Scalable Design of Tailored Soft Pulses for Coherent Control

Pinaki Sengupta and Leonid P. Pryadko

Department of Physics, University of California, Riverside, California 92521, USA

(Received 15 February 2005; published 15 July 2005)

We present a scalable scheme to design optimized soft pulses and pulse sequences for coherent control of interacting quantum many-body systems. The scheme is based on the cluster expansion and the time-dependent perturbation theory implemented numerically. This approach offers a dramatic advantage in numerical efficiency, and it is also more convenient than the commonly used Magnus expansion, especially when dealing with higher-order terms. We illustrate the scheme by designing 2nd-order self-refocusing π pulses and a 6th-order 8-pulse refocusing sequence for a chain of qubits with nearest-neighbor couplings. We also discuss the performance of soft-pulse refocusing sequences in suppressing decoherence due to low-frequency environment.

DOI: 10.1103/PhysRevLett.95.037202 PACS numbers: 75.40.Gb, 75.10.Jm, 75.30.Ds, 75.40.Mg

A control of coherent evolution of quantum systems is increasingly important in a number of research fields and applications [1–5]. Such control has long been a staple in nuclear magnetic resonance (NMR) spectroscopy, where a structural analysis of complex molecules requires the application of long sequences of precisely designed radio-frequency (rf) pulses [6]. Recently, coherent control has emerged as an important part of quantum information processing (QIP), spurring numerous studies on general properties and specific design of pulses and pulse sequences for application in NMR-based [7] and other potential implementations [8,9] of quantum computers (QCs).

The precision required for QIP is achieved most readily using shaped (also soft), typically narrow-spectrum, pulses. When properly constructed, such pulses allow excitation to be limited to a particular set of modes which results in better control fidelity and reduced incoherent losses (e.g., heating). The latter is especially important for putative solid-state QC implementations which are proposed to operate at cryogenic temperatures. Additionally, as we also discuss in this work, refocusing with carefully designed high-order pulses and pulse sequences can offer significantly better protection against nonresonant decoherence sources (e.g., low-frequency phonons) as compared to lower-order sequences.

Over some 40 years shaped pulses were utilized in NMR, a number of schemes were suggested for their design [6]. Most (although not all) rely on the average Hamiltonian theory [10], a perturbative scheme based on the cumulant (Magnus) expansion for the evolution operator. The expansion is done around the evolution in the applied controlling fields, while the chemical shifts (resonant-frequency offsets) and, ideally, interspin couplings, are treated perturbatively. The main drawback of the Magnus expansion [Eq. (9)] for numerics is multiple integrations appearing in higher orders; its use in calculations was almost always limited to quadratic order. The alternative scheme found in the literature is a simulation involving the full or partial Hamiltonian of a quantum system [11,12]. This scheme obviously lacks scalability, as the computational difficulty grows exponentially with the system size.

We present an efficient scalable scheme to design high-order soft pulses and soft-pulse sequences for controlling quantum many-body systems. Instead of using Magnus expansion or other effective Hamiltonian theories, we rely on the time-dependent perturbation theory (TDPT) implemented numerically. This allows an easy extension to higher orders (up to 9th in this work), while preserving the benefits of the cluster theorem [13] which limits the size of the system to be analyzed. The high-order calculation allows a straightforward classification of pulse sequences by order K, the number of terms in the TDPT for which the control remains perfect. We also discuss the performance of different-K sequences in suppressing decoherence due to low-frequency environment.

As an illustration, we consider a quantum spin chain with ''always-on'' nearest-neighbor (NN) interactions, where each qubit (spin) can be individually controlled. We construct a family of one-dimensional pulses with different degrees of self-refocusing with respect to the J_z coupling. The duration of a pulse, τ, is fixed to allow parallel execution of quantum gates in different parts of the system. To reduce the spectral width [14] of an arbitrary sequence of such pulses we also require a number of derivatives of the controlling fields to vanish at the ends of the cycle. We show that thus designed pulses work as drop-in replacement of hard pulses, and compare their performance with that of two commonly used shapes. We illustrate the performance of the method by doing an exhaustive search among two-sublattice eight-pulse refocusing sequences to produce a sequence of order $K = 6$ for the quantum Ising chain [refocusing errors scale as $(J_z\tau)^6$], order $K = 2$ for general xxz chain, where, in addition, each spin has an order $K \geq 2$ protection against phase decoherence due to low-frequency environment (Table I).

