Soft Quantum Control for Highly Selective Interactions among Joint Quantum Systems

J. F. Haase, Z.-Y. Wang,* J. Casanova, and M. B. Plenio[†]

Institut für Theoretische Physik und IQST, Albert-Einstein-Allee 11, Universität Ulm, D-89069 Ulm, Germany

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We propose a quantum control scheme aimed at interacting systems that gives rise to highly selective coupling among their near-to-resonance constituents. Our protocol implements temporal control of the interaction strength, switching it on and off again adiabatically. This soft temporal modulation significantly suppresses off-resonant contributions in the interactions. Among the applications of our method we show that it allows us to perform an efficient rotating-wave approximation in a wide parameter regime, the elimination of side peaks in quantum sensing experiments, and selective high-fidelity entanglement gates on nuclear spins with close frequencies. We apply our theory to nitrogen-vacancy centers in diamond and demonstrate the possibility for the detection of weak electron-nuclear coupling under the presence of strong perturbations.

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Introduction.-The ability to selectively manipulate and couple the constituents in an interacting quantum cluster is a fundamental requirement for a wide range of technological applications [1–3]. For instance, the *individual* addressing of magnetic nuclei in a target molecule with a quantum sensor, such as the nitrogen-vacancy (NV) center in diamond [4], is a crucial requirement to determine the 3D structure of single molecules of interest for biochemistry and medicine [5-12]. In addition, the selective coupling of the quantum sensor with nearby quantum registers would enhance the sensitivity and resolution of quantum sensing protocols [13–18]. From a different point of view, if the addressing operation does not disturb the other qubits surrounding a certain target register, namely the ¹³C and ²⁹Si nuclear spins that appear in diamond [19– 23] and silicon carbide [24,25], or Eu^{3+} ions in stoichiometric rare-earth crystals [26,27], one can use the available qubits for quantum information [28-30] or quantum simulation [31] tasks. Furthermore, nuclear gubits coupled to an electron spin are also important to build a robust optical interface for quantum networks [32,33].

The addressability problem can be reduced to the situation shown in Fig. 1(a) where a control qubit (CQ) interacts with multiple resource qubits (RQs) [34,35]. In order to exert control on a certain RQ the characteristic frequency ω_0 of the CQ is tuned to the resonance frequency ω_j of the RQ via a continuous drive that exploits the Hartmann-Hahn resonance [36–38] or the application of pulsed dynamical decoupling (DD) [39–43]. As we will show later, because of the time independent coupling c_j between the CQ and each RQ, the spectral responses are proportional to $c_j/\delta_{0,j}$ which decays slowly with the energy mismatch $\delta_{0,j} = \omega_0 - \omega_j$ (j > 0 for RQs), i.e., in a power-law manner. Therefore other off-resonant RQs will

considerably perturb the CQ and vice versa, see Fig. 1(b), prohibiting the high-fidelity addressing on the desired target RQ. This is particularly challenging for realistic settings where the RQs only slightly differ in their resonance frequencies.

In this Letter, we propose the idea of soft temporal quantum control which enables on-resonant coupling within a desired set of target systems, while efficiently avoiding unwanted off-resonant contributions coming from others. With the specific case of Gaussian soft control, off-resonant effects are exponentially suppressed by the mismatch $\delta_{0,j}$ as $\exp(-\sigma^2 \delta_{0,j}^2/2)$, see Fig. 1(c), achieving high-selective coupling. In addition, we develop an average Hamiltonian theory for our soft quantum control method. By using the quantum adiabatic theorem, we take high-order virtual transitions into account and provide an



FIG. 1. Advantages of temporal shaping of coupling. (a) Illustration for the control qubit and resource qubits. (b) For the case of constant coupling c_j , the off-resonant response decays slowly $c_j/\delta_{0,j}$ (blue lines) with the energy mismatch $\delta_{0,j}$. The overlaps (gray areas) on the frequency response prohibit high-fidelity selective coupling. (c) With the soft coupling proposed in this Letter the off-resonant response decays exponentially (see the orange lines), which allows high-fidelity addressing.

accurate description of the dynamics even for situations involving strong perturbations and long evolution times. We will show specific applications of our method such as the realization of an efficient rotating-wave approximation (RWA) and highly selective two-qubit gates for quantum sensing and computing.

