Research Article

Quantum Optimal Numerical Controlling for Yukawa Interaction of Couple Heavy Particles[†]Quan-Fang Wang^{a*}*^a Mechanical and Automation Engineering,
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Beyond the controlling of molecules and atoms, quantum control step forward to a new era of achieving control at nucleus scale. This work is to attempt the investigation of quantum controlling with the interaction between two heavy particles (e.g. nucleon and meson). The interaction, which expressed as coupled Schrödinger and Klein-Gordon equations, will be the target of controlling. Experiment demonstration illustrate that theoretical study combining with computational control is effected to performance.

Keywords: Quantum numerical control; Yukawa interaction; heavy particle

1 Preliminaries

Let's start with the quantum control literatures which reported in physics, chemistry and mathematics fields. Observing the existing contributions and research achievements Assion (1998), one can easily have the concluding remark. A variety of breakthroughs have been made in those areas together with their characterization and background. Scientists and researchers who working in quantum control as well as quantum physics field, have eventually solved a great deal problems at different standing points. The most should be highlighted milestone works including trapped cooling atom with laser technology see Chu (1991, 1998, 2002), controlling molecules rearrangement and dissociation see Rice (2000), controlling molecules within chemistry reaction (e.g. break the weak bond), feedback controlling and learning controlling (e.g. finding the optimal set instead of one particular shaped laser wave functions Rabitz (2000), and Warren (1993) so forth. From controlling motions of atoms and molecules to controlling of their structures, from controlling quantum qubit NOT gate to high logic quantum qubit computations. Such a mount of outstanding works make big progress of the realms from past to present, it would be have a great promise to boost the field forward to the future.

This work is try to predict controlling of nuclei even it's not very clear how to achieve them in real lab experiments at present stage. The continuously mutated study would provide the pathway for controlling such elementary particles anticipately. The establishing of physical model with multiplicated control terms, the controlling theory and the simulating in numerical experiments are contained in the contents.

The article is organized as follows. Section 2 is to state the current theoretical conclusion on the control of Yukawa interaction given by Schrödinger and Klein-Gordon system. Section 3 is to

[†]Related work see *Single particle quantum controlling in Yukawa interaction*, Quan-Fang Wang, Poster at European Science Foundation conference 'Chemical Control with Electrons and Photons', Austria, 2008

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show the numerical approach for couple heavy particle consisting of one nucleon and one meson. Particularly, simulation result is for above two particles in two dimension (2D) case. Section 4 is to conclude the summaries and future researches.

2 Quantum optimal control for couple heavy particles

Suppose Ω is an open bounded set of spatial space $\mathbf{R}^3$ and set $Q = (0, T) \times \Omega$ for time $T > 0$. For $(\mathbf{x}, t) \in Q$, the expression of nucleon particle is taken the form of the Schrödinger dynamics Schrödinger (1952)

$$i \frac{\partial \psi}{\partial t} + \frac{\partial^2 \psi}{\partial \mathbf{x}^2} + \phi \psi + u \psi = 0, \quad (1)$$

where ψ denote complex-valued function representing probability density of nucleon field with initial ground state $\psi(0) = \psi_0$. Klein-Gordon dynamics express the motion of meson as

$$\frac{\partial^2 \phi}{\partial t^2} - \frac{\partial^2 \phi}{\partial \mathbf{x}^2} + \phi = |\psi|^2 + v \phi, \quad (2)$$

where ϕ denote real-valued function representing probability density of meson field with initial ground states

$$\phi(0) = \phi_0, \quad \phi_t(0) = \phi_1.$$

The physics model (1) and (2) represent the motions of two heavy particles in presence of Yukawa interaction see Heisenberg (1952), Yukawa (1935, 1937, 1938a,b). The variables u and v represent control inputs corresponding to external ultrashort (e.g. femtosecond/attosecond) infrared laser pulse (e.g. terahertz) in real laboratory experiments refer Assion (1998), Rice (2000), Warren (1993). The shaped laser pulse might be suitable to be manipulated. Note that one nucleon and one meson pairing will be considered as controlling objective in this work.

If the control variables are time depended only functions, denote as $\mathbf{u}(t) = (u(t), v(t))$ for simplicity, its space denoted as $\mathcal{U} = L^2(0, T)^2$. Let $\mathcal{U}_{ad}$ be a closed and convex admissible set of $\mathcal{U}$. Introduce two Hilbert spaces $H = L^2(\Omega)$, $V = H_0^1(\Omega)$ with usual norm and inner products Lions (1971). Hence, two embeddings in Gelfand triple space $V \hookrightarrow H \hookrightarrow V'$ are continuous, dense and compact.

Let's define the weak solution and its space for system (1) and (2) with above given initial conditions.

