Simulation methods for open quantum many-body systems

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目录

1 Introduction

本文主要介绍开放量子多体系统 open quantum many-body systems (OQMS) 的数值模拟方法, 包括 mean-field stochastic methods, tensor networks, variational methods, quantum Monte Carlo methods, a truncated Wigner approximation, BBGKY hierarchy equations, linked-cluster expansions. 开放系统目前还有很多 open problems, 下面是几个例子

- Rydberg atoms in which the interaction is often long range
- 2D TN
- AFM order in the 3D dissipative Ising model
- Phase transitions and universality classes of dissipative models

本文主要参考 [1]. Keldysh 场论 [2] 这种解析方法不在我们的讨论范围之内, PT 对称 QM 作为另一个最近与之相关的有趣的领域也不在讨论范围内 [3].

2 Open Quantum System

2.1 The Markovian quantum master equation

开放系统中主要考虑的是密度矩阵的演化和稳态. 本文只讨论 Markovian systems, 即系统当前的演化只由上一步演化的结果决定, 而不由更久远的历史影响. 对于这种 Markovian systems, 我们说它构成了一个 dynamical semigroup, 可由 Lindblad 形式的量子主方程 quantum master equation 描述

$$\frac{d}{dt}\rho = \mathcal{L}[\rho] \tag{1}$$

where

$$\mathcal{L}[\rho] = -i[H + H_{\text{Lamb shift}}, \rho] + \sum_{\mu} \left(L_\mu \rho L_\mu^\dagger - \frac{1}{2}\{L_\mu^\dagger L_\mu, \rho\} \right) \tag{2}$$

$\mathcal{L}$ 称为超算符, ρ 可以视为 Fock-Liouville 中的矢量, $\{L_\mu, L_\mu^\dagger\}$ 就是 Lindblad operator,μ 表示不同的 dissipation channels. 事实上 quantum master equation 还可以有其他形式, 主方程的推导见 [4]. 在推导 Lindblad 的过程中需要用到几种近似, 包括 Born-Markov approximation(环境的 correlation time τ_E 远小于系统的 relaxation time τ_R) 和 rotating wave approximation(系统的本征频率之差 $\omega_s \gg \tau_R^{-1}$).

这些近似可以很好地在量子光学的系统中实现, 因此实验大多以此为平台. 此外量子光学系统还有一个好处, 即能引入含时的 laser fields 作为 dissipation channel. 在系统 Hamiltonian 中加入 an oscillatory driving term, 我们可以观察到不同于 steady state 即为 thermal state 的情况, 比如在 Rydberg states 上实现的 driven-dissipative quantum many-body systems. 此外还有一些其他的实验平台, 比如 semiconductor polaritonic systems 和 circuit-quantum electrodynamics (QED) systems (Bose-Hubbard lattices).

另一个值得注意的就是 Lindblad operator 通常被认为是 local 的, 但这只在 weak-coupling 极限下成立, 这进一步就是说: (1) a slow development of correlations between system and environment, (2) fast decay of excitations of the environment, and (3) neglect of fast-oscillating terms when making a comparison to the typical system timescale. 因此, 当我们处理 strongly correlated systems 时, local Lindblad dissipation 很有可能被破坏, 这种情况下如何修正 Lindblad operator 见 [5].

此外, non-Markovian dynamics 有时也很重要, 有关讨论见 [6]. 从 continuous measurement and feedback 的角度考虑: instantaneous feedback 对应于 Markovian dynamics (Lindblad form), 而 delayed feedback 对应于 non-Markovian dynamics.

2.2 Steady-state solution versus time evolution

研究 open quantum many-body systems, 我们主要关心 2 个问题: 一个是长时间极限下的稳态, 类似于封闭体系; 另一个是动力学演化问题, 根据初态的不同演化的结果可能有多个稳态. 尽管对于有限系统中的产生某个特殊稳态的要求已经明晰 [7], 更普遍的稳态性质仍有待研究, 其中的复杂性在于 the long time limit and the thermodynamic limit do not necessarily commute.

有时, 为了寻找稳态做 full time evolution 也是一个可选的方案, 可以捕捉到一些特殊的现象, 比如 it is possible for open many-body systems exhibiting a trivial steady state, while the relaxation behavior is dominated by complex glassy quantum dynamics[8].

2.3 Differences to equilibrium problems

对于 open quantum many-body systems, 有一些我们原来常用的方法不再适用, 其中之一就是 quantum Monte Carlo, 这是因为此时我们无法写出 partition function. 更进一步说, for the steady state of an open system it is unclear a priori whether the steady state of the system is a thermal state that can be described in terms of a partition function. Density functional theory 是另一个例子, 这是因为 steady state 通常不同于 ground state(即便是 infinitely weak dissipation), 因此无法 minimize the ground state energy.

幸运的是, 还有一些原来的分析方法仍适用, 比如 tensor network(将在后面详细说) 和 symmetries. 对后者的分析可以给出 classification of dissipative phase transitions in terms of their universality classes, 即在 open quantum many-body systems 中 (dynamics) 普适类仍然存在.

2.4 Paradigmatic models

和封闭系统类似, 在开放系统模拟中我们也主要针对几个典型的模型, 下面介绍两类.

2.4.1 dissipative Ising model

第一类是 dissipative Ising model, 以 the transverse field Ising model with longitudinal dissipation 为例

$$H = \frac{h}{2}\sum_i \sigma_i^x + \frac{V}{4}\sum_{\langle ij\rangle}\sigma_i^z\sigma_j^z \tag{3}$$

dissipation 由 jump operators $c_i = \sqrt{\gamma}\sigma^-$ 给出, with γ the rate of dissipative flips from the spin up to the spin down state.

一个重要的结果就是 the dissipation breaks the Z_2 Ising symmetry, 即 quantum master equation 不具有 Z_2 对称性. 用 mean-field theory 计算, 该模型展现了: 对于 a large range of h values, the system exhibits two stable steady states; the bistable region ends in a critical point that belongs to the Ising universality class (2014).