We consider the following simplified Hamiltonian,

$$H(t) = H_C(t) + H_S + H_V(t) + H_\sigma, \qquad (1)$$

with the first (main) term due to individual control fields,

TABLE I. Order K determining the scaling ($\propto \tau^K$) of the gate errors with the pulse duration τ for different refocusing sequences. 1: a single π pulse along the x axis on odd sites, "X_1^2"; 2: two π pulses along the x axis, odd sites only, $X_1^2X_1^2$; 4: $X_1^2Y_2^2\overline{X}_1^2\overline{Y}_2^2$ (bars for negative pulses, subscripts denote odd or even sites); 8: $X_1^2Y_2^2\overline{X}_1^2\overline{Y}_2^2Y_2^2\overline{X}_1^2Y_2^2X_1^2$. Asterisks mark odd-site refocusing. See text for description of the three models.

Model	Ising				*xxz*				Bath			
Sequence	1	2	4	8	1	2	4	8	1	2	4	8
Gauss [15]	0	1	1	2	0	0	0	1	0	1*	0	1
Herm [16] , S_1	1	1	3	4	0	0	1	1	1*	1*	1	1
Q_1	2	3	5	6	0	0	1	2	2*	2*	2	3

$$H_{\mathrm{C}}(t) = \frac{1}{2}\sum_n [V_n^x(t)\sigma_n^x + V_n^y(t)\sigma_n^y], \tag{2}$$

where σ_n^μ, $\mu = x, y, z$, are the usual Pauli matrices for the nth qubit (spin) of the 1D chain. The other terms describe the interactions between the qubits (NN xxz),

$$H_{\mathrm{S}} = \frac{1}{4}\sum_{\langle n,n'\rangle} [J_{n,n'}^z \sigma_n^z \sigma_{n'}^z + J_{n,n'}^\perp(\sigma_n^x\sigma_{n'}^x + \sigma_n^y\sigma_{n'}^y)], \tag{3}$$

and the coupling with the oscillator thermal bath,

$$H_V(t) = \sum_{n\mu} A_n^\mu V_n^\mu(t), \qquad H_\sigma = \frac{1}{2}\sum_n B_n^\mu \sigma_n^\mu. \tag{4}$$

In Eq. (4), $A_n^\mu \equiv A_n^\mu(p_i, q_i)$ account for the possibility of a direct coupling of the controlling fields V_n^μ with the bath variables q_i, p_i, while $B_n^\mu \equiv B_n^\mu(p_i, q_i)$ describe the usual coupling of the spins with the oscillator bath. Already in the linear response approximation, the bath couplings (4) produce a frequency-dependent renormalization of the control Hamiltonian $H_{\mathrm{C}}(t)$ [Eq. (2)], as well as the thermal bath heating via the dissipative part of the corresponding response function. Both effects become more of a problem with increased spectral width of the controlling signals V_n^μ. In this work we do not specify the explicit form of the coupling $H_V(t)$. Instead, we minimize the spectral width of the constructed pulses.

Closed system.—In a qubit-only system with the Hamiltonian $H(t) = H_{\mathrm{C}}(t) + H_{\mathrm{S}}$, the effect of the applied fields is fully described by the evolution operator $U(t)$,

$$\dot{U}(t) = -i[H_{\mathrm{C}}(t) + H_{\mathrm{S}}]U(t), \qquad U(0) = \mathbb{1}. \tag{5}$$

As usual, the TDPT is introduced by separating out the bare evolution operator,

$$U(t) = U_0(t)R(t), \qquad \dot{U}_0(t) = -iH_{\mathrm{C}}(t)U_0(t). \tag{6}$$

Then, the operator $R(t)$ obeys the equation

$$\dot{R}(t) = -i\tilde{H}_S(t)R(t), \qquad \tilde{H}_{\mathrm{S}}(t) \equiv U_0^\dagger(t)H_{\mathrm{S}}U_0(t), \tag{7}$$

which can be iterated to construct the standard expansion $R(t) = \mathbb{1} + R_1(t) + R_2(t) + \cdots$ in powers of (tH_{S}),

$$\dot{R}_{n+1}(t) = -i\tilde{H}_S(t)R_n(t), \qquad R_0(t) = \mathbb{1}. \tag{8}$$

