ITR/SY: Center for Modeling of Quantum Dynamics, Relaxation and Decoherence in Solid-State Physics for Information-Technology Applications

PI: Vladimir Privman, Clarkson University, DMR Award 0121146

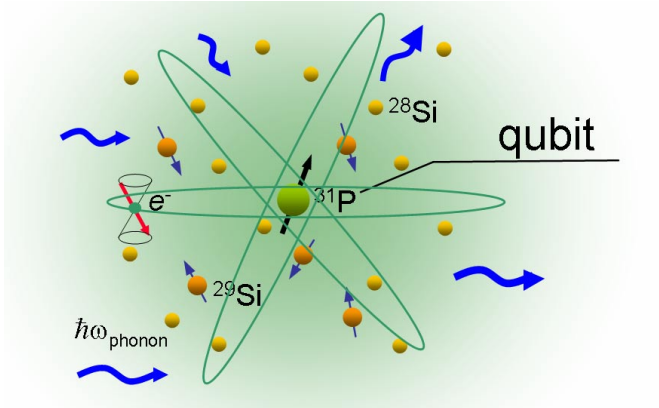
The main **objective** of our program has been to explore ***coherent quantum mechanical processes*** in novel solid-state semiconductor information processing devices, with components of atomic dimensions. These include quantum computers, spintronic devices, and nanometer-scale logic gates.

Our **achievements** to date include:

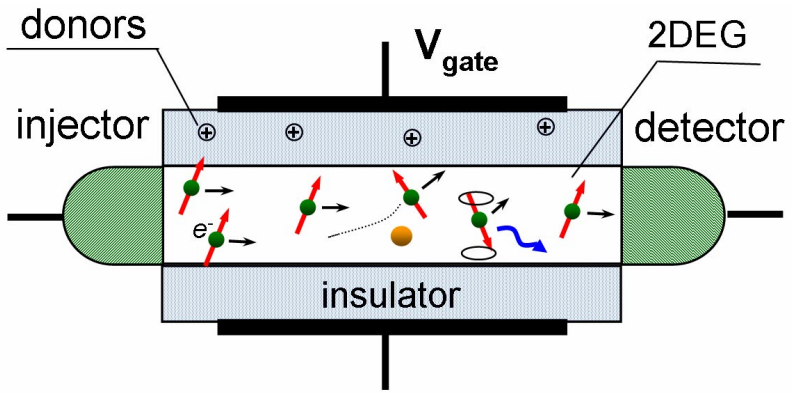
New measures of initial decoherence, and evaluation of decoherence for spins in semiconductors.

Evaluation of solid-state quantum computing designs, and studies of transport associated with quantum measurement.

Investigation of spin-polarized devices and role of nuclear spins in spintronics and quantum computing.



Donor electron spin in silicon decohers owing to interactions with phonons and nuclear spins



Spin-flip scattering in semiconductor nano-device

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Our program has involved four co-PIs: **M.-C. Cheng, M. L. Glasser, D. Mozyrsky, Ch. Tamon**, and extensive ***collaborations*** with leading experimental groups and with Los Alamos National Laboratory.

The **educational impact** has included training of 3 undergraduate students, 4 graduate students, 4 postdoctoral researchers, and development of a new course to introduce quantum device concepts to Physics and Electrical & Computer Engineering students.

Our **outreach program** has included sponsoring presentation events, and an international workshop *Quantum Device Technology*, held at Clarkson University in May of 2002.

Our results were published in several papers in refereed journals, and we set up a web site for outreach.

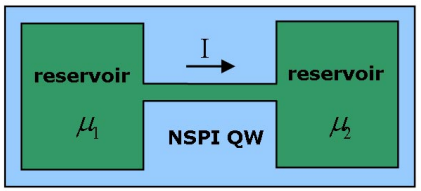
For a spin system in a bosonic bath, we find

$$\|\delta\| = \left[(\rho_{\uparrow\uparrow}(0) - \rho_{\downarrow\downarrow}(0)) \frac{(1 - e^{-B^2(t)})}{2} \right]^2 + \left[(1 - e^{-B^2(t)}) |\rho_{\uparrow\downarrow}(0)| \sin\left(\Omega/2\, t - \varphi_0 \right) \right]^2 =$$

