Quantum Dynamics and Coherence of Qubits

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Abstract—We review results in theoretical modeling of quantum systems in support of the studies of decoherence and qubit interactions for quantum information processing. The developed modeling tools have been applied to semiconductor materials and nanostructures that show promise for implementation of coherent, controlled quantum dynamics at the level of registers of several quantum bits (qubits), such as spins. Field-theoretical techniques have been utilized to address decoherence and more generally the origin and effects of quantum noise and the loss of entanglement in quantum dynamics of qubits and several-qubit registers. Qubit coupling mechanisms via the indirect exchange interaction have been investigated, and quantum computing designs have been evaluated for scalability. We also describe general and specific research challenges, the solution of which will advance the field of modeling "open quantum systems" to further our understanding of how environmental influences affect quantum coherence and its loss during quantum dynamics.

Keywords—*qubit; decoherence; exchange; entaglement.*

I.   INTRODUCTION

We review results in the field of "controlled quantum dynamics," aimed at investigating general aspects of quantum noise, as well as single- and multi-qubit decoherence, robustness of entanglement, and origins of two-qubit interactions, the latter mediated via the qubits' coupling with a many-body bath of modes (e.g., acoustic phonons, conductions electrons). Study of "open quantum systems," with new challenges suggested by the emerging field of quantum information, requires utilization and development of field-theoretical many-body techniques for the description of quantum dynamics. These studies have facilitated evaluation of scalability of existing and emerging quantum computing schemes, for instance, for spin- and quantum-dot based quantum computer designs.

Emergence of entanglement, by induced indirect-exchange Ruderman-Kittel-Kasuya-Yosida (RKKY) type interactions, and its loss due to quantum noise can be quantified by developed calculation techniques for the system's dynamics, with the environmental (bath) modes traced out, to describe the induced interaction and quantum noise in a unified treatment.

The reported research has been focused on the maintenance of coherence of quantum dynamics controlled by qubit-qubit interactions and quantum noise, both mediated by coupling to external baths, such as acoustic phonons or conduction electrons coupled to quantum-dot and impurity-atom *spin qubits* in semiconductor-material heterostructures. The latter, RKKY-type mechanism of spin-spin (qubit-qubit) interaction offers an approach to incorporate scalable control of entanglement into solid state quantum computing schemes. Calculations of bath-induced interactions and decoherence have been carried out for systems of relevance to the ongoing measurement and interaction experiments.

In Section II, we generally cite our modeling results. In Section II, we survey the status of research work in the field of evaluation of decoherence. In Section IV, we outline research challenges in the topics involving induced interactions (RKKY-type) and their interplay with quantum noise. Finally, in Section V we address some longer-term issues in the physics of open quantum systems subject to environmental noise.

II.   DECOHERENCE AND INDUCED INTERACTIONS

Decoherence (quantum phase noise) [1] and, for more than a single qubit, the associated loss of entanglement, are the main obstacles to scalable quantum computation. Theoretical evaluation of a quantum computing scheme includes identification of system parameter ranges for which the level of quantum noise is within the conditions for fault-tolerant quantum error correction. Coherent quantum control of systems and structures on the nanoscale, but larger than single atoms and molecules, has been explored in experiments that control quantum dynamics beyond the traditional energy-level spectroscopy. Reduction of quantum noise to maintain quantum coherence over the experimental time scales is key to probing processes and concepts that were until recently out of the reach of experimental observations, including such recent discoveries as observation of an electron spin resonance (ESR) signal from a single spin [2,3], or probing RKKY-type indirect exchange interaction that, via conduction electrons, influences the dynamics of two spins of electrons located in separate quantum dots [4].

Here we outline research to advance theoretical evaluation of decoherence, entanglement, and interactions. From the earlier focus on the quantum-Hall-effect systems [5-7], our research has extended to rather general results on decoherence [1,8-10] and, more recently, disentanglement

and RKKY-type interactions for two qubits [11-13], as well as to additive measures of decoherence for multi-qubit registers [1,14]. Model calculations have been carried out for a range of spin- and quantum-dot-based quantum computing schemes in semiconductor nanostructures, e.g., [1,10,15,16]. While the focus has been on semiconductor materials, most of these approaches apply to any qubit-based quantum computing scheme.