Definition 2.1: The Hilbert space $W(0, T; V, V')$, which called solution space, defined by

$$W(0, T; V, V') = \left\{ (\psi, \phi) \mid \begin{aligned} &\psi \in L^2(0, T; V), \psi' \in L^2(0, T; V'), \\ &\phi \in L^2(0, T; V), \phi' \in L^2(0, T; H), \phi'' \in L^2(0, T; V') \end{aligned} \right\}.$$

Definition 2.2: Let $T > 0$, the pairing (ψ, ϕ) are weak solutions of (1) and (2) if $\psi, \phi \in$

$W(0, T; V, V')$ satisfy

$$\begin{cases} \int_0^T \int_{\Omega} [-i\psi\eta_t - \psi_{\mathbf{x}}\eta_{\mathbf{x}} + i\alpha\psi\eta + \phi\psi\eta] d\mathbf{x}dt = \int_0^T \int_{\Omega} u\eta d\mathbf{x}dt + \int_{\Omega} i\psi_0\eta(0) d\mathbf{x} \\ \int_0^T \int_{\Omega} [\phi\rho_{tt} + \phi_{\mathbf{x}}\rho_{\mathbf{x}} + \phi\rho - \beta\phi\rho_t - |\psi|^2\rho] d\mathbf{x}dt \\ = \int_0^T \int_{\Omega} v\rho d\mathbf{x}dt + \int_{\Omega} \phi_1\rho(0)d\mathbf{x} - \int_{\Omega} \phi_0\rho_t(0)d\mathbf{x} + \beta \int_{\Omega} \phi_0\rho(0)d\mathbf{x} \end{cases} \quad (3)$$

for all $\bar{\eta} \in C^1(0, T; V)$, $\bar{\rho} \in C^2(0, T; V)$ and such that

$$\eta(T) = \rho(T) = \rho_t(T) = 0, \quad \text{a.e. } t \in [0, T].$$

The objective function associated with (1)-(2) is given by

$$J(\mathbf{u}) = \epsilon_1 \|\psi_f(\mathbf{u}) - \psi_{\text{target}}\|_V^2 + \epsilon_2 \|\phi_f(\mathbf{u}) - \phi_{\text{target}}\|_V^2 + (\mathbf{u}, \mathbf{u})_{\mathcal{U}}, \quad (4)$$

for all $\mathbf{u} \in \mathcal{U}_{ad}$, where $\psi_{\text{target}}, \phi_{\text{target}} \in V$ are target exciting states, $\psi_f(\mathbf{u}), \phi_f(\mathbf{u})$ are final observed quantum states, respectively. Here, ϵ_1 and ϵ_2 are penalty weighted coefficients for balancing the evaluates of system and running criteria.

The task of quantum optimal control is to sake quantum optimal control pairing $\mathbf{u}^* = (u^*, v^*)$ satisfying system (1)-(2) for given initial functions, and minimizing the objective function (4).

Theorem 2.3: *Given $\psi_0, \phi_0 \in V$ and $\phi_1 \in L^2(\Omega)$. Then there exists at least one quantum optimal control $\mathbf{u}^* = (u^*, v^*)$ for cost (4) subject to system (1)-(2) with initial functions (cf. Lions (1971)). Furthermore, the quantum optimal control $\mathbf{u}^*$ is characterized by simultaneously optimality system:*

$$\begin{cases} i\psi_t + \psi_{\mathbf{x}\mathbf{x}} + \phi\psi + u^*\psi = 0 & \text{in } Q, \\ \phi_{tt} - \phi_{\mathbf{x}\mathbf{x}} + \phi = |\psi|^2 + v^*\phi & \text{in } Q, \\ \psi(0) = \psi_0, \phi(0) = \phi_0, \phi_t(0) = \phi_1 & \text{on } \Omega. \end{cases} \quad (5)$$

$$\begin{cases} ip_t + p_{\mathbf{x}\mathbf{x}} + \psi q + \phi p = 0 & \text{in } Q, \\ q_{tt} - q_{\mathbf{x}\mathbf{x}} + q = 2|\psi|\phi p & \text{in } Q, \\ ip_f = \psi_f(\mathbf{u}^*) - \psi_{\text{target}} & \text{on } \Omega, \\ q_f = \phi_f(\mathbf{u}^*) - \phi_{\text{target}}, q'_f = 0 & \text{on } \Omega. \end{cases} \quad (6)$$

$$(\mathbf{u}^*, \mathbf{u} - \mathbf{u}^*)_{\mathcal{U}} + \int_Q p(\mathbf{u}^*)(u - u^*) d\mathbf{x}dt + \int_Q q(\mathbf{u}^*)(v - v^*) d\mathbf{x}dt \geq 0, \quad \forall \mathbf{u} = (u, v) \in \mathcal{U}_{ad}. \quad (7)$$

where $(p, q) \in W(0, T; V, V')$ are solutions of adjoint systems (6) corresponding to (ψ, ϕ) in (5) respectively. Clearly, the (7) is well known as the necessary optimality condition.

