^2 f_i \delta(t - t') \\
g_{ij}^>(t, t') &= -i \delta_{ij} 2\pi \mathcal{D}_i |V_i|^2 (1 - f_i) \delta(t - t')
\end{aligned}$$

Here  $f_i$  is the Fermi function and  $\mathcal{D}_i$  is a constant density of states in the  $i$ -th reservoir. Fermi functions take the values  $f_i = 0 (f_i = 1)$  for the drain (source) reservoir. With  $\Gamma_i = 2\pi \mathcal{D}_i |V_i|^2$  being the strength of the coupling to the reservoir, we can use the wideband approximations to derive the Schrödinger picture Lindblad equation [40],

$$\dot{\rho}_S = -i[H_S, \rho_S] - \frac{1}{2} \sum_i \Gamma_i [f_i \mathcal{L}_i^+ \rho_S + (1 - f_i) \mathcal{L}_i^- \rho_S], \quad (22)$$

with  $\mathcal{L}_i^+ \rho_S = c_i c_i^\dagger \rho_S + \rho_S c_i c_i^\dagger - 2c_i^\dagger \rho_S c_i$ , and  $\mathcal{L}_i^- \rho_S = c_i^\dagger c_i \rho_S + \rho_S c_i^\dagger c_i - 2c_i \rho_S c_i^\dagger$  codify the dissipative action of the reservoir to site  $i$ .

The integro-differential equation in 21 simplifies to a differential equation 22 with the wide-band approximation.

The vectorized system density matrix,  $\vec{\rho}_S = \text{vec}[\rho_S]$ , follow a numerically amenable differential equation [41].

$$\vec{\rho}_S(t) = e^{-i\mathcal{M}t} \vec{\rho}_S(0) \quad (23)$$

The  $\mathcal{M}$  matrix has the structure [40],

$$\begin{aligned}
\mathcal{M} &= \mathcal{M}_0 - i \frac{\Gamma}{2} \\
\mathcal{M}_0 &= I^{\otimes 3} \otimes H_S - H_S^T \otimes I^{\otimes 3}
\end{aligned}$$

$I$  being the 2d identity matrix. The structure of  $\mathcal{M}$  holds the signatures of NHH that is induced by the coupling to the reservoirs. A passing note on the numerics is that before integrating eq. 23, the fermionic operators have to be replaced by spin operators with the Jordan Wigner transformation.

## V. CORRELATED RADIANCE IN EMITTERS COUPLED TO NONLINEAR PHOTONIC CAVITY

Translational symmetry techniques can be availed of in computing dynamics problems involving nonlinear cavities which are always very demanding [42]. Two or multiple photon bound states can be used in ansatzes that carry the essential support of the wavefunction in certain dynamics problems[43, 44].

$H_B$  in eq. ?? with energy  $\omega_c$  and tunneling amplitude  $J$ ,

$$H_{ph} = \sum_n \omega_c a_n^\dagger a_n - \frac{U}{2} a_n^\dagger a_n^\dagger a_n a_n - J (a_n^\dagger a_{n+1} + H.c.)$$

N two Level System(TLS) are each coupled to a cavity of the one dimensional lattice.

$$H = H_{ph} + \frac{\omega_e}{2} \sum_{i=1}^N \sigma_i^z + g \sum_{i=1}^N (a_{n_i} \sigma_i^+ + a_{n_i}^\dagger \sigma_i^-) \quad (24)$$

For N=2, the essential physics is found in a subspace of wave-functions with two-photon bound states[43, 44].

$$\begin{aligned}
|\phi_2\rangle(t) &= e^{-2i\omega_e t} \left\{ c_e(t) \sigma_1^+ \sigma_2^+ + \sum_K c_K(t) B_K^\dagger \right. \\
&\quad \left. + \sum_k [c_{1k}(t) \sigma_1^+ + c_{2k}(t) \sigma_2^+] a_k^\dagger \right\} |g, g, vac\rangle, \quad (25)
\end{aligned}$$

with  $a_k^\dagger = \sum_n e^{ikn} a_n^\dagger / \sqrt{N_c}$  and  $B_K^\dagger$  is creation operator of a boundstate of two photons,  $|\Psi_K^b\rangle = B_K^\dagger |vac\rangle$ .