III. DECOHERENCE DURING QUANTUM GATE FUNCTIONS

It has been recognized that for times, t, larger than $\hbar/kT$, which is about 2.5×10^{-14} sec at room temperatures of 300K, Markovian approximation schemes, e.g., [17,18], can be used. For NMR/ESR, these have been utilized primarily for single-qubit calculations of the relaxation and dephasing time scales, T_1 and T_2, and of the asymptotic large-time properties of the density matrix elements of the qubit, with the environmental (bath) modes traced out.

Quantum information processing necessitates the development of techniques applicable for the "short-time" regime $t < \hbar/kT$, because most quantum-computation schemes are for systems at very low temperatures, for which gate times are shorter than or comparable to $\hbar/kT$. Then the bath mode correlations with the system of qubits cannot be entirely treated within the no-memory, immediate-rethermalization Markovian approximations. We have developed a new calculational approach designed for this regime, which *does not include* the Markovian assumption, and reported its applications, e.g., [8-10,16].

The level of quantum noise in the idling state, for a single qubit, as well as during the simplest quantum gates, has been well quantified [1,10,19-38]. The calculation involves evaluation of the qubit's density matrix, followed by calculation of numerical measures of the degree of decoherence. The calculations can be done within both our short-time and the Markovian approximations, and the largest (the worst-case scenario) noise measure values can then be used to test the system as candidate for scalable quantum computer designs.

We have introduced new quantitative measures of decoherence which are approximately *additive* [1,10,14] as long as the noise for each qubit is small (for the short duration of a quantum gate function), and therefore these measures can be used to further extend the results to *several-qubit quantum registers*, in terms of the noise measures of the individual qubits, even when these qubits are *strongly entangled*.

In these calculations, the Hamiltonian of the qubit system and bath of environmental modes, is modeled by

$$H = H_S(t) + H_B + H_{SB} , \qquad (1)$$

where

$$H_S(t) = H_i + H_g(t) . \qquad (2)$$

Here H_i is the Hamiltonian of the idling qubit register, while $H_g(t)$ represents time-dependent gate control. The Hamiltonian of the environment is given by H_B, and H_{SB}

is its interaction with the qubits. The environment is often modeled as a bath of bosonic quantum modes (e.g., phonons).

There have been few available results for evaluation of quantum noise *during general time-dependent* gate functions. The time dependence introduced by non-zero $H_g(t)$, requires time-ordering in the evaluation of the qubit evolution operator, which makes many standard techniques for dynamical calculations inapplicable. We initiated a new approach [39] yielding the first results for a gate-controlled qubit interacting with a boson bath of modes.

Recently reported first experimental successes in coherent control of single electron spins in quantum dots, e.g., [40], pose an interesting theoretical challenge to develop systematic modeling techniques for general-time-dependence gate-controlled qubits, as well as establish additivity criteria to enable evaluation of the level of noise for registers of several such controlled qubits.

IV. INDUCED INTERACTION AND QUANTUM NOISE

Modeling of an open quantum system within the Hamiltonian description, Eqs. (1)-(2), involves significant technical difficulties: While the system Hamiltonian can be just single- or two-spin, the bath-mode Hamiltonian involves many modes, in the simplest case a collection of noninteracting bosonic fields,

$$H_B = \sum_k \omega_k b_k^\dagger b_k . \qquad (3)$$

The qubit-bath interaction can involve terms of the form

$$H_{SB} = \Lambda_S \sum_k g_k b_k^\dagger + \Lambda_S^\dagger \sum_k g_k^* b_k + \dots , \qquad (4)$$

where Λ_S is a system operator, as well as more complicated expressions in the case of fermionic bath fields (e.g., electrons). There can usually be several interaction terms involved in Eq. (4), and also in Eq. (3), when more than one qubit is studied, and for various bosonic polarizations, for instance for acoustic phonons, or for more than one bath dominating the relaxation of the system.

However, and even more importantly, there are *physical assumptions* that have to be invoked to supplement this description. The open-quantum system dynamics cannot be entirely specified by the Hamiltonian for the system and the selected bath of external modes. We have to also model the effects of the thermalization imposed by the "rest of the universe" on the bath, as well as consider the choice of the initial conditions for the whole system, the latter an issue that represents an important challenge on its own, which will not be addressed here. These topics have a long history in the NMR and ESR literature, primarily for single, idling spins within Markovian approximations [17,18,41-44].