Generic model.—To explore the effects emerging from temporal control, we consider the Hamiltonian ($\hbar = 1$) $H = H_S + H_{int}$, where H_S is the Hamiltonian for the quantum registers and $H_{int} = \lambda(t) \sum_{\alpha} c_{\alpha} V_{\alpha}$ describes their interactions that we want to perform selective control. $\lambda(t)$ is a dimensionless, time-dependent global factor and V_{α} may be single-body or N-body operators with strength c_{α} (i.e., the norm of V_{α} is bounded to one).

In terms of the eigenvalues ω_j and the projection operators $\mathbb{P}(\omega_j)$ of the Hamiltonian $H_S = \sum_j \omega_j \mathbb{P}(\omega_j)$, we write

$$H_{\rm int} = \lambda(t) \sum_{\alpha,j,k} c_{\alpha} V_{\alpha}^{\omega_j,\omega_k},\tag{1}$$

where each $V_{\alpha}^{\omega_j,\omega_k} \equiv \mathbb{P}(\omega_j)V_{\alpha}\mathbb{P}(\omega_k)$ fulfils

$$[H_S, V_{\alpha}^{\omega_j, \omega_k}] = (\omega_j - \omega_k) V_{\alpha}^{\omega_j, \omega_k}.$$
 (2)

In coupled quantum networks, $V_{\alpha}^{\omega_j,\omega_k}$ would describe the interaction between quantum systems with an energy mismatch of $\delta_{j,k} \equiv \omega_j - \omega_k$. Our target is to suppress the terms $V_{\alpha}^{\omega_j,\omega_k}$ in Eq. (1) for which $\omega_j \neq \omega_k$, and to keep the energy conserving ones (i.e., those with $\delta_{j,k} = 0$) by shaping the parameter $\lambda(t)$ for the sake of enhanced selectivity.

Leading-order effects and soft quantum control.—In a rotating frame with respect to H_S , H_{int} becomes $H'_{\text{int}}(t) = \lambda(t) \sum_{\alpha,j,k} c_\alpha V_\alpha^{\omega_j,\omega_k} e^{i\delta_{j,k}t}$. In the absence of a modulation for λ , i.e., $\lambda(t) = \lambda_0$, unwanted terms in V_α can be neglected by the RWA provided that the $\delta_{j,k}$ is sufficiently large compared with $\lambda_0 c_\alpha$. To see how the modulation of $\lambda(t)$ improves this situation, we calculate the leading-order effective Hamiltonian in the rotating frame by using the Magnus expansion [44,45] for a time interval [-T/2, T/2]; it reads

$$\bar{H}_{\rm int}^{(1)} = \frac{1}{T} \int_{-T/2}^{T/2} dt H_{\rm int}'(t) = \sum_{\alpha,j,k} c_{\alpha} g(\delta_{j,k}) V_{\alpha}^{\omega_{j},\omega_{k}}, \qquad (3)$$

where the averaging factor

$$g(\delta_{j,k}) = \frac{1}{T} \int_{-T/2}^{T/2} dt \lambda(t) e^{i\delta_{j,k}t}$$
(4)

can be controlled by $\lambda(t)$.

For the conventional case of a constant $\lambda(t) = \lambda_0$, we have

$$g(\delta_{j,k}) = g_C(\delta_{j,k}) \equiv \lambda_0 \frac{\sin\left(T\delta_{j,k}/2\right)}{(T\delta_{j,k}/2)}.$$
 (5)

In this manner, unwanted terms in V_{α} are suppressed by a large energy mismatch $\delta_{j,k}$ to decrease the value of $g_C(\delta_{j,k})$ [46]. By selecting λ_0 sufficiently small, the off-resonant interactions can be more efficiently suppressed with the associated improvement in the addressing for the resonant terms. See Refs. [9,47] for a specific application of the latter to the case of NV centers in diamond surrounded by ¹³C nuclear spins. However, from Eqs. (3) and (5) the effects introduced by off-resonant terms decay slowly as a power law $\lambda_0 c_{\alpha}/\delta_{j,k}$ on the energy mismatch $\delta_{j,k}$ while, in addition, because $g(0) = \lambda_0$ a decrease on λ_0 also carries the undesired effect of reducing the intensity of the coupling with the resonant terms.