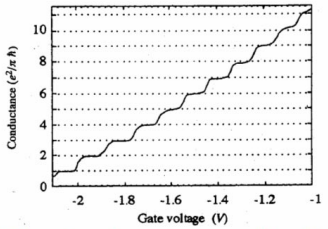
$$= \left(1 - e^{-B^2(t)}\right) \left(\frac{(\rho_{\uparrow\uparrow}(0) - \rho_{\downarrow\downarrow}(0))^2}{4} + |\rho_{\uparrow\downarrow}(0)|^2 \sin^2\left(\Omega/2\, t - \varphi_0 \right) \right)^{1/2}$$

where the norm for the density operator deviation is defined as

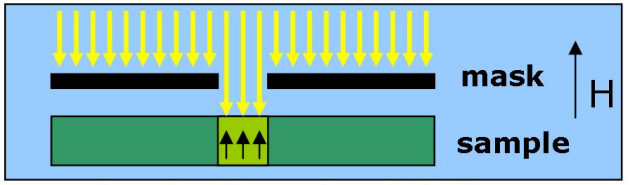
$$\|\delta\| = \sup_{\varphi \neq 0} \frac{\| (\rho - \rho^{(0)}) \,|\, \varphi > \|}{\| \varphi > \|}$$



Transport through NSPI QW



Conductance quantization



Local nuclear spin polarization

Quantum Dynamics, Relaxation and Decoherence in Solid State Physics

Vladimir Privman, Clarkson University, privman@clarkson.edu

The main **objective** of our program has been to explore ***coherent quantum mechanical processes*** in novel solid-state semiconductor information processing devices, with components of atomic dimensions. These include quantum computers, spintronic devices, and nanometer-scale logic gates.

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Evaluation of solid-state quantum computing designs, and studies of transport associated with quantum measurement.

Investigation of spin-polarized devices and role of nuclear spins in spintronics and quantum computing.

QC
- **designs**
- **specific material calculations**

Decoherence
- **general models**
- **specific results for QC-motivated solid-state systems**

Transport
- **measurement**
- **spintronics**

Describe in terms of a QC design and evaluation

This talk

Posters

Vladimir Privman, Clarkson University, privman@clarkson.edu

Why Quantum Computing?

IN

0110010

or

1100101

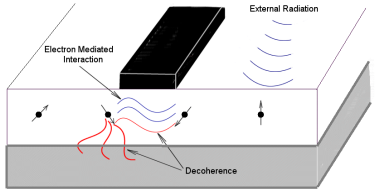
Irreversible "thermodynamic" gates $\longrightarrow$

RESULT

1100

or

0100



IN

$\alpha|0110010\rangle$

$+$

$\beta|1100100\rangle$

Reversible quantum gates $\longleftrightarrow$

RESULT?

$\alpha|1100011\rangle$

$+$

$\beta|0100100\rangle$

Vladimir Privman, Clarkson University, privman@clarkson.edu

Survey of Issues: Computer Science → Physics → Engineering

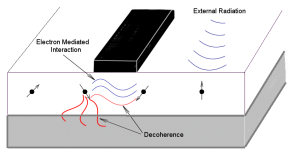
IN

$\alpha|0110010\rangle$

+

$\beta|1100100\rangle$

Reversible quantum gates ↕



- How to put together "quantum gates" and identify a universal set of few-qubit gates?
- Is quantum error correction possible?
- What is the equivalent of digital, copying, etc., QC?

RESULT ?

$\alpha|1100011\rangle$

+

$\beta|0100100\rangle$

- Can we utilize the power of quantum superposition for "parallel" information processing? Shor's algorithm (1994).

