1 Lecture 12: the time-dependent variational principle for dissipative dynamics

The time-dependent variational principle of Dirac is a powerful method to simulate the real and imaginary time dynamics of strongly correlated quantum systems. The original formulation has, as far as I can tell, only been formulated in the case of pure states. The generalisation to quantum systems undergoing dissipative dynamics is nontrivial and appears not to have been attempted. Here we describe a natural generalisation.

2 Notation

We denote by $\mathcal{M}_n(\mathbb{C})$ the set of all $n \times n$ complex matrices with entries in $\mathbb{C}$. There is a natural inner product $\langle A, B\rangle$ on $\mathcal{M}_n(\mathbb{C})$ provided by

$$\langle A, B\rangle = \mathrm{tr}(A^\dagger B), \quad A, B \in \mathcal{M}_n(\mathbb{C}). \tag{1}$$

The state space of a n-dimensional quantum space is given by the set $\mathcal{D}_n$ of all density operators, defined by

$$\mathcal{D}_n = \{\rho \in \mathcal{M}_n(\mathbb{C}) \,|\, \rho^\dagger = \rho, \rho \geq 0, \mathrm{tr}(\rho) = 1\}. \tag{2}$$

Throughout this lecture we regard $\mathcal{D}_n$ as a (n^2-1)-dimensional differentiable real manifold (with boundary) in the natural way, i.e., with a single coordinate chart provided by, e.g., the map

$$U : \mathcal{D}_n \to \mathbb{R}^{n^2-1}, \tag{3}$$

where $U(\rho) = (r_1, r_2, \ldots, r_{n^2-1})$, with

$$\rho = \frac{\mathbb{I} + \sum_{j=1}^{n^2-1} r_j \lambda^j}{n}, \tag{4}$$

and λ^j is an orthonormal basis of traceless hermitian operators, i.e., $\langle \lambda^j, \lambda^k\rangle = \delta^{jk}$.

The tangent space $T_\rho\mathcal{D}_n$ to $\mathcal{D}_n$ at $\rho \in \mathcal{D}_n$ may be straightforwardly identified with the set

$$\{A \in \mathcal{M}_n(\mathbb{C}) \,|\, A^\dagger = A, \mathrm{tr}(A) = 0\} \tag{5}$$

of traceless hermitian matrices. We give $\mathcal{D}_n$ the structure of a Riemannian manifold by choosing a positive bilinear form $M_\rho(A, B)$ on $T_\rho\mathcal{D}_n$ for all $\rho \in \mathcal{D}_n$.

Throughout we define a *variational class* simply to be a submanifold $\mathcal{V}$ of $\mathcal{D}_n$. We assume that the manifold $\mathcal{V}$ can be parametrised as

$$\mathcal{V} = \{\rho(\mathbf{x}) \,|\, \mathbf{x} \in \mathbb{R}^D\}, \tag{6}$$

where we assume the dependence on the parameters x^j to be analytic.

It is convenient to introduce the left and right multiplication operators $L_Y(X) = YX$ and $R_Y(X) = XY$, $X, Y \in \mathcal{M}_n(\mathbb{C})$, respectively. The *modular operator* is then defined to be

$$\Delta_{\rho,\sigma} = L_\rho R_\sigma^{-1}, \tag{7}$$

for all $\rho, \sigma \in \mathcal{D}_n$. We also define

$$\Omega_\rho(A) = R_\rho^{-1} k(\Delta_{\rho,\rho}), \tag{8}$$

where $k \in \mathcal{K}$ and

$$\mathcal{K} = k| - kisoperatormonotone, k(w^{-1}) = wk(w), andk(1) = 1. \tag{9}$$

3 Monotone Riemannian metrics

There is no canonical choice of Riemannian metric on $\mathcal{D}_n$. However, there are several canonical *families* of Riemannian metrics which naturally arise from information-theoretic considerations.

Here the natural condition is that the metric is *monotone*, meaning that $M_{T(\rho)}(T(A), T(A)) \leq M_\rho(A, A)$, where T is a CPT map. The reasoning here is that the distinguishability of two states infinitesimally close to ρ should only be decreased under the action of a channel. Petz showed there is a one-to-one correspondence between the set of monotone metrics and a special class of convex operator functions. A complete classification is now well understood (see, e.g., this paper for a quick overview). We do not express our results in the most general way available (although this is entirely straightforward once we understand a couple of examples), but instead focus on two special metrics defined as follows.