2.4.2 driven-dissipative Bose-Hubbard model

第二类是 driven-dissipative Bose-Hubbard model, 以有 dissipative particle loss 的 Bose-Hubbard model 为例

$$H = -J\sum_{\langle ij\rangle} b_i^\dagger b_j + \sum_i \left[\frac{U}{2}n_i^2 - \Delta\omega n_i + F(b_i + b_i^\dagger)\right] \tag{4}$$

U 表示 on-site interaction, $\Delta\omega$ is the chemical potential for the bosons, and F describes the coherent driving 来抵消 dissipation 的作用, jump operators $c_i = \sqrt{\gamma}b_i$.

与 dissipative Ising model 类似, the dissipation term also breaks the $U(1)$ symmetry of the conventional Bose-Hubbard model (虽然 symmetry

已经被 F term break 了). 其同样具有 mean-field phase diagram, 类似于 Mott lobes[9]. 解的 stability 可由密度矩阵的行为给出

$$\rho = \prod_i (\rho_i^{MF} + \delta\rho_i) \tag{5}$$

i 代表了多个 steady state. Expanding the quantum master equation up to first order in $\delta\rho_i$ allows one to evaluate the stability by checking whether none of eigenvalues of the Liouvillian have a positive real part.

3 Stochastic Methods

本节讨论随机过程方法. 不同于封闭系统的动力学演化, 在 open quantum many-body systems 中我们需要演化密度矩阵, 因此对于 d 维 Hilbert space 的系统, 演化的复杂度至少 $\sim O(d^2)$. 不过想到 initial density matrix 可以写成 a statistical ensemble of pure states, 我们有办法不演化整个密度矩阵而得到结果, 即 the key strategy is to propagate the individual trajectories consisting of pure states $|\psi\rangle$ to the time t and then calculate observables according to

$$\langle O\rangle = \mathrm{Tr}(O\rho) = \sum_i p_i \langle\psi_i|O|\psi_i\rangle \tag{6}$$

其中 p_i 可由 standard Monte Carlo techniques 给出, 这种方法称为 wave-function Monte Carlo. 如果要模拟 M 个 trajectories, 最简单的方案就是取 $p_i = 1/M_i$, 此时相对误差 $\sim 1/\sqrt{M}$, the entire computational cost is $O(Md)$. 一般取 M 在 1000 左右. 这种操作为并行计算提供了方便. 沿着这个思路, 下面介绍两种方法来描述 pure state 的演化.

3.1 Quantum state diffusion

在 quantum state diffusion approach 中, the incoherent dynamics from the Lindblad operators 可由随机薛定谔方程描述

$$d\psi_i(t) = -iH_{eff}\,|\psi_i(t)\rangle\,dt + \sum_j M_j\,|\psi_i(t)\rangle\,dW_j \tag{7}$$

where dW_j refers to the Wiener increments. The effective Hamiltonian H_{eff} describes the drift of the state vector in the Hilbert space

$$H_{eff} = H + \sum_j \left(2\langle c_j^\dagger\rangle c_j - c_j^\dagger c_j - \langle c_j^\dagger\rangle\langle c_j\rangle\right) \tag{8}$$

The diffusion operators M_j describe the random fluctuations arising from each associated jump operator c_j

$$M_j = c_j - \langle c_j\rangle \tag{9}$$

上述方程保证了 norm of state 不变, 之后可以使用 standard techniques for stochastic differential equations 求解.

3.2 Quantum jump method

quantum jump method 也是一个可选的演化方法, 详细介绍见 [10]. 在这个方法中, 动力学演化可以被分为两部分: 1. propagated under an effective non-Hermitian Hamiltonian H_{NH}, 例如

$$H_{NH} = H - \frac{i}{2}\sum_j c_j^\dagger c_j \tag{10}$$

2. Once the norm of the state drops below a previously drawn random number r, a quantum jump occurs. Jump 的概率分布为

$$p_j = N\,\langle\psi_i|c_j^\dagger c_j|\psi_i\rangle \tag{11}$$

其中 N 是归一化系数.

对于非平衡小系统, 需要加入其他方法来从有限尺寸外推热力学极限. 一种方法是先考虑各向异性系统以获得更多数据点, 从而做更可靠的有限尺度外推, 比如磁化率的外推公式 $\chi = N^{\alpha}\tilde{\chi}(\lambda)$, 其中 the reduced susceptibility $\tilde{\chi}$ is only a function of the anisotropy λ of the system and can be determined by symmetry considerations as well as numerical data.

4 Tensor Network Methods

TN 可以很好的描述 large system size 中的 quantum correlations. 对比 QMC, TN 没有 sign problem for fermionic or frustrated systems. 这些优点在 open quantum many-body systems 中也有体现.

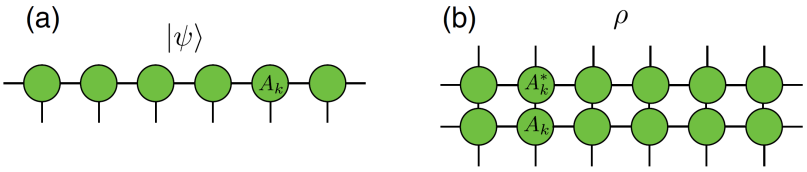
4.1 One spatial dimension

4.1.1 Matrix product density operators

在 open quantum many-body systems 中, 我们考虑的主要是 matrix product operators (MPOs) or matrix product density operators (MPDOs). 就像封闭系统那样, 我们可以定义 MPS with bond dimension D(or χ) and physical dimension d. A MPDO ρ of N d-level particles with $(D_1, D_2, \ldots, D_N)$-dimensional bonds is defined as

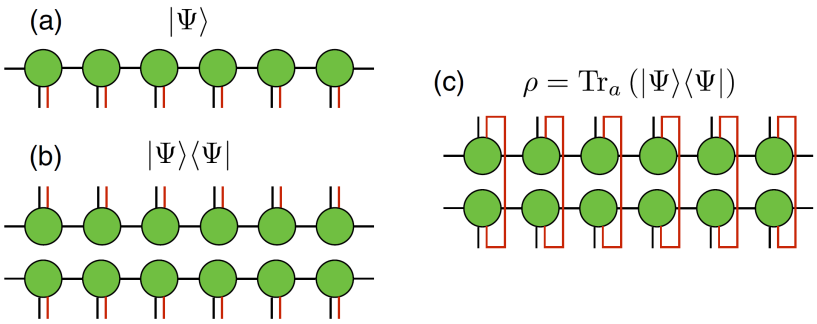
$$\rho = \sum_{\{s,s'\}=1}^{d} \prod_{k} M_k^{s_k,s'_k} |s\rangle \langle s'| \tag{12}$$

where $M_k^{s_k,s'_k}$ are $D_k^2 \times D_{k+1}^2$ matrices.



