Wave function regulation to accelerate adiabatic dynamics in quantum mechanics

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Abstract. The theory to accelerate system on quantum dynamics has been constructed to get the desired wave function on shorter time. This theory is developed on adiabatic quantum dynamics which any regulation is done on wave function that satisfy Schrödinger equation. As an example we show accelerated manipulation of WFs with use of a parameter-dependent asymmetric double-well potential. The theory is also applicable to macroscopic quantum mechanics described by non linear Schrödinger equation.

1. Introduction

A shorter time is become the main important factor that needed by manufacturing products (e.g., electronics, automotives, plants, etc.). If we try to fabricate a massive amounts of such nanoscale structures for manufacturing purposes in shorter time, we should fast-forward the dynamics of each atom or its wave function (WF) to speed up the fabrication. How can we speed up the motion of WF? The fast-forward concept is the answer. \cite{4} described the inverse engineering based on Lewis-Riesenfeld invariants method to ”shortcut to adiabaticity” and also described the connection to fast-forward approach. \cite{5} proposed a formula to fast-forward in a finite-dimensional Hilbert space. He found that the fast-forward potential can be understood as a counteradiabatic term. The fast-forward is defined as making state reach its future state, i.e., a target state, in a shorter time than a standard one, \cite{1}, \cite{2} and \cite{3}.

Let $\Psi_0(x,t)$ is a known function of space ($x$) and time ($t$) and is called a standard state, and $\Psi_\alpha(x,t)$ is called fast-forward state of $\Psi_0(x,t)$ by $\alpha$ times, i.e.,

$$|\Psi_\alpha(x,t)\rangle = |\Psi_0(x,t)\rangle(\alpha t)$$  \hspace{1cm} (1)

with $\alpha$ is time independent magnification factor of the fast-forward. Time evolution from WF is is speed up if $\alpha > 1$ and slowed down if $0 < \alpha < 1$. In general $\alpha$ can be time dependent $\alpha = \alpha(t)$. The time evolution of of WF is accelerated and decelerated when $\alpha(t)$ is increasing and decreasing, respectively, the fast forward state is defined as

$$|\Psi_\alpha(t)\rangle = |\Psi_0(t)\rangle(\Lambda(t))$$,  \hspace{1cm} (2)
where 
\[ \Lambda(t) = \int_0^t \alpha(t') dt' \]  
(3)

The atomic dynamic is described by Schrödinger equation
\[ i\hbar \frac{d}{dt} \langle \Psi_0(t) \rangle = \hat{H}_0 \langle \Psi_0(t) \rangle \]  
(4)

with
\[ \hat{H}_0 = \frac{\hat{p}^2}{2m_0} + \langle V_0(\hat{x}, t) \rangle \]  
(5)

To accelerate the WF is done through additional phase \( e^{if(x,t)} \) with
\[ |\Psi_{FF}(x,t)\rangle = \exp\left[if(x,t)\right]|\Psi_a(x,t)\rangle \]  
(6)

From [1], the driving potential \( V_{FF} \) is
\[ V_{FF} = V_a - \hbar \frac{\partial f}{\partial t} - \eta(\nabla f)^2 + Re[w\nabla^2 \Psi_a/\Psi_a + 2i\eta \nabla f \cdot \nabla \Psi_a/\Psi_a] \]  
(7)

2. Fast-Forward of Adiabatic Quantum Dynamics
An adiabatic process occurs when the external parameter of the Hamiltonian of the system is adiabatically changed. We propose a theory to accelerate the adiabatic dynamics in quantum mechanics and obtain, in any desired short time, the target state originally accessible after an infinite time through the adiabatic dynamics, [2]. The Schrodinger equation with a given potential \( V_0 = V_0(x,t) \) and nonlinearity constant \( c_0 \) (Appearing in macroscopic quantum dynamics)
\[ i\hbar \frac{d}{dt} \langle \Psi_0(x,t) \rangle = -\frac{\hbar^2}{2m_0} \nabla^2 \Psi_0 + V_0(x,t) \Psi_0 - c_0|\Psi_0|^2 \Psi_0 \]  
(8)