From Eq. (4), we find that by using a time-dependent soft modulation, i.e., $\lambda(t)$ is small at the beginning and at the end of quantum evolution, the nonresonant terms can be removed with greater fidelity. More specifically, we propose the Gaussian temporal modulation

$$\lambda(t) = \lambda_0 \exp\left[-t^2/(2\sigma^2)\right],\tag{6}$$

which has the corresponding factor

$$g(\delta_{j,k}) = g_M(\delta_{j,k}) \equiv \lambda_0 \eta(\sigma, T) \exp\left(-\frac{1}{2}\sigma^2 \delta_{j,k}^2\right), \quad (7)$$

where $\eta(\sigma,T) = \sqrt{\pi/2}(\sigma/T) \{ \operatorname{erf}[(T-2i\sigma^2\delta_{j,k})/(2\sqrt{2}\sigma)] + \operatorname{erf}[(T+2i\sigma^2\delta_{j,k})/(2\sqrt{2}\sigma)] \}$ and $\operatorname{erf}(x) = (2/\sqrt{\pi}) \times \int_0^x dz e^{-z^2}$. A simple inspection of Eq. (7) reveals that the effective couplings $g_M(\delta_{j,k})c_\alpha$ decay exponentially with $\delta_{j,k}$. Hence, we expect the selectivity to be dramatically improved. We want to remark that our temporal shaping scheme shares interesting similarities with the control by Gaussian pulses of classical fields [48]; however, in our case, the shaping is exerted on the coupling between quantum systems where quantum backaction plays a significant role on both sides [49].

Higher-order effects and adiabatic average Hamiltonian.—Although the leading-order average Hamiltonian $\bar{H}_{int}^{(1)}$ in Eq. (3) describes well the dynamics for $T \ll 1/\max |c_{\alpha}|$, if strong coupling constants are present, higher-order corrections [44,45] have to be included in order to have an accurate description of the dynamics for larger times.

While the evaluation of higher-order terms is involved in the general case, now we will show that our proposed soft quantum control scheme allows us to easily describe the system propagator including high-order corrections when executed in an adiabatic manner. To this end we first analyze the propagator $U_D = \exp(-i \int_{-T/2}^{T/2} H_D dt)$, where $H_D = H_S + \lambda(t) \sum_{\alpha} c_{\alpha} \sum_j V_{\alpha}^{\omega_j, \omega_j}$ includes the on-resonance desired interactions. In the latter all $V_{\alpha}^{\omega_j,\omega_j}$ operators commute with H_S ; see Eq. (2); hence H_D can be diagonalized in the common eigenstates $|\psi_n^D\rangle$ (n = 1, 2, ...) of H_S and $V_{\alpha}^{\omega_j,\omega_j}$. Therefore $U_D = \sum_n e^{-i\phi_n^D(T)} |\psi_n^D\rangle \langle \psi_n^D|$ is also diagonal in the basis $\{|\psi_n^D\rangle\}$ and the dynamic phases $\phi_n^D(T)$ include the effect of energy shifts coming from $V_{\alpha}^{\omega_j,\omega_j}$.

If the whole Hamiltonian *H* is considered, the timeordered evolution $U = \mathcal{T} \exp \left[-i \int_{-T/2}^{T/2} H(t) dt\right]$ is generally nondiagonal in the basis $\{|\psi_n^D\rangle\}$ and the noncommuting $V_{\alpha}^{\omega_j,\omega_k}$ terms would cause unwanted transitions between the different $|\psi_n^D\rangle$ states.