这样定义的密度矩阵自动满足正定性. 我们可以通过增大 MPS 的 local Hilbert 空间来纯化 density matrix, MPDO 可以借此被 MPS 表达

$$|\Psi\rangle = \sum_{\{s,a\}} \prod_i A_i^{s_i,a_i} |sa\rangle\,, \quad \rho = \mathrm{Tr}_a(|\Psi\rangle\langle\Psi|) \tag{13}$$



于是我们只需要演化一个维度较大的 MPS 就可以直接 trace 得到密度矩阵, 比如用 DMRG. 除此之外, such a purification scheme can be used for mixed state evolution under dissipation as well as for thermal equilibrium and can be implemented irrespective of periodic or open boundary conditions and finite or infinite systems. 在这种方案中, 主要的误差来自 Trotter 分解的误差和截断误差. 然而需要声明: a description of mixed states that is both efficient and locally positive semidefinite does not exist and that one can make only approximations. 我们上面提到的 local purification 方案并不能保证还原后的 MPDO 正定, locally purified MPS 的键维度并不会被 MPDO 的键维度 bound 住, 因此有时 local purification techniques can be much more costly.

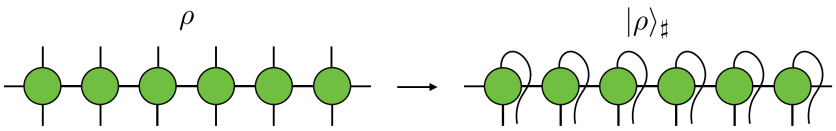
4.1.2 Vectorized density matrices

除了上面的纯化方案, 直接 vectorized density matrices 也是一个可行的方案, 其可以使用 TEBD 等算法 simulate the real time Markovian dynamics

given by a master equation. 向量化的核心操作就是 Choi isomorphism, 即把 MPDO ρ 直接同构到 $|\rho\rangle$

$$|\rho\rangle = \sum_{i_1=0}^{d^2-1} \cdots \sum_{i_N=0}^{d^2-1} c_{i_1 \cdots i_N} |i_1\rangle \otimes \cdots \otimes |i_N\rangle \tag{14}$$

其中 $|i_l\rangle$ 是 C^{d^2} 的 basis.



Further assuming that the Liouvillian superoperator $\mathcal{L}$ can be decomposed into terms involving at most nearest neighbors, i.e., $\mathcal{L}[\rho] = \sum_l \mathcal{L}_{l,l+1}[\rho]$, 因此 TEBD 就可以应用. 然而, 对于这类基于 Choi 同构的技术, the issue of positivity still remains at large. 为了解决这个问题, purification 依旧可行, 即 $\rho = XX^\dagger$ 分解出 purification operator 然后对其演化. Such an approach never required to contract the two TN layers (X and $X^\dagger$) together, thereby ensuring positivity at all times during the evolution. 此外, 该方法还能更好地控制 the approximation error with respect to the trace norm.

4.1.3 Direct MPO approaches

Direct MPO approaches 采用 variational method 来直接找到 the null eigenvector of $\mathcal{L}$ 即 steady state, 例如 finding the steady states of dissipative 1D systems[11]. 这种做法基于: if ρ_s is the steady state of the Lindbladian master equation satisfying $\mathcal{L}|\rho_s\rangle$, then $|\rho_s\rangle$ will also be the ground state of the nonlocal Hamiltonian $\mathcal{L}^\dagger\mathcal{L}$ (since it is Hermitian and positive semidefinite). 这种方案的好处在于避免了 imaginary time evolution, 保证了 steady state 的收敛 [12]; 可以使用类似于 DMRG 的做法. 这种方案甚至可以 work in the weakly dissipative regime by slowly tuning the dissipation rates along the sweeps, 然而其不能找到 transient state.

[13] 是一个很好的例子, 包括 infinite 1D systems (i.e., the thermodynamic limit) 和 hybrid technique of both imaginary and real time evolution. 他们取

$$\mathcal{H} = \sum_{r\in\mathbb{Z}} (\mathcal{L}_r^\dagger \mathcal{L}_r)^{1/k} \tag{15}$$

的基态, 其中 $\mathcal{L} = \sum_{r\in\mathbb{Z}} \mathcal{L}_r$, 取 k 次根只是为了快速收敛 (因为这可以提高半正定矩阵的能级差 if the gap between the two lowest eigenvalues < 1). 主要步骤包括一步 imaginary time evolution 和一步 real time evolution

$$|\rho_G\rangle \approx \lim_{\tau\to\infty} \frac{e^{-\mathcal{H}\tau}|\rho_0\rangle}{||e^{-\mathcal{H}\tau}|\rho_0\rangle||} \tag{16}$$

$$\to |\rho_S\rangle \approx \lim_{\tau\to\infty} \frac{e^{\mathcal{L}T}|\rho_S\rangle}{||e^{-\mathcal{L}T}|\rho_S\rangle||} \tag{17}$$

Imaginary time evolution in step (i) ensures that one does not pass through a highly entangled transient regime. Step (ii) improves the accuracy of the stationary state. 对于非马尔可夫过程的 MPS 方法, 可以参考 [14][15].