Recent experimental efforts to create and maintain entanglement of two electron spins in gate-formed double quantum dots with interaction mediated by electrons in conducting channels [4,45], have drawn interest to a new set

of problems. The bath modes, while serving as the main source and mediator of the quantum noise causing decoherence, will also cause loss of entanglement of two (and more) spins. However, the same modes, via their interactions with the qubits can also mediate an indirect exchange (RKKY-type) interaction. The latter can create entanglement and, for appropriate initial conditions, drive the approximately coherent quantum dynamics for some time. Ultimately, for long enough times the quantum noise effects will dominate and cause thermalization (unless the qubits are perturbed by quantum-control gate function external potentials).

Let us remark that the original RKKY calculation corresponds to the zero-temperature evaluation of the coupling induced between localized magnetic moments by a "bath" of conduction electrons. The ideas to utilize various solid-state excitations as a medium to couple qubits for quantum information processing have been advanced by several groups [5-7,12,13,46-50]. The main advantage of such coupling is that it should allow for larger distances between qubits and therefore for their easier fabrication and control.

Besides the need to properly incorporate the *physics* of the environmental influences in the open-quantum-system description, which is not a fully understood problem and is usually handled within phenomenological approaches, one should also aim at *tractability* of the resulting equations for the quantities of interest, for instance, the density matrix of the qubits, ρ_S, after the environmental effects were traced out. Typically, a Markovian approximation scheme can lead to a quantum Liouville equation of the type

$$i\hbar\dot\rho_S = \left[H_S, \rho_S\right] + \text{coherent terms} + \text{noise terms} . \quad (5)$$

The hope is to be able to derive the "coherent" terms, which correspond to Hermitian additions to H_S in the commutator, and the noise terms due to the bath modes.

The added terms in Eq. (5), induced by the system's interactions with the bath modes, are usually evaluated within the second-order (in the interaction strength) expansion, as well as other approximations [12,13,18,50] aimed at making the results tractable for calculations. For more than one qubit, the qubit-qubit entanglement is created both by the internal qubit-qubit interactions in H_S, and by the induced interactions, which are part of the coherent terms, whereas other coherent terms involve for instance single-qubit operators and represent Lamb shifts.

The noise terms, however, act to unravel the entanglement. Indeed, results have been reported for a system of two qubits, suggesting that the noise-induced decoherence of two entangled noninteracting qubits and their disentanglement are closely related [11,51], with the suppression of entanglement taking place at least as fast as the product of the factors that describe the suppression of each qubit's coherence. These results were obtained both for a Markovian-type noise model and for the short-time regime, but limited to uncorrelated noise sources for each qubit.

We have reported the first systematic calculations [12,13,50] of the combined effects of the induced interaction and quantum noise due to the phonon or (interacting, correlated) conduction electron bath, with applications for qubit geometries suggested by possible experiments [2-4,45]. While the actual calculations are quite formidable, the expression for the induced interaction is relatively compact, because it only involves components of two spin operators. As an illustration, here is the result for the calculated [50] indirect exchange interaction between two spins at separation $\mathbf{d}$, mediated by acoustic phonons,

$$H_{\text{int}}(t) = \\ -\sum_{m=x,y,z} \alpha_{n_m}^m \omega_c^{n_m} \sigma_m^{(1)} \sigma_m^{(2)} \frac{2\Gamma(n_m)\,\text{Re}\left(1 + i\,\omega_c\,|\mathbf{d}|/c_s\right)^{n_m}}{\left[1 + \left(\omega_c\,|\mathbf{d}|/c_s\right)^2\right]^{n_m}} . \quad (6)$$

Here $\sigma_{m=x,y,z}^{(1),(2)}$ are the Pauli matrixes of the qubits, c_s is the speed of sound, and ω_c is the phonon cut-off frequency. For a system of two spins (of outer electrons) of P-donor impurities, placed in bulk Si at a distance $\mathbf{d}$ apart, and subject to a constant uniform magnetic field, H_z, the exchange interaction is primarily due to the longitudinal acoustic phonons [50]. The coupling is super-Ohmic: we can assume that $n_m = 3$ in Eq. (6), for the small-frequency dependence of the standard Caldeira-Leggett spectral function, and that the coupling parameters due to the spin-orbit interaction, satisfy $\alpha_{n_x}^x = \alpha_{n_y}^y \ll \alpha_{n_z}^z$, with $\alpha_3^z \omega_c^2 \simeq 8.4 \cdot 10^{-10}$. The cut-off frequency is due to the localization of the wave function, $\omega_c = c_s/a_B \simeq 9.3 \times 10^{12}\,\text{s}^{-1}$, which in this case is much smaller than the lattice Debye cut-off ($a_B \simeq 10^{-9}$m is half of the effective Bohr radius of an electron at the P-impurity).