However, when the soft control is included one can efficiently eliminate the unwanted interactions caused by $V_{\alpha}^{\omega_{j},\omega_{k}}$, even for long evolution times *T*. At the boundaries of the interaction times (-T/2 and T/2), $\lambda(t)$ has negligible values and therefore the system's eigenstates coincide with those of H_{D} . More precisely, under the condition of adiabatic evolution [50,51], there are no transitions among the states $|\psi_{n}^{D}\rangle$ and the propagator at the end of the evolution is $U \approx \sum_{n} e^{-i\phi_{n}(T)} |\psi_{n}^{D}\rangle \langle \psi_{n}^{D}| \equiv \overline{U} \equiv e^{-i\overline{H}T}$, where $\phi_{n}(T)$ are the dynamic phases, while the geometric phases vanish because $\lambda(t)$ returns to its original value [52]. In this manner *U* takes the same form as U_{D} and the adiabatic average Hamiltonian for the soft quantum control scheme

$$\bar{H} = \sum_{n} [\phi_n(T)/T] |\psi_n^D\rangle \langle \psi_n^D|, \qquad (8)$$

is diagonal in the same basis as H_D and includes all the high-order energy shifts. In the following, we illustrate our general theory via two important applications.

Improved RWA.—Here we demonstrate how the soft quantum control mechanism efficiently eliminates the nonenergy-conserving (or counterrotating) terms over a continuous time interval even for long evolution times. The existence of the nonenergy-conserving terms is due to the limit of available resources for selective control on realistic quantum systems (e.g., singlet-triplet qubits in semiconductor quantum dots [53,54]). As an example, we consider a control qubit (0) and two equally strong coupled resource qubits (1,2) (e.g., singlet-triplet qubits [53,54]) with the interaction

$$H_{\rm int} = c\lambda(t)\sigma_0^x(\sigma_1^x + \sigma_2^x) = c\lambda(t)(P_{0,1} + Q_{0,1} + \sigma_0^x\sigma_2^x),$$
(9)

where σ_j^{α} ($\alpha = x, y, z$) denotes a Pauli operator for the *j*th qubit, $P_{0,1} = \sigma_0^+ \sigma_1^- + \text{H.c.}$ with $2\sigma_j^\pm = \sigma_j^x \pm i\sigma_j^y$, and $Q_{0,1} = \sigma_0^+ \sigma_1^+ + \sigma_0^- \sigma_1^-$. The coexistence of $P_{0,1}$ and $Q_{0,1}$ can be due to the nature of systems (see [54] for a realistic example). We aim to interact qubit 0 purely with qubit 1 via the flip-flop term $P_{0,1}$ without involving the perturbation



FIG. 2. Fidelities under RWA. (a) Fidelity to the target evolution without unwanted coupling by using the constantamplitude coupling. (b) As in (a) but using a Gaussian soft coupling with $\sigma = T/(4\sqrt{2})$ and $1/\lambda_0 = \sqrt{2\pi\sigma} \text{erf}[T/(2\sqrt{2}\sigma)]$ such that we obtain the same target evolution. Curves in (c) and (d) show cross-sectional plots in the constant-amplitude case of (a) [red solid lines], or for the Gaussian shaped coupling case of (b) [blue dashed lines]. It is easy to see that the soft quantum control scheme keeps a high fidelity even for a relatively large ratios c/ω at long evolution times *T*.

 $Q_{0,1}$. Therefore the energies $H_S = (\omega/2)(\sigma_0^z + \sigma_1^z) + (\omega_2/2)\sigma_2^z$ are chosen such that qubit 2 is off resonant with $\omega_2 = 3\omega$. The corresponding target Hamilton

$$H_{\text{target}} = \frac{1}{2}\tilde{\omega}(\sigma_0^z + \sigma_1^z) + \frac{1}{2}\tilde{\omega}_2\sigma_2^z + \tilde{c}(\sigma_0^+\sigma_1^- + \text{H.c.}),$$
(10)

with the associated propagator $U_{\text{target}} = e^{-iH_{\text{target}}T}$ can be used to generate high-fidelity swap gate between qubits 0 and 1. The corrected energies and interaction marked with a tilde can be obtained by using the adiabatic average Hamiltonian according to Eq. (8).