4.2 Extensions to higher dimensions

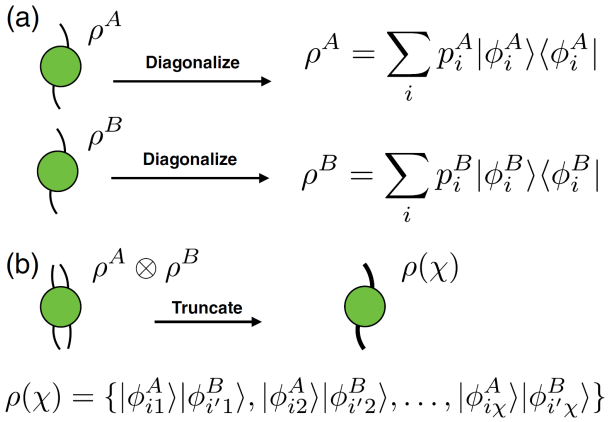
高维情况的 TN 有直接的推广, 即 PEPS. 为了解决 PEPS 的精确收缩问题, 我们需要 additional PEPS contraction algorithms, 这对于 gapped 系统尤其有效, 然而其只能成功计算基态、部分热态以及一部分时间演化问题. 与前面的封闭系统不同, 到目前为止, 在开放系统中成功应用的只有一种 PEPS 方法和一种 corner space renormalization method, 详细介绍如下.

4.2.1 Corner space renormalization method

The corner space renormalization method starts by finding the steady-state density matrix for small lattice systems, 见 [16]. Steady state 可以对角化

$$\rho^A = \sum_i p_i^A |\psi_i^A\rangle\langle\psi_i^A|, \quad \rho^B = \sum_i p_i^B |\psi_i^B\rangle\langle\psi_i^B| \tag{18}$$

当 AB 合并, 我们可以截断到前 χ 个最大可能的 product states, 张成 corner space. The steady state of the density matrix in this corner space can be determined by using either direct numerical integration in time (for small χ) or a stochastic wave-function Monte Carlo algorithm for large χ. 当增大 corner space 时, 可以观察到物理量的收敛行为. 更大的系统可以取更多的小系统同时合并.



The size of the lattice that can be simulated using this technique depends on the entanglement of the steady state. 另一个有趣的 point 是该方法中的 density operator 结构正是 TTN(tree tensor network), 因此这种方法恰好适用于 driven-dissipative systems of finite size, 处理 nondriven nondissipative systems 还需要更 general 的 TN 方法.

4.2.2 Vectorized projected entangled pair operators

第二种方法依旧是 vectorized PEPOs. 和 1D 情况一样, 这种方法并不能保证正定性, 但 for simulations targeting the steady states, this lack of exact positivity is not a bottleneck if the fixed point is not highly entangled. 和 1D 一样做 Choi's isomorphism $|\dot{\rho}\rangle = \mathcal{L}|\rho\rangle$,

$$\mathcal{L} = -i(H \otimes 1 - 1 \otimes H^T) + \sum_\mu \left(L_\mu \otimes L_\mu^\dagger - \frac{1}{2} L_\mu^\dagger L_\mu \otimes 1 - \frac{1}{2} 1 \otimes L_\mu^\dagger L_\mu \right) \quad (19)$$

The tensor product $\otimes$ separates the operator acting on the ket and bra index of ρ before the vectorization. 做演化 $|\rho(t)\rangle = e^{\mathcal{L}t}|\rho(0)\rangle$, in the limit of $t \to \infty$, we obtain the nonequilibrium steady state (NESS) $|\rho_s\rangle$ as the fixed point of the master equation. 如果做 TEBD, 这就相当于 the iPEPS to compute ground states of local Hamiltonians in 2D in the thermodynamic limit, 因此 iPEPS 从原理上可以求解任意 2D dissipation and steady states.

Ground states	Steady states
$H = \sum_{\langle i,j\rangle} h^{[i,j]}$	$\mathcal{L}_\sharp = \sum_{\langle i,j\rangle} \mathcal{L}_\sharp^{[i,j]}$
e^{-Ht}	$e^{\mathcal{L}_\sharp t}$
$\|e_0\rangle$	$\|\rho_s\rangle_\sharp$
$\langle e_0\|H\|e_0\rangle = e_0$	${}_\sharp\langle\rho_s\|\mathcal{L}_\sharp\|\rho_s\rangle_\sharp = 0$
Imaginary time	Real time

然而, 实时演化中 $\mathcal{L}$ 包含 H 和 L_μ 驱动项, 前者增大纠缠而后者减小纠缠, 耗散强度决定了到达稳态的时间. 一般来说演化到一定时间,bond dimension 就会增大到无法处理, 除非在到达临界点之前耗散就能把系统驱动到 steady state. In fact, even if there is too much entanglement for the TN at intermediate times, the dissipation may still drive the evolution toward a good approximation of the correct steady state. 总而言之,dissipation limits the growth of entanglement if the fixed point attractor is strong enough. 另一个想法是 maximizing the fidelity 来优化 steady state[17].

Dissipative Ising and the XYZ model 已经使用 iPEPS 做了计算. 其给出了 Ising 的一级相变以及其平均场近似 (bistability), 横场情况无 AFM phase 等结果. 其中的平均场方法将在后面叙述. 这种方法中, contributions of negative eigenvalues of the reduced density matrices are small in most of the regimes, 因此正定性问题并不显著, 这可能源于 entanglement monogamy, 即 correlation 在 2D 有更多的 bonds 可以分布, 只需要 small bond dimension

就可以描述.

4.2.3 Preserving positivity of the density matrix

最后我们来讨论如何保证 2D 中 density martix 的正定性. 这依然可以通过分解密度矩阵然后分别演化两个 PEPO 来解决, 也可以使用 [18] 提出的 positivity preserving algorithm 构造 PEPDO(需要 high bond dimension). 另一种方法是求解 the Hermitian and positive semidefinite operator $\mathcal{L}^\dagger\mathcal{L}$ 的基态, 比如做 time evolution imaginary. 然而有一个问题: The crossed products are nonlocal, 因此实际计算需要做额外的近似. 另一个选择是近似计算基态, 虽然由于非局域性难以进行, 比如 DMRG in 1D 和 variational PEPS in 2D. 此外直接计算 PEPO $\mathcal{L}^\dagger\mathcal{L}$ 也会引入 a large bond dimension. 最后还有一个想法, target the variational minimization of the real part for the expectation value of $\mathcal{L}$.

