Scalable design of tailored soft pulses for coherent control

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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 $\pi$-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.

A control of coherent evolution of quantum systems is increasingly important in a number of research fields and applications. Such control has long been a staple in nuclear magnetic resonance (NMR) spectroscopy, where determination of the structure of complex molecules like proteins require the application of long sequences of precisely designed radio-frequency (r.f.) pulses. Recently, coherent control (CC) 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 and other potential implementations of quantum computers (QCs). This progress is closely followed by applications of coherent control in atomic physics, quantum optics, laser induced chemical reactions, data communications, and biomedical applications.

The precision required for QIP in particular, and for contemporary applications of CC in general, is achieved most readily using shaped (also, soft), typically narrow-band, 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 non-resonant decoherence sources (e.g., low-frequency phonons) as compared to lower-order sequences.

Over some forty years the shaped pulses were utilized in NMR, a number of analytical and numerical schemes were suggested for their design. Most (although not all, see Ref. 9) rely on the average Hamiltonian theory, 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, inter-spin couplings are treated perturbatively. The main drawback of the Magnus expansion [see Eq. (9) below] for numerics is the multiple integration appearing in higher orders; its use in actual calculations was almost always limited to quadratic order.

The alternative scheme found in the literature is a simulation involving the full Hamiltonian of a quantum system. In particular, such a calculation was done to optimize pulse shapes for a three-level Hamiltonian of a current-biased superconducting qubit. This approach guarantees precision of custom-designed shapes, but it obviously lacks scalability, as the computational difficulty grows exponentially with the size of the system.

In this paper, 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 the Magnus expansion or other form of the effective Hamiltonian theory, we rely directly on the time-dependent perturbation theory implemented numerically. This allows an easy extension to higher orders (up to 9th in this work), at the same time preserving the benefits of the cluster theorem 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 time dependent perturbation series for which the control remains perfect.

To be specific, and also as an illustration, we consider a quantum spin chain with each spin (qubit) individually controlled and “always-on” nearest-neighbor (n.n.) interactions. Assuming the Ising coupling is dominant, $J_{\perp}$, we construct a family of one-dimensional $\pi$-pulses [with different degrees of self-refocusing with respect to the $J_{\perp}$ coupling. The duration of a pulse, $\tau$, is chosen to be fixed, so as to allow parallel execution of quantum gates in different parts of the system. To reduce the spectral width 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 in several pulse sequences and composite pulses with that of two commonly used shapes. In particular, we present an eight-pulse refocusing sequence of order $K = 6$ for the quantum Ising model [refocusing errors scale as $(J_{\perp} \tau)^6$], order $K = 2$ for general $XXZ$ model, where, in addition, each spin has an order $K \geq 2$ protection against phase decoherence due to low-frequency environment (TAB. I).

We consider the following simplified Hamiltonian

$$H(t) = H_C(t) + H_S + H_V(t) + H_\sigma,$$ (1)
For a finite system of $n$ qubits and a given maximum order $K$ of the expansion, Eqs. (6), (7), and (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.

$$R(t) = \exp(C_1 + C_2 + \cdots), \quad C_1 = -i \int_0^t dt_1 \tilde{H}_S(t_1),$$
$$C_2 = -\frac{1}{2} \int_0^{t_1} dt_2 \int_0^{t_1} dt_1 [\tilde{H}_S(t_1), \tilde{H}_S(t_2)], \quad \cdots$$

Generally, the term $C_k$ contains a $k$-fold integration of the commutators of the rotating-frame Hamiltonian $H_S(t_1)$ at different time moments $t_1$ and has an order $(t H_S)^k$. 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 $k$-th 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 $K$-th order, one needs to analyze all distinct clusters with up to $K + 1$ vertices. For an infinite chain with n.n. couplings, these are finite chains with up to $K$ bonds and $K + 1$ vertices.

The discussed cluster theorem\textsuperscript{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 $C_1 = \ldots = C_K = 0$ is formally equivalent to

$$R_1 = R_2 = \ldots = R_K = 0.$$  

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 $K$-th 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 library\textsuperscript{15} 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,

$$V(t + \tau/2) = A_0 + \sum_m A_m \cos(m \Omega t) + B_m \sin(m \Omega t),$$
where the angular frequency $\Omega = 2\pi/\tau$ is related to the full pulse duration $\tau$. 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 (typically, eight digits or more).

As the simplest application of the formalism, we designed a number of inversion ($\pi$-) pulse shapes\textsuperscript{14}, self-refocusing to various degrees with respect to the Ising interaction; their coefficients are listed in TAB. II. To reduce the bandwidth 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\textsuperscript{16} as a drop-in replacement of hard (or short Gaussian) pulses. We note that in our setup there is no gap between subsequent pulses, the pulses follow back to back with the repetition period $\tau$. The system is “focused” at the end of each time interval. Such a scheme with a common “clock” time $\tau$ 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), (7), and (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 $\propto N^{K+1} = \tau^K$; the corresponding gate fidelity (defined as the probability of error, either average or maximum) would scale as $1 - O(\tau^2 K)$.