Suppose for any given $\rho \in \mathcal{D}_n$, and $A, B \in T_\rho \mathcal{D}_n$, the bilinear form defining the metric is given by

$$M_\rho(A, B) = \langle A, \Omega_\rho(B) \rangle. \tag{10}$$

(It turns out that all monotone metrics have this form.) The two examples we study are furnished by the *Bures metric*

$$\Omega_\rho^{\text{Bures}} = 2(R_\rho + L_\rho)^{-1} \tag{11}$$

and

$$\Omega_\rho^0 = \frac{1}{2}(R_\rho^{-1} + L_\rho^{-1}). \tag{12}$$

4 The time-dependent variational principle for dissipative dynamics

In this section we formulate the time-dependent variational principle for dissipative dynamics generated by equations of the form

$$\frac{d\rho}{dt} = \mathcal{L}[\rho] \tag{13}$$

with respect to a general variational class $\mathcal{V} \subseteq \mathcal{D}_n$ and a monotone Riemannian metric $M_\rho(A, B)$.

The setup is identical to the pure-state case: we aim to find the optimal path $\rho(t) \in \mathcal{V}$ generated by the vector field induced by finding the optimal element $A \in T_{\rho(t)}\mathcal{V}$ which is closest to the RHS of (13), where we use the quadratic form $M_{\rho(t)}(A, B)$ to measure the distance, i.e., we aim to solve

$$\inf_{A \in T_{\rho(t)}\mathcal{V}} M_{\rho(t)}(A - \mathcal{L}[\rho(t)], A - \mathcal{L}[\rho(t)]). \tag{14}$$

This is equivalent to minimising

$$\inf_{A \in T_{\rho(t)}\mathcal{V}} \langle A - \mathcal{L}[\rho(t)], \Omega^k_{\rho(t)}(A - \mathcal{L}[\rho(t)])\rangle. \tag{15}$$

Writing this in terms of the explicit parametrisation $\rho(\mathbf{x})$, we see that we need to minimise

$$\inf_{\mathbf{v} \in \mathbb{R}^D} \langle v^j \partial_j \rho(\mathbf{x}(t)) - \mathcal{L}[\rho(\mathbf{x}(t))], \Omega_\rho(v^k \partial_k \rho(\mathbf{x}(t)) - \mathcal{L}[\rho(\mathbf{x}(t))])\rangle. \tag{16}$$

This may be rewritten as

$$\inf_{\mathbf{v} \in \mathbb{R}^D} \mathbf{v}^T \mathbf{G}_\rho \mathbf{v} - \mathbf{v}^T \boldsymbol{\ell}_\rho - \boldsymbol{\ell}_\rho^T \mathbf{v} + c_0, \tag{17}$$

where

$$(\mathbf{G}_\rho)_{jk} = \langle \partial_j \rho(\mathbf{x}(t)), \Omega_\rho(\partial_k \rho(\mathbf{x}(t)))\rangle \tag{18}$$

is the *Gram matrix* and

$$(\boldsymbol{\ell}_\rho)_j = \langle \partial_j \rho(\mathbf{x}(t)), \Omega_\rho(\mathcal{L}[\rho(\mathbf{x}(t))])\rangle. \tag{19}$$

The minimum is easily found to satisfy

$$\mathbf{v} = \mathbf{G}_\rho^{-1} \boldsymbol{\ell}_\rho. \tag{20}$$

5 The TDVP applied to a Lindblad equation

In this section we focus on the TDVP applied to the specific example

$$\frac{d\rho}{dt} = -i[K, \rho] - \frac{1}{2}\sum_\alpha \left(R_\alpha^\dagger R_\alpha \rho - 2R_\alpha \rho R_\alpha^\dagger + \rho R_\alpha^\dagger R_\alpha\right) \tag{21}$$

using the monotone metric based on Ω^0_ρ. In this case we find that the Gram matrix is given by (we suppress the arguments of ρ for clarity)

$$(\mathbf{G}_\rho)_{jk} = \frac{1}{2}\langle \partial_j \rho, (\partial_k \rho)\rho^{-1})\rangle + \frac{1}{2}\langle \partial_j \rho, \rho^{-1}(\partial_k \rho))\rangle \tag{22}$$

$$= \frac{1}{2}\mathrm{tr}(\rho^{-1}\{\partial_j \rho, \partial_k \rho\}). \tag{23}$$

We also find that

$$(\boldsymbol{\ell}_\rho)_j = \frac{1}{2}\mathrm{tr}(\partial_j\rho\mathcal{L}[\rho]\rho^{-1}) + \frac{1}{2}\mathrm{tr}(\partial_j\rho\rho^{-1}\mathcal{L}[\rho]) \tag{24}$$

$$= \frac{i}{2}\mathrm{tr}\left(\partial_j\rho(\rho K\rho^{-1} - \rho^{-1}K\rho)\right) \tag{25}$$

$$-\frac{1}{4}\sum_\alpha \mathrm{tr}\left(\partial_j\rho(2R_\alpha^\dagger R_\alpha - R_\alpha\rho R_\alpha^\dagger\rho^{-1} - \rho^{-1}R_\alpha\rho R_\alpha^\dagger + \rho R_\alpha^\dagger R_\alpha\rho^{-1} + \rho^{-1}R_\alpha^\dagger R_\alpha\rho)\right) \tag{26}$$