5 Variational Methods

正如我们前面所说, 传统的变分方法不适用于 OQMS, 不过这里仍有一些补救措施.

5.1 The variational principle for open quantum systems

5.1.1 Steady-state solution

变分方法大体分为两步: 1. parametrization of the state of the system in terms of a set of variational parameters $\{\alpha_i\}$; 2. identify a suitable functional that can be optimized by tuning the variational parameters. 这在 OQMS 中对应于 $\rho = \rho(\{\alpha_i\})$ 和 $\dot{\rho} = 0$. 由于 the exact steady state 很可能落在变分参

数流形之外, 因此最佳策略就是 minimize the functional $||\mathcal{L}\rho||$ for a suitable norm. 一种 norm 的选择是 trace norm $||\mathcal{L}\rho|| = \mathrm{Tr}(|\dot{\rho}|)$, 即密度矩阵的所有特征值的绝对值之和. 选择 trace norm 有两个 motivation: 1. First, the trace distance, being the natural distance measure for density matrices, is highly suggestive of the trace norm being the natural norm for the tangent space $\dot{\rho}$; 2. 和其他 norm 对比, trace norm 最合理. 后者是因为 Schatten p norms of the form $[\mathrm{Tr}(|\dot{\rho}|^p)]^{1/p}$ 偏向于最大混合态 ($p > 1$), 而 $p < 1$ 不能构成严格的 norm, 只剩下 $p = 1$. One can also understand the variational principle as a direct solution of the overdetermined steady state equation $\mathcal{L}\rho = 0$ in terms of a trace norm minimization. 不过因为 trace norm 需要对角化 ρ, the evaluation of the variational functional is still an exponentially difficult problem. 这可以通过引入 upper bounds 解决 (即便在相变附近也误差也不大), 其取决于 the degree of additional correlations that can be built up by applying the Liouvillian to states within the variational manifold[19]. 比如 [19] 给出 $||\mathcal{L}\rho||$ 的 upper bound 形式 (只考虑近邻相互作用, 即两体关联)

$$D = \sum_{ij\in\mathcal{T}} \mathrm{Tr}(|\dot{\rho}_{ij}|), \quad \rho = \prod_i \rho_i \tag{20}$$

where $\mathcal{T}$ contains pairs of sites that are connected to each other by the Liouvillian. 值得一提,[20] 在 two-dimensional Jordan-Wigner transformation 之后, 通过选择合适的变分流形排除了 nonlocal Wigner strings 的出现.

5.1.2 Field-theoretical treatment of fluctuations

回忆标准的 Ginzburg-Landau theory, 其在自由能泛函中引入空间涨落项. 在 OQMS 中, 自然想到构造 dissipative Ginzburg-Landau theory based on the variational principle[21]. 上面计算得到的 upper bound 是在 product states 的假设下写出的, 为了捕捉 fluctuations 我们可以在连续极限下展开

upper bound

$$D[\phi] = \int dx \left[\sum_m v_m [\nabla \phi(x)]^m + \sum_n u_n [\phi(x)]^n \right] \tag{21}$$

其中系数可由 microscopic quantum master equation 计算得出, 截断到 m, n 阶. Dynamical symmetry 可以给出符合热力学统计形式的 steady state[22], 于是可以构造 Ginzburg-Landau-Wilson functional integral for an effective partition function

$$Z_{eff} = \int \mathcal{D}\phi \exp(-\beta_{eff} D[\phi]) \tag{22}$$

其中 β_{eff} can be derived from the u_0. 之后可以使用诸如 perturbative renormalization group 等技术分析.

5.1.3 Time evolution

最后来讨论 full time evolution. 比如 in the lowest-order Euler approximation,

$$D = \mathrm{Tr}(|\rho(t+\tau) - \rho(t) - \tau \mathcal{L}\rho(t)|) \tag{23}$$

即 the variational functional is replaced by a variational integration of the quantum master equation for small time steps τ. 如 rk45 等更高阶的近似也可以应用, 注意要考虑 upper bound 中的高阶关联. 一个比较好用的近似是 implicit midpoint method.

5.2 Comparison with mean-field methods

For equilibrium problems, the variational method based on product states is exactly equivalent to a mean-field decoupling of the interaction terms. 但是上面的描述对 OQMS 并不成立, 其主方程组为

$$\frac{d}{dt}\rho_i = \mathrm{Tr}_{j \neq i} \left(\frac{d}{dt} \rho \right) = -i[H_i^{MF}, \rho_i] + \mathcal{D}_i(\rho_i) \tag{24}$$

后一项是 the mean-field dissipators. 这组方程是 self-consistently, 因此可以递归求解, 特别的对于平移不变的系统只需要解 an effective single site problem. 下面介绍一些 mean-field 的结果.

5.2.1 Mean-field bistability

因为平均场方程的的非线性结构, 系统可以存在多个稳态解, 其稳定性需要从变分的角度分析. The solutions according to the variational principle and mean-field theory are identical only in the limit of infinite dimensions, where both approaches become exact. 目前, mean-field bistability has been found in the absence of symmetries in the underlying master equation; i.e., the two solutions are not connected by a symmetry transformation. 这类似于封闭系统的简并态和自发对称性破缺. 然而进一步利用 the variational principle 和 Keldysh formalism 发现 bistability will be replaced by a first-order transition both in the dissipative Ising and in the driven-dissipative Bose-Hubbard model. 因此, 在 OQMS 中平均场理论在高维定性正确的结论似乎被打破了, 取而代之的是变分原理, 这提示我们要小心的看待可能出现的 bistability. 此外, the situation is similar when it comes to limit cycles of open quantum many-body systems[23][24].

5.2.2 Extensions of mean-field theory

One systematic extension of mean-field theory is cluster mean-field theory. 直观上理解就是将 N 个单粒子平均场运动方程约化成 N/L 个 cluster 运动方程. 有趣的是, cluster mean-field approaches treat the short-range physics more accurately than bare mean-field theory, leading to better quantitative estimates for phase transitions. 但本质上平均场方法无法捕捉 long range fluctuations.

