

Approach for Controlling Nano-scale Quantum Systems

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ナノスケール系での量子状態制御を実現するための新しいアプローチを提示する。ここで提示する Hybrid Control Scheme には、我々が導出した複雑な系での多準位状態制御のための解析的最適外場 [T. Takami and H. Fujisaki, J. Phys. Soc. Jpn. **73** (2004), 3215] を利用する。

1 Coarse Grained Picture for Controlling Complex Systems

Controlling quantum states has been studied for a long time in various chemical reaction systems [1] by the use of physical properties such as quantum interference, resonant transitions between eigen-levels, adiabatic passage in stimulated Raman spectroscopy (STIRAP), etc.

Recently, we have developed a coarse-grained approach [2, 3] where a control field

$$\varepsilon(t) = \frac{\pi\hbar}{\bar{V}^2 T} \text{Re} \left[e^{-i\theta} \langle \varphi_0 | \hat{U}_0(0, t) V \hat{U}_0(t, T) | \varphi_T \rangle \right] \quad (1)$$

is obtained analytically. It is shown that the field (1) almost exactly steers $|\varphi_0\rangle$ at $t = 0$ to $|\varphi_T\rangle$ at $t = T$ when the target time T and the system size N are large. The controllability by the field for a fixed T and N is related to the value of the coarse-grained transition element [2, 3]

$$\bar{V}^2 \equiv \frac{1}{T} \int_0^T |\langle \varphi_0 | \hat{U}_0(0, t) V \hat{U}_0(t, T) | \varphi_T \rangle|^2 dt \quad (2)$$

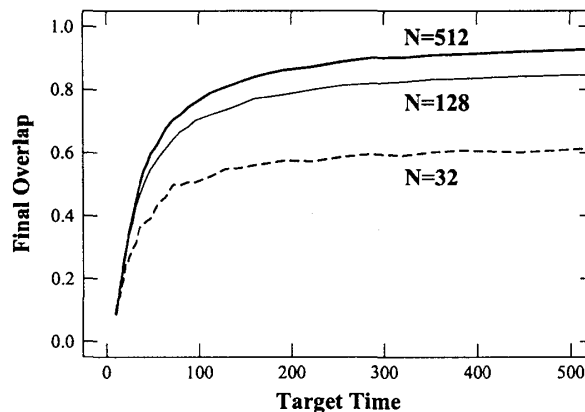


Figure 1: Final overlap by analytic external field in random matrix systems.

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which plays an important role in the hybrid control scheme described in the next section.

In Fig. 1, we show the result of final overlaps obtained by the analytic control field (1). It can be seen that the final overlap becomes large in the limit of T , $N \rightarrow \infty$.

2 Hybrid Control Scheme for Large Systems

We consider an application of the analytic control field (1) to nano-scale large quantum systems. From the analyses in model systems, it is known that, for a set of initial and target states with a fixed T and N , the coarse-grained transition element \bar{V}^2 must be increased in order to obtain a large final overlap. With this property, we introduce a control scheme on a Hamiltonian with two external fields $\mathcal{E}(t)$ and $\varepsilon(t)$,

$$H(\mathcal{E}(t), \varepsilon(t)) = H_0 + \mathcal{E}(t)W + \varepsilon(t)V, \quad (3)$$

where $\varepsilon(t)$ is an analytic control field defined by (1), and $\mathcal{E}(t)$ is another control field introduced to increase $\bar{V}_{\mathcal{E}}^2$ defined by

$$\bar{V}_{\mathcal{E}}^2 = \frac{1}{T} \int_0^T dt \left| \langle \varphi_0 | \hat{U}_{\mathcal{E}}(0, t) V \hat{U}_{\mathcal{E}}(t, T) | \varphi_T \rangle \right|^2. \quad (4)$$

This scheme is divided into two steps: At first, we search for a slowly varying field $\mathcal{E}(t)$ which makes $\bar{V}_{\mathcal{E}}^2$ large enough. In the next step, the analytic field $\varepsilon(t)$ is obtained by (1). The effectiveness of $\varepsilon(t)$ is already guaranteed because $\bar{V}_{\mathcal{E}}^2$ is large. The initial state $|\varphi_0\rangle$ is steered to the target state $|\varphi_T\rangle$ by the use of those two fields, $\mathcal{E}(t)$ and $\varepsilon(t)$.

Computation for the first step can be performed by large scale classical dynamics under the optimal control theory or the genetic algorithm. On the other hand, the solution of the second step is given analytically by (1). Because of the combination of a couple of external fields based on the different control schemes, we have called the scheme “hybrid.”

3 Conclusion

We introduced a “hybrid control scheme” for large systems by the use of our analytic approach for complex systems. This scheme should be validated through large scale computation for controlling complex systems, and is expected to be applied to large systems like bio-molecules, nano-scale physical devices, etc.

References

- [1] S. A. Rice and M. Zhao, *Optical Control of Molecular Dynamics* (John Wiley & Sons, NY, 2000).
- [2] T. Takami and H. Fujisaki, *J. Phys. Soc. Jpn.* **73** (2004), 3215.
- [3] T. Takami, H. Fujisaki and T. Miyadera, *Adv. Chem. Phys.* **130** part A (2005), 435.