For a finite system of n qubits and a given maximum order K of the expansion, Eqs. (6)–(8) are a set of coupled first-order ordinary differential equations for the $2^n \times 2^n$ matrices $U_0, R_1, R_2, \ldots, R_K$, and can be integrated efficiently using any of the available extrapolation schemes. Obviously, for a given system, solving the full equations (5) is simpler by a factor of at least $(K + 1)$. However, it is the analysis of the perturbative expansion that is the key for achieving the scalability of the results.

The standard Magnus expansion can be readily obtained by integrating Eqs. (8) formally and rewriting the result in terms of cumulants,

$$R(t) = \exp(C_1 + C_2 + \cdots), \qquad C_1 = -i\int_0^t dt_1 \tilde{H}_{\mathrm{S}}(t_1),$$
$$C_2 = -\frac{1}{2}\int_0^t dt_2 \int_0^{t_2} dt_1 [\tilde{H}_{\mathrm{S}}(t_1), \tilde{H}_{\mathrm{S}}(t_2)], \ldots \tag{9}$$

Generally, the term C_k contains a k-fold integration of the commutators of the rotating-frame Hamiltonian $\tilde{H}_{\mathrm{S}}(t_i)$ at different time moments t_i and has an order $(tH_{\mathrm{S}})^k$. The advantage of the cumulant expansion is that it does not contain the disconnected terms arising from different parts of the system. For an arbitrary lattice model of the form (3), with bonds representing the qubit interactions, the terms contributing to kth order can be represented graphically as connected clusters involving up to k lattice bonds; generally such clusters cannot have more than $n = k + 1$ vertices. Thus, to obtain the exact form of the expansion up to and including Kth order, one needs to analyze all distinct clusters with up to $K + 1$ vertices. For an infinite chain with NN couplings, these are finite chains with up to K bonds and $K + 1$ vertices.

The discussed cluster theorem [13] appears to offer a distinct advantage to the Magnus expansion compared with the regular perturbation theory. On the other hand, evaluation of multiple integrals (9) directly is computationally challenging, which limits the use of higher-order Magnus expansions for numerics. We note, however, that the order-K universal self-refocusing condition $C_1 = C_2 = \ldots = C_K = 0$ is formally equivalent to

$$R_1 = R_2 = \ldots = R_K = 0. \tag{10}$$

The matrices R_k in the latter condition are much easier to evaluate numerically using Eqs. (6)–(8). Yet the benefits of the cluster theorem remain: to Kth order only clusters with up to $K + 1$ vertices need to be analyzed.

We implemented the described scheme using the standard fourth-order Runge-Kutta algorithm for solving coupled differential equations and the GSL [17] numerical package for matrix operations. The coefficient optimization was done using a combination of simulated annealing and the steepest descent method. The trial pulse shapes were encoded in terms of their Fourier coefficients [18],

$$V(t+\tau/2) = A_0 + \sum_m A_m \cos(m\Omega t) + B_m \sin(m\Omega t), \quad (11)$$

where the angular frequency $\Omega = 2\pi/\tau$ is related to the pulse duration τ. The target function for single-pulse optimization included the sum of the magnitudes squared of the matrix elements of the zeroth-order mismatch matrix $[U_0(\tau) - U_{\text{target}}]$, and of the matrices $R_k(\tau)$, $k = 1, \ldots, K$. The minimization continued until these contributions went down to zero with the numerical precision.

As the simplest application of the formalism, we designed a number of inversion (π-) pulse shapes [19], self-refocusing to various degrees with respect to the Ising interaction; their coefficients are listed in Table II. To reduce the spectral width of an arbitrary sequence of such pulses, we required additionally that the function (11) vanishes along with a number of its derivatives $V^{(l)}(t)$, $l = 1, 2, \ldots, 2L-1$, at the ends of the interval, $t = 0, \tau$.