Writing the photon number conserving bose Hubbard model in the  $k$ -space, all the different  $k$ -s decouple. the cross terms of the Hamiltonian are zero because it is particle number conserving. The first term with no explicit  $k$ -dependence can have diagonal in  $k$ - resolution as well,

$$1 \equiv \sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k}| \quad (26)$$

Therefore it is possible to solve the individual  $k$ -value dynamics separately as the interactions are decoupled in  $k$ .

## VI. NON-HERMITIAN DYNAMICS

There are works that treat NHH as a focussed view of a larger physical system where all the rules of Conventional Quantum Mechanics(CQM) hold and the NHH problem boils down to mapping the given problem to valid choices (not unique) extended systems that follow CQM [3]. But there have been efforts to trat NHH as fundamental objects and fundamental physics in their own right. As was explained in [45], for neutral meson systems, NHHs were used in [46, 47]. A general NHH,  $\hat{H}$  can be split into Hermitian ( $\hat{H}_+$ ) and non-Hermitian ( $\hat{H}_-$ ) parts i.e.  $\hat{H} = \hat{H}_+ + \hat{H}_-$ . They are simply,  $\hat{H}_\pm = (\hat{H}_+ \pm \hat{H}_-)/2$ . With the definitions,  $\hat{M} = \hat{H}_+$ , and  $\hat{\Gamma} = 2i\hat{H}_-$  ( $\hat{M}$  and  $\hat{\Gamma}$  both Hermitian with positive eigenvalues), NHH are often put in the Weisskopf-Wigner form,  $\hat{H} = \hat{M} - i\hat{\Gamma}/2$  ( $\hat{M}$  and  $\hat{\Gamma}$  are both Hermitian). With a NHH, the Liou-villian equation for the density matrix, eq. 3 no longer preserves the trace. Ref.s [48–50] introduces the normalized density matrices,  $\hat{\rho}_N(t) = \hat{\rho}(t)/\text{Tr}[\hat{\rho}(t)]$  leading to the redefinition of the expectation value of an observable  $\hat{O}(t)$  as,  $\langle \hat{O}(t) \rangle = \text{Tr}[\hat{\rho}_N(t)\hat{O}(t=0)]$ . The proposed master equation is the following,

$$i\partial_t \hat{\rho}_N = [\hat{M}, \hat{\rho}_N] - \frac{i}{2}\{\hat{\Gamma}, \hat{\rho}_N\} + \frac{i}{2}\text{Tr}[\hat{\Gamma}\hat{\rho}_N]\hat{\rho}_N, \quad (27)$$

instead of the usual Liouville-von Neumann equation,

$$i\partial_t \hat{\rho} = [\hat{H}_{eff}, \hat{\rho}] = [\hat{M}, \hat{\rho}_N] - \frac{i}{2}\{\hat{\Gamma}, \hat{\rho}_N\}, \quad (28)$$

with an effective Hamiltonian  $\hat{H}_{eff}$  (which is Non-Hermitian). The corresponding Schrödinger equation to the master equation eq. 27 was also defined in [48].

$$i\frac{\partial}{\partial t}|\psi'\rangle = \left(\hat{H}_+ + \hat{H}_- - \langle \hat{H}_- \rangle\right)|\psi'\rangle, \quad (29)$$

with  $\langle \hat{H}_- \rangle \equiv \langle \psi' | \hat{H}_- | \psi' \rangle = \langle \psi' | \hat{H} - \hat{H}_+ | \psi' \rangle$ . Ref. [48] succeeded in finding an equation of motion for the determinant of the density matrix  $\hat{\rho}(t)$ .

$$\frac{\partial}{\partial t} \det \hat{\rho}(t) = -\frac{1}{\hbar} \det \hat{\rho}(t) \text{tr}[\hat{\Gamma}] \quad (30)$$

Eq. 30 can be integrated

$$\det \hat{\rho}(t) = \det \hat{\rho}(0) e^{-\frac{1}{\hbar} \text{tr}[\hat{\Gamma}]t} \quad (31)$$

Eq. 31 reveals the asymptotic dynamics of the determinant of the density matrix. For example for a  $\hat{\Gamma}$  with trace 0,  $\det \hat{\rho}(t)$  is a conserved quantity.