The expression for the noise effects is much more cumbersome [13,50], and is model-assumption dependent. The interplay of the induced interaction and quantum noise can be used to control the creation of time-dependent entanglement, as illustrated in Figure 1. The obtained results suggest future research into both the buildup of the entanglement and its unraveling, for interacting (and ultimately also controlled via time-dependent external "gate-function" interactions) qubits subject to quantum noise due to various bosonic and fermionic bath modes, in both the short-time and Markovian regimes. Entanglement should be explored as a fragile resource for quantum information processing, and for the relation [11,51] of disentanglement to decoherence.

The concurrence is by now a generally accepted, calculable in closed form measure of quantum-information content of two-qubit entanglement [52]. For the dynamics of two spins interacting with an acoustic-phonon environment, the concurrence as a measure of entanglement can reveal a rather nontrivial behavior; see Figure 1. We point out,

however, that with the full reduced density matrix of the system available, other quantities can also be calculated as needed, e.g., [53].
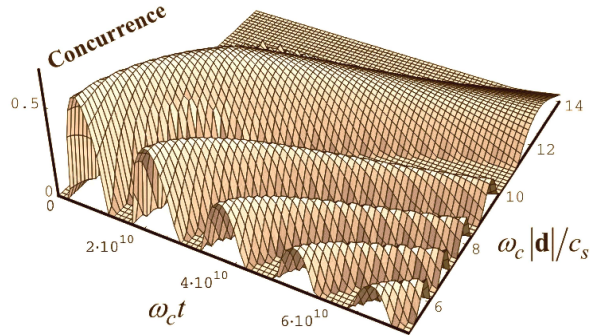
Figure 1. The concurrence as a function of time for various qubit separations, here quantifies the entanglement of two spin-1/2 qubits, due to the interaction and quantum noise induced by a bath of acoustic phonons. The parameters were for P-donor electrons in Si, at $T = 1$ K, in external magnetic field $H_z = 3 \times 10^4$ G. In terms of the single-spin basis $|\pm\rangle \propto |\uparrow\rangle \pm |\downarrow\rangle$; the two spins were initially in $|++\rangle$; the bath was initially thermalized at the temperature T.

V. CHALLENGES

With the actual experimental probes now being carried out at the nanoscale, long-standing open problems have become more pressing, and some new ones have been suggested by experimental developments. For definiteness, we consider time-independent H_S from now on.

Perhaps the most fundamental of these problems is the matter of thermalization vs. bath-induced coherent-dynamics effects in open quantum systems. The "textbook" approach to thermalization [17,42-44] has been to assume that, for large enough times the time evolution of the system plus bath is not just controlled by the combined Hamiltonian, but is supplemented by the instantaneous loss-of-memory (Markovian) approximation, which introduces irreversibility and imposes the bath temperature on the reduced system dynamics in the infinite-time limit, which is then approached as the density matrix elements assume their thermal values:

$$\rho_S(t) \rightarrow e^{-H_S/kT} \Big/ \mathrm{Tr}\left(e^{-H_S/kT}\right), \qquad (7)$$

with the exponential relaxation (diagonal) and decoherence (off-diagonal) rates defining the time scales $T_{1,2}$.

However, it turns out that the traditional phenomenological no-memory approximations, yielding thermalization and the Fermi golden rule for the transition rates, etc., assume in a way too strong a memory loss: They erase the possible bath contributions to the coherent part of the dynamics at shorter times, such as the Lamb shift for a single qubit as well as the induced RKKY interactions for a

bi-partite system. Indeed, while relaxation leading to Eq. (7) is driven by the "on-shell" exchanges with the bath, it is the memory of (correlation, entanglement with) the bath modes that drives the induced interaction via virtual exchanges. Actually, the "on-shell" condition (imposed by the so-called secular approximation, see Section 8.1.3 in [17]) also underestimates additional decoherence at short times: the "pure" or "adiabatic" contribution to the off-diagonal dephasing, that has been estimated by using other approaches [1,8,9,16,33].

Perhaps the simplest way to recognize the ambiguity is to ask if the Hamiltonian in Eq. (7) should have included the bath-induced interaction terms (not shown)? Should the final Boltzmann distribution correspond to the energy levels / basis states of the original "bare" system or the one with the RKKY-interaction / Lamb shifts added, and more generally, a bath-renormalized, "dressed" system?