These shapes can work in known high-order pulse sequences [20] as a drop-in replacement of hard pulses. We note that in our setup there is no gap between subsequent pulses; the pulses follow back to back with the repetition period τ. The system is ''focused'' at the end of each time interval. Such a scheme with a common ''clock'' time τ is convenient, e.g., for parallel execution of quantum gates in different parts of the system. For each qubit, various pulses (or intervals of no signal) can be executed in sequence. The performance of such sequences can be analyzed in the same manner as that of a single pulse. Namely, we integrate Eqs. (6)–(8) over the full duration t of the pulse sequence; the order of the sequence is the number K of the exactly cancelled terms in the perturbative expansion of $R(t)$. After $N = t/\tau$ steps, the error in the unitary evolution matrix would scale as $\propto N\tau^{K+1} = t\tau^K$; the corresponding gate fidelity (defined as the probability of error, either average or maximum) would scale as $1 - \mathcal{O}(\tau^{2K})$.

In Table I, we illustrate the quality of the obtained pulses by comparing their performance in several refocusing sequences for different models. ''Ising'': the Ising-only interaction [Eq. (3) with all $J^\perp = 0$]; ''xxz'': the xxz spin chain with both J^z and $J^\perp$ nonzero; ''bath'': Ising spin chain coupled to a thermal bath generating slow (compared to τ) phase modulation, simulated as H_σ [Eq. (4)] with random time-independent coefficients B_n^z (see further discussion on open systems below). The pulse sequences are listed in the caption; these are ''best'' sequences at given length for all three pulse shapes found by exhaustive search. The fact that such a brute-force optimization approach works is entirely due to the efficiency of the method.

The most interesting is the length-8 sequence ''$\mathrm{X}_1^2\mathrm{Y}_2^2\overline{\mathrm{X}}_1^2\mathrm{Y}_2^2\overline{\mathrm{Y}}_2^2\overline{\mathrm{X}}_1^2\mathrm{Y}_2^2\mathrm{X}_1^2$,'' where X_1^2 is a π pulse in x direction applied on every odd site, $\overline{\mathrm{Y}}_2^2$ is a π pulse in negative y direction on even sites, etc. This sequence is the best among the length-8 sequences for both the Ising and the xxz ($J^\perp \neq 0$) models, and, additionally, it protects every qubit from phase decoherence due to low-frequency noise. Our second-order self-refocusing pulses are clearly advantageous, especially if the Ising coupling is dominant. The corresponding errors scale as $(J_z\tau)^6$ compared with that for the standard (first-order) Hermitian pulse where gate error scales as $(J_z\tau)^4$ [the gate fidelities differ from unity by $\mathcal{O}((J_z\tau)^{12})$ and $\mathcal{O}((J_z\tau)^8)$].

These pulses were designed for systems with dominant NN Ising coupling, and this is the situation where they are most useful as a replacement of, say, Gaussian pulses. For example, when the pulse Q_1 along with analogously designed second order $\pi/2$ and 2π pulses were used to simulate the BB_1 composite pulse [21] designed to compensate for amplitude errors to third order, the results for a single spin were essentially identical to those with Gaussian pulses, with errors cubic in the amplitude mismatch. However, when used in an Ising chain, the performance of the BB_1 sequence with Gaussian pulses deteriorated linearly in $J_z\tau$ already with zero amplitude mismatch, while for our second-order pulses the additional error was smaller, scaling as the product of $(J_z\tau)$ and the amplitude mismatch. Clearly, if the two sources of errors are comparable, combining high-accuracy BB_1 composite pulse and the second-order pulses may be superficial; simpler pulse sequence and/or pulses with first-order compensation could give a comparable accuracy.

Open systems.—Qualitatively, the effect of the refocusing pulses on the thermal bath coupling H_σ [Eq. (4)] can be most readily understood in the rotating frame defined by the bare evolution operator $U_0 \equiv U_0(t)$ [Eq. (6)],

$$\tilde{H}_\sigma(t) = U_0^\dagger H_\sigma U_0 = \frac{1}{2}\sum_{n,\mu,\mu'} B_n^\mu(p_i, q_i) Q_n^{\mu\mu'}(t)\sigma_n^{\mu'}. \quad (12)$$

For refocusing, the rotation matrices $Q_n^{\mu\mu'}(t)$ are periodic with the full sequence period $\tilde{\tau}$; they can be written as a

TABLE II. Fourier coefficients A_m [Eq. (11)] for the constructed pulses (pulses are symmetric; all $B_m = 0$). Shapes S_L and Q_L, respectively, are first ($K = 1$) and second ($K = 2$) order self-refocusing inversion pulses for the Ising coupling, with $2L$ derivatives vanishing at the ends of the interval. The fixed-time errors scale with the duration of the pulse as $\propto (\tau J_z)^K$.