Eq. 27 is sometimes also put in the form,

$$i\partial_t \hat{\rho}_N = [\hat{M}, \hat{\rho}_N] - \frac{i}{2}\{\hat{\Gamma}, \hat{\rho}_N\}, \quad (32)$$

where,

$$\hat{\Gamma}_{\hat{\rho}} = \hat{\Gamma} - \text{Tr}[\hat{\Gamma}\hat{\rho}_N]1 \quad (33)$$

$\text{Tr}[\hat{\Gamma}\hat{\rho}_N]$  is responsible for a state-dependence in the effective Hamiltonian which codifies a feedback over the dynamics. The Gisin equation of [51] is obtained with the substitution  $\hat{M} = \frac{\hat{\Gamma}}{2}$ . [52] showed the derivation of classical Landau-Lifshitz equation from the quantum mechanical equation eq. 32.

$$\partial_t \text{Tr}[\hat{\rho}_N] = -\text{Tr}[\hat{\Gamma}\hat{\rho}_N] \quad (34)$$

The non-linear term  $\frac{i}{2}\text{Tr}[\hat{\Gamma}\hat{\rho}_N]\hat{\rho}_N$  comes from the time derivative of  $\text{Tr}[\hat{\rho}_N]$  (eq. 34) and helps preserve the trace over time evolution [50]. Dropping the term we simply get the eq. 28 which is linear and has some use in the theory despite the decay of the trace over time. Eq. 27 has been used in the context of symmetry breaking [50], criticality in  $\mathcal{PT}$  symmetric systems [53], quantum speed limits [54, 55], in the development of ‘biorthogonal quantum mechanics’ [56]. Both eq. 32 and 27 can have additive Lindblad dissipators  $\mathcal{D}[\hat{L}_j](\hat{L}_j$  being some collapse operator) on the right hand side in the presence of further dissipative interactions [57].

Ref. [58] discusses the evolution of entropy in the NH approach. The usual definition of von-Neumann entropy leads to more interesting features when applied to the Non-Hermitian systems.

$$S_{vN} \equiv -k_B \langle \ln \hat{\rho}_N \rangle = -k_B \text{Tr}[\hat{\rho}_N \ln \hat{\rho}_N] \quad (35)$$

If  $\hat{\Gamma} \rightarrow 0$  and  $\hat{H}_{eff} \rightarrow \hat{M}$ , under unitary dynamics, we simply obtain an unevolving von Neumann entropy [58],

$$\partial_t S_{vN} = -k_B \text{Tr}[\partial_t \hat{\rho}_N \ln \hat{\rho}_N] = 0 \quad (36)$$

For the Non Hermitian case, however, the evolution of  $S_{vN}$  can be found in the form,

$$\partial_t S_{vN} = \frac{2k_B}{\hbar} \text{Tr}[\hat{\Gamma}\hat{\rho}_N \ln \hat{\rho}_N] + \frac{2}{\hbar} \text{Tr}[\hat{\Gamma}\hat{\rho}_N] S_{vN} \quad (37)$$

Therefore, it can be observed that, the non-unitary evolution codified in eq. 27 in general leads to entropy production or increase unlike the unitary evolution. Considering the presence of nonequilibrium processes that may lead to the Non Hermitian physics, such a behaviour is not invalid. A second definition of entropy entertained

in [58] is based on taking the statistical average of the logarithm of the non-normalized density operator,

$$\begin{aligned} S_{NH} &= -k_B \langle \ln \hat{\rho} \rangle = -k_B \text{Tr}[\hat{\rho}_N \ln \hat{\rho}] \\ &= -k_B \frac{\text{Tr}[\hat{\rho} \ln \hat{\rho}]}{\text{Tr}[\hat{\rho}]} \end{aligned} \quad (38)$$

with a curious result for the difference between the two entropies,

$$S_{NH} = S_{vN} - k_B \ln[\text{Tr}[\rho]],$$

$k_B$  being the Boltzmann constant.