DMFT 方法是一种 mean-field approximation 的推广和超越. DMFT

is a mapping of a many-body lattice model onto a single impurity problem that has to be solved in a self-consistent way, 如标准 Kondo effect. Within DMFT, the approach is to start with an effective dynamical Green's function $\mathcal{G}_0$, which serves as a time-dependent version of a mean-field coupling. 例如 Fermi-Hubbard models

$$S_{eff} = -\int_0^\beta \int_0^\beta d\tau' \sum_\sigma f_\sigma^\dagger(\tau)\mathcal{G}_0^{-1} f_\sigma(\tau') + U\int_0^\beta f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow \tag{25}$$

The central idea of DMFT is to consider a self-consistent solution that reproduces the dynamical Green's function $\mathcal{G}_0$. 考虑 the local Green's function G_0

$$G_0(i\omega_n) = \langle c_\sigma(i\omega_n) c_\sigma^*(i\omega_n)\rangle_{S_{eff}} \tag{26}$$

$$= \frac{1}{\mathcal{G}_0^{-1}(i\omega_n) - \Sigma(i\omega_n)} \tag{27}$$

$$= \int d\epsilon \frac{N(\epsilon)}{i\omega_n + \mu - \Sigma(i\omega_n) - \epsilon} \tag{28}$$

where μ is the chemical potential, $N(\epsilon)$ is the density of states, ω_n 是费米子的 Matsubara frequencies. The first step in bringing DMFT to open systems was to use effective Lindblad master equations to describe quantum transport in closed quantum systems using DMFT.

另一个推广 mean-field theory 的方法是 projection operator methods. The central idea is to consider a single site of the many-body problem, with the rest of the system forming a non-Markovian environment. This non-Markovian master equation is then solved using standard projection operator techniques such as the Nakajima-Zwanzig method or the time-convolutionless master equation[25]. 例如, 对于无时间卷积主方程 the time-convolutionless master equation, the initial step is to introduce corrections $\Delta\mathcal{L}$ to the mean-field Liouvillian $\mathcal{L}_{MF}$. The projection $\mathcal{P}$ removes all correlations and projects

the system onto a product state.

$$\mathcal{L} = \mathcal{L}_{MF} + \Delta\mathcal{L} \tag{29}$$

考虑直积态作为初态, 有 the projected Lindblad master equation

$$\mathcal{P}\frac{d}{dt}\rho(t) = \mathcal{L}_{MF}\mathcal{P}\rho(t) + \mathcal{P}\Delta\mathcal{L}\int_0^t dt'\mathcal{K}(t,t')\mathcal{P}\rho(t') \tag{30}$$

The generator $\mathcal{K}$ may then be expanded in terms of a power series of the beyond mean-field corrections $\Delta\mathcal{L}$ [25].

5.3 Variational tensor network methods

高阶方法本质是做融合怪, 比如 TN 和 variational method. 然而这样有一个严重的问题, the natural trace norm for constructing the variational principle cannot be calculated efficiently in a tensor network representation, 于是我们不得不考虑其他的 norm 来补救. Non-natural norm 带来了不受 variational algorithm 控制的 error, 不过 the choice of the norm is not really relevant if the value of the norm is low. 实际操作中, 越高的维度、越长的 relaxation times, 这种问题会越明显, 前者是因为 bond dimensions 受限而后者是因为可能无法达到任意低的 norm.

一种解决方法是 representing the density matrix in terms of an ensemble of pure states and use a variational tensor network formulation for these pure states

$$\rho = \int p(\alpha,\tilde{\alpha})\,|\psi(\alpha)\rangle\,\langle\psi(\alpha)|\,d\alpha d\tilde{\alpha} \tag{31}$$

此时 variational norm 为

$$D_H = |H_{eff}\,|\psi(\alpha)\rangle\,|^2, \quad H_{eff} = H - \frac{i}{2}\sum_i c_i^\dagger c_i \tag{32}$$

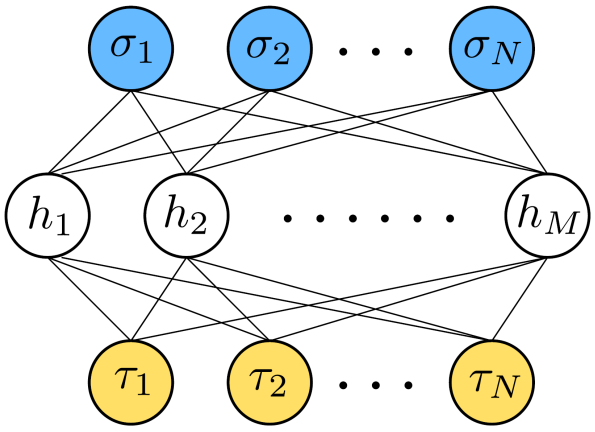
jump operator 也可以类似处理.

5.4 Variational quantum Monte Carlo methods

The central idea behind variational quantum Monte Carlo methods is to rewrite a quantum many-body problem in terms of a sampling over a classical probability distribution. 然而 sign problem 仍然存在, 尤其是在 OQMS 中 Liouvillian can be complex. 最近在 OQMS 中引入的 vQMC 是在神经网络模拟的背景下引入的, 基础是 restricted Boltzmann machines (RBMs) 的 variational wave functions. 对于某个自旋构型 $\{\sigma, \tau\}$, the vectorized density matrix 表示为

$$\rho(\sigma,\tau) = \frac{1}{Z}\sum_{\{h_j\}} \exp\left[\sum_{ij}\left(W_{ij}\sigma_i + W_{ij}^*\tau_i\right)h_j\right] \exp\left[\sum_i\left(a_i\sigma_i + a_i^*\tau_i\right) + \sum_j b_j h_j\right] \tag{33}$$

where an additional hidden layer introduces variational parameters associated with the quantum correlations of the many-body state and W_{ij}, a_i, b_j are the variational parameters. RBMs are potentially capable of describing long-range entangled quantum states.