Vladimir Privman, Clarkson University, privman@clarkson.edu

First Proposals for Solid-State Quantum Computers in Semiconductor Structures

Approach: Quantum Dots

D. Loss, D. P. DiVincenzo, Phys. Rev. **A57**, 120 (1998)

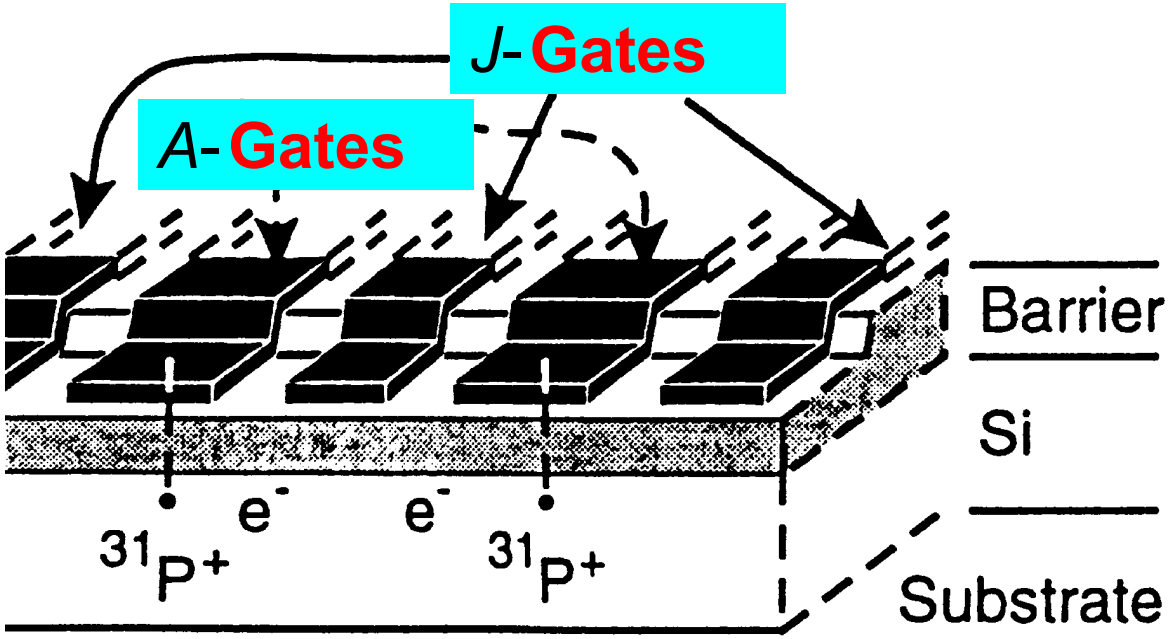
Approach: Nuclear Spins in the Quantum-Hall-State Semiconductor Heterostructures

V. Privman, I. D. Vagner, G. Kventsel, Phys. Lett. **A239**, 141 (1998)

Approach: Nuclear and Electronic Spins in Semiconductor Heterostructures, Control by Gates

B. E. Kane, Nature **393**, 133 (1998)

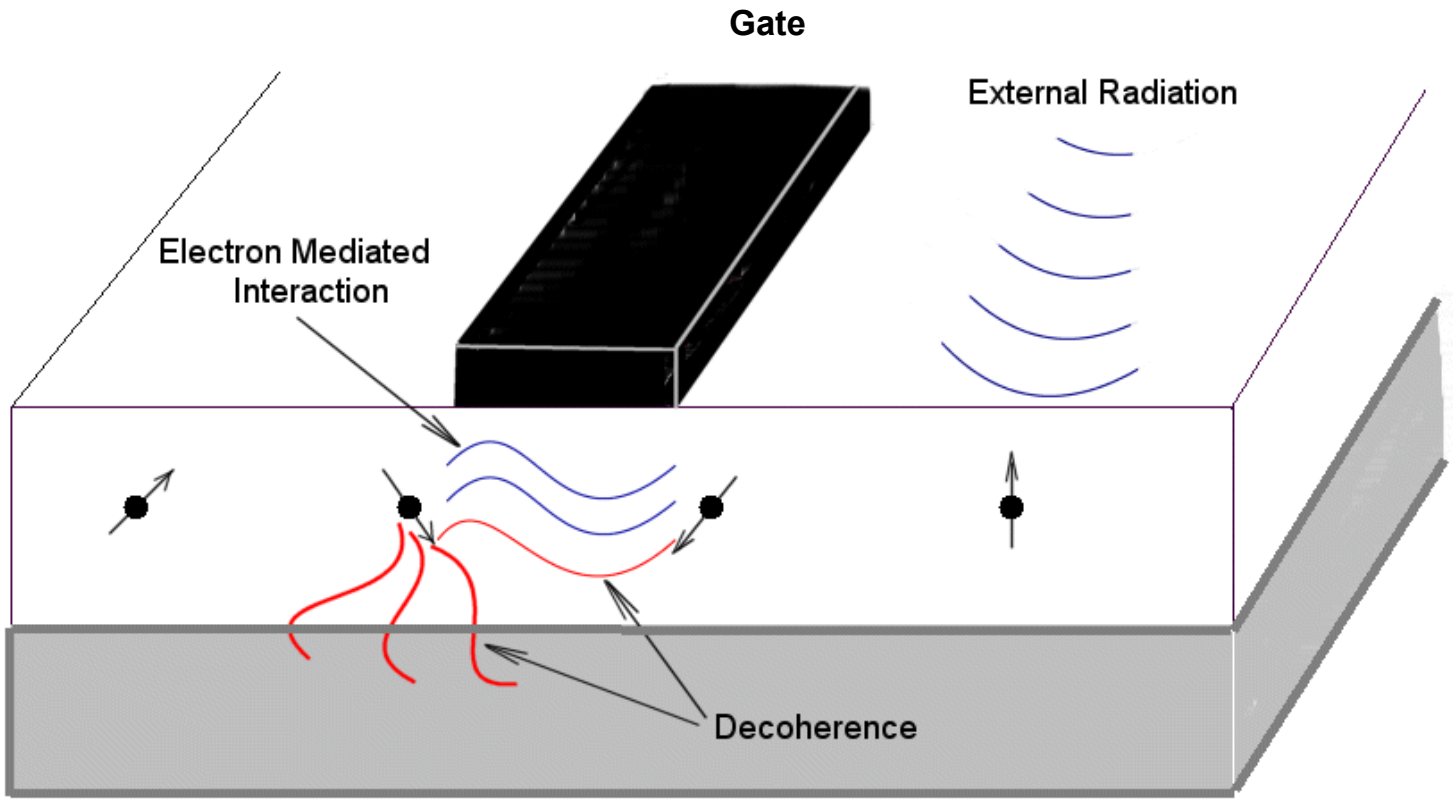
Vladimir Privman, Clarkson University, privman@clarkson.edu