Since,  $\ln[\text{Tr}[\rho]]$  is a measure of the loss in the trace in the linear evolution, the difference of the two entropies in a sense quantifies the loss. Problematically, the entropy  $S_{NH}$  is not invariant under constant shifts of the Hamiltonian which is not supposed to change any of the physical properties [58].

$$\begin{aligned} \hat{\Gamma} &\rightarrow \hat{\Gamma} + \frac{1}{2}\alpha \mathbf{1} \\ S_{vN} &\rightarrow S_{vN}, \\ S_{NH} &\rightarrow S_{NH} + k_B \alpha t \end{aligned}$$

The dynamics of von-Nwemann entropy is indeed very rich and deserves attention in the context of specific examples. Ref. [59] investigated the dynamics of coupled nonlinear oscillators with the non-Hermitian master equation eq. 27 specifically with the example of resonant cavities coupled by a chiral mirror. The number non-conserving physics is relevant to the  $\mathcal{PT}$ -symmetric lasers and anti-lasers [60–63] and simulation of double-well non-Hermitian Bose condensate models. The dynamics of von Neumann entropy was found to be rich and illuminating. While nonlinearity induces entanglement, its dynamics and amount was controllable by the asymmetry of the non-Hermitian interaction.

Ref. [64] investigated the evolution of purity in the non-linear evolution eq. 27, demonstrating that quantum fluctuations may destabilize initial pure states evolving into mixed states unlike the Hermitian master equations which preserve the purity of an initial pure state. Ref. [48] also finds an equation of motion for the purity defined in the habitual form,

$$\begin{aligned} \tilde{\mathcal{P}}(\hat{\rho}) &\equiv \text{tr}(\hat{\rho}'^2) = \text{tr}(\hat{\rho}^2)/(\text{tr}(\hat{\rho}))^2 \\ \frac{\partial}{\partial t} \tilde{\mathcal{P}}(\hat{\rho}) &= \mathcal{R}(\hat{\rho}, \hat{\Gamma}), \\ \mathcal{R}(\hat{\rho}, \hat{\Gamma}) &= 2\text{Tr}[\hat{\rho}'\hat{\Gamma}]\text{Tr}[\hat{\rho}'^2] - \text{Tr}[\hat{\rho}'^2\hat{\Gamma}] \end{aligned}$$

So, the purity is conserved over time if the function,  $\mathcal{R}(\hat{\rho}, \hat{\Gamma})$  is 0.

The time correlation functions need to be defined and understood since properties of correlation functions are related to linearity and we have master equations generalized to nonlinearity. Ref. [49] entertains multiple

definitions. The hermitian correlation function can only be defined with the Hermitian part of the Hamiltonian,  $\hat{M}$ . For two arbitrary operators  $\hat{\chi}$  and  $\hat{\xi}$ ,

$$C_{\chi\xi} = \text{Tr} \left\{ \hat{\chi} \exp \left[ -i(t_2 - t_1)\hat{M} \right] \hat{\xi} \hat{\rho}_{\hat{M}} \exp \left[ i(t_2 - t_1)\hat{M} \right] \right\} \quad (39)$$

The correlation function from Eq. 39 is generalized in the non-Hermitian case,

$$\begin{aligned} C_{\chi\xi}(t_1, t_2) &= \text{Tr} \left\{ \hat{\chi} \mathcal{K}(t_2, t_1) \hat{\xi} \mathcal{K}(t_1, t_0) \hat{\rho}_N(t_0) \right\} \\ &= \text{Tr} \left\{ \hat{\chi} \mathcal{K}(t_2, t_1) \hat{\xi} \hat{\rho}_N(t_1) \right\} \\ &= \text{Tr} \left\{ \hat{\chi} \mathcal{K}(t_2, t_1) \hat{\xi} \hat{\rho}(t_1) / \text{Tr}[\hat{\rho}(t_1)] \right\}, \end{aligned} \quad (40)$$

$\hat{\chi}$  and  $\hat{\xi}$  are Schrödinger picture operators,  $\mathcal{K}$  is the generalized evolution operator evolving the density operator from a point in time to other,  $\mathcal{K}(t_b, t_a) \hat{\rho}(t_a) = \hat{\rho}(t_b)$ .