There is presently no consistent treatment that will address in a satisfactory way all the expected *physics* of the bath-mode effects on the dynamics. The issue is partly technical, because we are after a *tractable*, rather than just a "foundational" answer. It is well accepted that the emergence of irreversibility cannot be treated within tractable and calculationally convenient approaches derived directly from the microscopic dynamics: phenomenology has to be appealed to. However, even allowing for phenomenological solutions, all the known tractable schemes yielding the indirect exchange interaction, treat thermalization in a cavalier way, resulting typically in noise terms corresponding to getting the infinite temperature limit at large times, which thus artificially avoids the issue of which H_S should enter in Eq. (7), whereas the established schemes that yield thermalization at large times, lose some intermediate- and short-time dynamical effects.

We have just discussed the challenges in formulating unified treatments that will cover all or most of the interesting dynamical effects for various time scales, from short to intermediate (for induced interaction effects and pure decoherence) to large (for the onset of thermalization), providing a tractable calculational (usually perturbative, many-body) scheme. This discussion also alludes to several other interesting conceptual challenges in the theory of open quantum systems.

Let us presently comment on the issue of the bath-mode interactions with each other, as well as with impurities, the latter particularly important and experimentally relevant [45,54] for conduction electrons as carriers of the indirect-exchange interaction. Indeed, the traditional treatment of open quantum systems has assumed noninteracting bath modes. When the bath mode interactions had to be accounted for, we have treated the added effects either perturbatively [6], or, for strong interaction, such as Luttinger-liquid electrons in a 1D channel, we took [12] the collective excitations as the new "bath modes." Generally, however, especially in Markovian schemes, one has to seek approaches that do not involve certain double-counting. Indeed, the assumption that the bath modes are at a fixed

temperature, could be possibly considered as a partial accounting for the effects of the mode-mode and mode-impurity interactions, because these interactions can contribute to themalization of the bath, on par with other influences external to the bath. This may be particularly relevant for phonons that always have strong anharmonicity for any real material. In a way this problem fits with the previous one: We are dealing with effects that can be, on one hand, modeled by added terms in the total Hamiltonian but on the other hand, may be also mixed up in the process of thermalization that is modeled by actually departing from the Hamiltonian description and replacing it with Liouville equations that include noise effects. Recent experimental advances bring these long-standing challenges to the level of application that requires tractable solutions that can be confronted with experimental data.

There are other interesting topics to be considered, for instance, the question of whether additional sources of quantum noise are important? It has recently been established [55] that potential difference between two leads (reservoirs, or baths, of electrons) can be a source of quantum noise, with the potential difference magnitude playing the role of the temperature parameter. What, then, about a system (qubit) coupled to two thermal baths at different temperatures? Will the resulting heat transfer (energy flow between the bath via the system) generate added quantum noise?

As an example of a more practical issue, let us mention the possible effect of the sample geometry on phonon and conduction electron induced relaxation and interactions. We have already explored [12] the one-dimensional aspect of the electron gas in a channel. Indeed, electrons are easy to confine by gate potentials. The situation for phonons, however, is less clear: can geometrical effects modify, and particularly reduce, their quantum-noise generation capacity, or change the induced interactions? Our preliminary studies [50] seem to indicate strong overall geometry dependence. However, the situation is not entirely clear, especially for the strength of the noise effects, and suggests future explorations because recent experiments with double dot nanostructures in Si membranes [56] indicate that true nanosize confinement (due to the sample dimensions) of otherwise long-wavelength modes (in the transverse sample dimensions) is now possible and will have dramatic effect on the phonon spectrum and, as a result, on those physical phenomena that depend on the phonon interactions with electron spins.

Finally, we point out that several recent experiments, e.g. [57-62], have explored aspects of coherence and control in semiconductor nanostructures for quantum computing. While the progress has been impressive, there is no clear "winner" system. It is likely that the future promising designs will be hybrid, based on the presently explored schemes. It is notable that the ensemble-NMR quantum computing approaches have presently reached partial control and manipulation of 12 qubits [63], which allows consideration of "algorithmic" concepts in multi-qubit system design while the other approaches catch up.

To summarize, we have outlined ongoing theoretical research and a selection of challenging open problems to address, in support of the emerging field of quantum information, ultimately aimed at achieving quantum control of multi-qubit systems.

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