From: **B. E. Kane**, *Nature* 393 (May 14, 1998) p. 133-137

Quantum Dynamics, Relaxation and Decoherence in Solid State Physics

Vladimir Privman, Clarkson University, privman@clarkson.edu



Vladimir Privman, Clarkson University, privman@clarkson.edu

Quantum Hall Quantum Computing

V. Privman, I. D. Vagner, G. Kventsel, Phys. Lett. A239, 141 (1998)

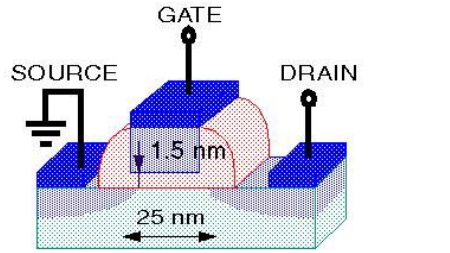
Nuclear spin qubits immersed in the 2D electron gas which is in the nondissipative integer quantum Hall effect (QHE) state

Qubits: spins (nuclear, or bound-electron)

Coupling: via 2D electron gas (2DEG)

Low temperatures & high magnetic field — to decrease decoherence and quantize the 2D conduction electron motion

The 2DEG (with added "gate" ideas borrowed from Kane) and superconducting QC schemes are probably the closest to the next-generation "classical" computer component technology:



Nanoscale Metal Oxide Semiconductor Field Effect Transistor (MOSFET)

For QC:

embed and control single spins
$T \to 0$
B – large
isotope purification
…

Vladimir Privman, Clarkson University, privman@clarkson.edu

Evaluation and Design of QC Models

Initialize

Control and
Evolve in time

Measure

Time Scales of Quantum Dynamical Processes

Review: **V. Privman, D. Mozyrsky, I. D. Vagner, Computer Phys. Comm. (July 2002)**

Control qubits: T_{ext}

Control interactions: T_{int} $(> T_{ext})$

Avoid thermalization: T_1

Avoid decoherence: T_2 $(< T_1)$

Goal: T_{ext} , $T_{int} << T_2$, T_1

Vladimir Privman, Clarkson University, privman@clarkson.edu

Time Scales of Quantum Dynamical Processes

Evaluation of T_1 and T_2 can be done initially for a single-qubit system interacting with the excitations of the 2DEG which have a spectral gap (owing to the Zeeman splitting). Because of the spectral gap, we have $T_2 \ll T_1$, and the physics of these processes is different: relaxation (T_1) requires energy exchange, whereas decoherence (T_2) is due to virtual excitations. Both are impurity driven.

D. Mozyrsky, V. Privman, I. D. Vagner, Phys. Rev. B 63, 085313 (2001)

Calculation of T_{int} requires consideration of two qubits and their interactions via the excitations of the 2DEG.