The Schrodinger equation for \( \Psi_{FF} \) is given by
\[ i\hbar \frac{d}{dt} \langle \Psi_{FF}(x,t) \rangle = -\frac{\hbar^2}{2m_0} \nabla^2 \Psi_{FF} + V_0(x,t) \Psi_{FF} - c_0|\Psi_{FF}|^2 \Psi_{FF} \]  
(9)

The driving potential of the fast forward \( V_{FF} \) from equation 7
\[ V_{FF} = \alpha V_0 - \hbar \frac{df}{dt} - \frac{\hbar^2}{2m_0} (\nabla f)^2 + Re \left[ -\frac{\hbar}{2m_0} \frac{\nabla^2 \Psi_a}{\Psi_a} + i \frac{\hbar^2}{m_0} \nabla f \cdot \frac{\nabla \Psi_a}{\Psi_a} \right] - (\alpha - 1) c_0 |\Psi| \alpha |^2 \]  
(10)

From [2] \( f \) is given by
\[ f(x,t) = (\alpha(t) - 1) \eta(x, \Lambda(t)) \]  
(11)

However, in the fast forward of the adiabatic dynamics, we shall use infinitely large \( \alpha \). Then the expression of \( V_{FF} \) in equation 10 and \( f \) in equation 11 should diverge. This difficulty will be overcome by regularization of the standard potential and wave functions. The regularization means that we have to determine \( \theta \) dan \( \hat{V} \) After regularization we can write, \( \Psi_{0\text{reg}} \) as a regularized standard state and the potential \( V_{0\text{reg}} \) in the regularized Hamiltonian is given as
\[ V_{0\text{reg}}(x,t) = V_0(x,R(t)) + e\hat{V}(x,t) \]  
(12)

where \( R \) is time dependent adiabatic parameter that written as
\[ R(t) = R(0) + ct \]  
(13)
which $\epsilon \ll 1$. Suppose the regularized standard state is represented as

$$
\Psi_0^{\text{reg}}(x, t, R(t)) = \phi_n(x, R(t)) e^{-i/\hbar} \int_0^t E_n(R(t')) dt' e^{i\theta(x, t)}
$$

(14)

where $\theta$ is a real function of $x$ and $t$. Here we shall obtain $\theta$ and $\tilde{V}$. From [2] the equation for $\theta$ written as

$$
(\nabla^2 \theta) |\phi_n|^2 + 2 \text{Re}[\phi_n \nabla \phi_n^*] \cdot \nabla \theta + \frac{2m_0}{\hbar} \text{Re} \left[ \phi_n \frac{\partial \phi_n^*}{\partial R} \right] = 0
$$

(15)

and the driving potential $V_{\text{FF}}$ to fast-forward the regularized standard state $\Psi_0^{\text{reg}}$ is

$$
V_{\text{FF}} = \alpha \tilde{V} + V_0 - \hbar \frac{d\alpha}{dt} e\theta - \hbar e^2 \alpha^2 \frac{\partial \theta}{\partial R} - \frac{\hbar^2}{2m_0} e^2 \alpha^2 (\nabla \theta)^2
$$

(16)

3. Example

This is an example of the fast-forward of adiabatic processes in the linear regime ($c_0 = 0$). We show the fast-forward of the adiabatic transport with use of a parameter-dependent asymmetric double-well potential. For zero energy ($E_0 = 0$) eigen function is defined by

$$
\Psi_0 = h(R) \left[ (1 - R)e^{-x^2/2a} + \text{Re}^{-i(x-d)^2/2a} \right]
$$

(17)

in the parameter range $0 \leq R \leq 1$ with $R = \epsilon t$ an adiabatic parameters. The standard potentials written as

$$
V_0(x) = \frac{\hbar^2}{2m} \frac{R(x-d)^2 e^{-i(x-d)^2/2a} + (1-R)x^2 e^{-x^2/2a} - \text{Re}^{-i(x-d)^2/2a}}{\text{Re}^{-i(x-d)^2/2a} + (1-R)e^{-x^2/2a}}.
$$

(18)

Normalization factor $h(R)$ determined by $\int_{-\infty}^{\infty} |\Psi|^2 = 1$ is given by

$$
h(R) = \frac{1}{(\pi a)^{1/4}} (1 - 2R + 2R^2 + 2R(1 - R)e^{-d^2/2a})^{-1/2}.
$$