In Fig. 2(a) and with the red solid lines in (c) and (d), we show the gate fidelities $F = |\text{Tr}(U_{\text{target}}U^{\dagger})|/\text{Tr}(UU^{\dagger})$ [55] [here $U = T e^{-i \int_{-T/2}^{T/2} (H_S + H_{int}) dt}$] with respect to the target evolution U_{target} for the standard coupling $\lambda(t) = 1$, while in Fig. 2(b) and with the blue dashed lines in (c) and (d) the fidelities are plotted for a situation involving the soft quantum modulation in Eq. (6). An inspection of these plots reveals that the soft coupling approach results in much higher fidelities in a wide range of parameters, even for strong coupling regimes $(c > \omega)$ and a wide range of evolution times. In contrast, the standard approach does not achieve a high fidelity to the target Hamiltonian because an efficient elimination of the oscillating terms requires weak couplings and longer averaging periods. Naturally during these times, relaxation and decoherence processes will decrease the fidelity further. Furthermore, locating the



FIG. 3. (a)-(c) Signal of transition probabilities, originating from two nuclear spins ($\omega_1 = 2\pi \times 441.91$ kHz and $\omega_2 = 2\pi \times 437.54$ kHz, see [56] for more details). (a) Hartmann-Hahn resonance spectrum with a total sensing time $T \approx$ 54 μ s (red) or $T \approx 435 \ \mu$ s (blue). (b) Signal for AXY sequences (red solid line) at the third harmonic with 128 composite pulses each has five elementary π pulses). The single-spin contributions are drawn with dashed lines and corresponding shading, and $f_3 =$ 0.271 is chosen to maximize the one from the first spin. The target signal centered at the vertical dashed-dotted line is destroyed by the strong perturbation from the unwanted second spin. (c) Varying f_3 of the AXY sequences in (b) according to the Gaussian shape clearly resolves the two spins. (d) The fidelity (blue solid curve) of the gate $U_{\text{target}}=e^{-i(\pi/4)\sigma_0^z\sigma_1^x}\otimes\mathbb{I}_2$ as a function of the microwave detuning error Δ by using the Gaussian AXY sequence with a Rabi frequency $\Omega = 2\pi \times 20$ MHz in the rectangular pulses. The red dashed line is the case for a mismatch of 5% in Ω . To realize the gate U_{target} , f_3 has been reduced by a factor of 2 when using the parameters indicated by the vertical dash-dotted line in (c).

points of high fidelity in the standard approach becomes increasingly difficult when more qubits are involved (cf. the two-qubit example in the Supplemental Material [56]).

Note that our approach is fundamentally different from adiabatic elimination [60,61]. Adiabatic elimination is aimed at *coupling* certain target levels by a virtual transfer of excitations through other mediator states that are removed from the dynamics, thus generating an evolution in the *reduced* Hilbert space of the target states. Instead our objective is to efficiently *suppress* unwanted interaction terms in the Hamiltonian through a soft modulation of the coupling constants, without reducing the dimension of the whole Hamiltonian and without having to use other states as mediators. Hence our method allows us to switch off unwanted interactions among the qubits in a highly selective manner and to perform high-fidelity quantum gates as we will demonstrate later.

Selective qubit addressing.—The soft quantum control mechanism allows high-fidelity interactions between weakly coupled qubits while it avoids perturbations that arise from the presence of strongly coupled qubits. Since the NV center in diamond is an excellent platform for quantum information processing [28–30], quantum networks [32,33], and quantum sensing [5,6], we consider a network consisting of an NV electron spin and its surrounding 13 C nuclear spins (see [56] for details of the model).

The electron-nuclear hyperfine coupling offers a medium to control the ¹³C nuclear spins via the NV electron. Under pulsed DD [41–43,47] or a continuous drive [37,38] on the NV electron states $m_s = 0$ and, say, $m_s = -1$, the ¹³C Larmor frequencies ω_j are shifted by hyperfine coupling, providing the frequency differences $\delta_{j,n} = \omega_j - \omega_n$ for selective addressing [56]. However, the differences $\delta_{j,n}$ and the electron-nuclear interactions are typically of the same order of magnitude, imposing a challenge on highly selective coupling.