A different correlation function was also defined in terms of the linear non-trace preserving eq. 28,

$$\begin{aligned} C_{\chi\xi}^{(L)}(t_1, t_2) &= \text{Tr} \left\{ \hat{\chi} \mathcal{K}_L(t_2, t_1) \hat{\xi} \mathcal{K}_L(t_1, t_0) \hat{\rho}(t_0) \right\} / \text{Tr}[\hat{\rho}(t_2)], \\ &= \text{Tr} \left\{ \hat{\chi} \mathcal{K}_L(t_2, t_1) \hat{\xi} \hat{\rho}(t_1) \right\} / \text{Tr}[\hat{\rho}(t_2)], \end{aligned} \quad (41)$$

For relaxation in spin-ensembles, the redfield approach had always been the *modus operandi* [65–67] until recent years. For the description of nonlinear processes taking place in NMR experiments, more sophisticated phenomenological approaches have been developed with NHHs. A direct application of Liouvillian-von Neumann equation is not sensible because of the non-preservation of the trace over the evolution. A Liouvillian equation has also been defined for  $\eta$ -pseudo-Hermitian ( $\eta H \eta^{-1} = H^\dagger$  with  $\eta$  being a Hermitian metric operator in Hilbert space [68]) Hamiltonians in [69, 70]. For the generalized density matrix,  $\rho_G(t) = \rho(t)\eta$ , the proposed generalized density matrix evolution equation,

$$\begin{aligned} \frac{\partial}{\partial t} \rho_G &= -i[H, \rho_G] \\ &+ \sum_{j=1}^{N^2-1} \left( L_j \rho L_j^\dagger - \frac{1}{2} L_j^\dagger L_j \rho_G - \frac{1}{2} \rho_G L_j^\dagger L_j \right) \end{aligned} \quad (42)$$

where  $L_j^\dagger = \eta^{-1} L_j^\dagger \eta$  embodies the adjoint of  $L_j^\dagger$  with respect to the pseudo-inner product constructed by  $\eta$ . A similarity transformation is used to convert the  $\eta$ -pseudo Hermitian Hamiltonian to its Hermitian counterpart, which satisfies the regular Liouvillian master equation (eq. 3 for example). Eq. 42 is finally obtained by reverting back to the original basis.

Among the  $\eta$ -pseudo-Hermitian Hamiltonians,  $\mathcal{PT}$ -symmetric Hamiltonians have attracted substantial attention. Initiated by the original discovery by Bender and Boettcher in 1988 that the eigenvalues of Hamiltonians with  $\mathcal{P}$ :parity-inversion plus  $\mathcal{T}$ :Time reversal symmetry are all real [71], a revolution has taken place leading to the theory of Non-Hermitian Quantum Mechanics (NHQM) [68, 72–75]. The interest in unravelling

the physics of  $\mathcal{PT}$ -symmetry disseminated the borders of quantum and classicality [75] to semi-classical as well as classical physics. One important issue debated is the validity of non-Hermitian physics as a fundamental theory. Certain works are cautiously pessimistic about it since important cornerstones of physics seems to be in contradiction to it. [76] argues that local  $\mathcal{PT}$ -symmetry facilitates the perfect discrimination of non-orthogonal states and the violation of the no-signaling principle. Ref. [77] showed that entanglement under local operations can be increased. And ref. [78] showed entanglement under local unitary operations to be not invariant under local  $\mathcal{PT}$ -symmetric unitary operations.

The difficulty in formulating Non Hermitian Quantum Mechanics (NHQM) as a fundamental theory was noted to be intertwined with proper definition of the Hilbert space (mostly the inner product) [56, 79–83]. To make the trace time invariant, instead of keeping it fixed at 1, the metric of the Hilbert space could be redefined [84]. Ref. [84] focusses on finite-dimensional state spaces with a Hilbert space metric and generalized operator definitions that fixes the problems of violation of the no-go theorems argued in [76–78].  $|\psi\rangle(t)$  is parallel transported in the direction of time and inner products between parallel transported vectors are fixed in time. To differentiate from the conventional inner product it is written as  $\langle\langle\psi_1(t)|\psi_2(t)\rangle\rangle$ . New vector  $|\psi\rangle(t)$  is the same as  $|\psi\rangle(t)$  and follows the Schrödinger equation,  $\partial_t|\psi(t)\rangle = -iH(t)|\psi(t)\rangle$ . Dual vectors are not simply the Hermitian conjugates, but also are subject of a linear map,