(19)

From equation 15, $\theta$ is written as

$$
\theta = \sqrt{\pi} \sqrt{a} \frac{(4(R-1)^2 + 2)e^{d^2/2a} - 4(R-1)Re^{d^2/2a}}{e^{d^2/2a - 4a} \int_{-\frac{d}{\sqrt{a}}}^{\frac{d}{\sqrt{a}}} \left( (R-1) \left( e^{x^2/2a} - 1 \right) + 1 \right) erf \left( \frac{x}{\sqrt{a}} \right) dx}
$$

$$
+ \int_{-\frac{d}{\sqrt{a}}}^{\frac{d}{\sqrt{a}}} \left( (R-1)e^{d^2/2a - Re^{d^2/2a}} \right) erf \left( \frac{x-d}{\sqrt{a}} \right) + (1-2R)erf \left( \frac{2x-d}{2\sqrt{a}} \right) \left( (R-1)e^{d^2/2a - Re^{d^2/2a}} \right) dx.
$$

(20)

The regularized standard state written as

$$
\Psi_0^{\text{reg}} = h(R) \left[ (1 - R)e^{-x^2/2a} + \text{Re}^{-i(x-d)^2/2a} \right] e^{i\theta}
$$

(21)
Note that $\tilde{V}$ vanishes owing to the absence of the space dependent phase of $O(1)$
$(\text{Im}((\partial \phi_n/\partial R)/\phi_n) = \text{Im}((\partial \phi_n/\partial x)/\phi_n) = 0$ then we can write

$$V_0^{\text{reg}} = V_0(x)$$

(22)

and fast-forward state is

$$\Psi_{\text{FF}} = e^{i f(x,t)} h(R) \left[ (1 - R)e^{-\frac{x^2}{2\alpha}} + Re^{-(x-d)^2/2\alpha} \right] e^{i \epsilon \theta}$$

(23)

then the driving potential

$$V_{\text{FF}} = V_0(x) - \hbar \frac{d \alpha}{dt} e^{\epsilon \theta} - \hbar \epsilon^2 \alpha^2 \frac{\partial \theta}{\partial R} - \frac{\hbar^2}{2m_0} \epsilon^2 \alpha^2 (\nabla \theta)^2.$$  

(24)

where $f(x)$ is correspond to equation 11. The magnification factor $\alpha$ is commonly choosen for 
$0 \leq t \leq T_F$

$$\alpha(t) \epsilon = \bar{v} \cos \left( \frac{2\pi}{T_F} t + \pi \right) + \bar{v},$$

(25)

where $\bar{v}$ is the time average of $\alpha(t)\epsilon$ during the fast forwarding, and the final time of the fast-
forward $T_F$ is related to the standard final time $T$ as $T_F = \epsilon T/\bar{v}$. The standard final time $T$ is
taken as $T = 1/\epsilon$ and $R(0) = 0$ The spatio-temporal dependence of $V_{\text{FF}}$ and $|\Psi_{\text{FF}}|$ are shown
in figure 1 and 2. The 3D plot for $V_{\text{FF}}$ and $\Psi_{\text{FF}}$ are

Figure 1 $V_{\text{FF}}$ on (x,t) plane, with $\epsilon T = 1$, $T_F = 0.025$, $\hbar/m_0 = 1$, $a = 1$, dan $d = 3$

Figure 2 $|\Psi_{\text{FF}}|^2$ on (x,t) plane with the same parameters as in figure 1
4. Conclusion
The method to accelerate adiabatic dynamics in quantum mechanics is shown, using an infinitely large magnification factor of fast-forward and the regularization of standard states and a Hamiltonian. Typical example of the fast-forward of adiabatic dynamics, e.g asymmetric double well-potential. The WP is rapidly transported to the adiabatically accessible targeting position, leaving neither a disturbance nor oscillation after the transport; the WF function becomes stationary again in the confining potential at the end of fast-forward.

Acknowledgments
This work is funded by Riset KK ITB 2015 and Hibah Desentralisasi ITB 2015.

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