Using the definitions of weak solution and weak form (3) under solution space $W(0, T; V, V')$, one can easily get the complete proof as the manipulation citing Wang (2006, 2007).

3 Numerical approach

In order to obtain the quantum optimal pairing u^* and v^* , the preformed algorithm could be found in Wang (2006) and Wang (2007). That is, finite element method is used in the computational approach based on the variational method in Hilbert space. Quadratic base function is adopted in finite element approximate. Furthermore, the modified nonlinear conjugated gradient method is utilized in optimality minimization.

Consider two particles motions in two dimensional spatial space $[0, X] \times [0, Y]$, where $X = 50(\mu m)$ and $Y = 50(\mu m)$. Take $t_0 = 0.0(\text{fs})$, $T = 20.0(\text{fs})$ and time interval $\Delta t = 2.0(\text{fs})$. Assume the stop criteria $\varepsilon = 10^{-2}$ in minimization scheme. Define two appendix functions for initial states configuration as follows:

$$\Psi(x, t, v_1) = \frac{3\sqrt{2}}{4\sqrt{1-v_1^2}} \sec^2 \frac{1}{2\sqrt{1-v_1^2}}(x - v_1 t - x_0) \times \exp\left(i(v_1 x + \frac{(1-v_1^2+v_1^4)}{2(1-v_1^2)}t)\right),$$

$$\Phi(x, t, v_2) = \frac{3}{4(1-v_2^2)} \sec^2 \frac{1}{2(1-v_2^2)}(x - v_2 t - x_0),$$

where v_1 and v_2 are velocities of nucleon and meson, respectively. Setting x coordinate location center is $x_0 = 25.0(\mu m)$, two particles locations at y coordinate are $y_{10} = 15.0(\mu m)$ and $y_{20} = 35.0(\mu m)$. Their wave propagation velocities $v_1 = 5/11$ and $v_2 = -5/11$. Therefore, the initial ground states can be given and expressed by

$$\psi_0 = \Psi(\sqrt{(x-x_0)^2 + (y-y_{10})^2}, 0, v_1) + \Psi(\sqrt{(x-x_0)^2 + (y-y_{20})^2}, 0, v_2),$$

$$\phi_0 = \Phi(\sqrt{(x-x_0)^2 + (y-y_{10})^2}, 0, v_1) + \Phi(\sqrt{(x-x_0)^2 + (y-y_{20})^2}, 0, v_2).$$

The graphics of $\psi(0)$ and $\phi(0)$ are plotted in (a), (b) of Figure 1, respectively. Take target

Figure 1. (a). $\psi(0)$.

(b). $\phi(0)$

quantum excited states

$$\psi_{\text{target}} = \Psi(\sqrt{(x-x_0)^2 + (y-y_{10})^2}, T, v_1) + \Psi(\sqrt{(x-x_0)^2 + (y-y_{10})^2}, T, v_2),$$

$$\phi_{\text{target}} = \Phi(\sqrt{(x-x_0)^2 + (y-y_{10})^2}, T, v_1) + \Phi(\sqrt{(x-x_0)^2 + (y-y_{10})^2}, T, v_2).$$

Assume the iteration step n , and define Gaussian enveloped function

$$s[n] = \exp\left(-\frac{\pi}{2}(t - (n-1)\Delta t)^2\right).$$

By updated gradient conjugate method, the employed control functions (e.g. laser pulses) at

each iteration are calculated as:

$$\begin{aligned}
 u[1] &= s[1][1.9285 + 2 \sin(300t + \pi/6)], \\
 v[1] &= s[1][26.3797 + 2 \sin(240t + \pi/3)]. \\
 u[2] &= s[2][0.00409813 + 0.994788 \sin(300t + \pi/6)], \\
 v[2] &= s[2][-0.0732996 + 0.994788 \sin(240t + \pi/3)]. \\
 u[3] &= s[3][0.0011282 + 0.994742 \sin(300t + \pi/6)], \\
 v[3] &= s[3][-0.0738101 + 0.994742 \sin(240t + \pi/3)]. \\
 u[4] &= s[4][0.00338029 + 0.99469 \sin(300t + \pi/6)], \\
 v[4] &= s[4][-0.00268291 + 0.994691 \sin(240t + \pi/3)]. \\
 u[5] &= s[5][0.00337783 + 0.994685 \sin(300t + \pi/6)], \\
 v[5] &= s[5][0.00211341 + 0.994686 \sin(240t + \pi/3)]. \\
 u[6] &= s[6][-0.00314005 + 0.994685 \sin(300t + \pi/6)], \\
 v[6] &= s[6][0.002106 + 0.994686 \sin(240t + \pi/3)]. \\
 u[7] &= s[7][-0.00315287 + 0.994685 \sin(300t + \pi/6)], \\
 v[7] &= s[7][-0.00334883 + 0.994686 \sin(240t + \pi/3)]. \\
 u[8] &= s[8][-0.00296492 + 0.994685 \sin(300t + \pi/6)], \\
 v[8] &= s[8][0.00388112 + 0.994686 \sin(240t + \pi/3)]. \\
 u[9] &= s[9][-0.00313307 + 0.994685 \sin(300t + \pi/6)], \\
 v[9] &= s[9][-0.00259537 + 0.994686 \sin(240t + \pi/3)]. \\
 u[10] &= s[10][-0.00305381 + 0.994685 \sin(300t + \pi/6)], \\
 v[10] &= s[10][0.00456821 + 0.994686 \sin(240t + \pi/3)].
 \end{aligned}$$