	A_0	A_1	A_2	A_3	A_4	A_5
S_1	0.5	−1.2 053 194 466	0.4 796 460 175	0.2 256 734 291		
S_2	0.5	−1.1 950 755 990	0.7 841 246 569	0.0 738 054 432	−0.1 628 545 011	
Q_1	0.5	−1.1 374 003 264	1.5 774 784 244	−0.6 825 954 606	−0.2 574 826 374	
Q_2	0.5	−1.0 965 122 417	1.5 309 957 409	−1.1 470 791 601	0.0 020 722 004	0.2 105 234 605

sum of harmonics with the main frequency $\tilde{\Omega} = 2\pi/\tilde{\tau}$,

$$Q_n^{\mu\mu'}(t) = \sum_m C_{nm}^{\mu\mu'} e^{-i\tilde{\Omega}_m t}, \qquad \tilde{\Omega}_m \equiv m\tilde{\Omega}. \tag{13}$$

The constant-field first-order refocusing condition (average Hamiltonian vanishes to leading order) is equivalent to a cancellation of some linear combinations of $C_{n0}^{\mu\mu'}$ (e.g., $C_{n0}^{z\mu'} = 0$ for phase noise assumed for thermal bath in Table I). As a result, the environmental modes at low frequencies get modulated and are effectively replaced by those at higher frequencies, $\omega \to \omega + \tilde{\Omega}_m$, $m \neq 0$, leading to a significant reduction of the decoherence caused by resonant decay processes [22–24]. On the other hand, fast modes are mostly unaffected; modulation has essentially no effect on a "fast" (e.g., δ-correlated) thermal bath.

Quantitatively, the effect of refocusing can be understood with the quantum kinetic equation (QKE) in the rotating frame, with the kernel accurate at least to order K to analyze order-K refocusing [25]. For large $\tilde{\Omega}$, the density-matrix dynamics separates onto sectors with frequencies around $\tilde{\Omega}_m$. The slow sector, $m = 0$, carries the main part of the total weight, with that of the remaining (generally, rapidly-decaying) sectors totaling $\sim\Delta(0)/\tilde{\Omega}^2$, where $\Delta(t - t') \equiv ||\langle B^{\mu}(t)B^{\mu'}(t')\rangle||$ is a norm of the correlation matrix of the fluctuating field. Only the dynamics in the slow sector is protected by the refocusing. In particular, the analysis of the QKE with the leading second-order kernel shows that already with first-order ($K = 1$) constant-field refocusing direct decay processes require excitations at frequencies $\omega \gtrsim \tilde{\Omega}$, which may dramatically reduce the dissipative part of the QKE kernel. The nonresonant reactive processes are also suppressed: the rate of phase errors is $\sim\Delta(0)/\tilde{\Omega}$ with $K = 1$ refocusing and $\sim|\Delta''(0)|/\tilde{\Omega}^3$ (primes denote time derivatives) with $K \geq 2$ refocusing, as, e.g., for length-8 sequence in Table I. Generally, these results [25] apply equally for soft- and hard-pulse refocusing, and are consistent with established results on kinetics of few-level systems in rf field [22], and with the properties of hard-pulse sequences for low-frequency environment [24,26].

To conclude, we presented an efficient scheme for designing high-order soft pulses and soft-pulse sequences in a scalable fashion, without the need for solving the full Hamiltonian. Soft (narrow-spectrum) pulses are indispensable for their selectivity and reduced coupling to environmental modes, which in turn suppresses signal distortions and heating. Use of high-order pulses is especially efficient if one interaction (e.g., the Ising term) is dominant. High-order pulse sequences generally offer better accuracy and can dramatically reduce the decoherence due to coupling with low-frequency environment.

We thank M. I. Dykman and D. Lidar for encouragement and illuminating discussions.