To demonstrate the advantages of the soft quantum control, we compare different protocols in Fig. 3 by using a model with two spectrally close nuclear spins (their coupling is small but is taken into account in simulations). As shown in Fig. 3(a) a frequency scan obtained via a continuous, constant drive [37,38] does not resolve the two ¹³C nuclei even for a longer sensing time *T* because of the slow power-law-decay of the signal around the resonance position.

Because pulsed DD sequences can be implemented easily in current experimental setups and coherent control on NV electron and nuclear spins longer than one second has been experimentally implemented with over ten thousands of DD pulses [30], we apply a DD sequence to preserve the coherence of the NV electron qubit and to realize the Hamiltonian [56]

$$H = -\frac{1}{8} f_{k_{\rm DD}} \sigma_0^z \sum_{j>0} a_j^{\perp} \sigma_j^x - \sum_{j>0} \frac{1}{2} \delta_{j,n} \sigma_j^z, \qquad (11)$$

for addressing the nuclear frequency ω_n . Both $\delta_{j,n}$ and a_j^{\perp} are determined by the hyperfine coupling at the nuclear locations.

The DD protocol of adaptive-XY (AXY) sequences [47] provides better performance [9,47] over standard DD sequences [39,40] because it has strong robustness against control errors and allows us to tune $f_{k_{DD}}$ in a desirable manner. As shown in Fig. 3(b), by using a smaller $f_{k_{DD}}$ more signal details are revealed. However, this approach also reduces the coupling to the target spins.

By changing $f_{k_{\rm DD}}$ in the AXY sequences for every unit with four composite pulses, we implement the Gaussian soft modulation $\lambda(t)$ in a digitized manner while preserving the robustness of the sequences against experimental control errors (see [56] for details). The resulting Gaussian AXY significantly enhances and resolves the weak spin signal by using the soft modulation to eliminate the strong unwanted perturbation [see Fig. 3(c)]. In addition, it removes all the side peaks around the spin resonances, which is of great advantage when fitting dense signals [22] and avoids false identification of the signal peaks, in particular at the presence of spurious resonances [62–64]. Furthermore, it allows robust, high-fidelity quantum gates on the desired nuclear qubits. We calculate the fidelity for the gate $U_{\text{target}} = \exp(-i\pi\sigma_0^z \sigma_1^x/4) \otimes \mathbb{I}_2$ for the same parameters as the spectrum given in Fig. 3(c), but choose f_3 such that the target spin only performs a half rotation. We include an energy shift of the strongly coupled nuclear spin equivalent to the first example above. The fidelity is shown in Fig. 3(d) for different values of possible pulse errors. It is always well above 99%. On the contrary, the fidelities achieved by the Hartmann-Hahn or AXY protocol under the same condition are very low (e.g., 57%) for AXY) because of the poor spin addressing [see Figs. 3(a) and 3(b)]. Note that the enhanced spectral resolution by the soft control can be used to improve the controllability of interacting spin clusters [7-9,16,30] and nuclear-spin decoherence-free subspace [29].

Conclusions.—We proposed the mechanism of soft quantum control which enables highly selective coupling between different on-resonance constituents of composite quantum systems. The method introduces a time-dependent modulation of the coupling constants in addition to the matching of resonance frequencies. This results in an exponentially improved suppression of off-resonant couplings. Furthermore, we establish an adiabatic average Hamiltonian theory to describe interacting systems even under the presence of strong coupling terms to undesired parts of the Hilbert space. We showed two direct applications of our protocol: an improved RWA and, when combined with DD techniques, the addressing of weakly coupled nuclear spins under the presence of strong perturbations, originating from impurities with close resonance frequencies. The method is of general applicability and can be useful for the coherent manipulations of quantum registers and spectroscopic challenges in a wide range of systems such as stoichiomeric rare earth ion systems, spin defects, and single dopants in solids, as well as spin-boson systems.

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J. F. H. and Z.-Y. W. contributed equally to this work.

zhenyu3cn@gmail.com

^Tmartin.plenio@uni-ulm.de

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