...after a lengthy calculation, we get

$$H_{ex} = \frac{1}{2}\sum_{\mathbf{k}} \left[W_{\mathbf{k}} |\uparrow_e\rangle\langle\downarrow_e| S_{\mathbf{k}} + W^*_{\mathbf{k}} |\downarrow_e\rangle\langle\uparrow_e| S^\dagger_{\mathbf{k}} \right] \quad (4)$$

where $|\uparrow_e\rangle\langle\downarrow_e| = b^\dagger_\uparrow b_\downarrow$ in the appropriate subspace, and

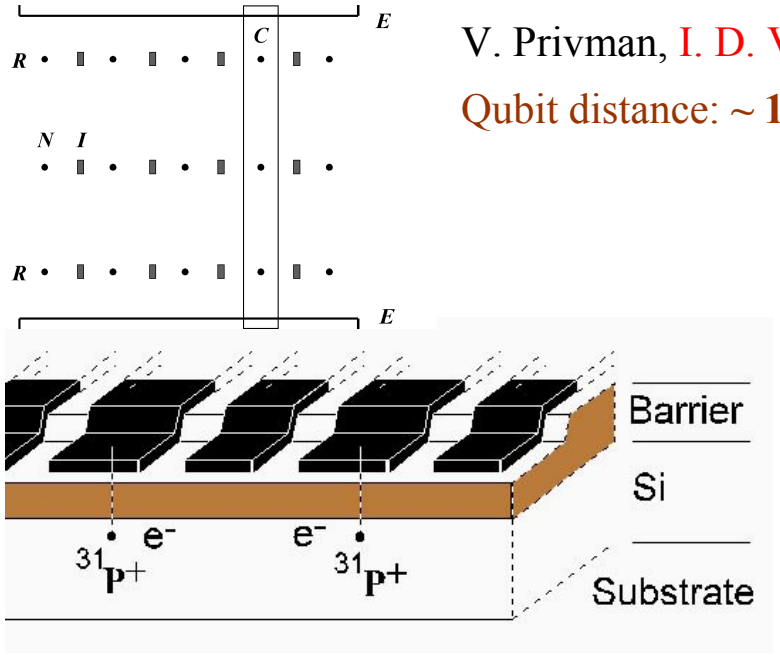
$$W_{\mathbf{k}} = \frac{1}{\ell(2\pi L_x L_y)^{1/2}} \int d^3\mathbf{R}_1 d^3\mathbf{R}_2 \Psi^*_0(\mathbf{R}_1)\Psi_0(\mathbf{R}_2) U(\mathbf{R}_1 - \mathbf{R}_2)\chi^*(z_2)\chi(z_1) C_{\mathbf{k}}(\mathbf{r}_1,\mathbf{r}_2) \quad (5)$$

$$C_{\mathbf{k}}(\mathbf{r}_1,\mathbf{r}_2) \equiv \exp\left\{ -\frac{1}{4\ell^2}\left[(x_1-x_2)^2 + (y_1-y_2)^2 - 2i(x_1-x_2)(y_1+y_2) \right] \right\} \times$$

$$\exp\left[-\frac{\ell^2}{4}(k_x^2+k_y^2) - \frac{k_y}{2}(iy_1+iy_2-x_1+x_2) - \frac{k_x}{2}(ix_1+ix_2+y_1-y_2) \right] \quad (6)$$

D. Mozyrsky, V. Privman, M. L. Glasser, Phys. Rev. Lett. 86, 5112 (2001)

Improved QC Design: Kane + QHE → 0.1 μm Gate Separation



V. Privman, I. D. Vagner, G. Kventsel, Phys. Lett. A239, 141 (1998)

Qubit distance: ~ **10** nm (of the order of the magnetic length).

B. E. Kane, Nature 393, 133-137 (May 14, 1998)

Qubit distance: realistically, must be ~ **4** nm.
Interaction can be oscillatory.

D. Mozyrsky, V. Privman, M. L. Glasser, Phys. Rev. Lett. 86, 5112 (2001)

Couple nuclear spin qubits indirectly via their hyperfine interaction with the outer bound electrons (as in Kane's scheme) which in turn interact via the 2DEG. Qubit distance: ~ **100** nm = **0.1** μm.