换言之 RBMs wave functions 能高效描述的态比 MPS 的多. For the variational Monte Carlo samplings, different norms have been put forward, 比如 Hilbert-Schmidt norm of the time evolution or the steady state ($D = \mathrm{Tr}(\dot{\rho}^2)/\mathrm{Tr}(\rho^2)$) 或 minimize the Hermitian $\mathcal{L}^\dagger\mathcal{L}$. 与 TN 不同, RBMs 能直接

用于 2D 情况, 因此 it will be interesting to see how these methods perform for the investigation of dissipative phase transitions, particularly in critical systems.

6 Phase-Space and Related Methods

6.1 Truncated Wigner approximation

The truncated Wigner approximation is a semiclassical approximation of the dynamics of an open system obtained by replacing Moyal's equation, which governs the dynamics of operators in phase space, with the classical Liouville's equation[26]. 考虑一个例子: driven-dissipative microcavity polariton system coherently driven into the optical parametric oscillator regime, 其具有 2D driven-dissipative nonequilibrium phase transition

$$H = \int d\boldsymbol{r} \begin{pmatrix} \psi_X^\dagger & \psi_C \end{pmatrix} \begin{pmatrix} -\frac{\nabla^2}{2m_X} + \frac{g_X}{2}|\psi_X|^2 & \frac{\Omega_R}{2} \\ \frac{\Omega_R}{2} & -\frac{\nabla^2}{2m_C} \end{pmatrix} \begin{pmatrix} \psi_X \\ \psi_C \end{pmatrix} \tag{34}$$

其中 $\psi_{X,C}(\boldsymbol{r},t)$ 分别是 cavity and photon field operators, $m_{X,C}$ 是 exciton and photon masses, g_X 是 exciton-exciton interaction strength, Ω_R 是 Rabi splitting. 为了抵消 incoherent decay 的影响, 我们需要引入 external drive (pump), 这对应着 system-bath (SB) Hamiltonian

$$H_{SB} = \int d\boldsymbol{r} \left[F(\boldsymbol{r},t)\psi_C^\dagger(\boldsymbol{r},t) + h.c.\right] + \sum_{\boldsymbol{k}} \sum_{l=X,C} \left\{\xi_{\boldsymbol{k}}^l \left[\psi_{l,\boldsymbol{k}}^\dagger(t) B_{l,\boldsymbol{k}} + h.c.\right] + \omega_{l,\boldsymbol{k}} B_{l,\boldsymbol{k}}^\dagger B_{l,\boldsymbol{k}}\right\} \tag{35}$$

其中 B 是 the bath's bosonic annihilation and creation operators with energy ω. 后一项描述了 the decay for both excitons and cavity photons, 前一项的 external homogeneous coherent pump $F(\boldsymbol{r},t) = f_p \exp\left[i(\boldsymbol{k}_p \cdot \boldsymbol{r} - \omega_p t)\right]$ 相当于往系统里补充 polaritons with momentum $\boldsymbol{k}_p$ and energy ω_p.

量子光学方法中, bath 被 trace 掉后做 Markovian approximation 得到主方程. 但是我们也可以从 phase-space 的角度求解. In particular, one can represent the quantum fields as quasiprobability distribution functions. The Fokker-Planck partial differential equation that governs the dynamics of such distributions can be mapped to a stochastic differential equation, which can be solved using different techniques. 比如在该例子中需要用 Wigner distribution 在有限格点 a 上做计算. By truncating the corresponding Fokker-Planck equation in the limit $g_X/(\kappa_{X,C}a^2) \ll 1$, with $\kappa_{X,C}$ the exciton and photon decay rates, and keeping up to second order derivatives only, one obtains the stochastic differential equation

$$i\mathrm{d}\begin{pmatrix}\psi_X\\ \psi_C\end{pmatrix} = \left[H'_{MF}\begin{pmatrix}\psi_X\\ \psi_C\end{pmatrix} + \begin{pmatrix}0\\ F\end{pmatrix}\right]\mathrm{d}t + i\begin{pmatrix}\sqrt{\kappa_X}\mathrm{d}W_X\\ \sqrt{\kappa_C}\mathrm{d}W_C\end{pmatrix} \tag{36}$$

其中 $\mathrm{d}W_{l=X,C}$ are Wiener noise terms,

$$H'_{MF} = \begin{pmatrix}-\frac{\nabla^2}{2m_X} + g_X(|\psi_X|^2 - \frac{1}{a^2}) - i\kappa_X & \frac{\Omega_R}{2}\\ \frac{\Omega_R}{2} & -\frac{\nabla^2}{2m_C} - i\kappa_C\end{pmatrix} \tag{37}$$

最近的发展包括 the discrete sampling of the Wigner function, the explicit calculation of the quantum corrections, generalization to spin systems.

6.2 BBGKY hierarchy equations

Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy is a set of coupled equations of motion for the reduced density matrices of the system[27]. 原理很简单, 考虑 one lattice site 和 two lattice sites 密度矩阵, separate the correlated parts

$$\rho_{\mu\nu} = \rho^c_{\mu\nu} + \rho_\mu\rho_\nu \tag{38}$$

$$\rho_{\mu\nu\lambda} = \rho^c_{\mu\nu\lambda} + \rho^c_{\mu\nu}\rho_\lambda + \rho^c_{\mu\lambda}\rho_\nu + \rho^c_{\nu\lambda}\rho_\mu + \rho_\mu\rho_\nu\rho_\lambda \tag{39}$$

后者常做截断 $\rho^c_{\mu\nu\lambda} \simeq 0$. Scaling hierarchy of correlations

$$\rho^c_{\mathcal{S}} = O(Z^{1-|\mathcal{S}|}) \tag{40}$$

with $|\mathcal{S}|$ the number of lattice sites in set $\mathcal{S}$. 生成泛函定义为

$$\mathcal{F}(\alpha_\mu) = \ln\left\{\mathrm{Tr}\left[\rho\prod_\mu(1_\mu+\alpha_\mu)\right]\right\} \tag{41}$$

with α_μ an arbitrary operator acting on an on-site μ. 密度矩阵可以由生成泛函求出

$$\rho_\mu = \frac{\partial\mathcal{F}}{\partial\alpha_\mu}\mid_{\alpha=0}, \quad \rho^c_{\mu\nu} = \frac{\partial^2\mathcal{F}}{\partial\alpha_\mu\partial\alpha_\nu}\mid_{\alpha=0} \tag{42}$$