The graphics of $u(t)$ and $v(t)$ at all iterations are plotted in Figure 2-3.

Figure 2. All $u(t)$, $n = 1, 2, \dots, 10$

Then obtained quantum optimal control variables as (at step $n = 4$)

$$\begin{aligned}
 u^* &= s[t][0.00338029 + 0.99469 \sin(300t + \pi/6)], \\
 v^* &= s[t][-0.00268291 + 0.994691 \sin(240t + \pi/3)].
 \end{aligned}$$

See (a) and (b) in Figure 4 for their graphics.

Figure 3. All $v(t)$, $n = 1, 2, \dots, 10$

Figure 4. (a). $u^*(t)$. (b). $v^*(t)$

Figure 5-6 given the states transition of nucleons and its contour plot.

Figure 5. $\psi(t)$ at iteration, $n = 1, 2, \dots, 10$

Figure 7 show the propagation of meson states, their contour plot is plotted in Figure 8.

Figure 6. Contour plots of $\psi(t)$, $n = 1, 2, \dots, 10$

Figure 7. $\psi(t)$ at iteration, $n = 1, 2, \dots, 10$

Figure 8. Contour plots of $\phi(t)$, $n = 1, 2, \dots, 10$

The cost values $J(\mathbf{u})$ and error values $eJ(\mathbf{u})$ are shown in (a) and (b) of Figure 9, respectively.

Figure 9. (a). $J(\mathbf{u})$

(b). $eJ(\mathbf{u})$

Clearly, laser pulses u and v drive the two particles to attain optimal states at step 4 in Figures 5 and 7. The optimality value $J(\mathbf{u}^*) = 2.74375$ and minimization error $eJ(\mathbf{u}^*) = 1.00524$.

After iteration step 4, the one nucleon and one meson are “recoiled” (forced interaction) with each other in nuclear “collision” (as a kinds of colision or nuclear event). Obviously, the energy is not conserved at whole control process. The objective functions at iteration step, see Table 1.

Table 1. Objective functions values

iteration	$J(\mathbf{u})$	iteration	$J(\mathbf{u})$
n=1	17.4019	n=2	10.7635
n=3	3.74899	n=4	2.74375
n=5	5.69131	n=6	163.554
n=7	254.802	n=8	25.4782
n=9	4.69623	n=10	189.72.

The iteration errors at each step are listed in Table 2.

Table 2. Error values at each iteration

iteration	error	iteration	error
n=1	17.4019	n=2	6.63841
n=3	7.01451	n=4	1.00524
n=5	2.94757	n=6	157.863
n=7	91.2481	n=8	229.324
n=9	20.782	n=10	185.024

The total computing time 5702.65 second. The used maximum memory is 7661.417808 bytes.

Remark 1: Further configurations are needed for real laboratory experiments, the corresponding atom units should be adopted appropriately. The intensity of shaped laser pulse and objectives functions should be adequately adjusted to make physical sense in nuclear scale.

Remark 2: Indeed, at current lab experiment on mixed frequency of laser pulse, instead of calculating the best sequence of frequencies, it randomly mixes frequencies and check out one work better than another. It is urgently demanded that theoretical study would make the experiment controlling clear with efficient laser selection.

4 Conclusions

In summary, this work addressed two dimension controlling of couple heavy particles under Yukawa interaction in nucleus. The theoretic analysis and experiment demonstration evident that it is reasonable to execute the quantum controlling with the advanced laser (photonic and electronic) technology. The presented study would provide a promising outlook for quantum nuclei controlling in real sense.

In the future work, the proposed computational approach would be developed to a realistic methodology in theoretical study and laboratory experiments for a board class of quantum system controlling in high dimension case (cf. Wang (2008)). In particular, the expected application to control of nucleus is a direction for enhancement.

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