$$\langle\langle\psi(t)| = \langle\psi(t)|G(t),$$

$G(t)$  is the solution (Hermitian, positive-definite) of the following equation

$$\partial_t G(t) = i [G(t)H(t) - H^\dagger(t)G(t)],$$

and we get a time dependent metric. In the special case the metric is time independent, we get the pseudo-Hermitian Hamiltonian,  $GH = H^\dagger G$ . The definition of unitary operators from CQM,  $U(t)^\dagger U(t) = \mathbf{1}$  changes to the condition of keeping the metric unchanged  $\mathcal{U}^\dagger G(t)\mathcal{U} = G(t)$  in NHQM. The generalized density matrix operator,  $\hat{\rho} = \sum_i p_i |\psi_i(t)\rangle\rangle\langle\langle\psi_i(t)|$  and expectation values of the generalized operators ( $\langle\langle\mathcal{O}\rangle\rangle = \sum_i p_i \langle\langle\phi(t)|\mathcal{O}|\phi_i(t)\rangle\rangle = \text{Tr}[\langle\phi(t)\rangle\rangle\langle\langle\phi(t)|\mathcal{O}\rangle\rangle$ ) have the habitual forms.

#### A. $\mathcal{PT}$ - symmetry

For a review, see [85] and a recent one for  $\mathcal{PT}$ -symmetry in photonic systems, see [86].

#### 1. Two Level

#### 2. Lattice

Functions to form the lattice from the k-space Hamiltonian?

### Appendix A: Quantum Stochastic Differential Equations

Landau's Density operator equations was originally showed to obtain diffusion or Fokker Planck equations (equivalently Wiener processes) in [88–90].

We follow a few of the derivations from [3, 90] to obtain quantum state diffusion equations for NHH models. Quantum State Diffusion (QSD) is a special form of ‘unravelling’ in that the unitary equivalence of all QSD choices hold just like the master equation for the density matrix. In other words, unitary transformations of the Lindblad operators do not alter the physics of the master equation or the QSD stochastic equation. Other stochastic diffusion equations do not possess that property [91]. For the uniqueness condition of QSD, see [90, 91]. General theory of Quantum Stochastic Process(QSP) based on Quantum Stochastic Differential Equations(QSDE) was developed [92]. The stochasticity originates from the interaction with external fields modelled as ‘Markovian heat bath’s (quantum Wiener processes). QSDEs were quickly adopted for continuous quantum measurement descriptions [93].

### Appendix B: Quantum State Diffusion for a Lattice of particles

Drift-diffusion models (with an associated Fokker-Planck equation) or quantum state diffusion models were developed earliest in [88–90, 93]. Early work on QSD models on open system dynamics include [94, 95]. The differential form of the stochastic equation of motion for the state vector  $|\psi\rangle$ ,

$$\begin{aligned} |d\psi\rangle = & -\frac{i}{\hbar}H|d\psi\rangle dt + \sum_m (2\langle L_m^\dagger \rangle_\psi L_m \\ & - L_m^\dagger L_m - \langle L_m^\dagger \rangle_\psi \langle L_m \rangle_\psi) |\psi\rangle dt \\ & + \sum_m (L_m - \langle L_m \rangle_\psi) |\psi\rangle d\xi_m, \end{aligned}$$

with  $\langle L_m \rangle_\psi = \langle\psi|L_m|\psi\rangle$  being the expectation value of  $L_m$  for the state  $|\psi\rangle$ . The last term on the right hand side embody the fluctuations/diffusion of the state vector (the other terms represent the ‘drift’).  $d\xi_m$  are independent complex differential random variables embodying a complex normalized Wiener process,

$$\begin{aligned} M(\text{Re}(d\xi_n)\text{Re}(d\xi_m)) &= M(\text{Im}(d\xi_n)\text{Im}(d\xi_m)) = \delta_{nm}dt \\ Md\xi_m &= 0, \quad M(\text{Re}(d\xi_n)\text{Im}(d\xi_m)) = 0, \end{aligned}$$



with  $M$  being the mean over the probability distribution.

From the treatment of state vectors as abstract mathematical quantities, QSD and quantum jump lend association with reality to quantum evolution in the method of QSPs. The stochastic reduction of the quantum state during the process of measurement is a process based in

physical reality [90].

For interpretation of the QSD (as well as quantum jump approach), see [18, 20] In fact the stochastic generalization of the Schrödinger equation was showed to be have better prospects of compatibility with the theory of relativity [89].

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