In Tab. 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 $J^L = 0$]; “$xxz$”: the $xxz$ spin chain with both $J^L$ and $J^L$-non-zero; “bath”: Ising spin chain coupled to a thermal bath generating slow (compared to $\tau$) phase modulation, simulated as $H_{\tau}$ [Eq. (4)] with random time-independent coefficients $B\tau$ (see further discussion on open systems below). The pulse sequences are listed in the caption; these are “best” sequences at given length for all pulse shapes found by exhaustive search (high-order sequences\textsuperscript{16} equivalent for hard pulses do not necessarily have equal orders here). 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 “$X_1^2 Y_2^2 X_1 Y_2^2 Y_1^2 X_1 Y_2^2 X_1^2$”, where $X_1^2$ is a $\pi$-pulse in $x$-direction applied on every odd site, $Y_2^2$ is a $\pi$-pulse in negative $y$-direction on even sites, etc. This sequence is the best among the length-eight sequences for both the Ising and the $xxz$ ($J^L \neq 0$) 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 $(J_2 \tau)^6$ compared with that for the standard (first-order) Hermitian pulse where gate error scales as $(J_2 \tau)^4$ [the gate fidelities differ from unity by $O((J_2 \tau)^{12})$ and $O((J_2 \tau)^8)$ respectively].

These pulses were designed for use in systems with dominant 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 $2\pi$ pulses were used to simulate the BB\textsubscript{1} composite pulse\textsuperscript{17} 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\textsubscript{1} sequence with Gaussian pulses deteriorated linearly in $J_2 \tau$ already with zero amplitude mismatch, while for our second-order pulses the additional error was smaller, scaling as the product of $(J_2 \tau)$ and the amplitude mismatch. Clearly, if the two sources of errors are comparable, combining high-accuracy BB\textsubscript{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 $H_{\sigma}$ [Eq. (4)] can be most readily understood in the rotating frame defined by the bare evolution operator $U_0(t)$ [Eq. 6],

$$\tilde{H}_\sigma(t) = U_0^\dagger(t) H_\sigma U_0 = \frac{1}{2} \sum_n B^\sigma_n(p_i, q_i) Q_\sigma^{\mu\nu}(t) \sigma_\nu \equiv m\tilde{\Omega}.$$ (12)

For refocusing, the rotation matrices $Q_\sigma^{\mu\nu}(t)$ are periodic with the full sequence period $\tilde{\tau}$; they can be written as a sum of harmonics with the main frequency $\tilde{\Omega} = 2\pi/\tilde{\tau}$,

$$Q_\sigma^{\mu\nu}(t) = \sum_m C_m^{\mu\nu} e^{-i\tilde{\Omega} t} \equiv m\tilde{\Omega}.$$ (13)

The constant-field first-order refocusing condition (average Hamiltonian vanishes to leading order) is equivalent to a cancellation of some linear combinations of $C_{n0}^{\mu\nu}$ (e.g., $C_{n0}^{\mu\nu} = 0$ for phase noise assumed for thermal bath in Tab. I). As a result, the environmental modes at low frequencies get modulated and are effectively replaced by those at higher frequencies, $\omega \rightarrow \omega + \Omega_m$, $m \neq 0$, leading to a significant reduction of the decoherence caused by resonant decay processes\textsuperscript{18–20}. On the other hand, fast modes are mostly unaffected; modulation has essentially no effect on a “fast” (e.g., $\delta$-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\textsuperscript{21}. For large $\Omega$, the density-matrix dynamics separates onto sectors with frequencies around $\Omega_m$. The slow sector, $m = 0$, carries the main part of the total weight, with that of the remaining (generally, rapidly-decaying) sectors totalling
TABLE II: Fourier coefficients for the constructed pulses, see Eq. (11). Shapes $S_L$ and $Q_L$ respectively are first ($K = 1$) and second ($K = 2$) order self-refocusing inversion pulses for the Ising spin coupling; the fixed-time errors scale with the duration of the pulse as $\alpha (\tau J_s)^K$ [cf. Eq. (3)]. These shapes have $2L$ derivatives vanishing at the ends of the interval.

| $A_0$ | $A_1$ | $A_2$ | $A_3$ | $A_4$ | $A_5$ |
|-------|-------|-------|-------|-------|-------|
| $S_1$ | 0.5   | -1.2053194466 | 0.4796460175 | 0.2256743291 |       |
| $S_2$ | 0.5   | -1.1950755990 | 0.7841246509 | 0.0738054432 | -0.1628545011 |
| $Q_1$ | 0.5   | -1.1374003264 | 1.5774784244 | -0.6829545606 | -0.2574826374 |
| $Q_2$ | 0.5   | -1.0965122417 | 1.5309957409 | -1.1470791601 | 0.00020722004 |

\[ \sim \Delta(0)/\tilde{\Omega}^2, \text{ where } \Delta(t-t') \equiv \| B_\mu(t) B_\nu(t') \| \] 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 non-resonant 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 $K = 2$ refocusing, as, e.g., for length-8 sequence in Tab. I. Generally, these results apply equally for soft- and hard-pulse refocusing, and are consistent with established results on kinetics of few-level systems in r.f. field, and with the properties of hard pulse sequences for low-frequency environment.

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-band) 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.

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