[1] C. E. Weiman, Rev. Mod. Phys. **71**, S253 (1999).
[2] I. Osborne and R. Coontz, Science **298**, 1353 (2002).
[3] D. Goswami, Phys. Rep. **374**, 385 (2003).
[4] A. Neogi, H. Yoshida, T. Mozume, and O. Wada, Opt. Commun. **159**, 225 (1999).
[5] A. D. Mehta *et al.*, Science **283**, 1689 (1999).
[6] C. P. Slichter, *Principles of Magnetic Resonance* (Springer-Verlag, Berlin, 1992), 3rd ed.; R. Freeman, Prog. NMR Spectr. **32**, 59 (1998); P. Hodgkinson and L. Emsley, Prog. NMR Spectr. **36**, 201 (2000); L. M. K. Vandersypen and I. L. Chuang, Rev. Mod. Phys. **76**, 1037 (2005).
[7] L. M. K. Vandersypen *et al.*, Nature (London) **414**, 883 (2001); C. S. Yannoni *et al.*, Appl. Phys. Lett. **75**, 3563 (1999); G. M. Leskowitz, N. Ghaderi, R. A. Olsen, and L. J. Mueller, J. Chem. Phys. **119**, 1643 (2003).
[8] P. M. Platzman and M. I. Dykman, Science **284**, 1967 (1999); M. I. Dykman, P. M. Platzman, and P. Seddighrad, Phys. Rev. B **67**, 155402 (2003).
[9] A. J. Berkley *et al.*, Science **300**, 1548 (2003).
[10] J. S. Waugh, L. M. Huber, and U. Haeberlen, Phys. Rev. Lett. **20**, 180 (1968); J. S. Waugh, C. H. Wang, L. M. Huber, and R. L. Vold, J. Chem. Phys. **48**, 662 (1968).
[11] G. D. Sanders, K. W. Kim, and W. C. Holton, Phys. Rev. A **59**, 1098 (1999); P. Hodgkinson, D. Sakellariou, and L. Emsley, Chem. Phys. Lett. **326**, 515 (2000); A. O. Niskanen, J. J. Vartiainen, and M. M. Salomaa, Phys. Rev. Lett. **90**, 197901 (2003).
[12] M. Steffen, J. M. Martinis, and I. L. Chuang, Phys. Rev. B **68**, 224518 (2003).
[13] J. G. A. Baker, *Quantitative Theory of Critical Phenomena* (Academic, New York, 1990).
[14] P. Borgnat, A. Lesage, S. Caldarelli, and L. Emsley, J. Magn. Reson., Ser. A **119**, 289 (1996).
[15] C. Bauer *et al.*, J. Magn. Reson. **58**, 442 (1984).
[16] W. S. Warren, J. Chem. Phys. **81**, 5437 (1984).
[17] M. Galassi *et al.*, *GNU Scientific Library Reference Manual* (Network Theory Limited, Bristol, UK, 2003), 2nd ed., http://www.gnu.org/software/gsl.
[18] H. Geen and R. Freeman, J. Magn. Reson. **93**, 93 (1991).
[19] We also designed several narrow-spectrum shapes replacing refocusing sequences of various order with respect to Ising coupling J_z. The advantage of individual pulses is the flexibility in canceling the additional interactions, and the ability of using known high-order sequences.
[20] K. R. Brown, A. W. Harrow, and I. L. Chuang, Phys. Rev. A **70**, 052318 (2004); K. Khodjasteh and D. A. Lidar, Phys. Rev. Lett. **89**, 197904 (2002).
[21] S. Wimperis, J. Magn. Reson., Ser. A **109**, 221 (1994).
[22] M. I. Dykman, Fiz. Nizk. Temp. **5**, 186 (1979); [Sov. J. Low Temp. Phys. **5**, 89 (1979)].
[23] A. G. Kofman and G. Kurizki, Phys. Rev. Lett. **87**, 270405 (2001); **93**, 130406 (2004).
[24] K. Shiokawa and D. A. Lidar, Phys. Rev. A **69**, 030302(R) (2004); L. Faoro and L. Viola, Phys. Rev. Lett. **92**, 117905 (2004).
[25] L. P. Pryadko *et al.* (to be published).
[26] P. Facchi *et al.*, Phys. Rev. A **71**, 022302 (2005).