Next the Liouville operators acting on one and two sites are introduce via the dissipation equation

$$i\partial_t\rho = [H,\rho] + \sum_\mu \mathcal{L}_\mu\rho + \frac{1}{Z}\sum_{\mu\nu}\mathcal{L}_{\mu\nu}\rho \tag{43}$$

with Z the coordination number of the Hamiltonian. 从上面的等式中可以推出 $\mathcal{F}$ 的时间演化方程, 经过一些计算可以给出不同层级的密度矩阵的时间演化, 比如

$$i\partial_t\rho_\mu = \mathcal{L}_\mu + \frac{1}{Z}\sum_k \mathrm{Tr}_k\left(\mathcal{L}^S_{\mu k}\rho_{\mu k}\right) \tag{44}$$

$$i\partial_t\rho_{\mu\nu} = \mathcal{L}_\mu\rho^c_{\mu\nu}\frac{1}{Z}\mathcal{L}_{\mu\nu}\rho_{\mu\nu} + \frac{1}{Z}\sum_{k\neq\mu,\nu}\mathrm{Tr}_k\left[\mathcal{L}^S_{\mu k}\left(\rho^c_{\mu\nu k}+\rho^c_{\mu\nu}\rho_k+\rho^c_{\nu k}\rho_\mu\right)\right] - \frac{\rho_\mu}{Z}\mathrm{Tr}_\mu\left(\mathcal{L}^S_{\mu\nu}\rho_{\mu\nu}\right) + (\mu\leftrightarrow\nu) \tag{45}$$

with $\mathcal{L}^S_{\mu\nu} = \mathcal{L}_{\mu\nu} + \mathcal{L}_{\nu\mu}$ 方程组可以保证时间平移不变. 结合 scaling hierarchy of correlations, one can expand in powers of $1/Z$ and obtain different approximations for the one- and two-particle behavior. 这种方法好在其不受维度的影响.

7 Linked-Cluster Expansion Methods

目前该方法发展的不多. The method numerically targets expectation values of observables in the steady state at long times of the master equation[28]. 下面简单介绍一下操作步骤.

首先 expand the Liouvillian as a sum of quasilocal terms

$$\mathcal{L} = \sum_{\langle k \rangle} \alpha_k \mathcal{L}_k \tag{46}$$

with α_k a local coupling strength and k a combined index that runs over all sites taking part in the respective interaction. The expectation value 也可以展开

$$O(\{\alpha_k\}) = \sum_{\{n_k\}} O_{\{n_k\}} \prod_k \alpha_k^{n_k} \tag{47}$$

with running over all non-negative integers for all k. 上式可以重整为 clusters 之和

$$O = \sum_c W_{[O]}(c) \tag{48}$$

c 表示 clusters, 是 k 的非空集合; W 表示 clusters 中的期望值, 其中只含有 clusters 内的 α_k 多项式. 类似于 finite cluster RG, 有 recurrence relation

$$W_{[O]}(c) = O(c) - \sum_{s \subset c} W_{[O]}(s), \quad O(c) = \mathrm{Tr}\left[\hat{O}\rho_s(c)\right] \tag{49}$$

其中 $\rho_s(c)$ 是 steady state for the finite cluster c. 考虑到 symmetries, 热力学极限下的算符期望值密度表示为

$$\frac{O}{L} = \sum_{n=1}^{\infty} \left(\sum_{c_n} l(c_n) W_{[O]}(c_n) \right) \tag{50}$$

with $L \to \infty$ the size of the system, the outer sum running over all possible cluster sizes n, and the inner sum running over all topologically different clusters c_n of size n, with $l(c_n)$ their multiplicity. 实际计算中需要把 clusters 的大小截断到某个 R.

8 一些补充

The most confidence in a simulation result can be achieved if it is reproducible when using a complementary simulation approach. Despite these caveats, one can make several key observations about the particular methods covered in this review. The first observation is that mean-field methods are considerably less reliable for open systems than their counterparts for closed systems, although the reason for this discrepancy is still an open question. Furthermore, tensor network methods have demonstrated their ability to successfully tackle many hard problems surrounding open many-body systems and resolve long-standing open questions. A particularly interesting and promising case is that of open 2D systems, which are unexplored territory to a large extent. As for the variational methods discussed in this review, there appears to be a trade-off between the formal suitability of the norm and its efficient computability.

TABLE II. Comparison of the different simulation methods discussed in this review. We differentiate the methods by the system sizes that can be simulated, the spatial dimensions, constraints on the local Hilbert space dimension, whether or not fermionic systems can be treated, the simulation performance for inhomogeneous systems, and whether or not the correct critical exponents of phase transitions can be obtained.

	WFMC[a]	TN[b]	Variational principle	VQMC[c]	CMF[d]	TWA[e]
System size (in qubits)	20	TDL[f]	TDL	16	TDL	400
Dimensions	One, two	One, two	Any[g]	Any	Any[h]	Any
Local Hilbert space	Small	Small	Large	Large	Small	Large
Fermionic systems	Yes	Yes	Partially	No	Partially	Unknown
Inhomogeneous systems	Good	Good	Bad	Good	Good	Good
Critical exponents	Good	Good	Good[i]	Unknown	Bad	Unknown
Time-dependent $\mathcal{L}$	Yes	Yes	Yes	Yes	Yes	Yes

[a]Wave-function Monte Carlo.
[b]Tensor networks.
[c]Variational quantum Monte Carlo.
[d]Cluster mean field.
[e]Truncated Wigner approximation.
[f]Systems in the thermodynamic limit.
[g]Works better in higher dimensions.
[h]Works better in higher dimensions.
[i]For states with thermal statistics.

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