Quantum Dynamics, Relaxation and Decoherence in Solid State Physics

Vladimir Privman, Clarkson University, privman@clarkson.edu

Illustration of Type of Results for a QC Scheme

Time Scales

T_{ext}	O(10^{-5}) sec	Single-qubit external NMR-radiation control time
T_{int}	O(10^{-2}) sec	Time scale defined by the two-qubit interactions
T_1	O(10) sec	Time scale associated with energy relaxation
T_2	O(10^{-1}) sec	Intrinsic quantum-mechanical decoherence time

Qubit-Qubit Interactions

$$H_{1,2} = J|0_1 1_2\rangle\langle 1_1 0_2| + J^*|1_1 0_2\rangle\langle 0_1 1_2|$$

$$d = (E_c/2\Delta)^{1/2}\,\ell$$

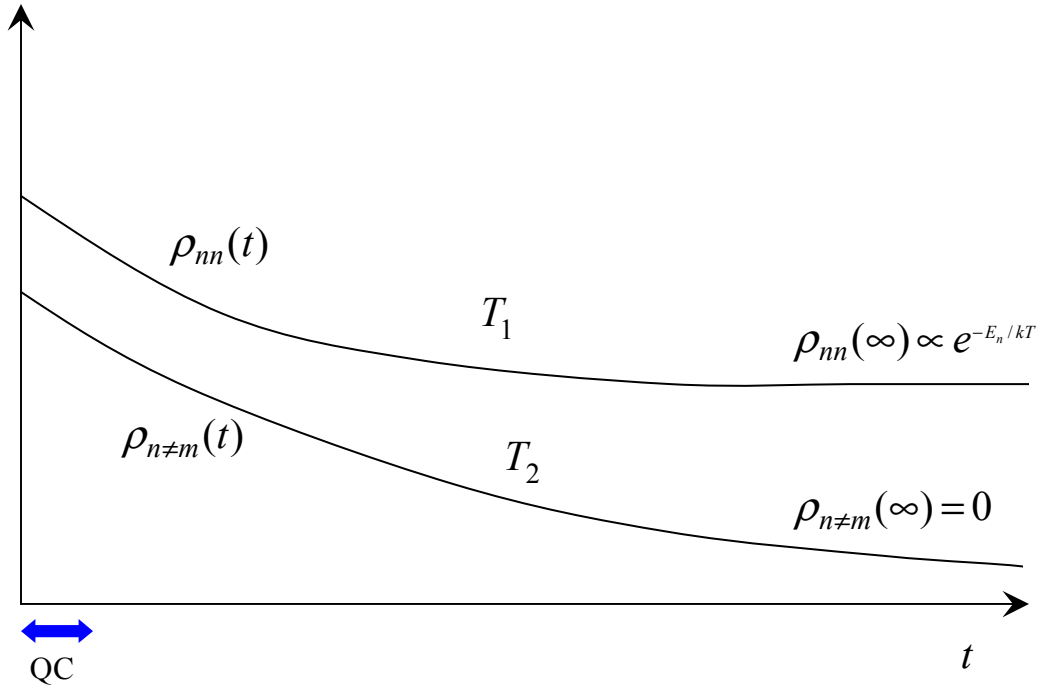
$$J = \left(\frac{A}{\Delta}\right)^2 \frac{|Z|^2}{(2\pi)^{1/2}E_c\ell^2}\left(\frac{d}{r}\right)^{1/2}\exp\left(-\frac{r}{d}\right), \qquad (r > \ell)$$

Quantum Dynamics, Relaxation and Decoherence in Solid State Physics

Vladimir Privman, Clarkson University, privman@clarkson.edu

Short Time Decoherence and Deviation from Pure Quantum States: Can we escape the T_1-T_2 paradigm?

V. Privman: quant-ph/0205037



We have developed a new short-time approximation scheme for evaluation of decoherence. At low temperatures, the approximation is argued to apply at intermediate times as well. It then provides a tractable approach complementary to Markovian approximations, and is appropriate for evaluation of deviations from pure states in quantum computing models.

Quantum Dynamics, Relaxation and Decoherence in Solid State Physics

Vladimir Privman, Clarkson University, privman@clarkson.edu

$$\sqrt{\pi}\,\rho(t) = \int dy\, e^{-y^2}\, e^{-iH_S t/2}\, e^{i[yB(t)\Lambda_S - C(t)\Lambda_S^2]}\, e^{-iH_S t/2}\, \rho(0)\, e^{iH_S t/2}\, e^{-i[yB(t)\Lambda_S - C(t)\Lambda_S^2]}\, e^{iH_S t/2}$$

$$B^2(t) = 8\sum_K \frac{|g_K|^2}{\omega_K^2} \sin^2\frac{\omega_K t}{2} \coth\frac{\beta\omega_K}{2}$$

$$C(t) = \sum_K \frac{|g_K|^2}{\omega_K^2}\,(\omega_K t - \sin\omega_K t)$$

For $\rho(0) = |\uparrow\rangle\langle\uparrow|$ or $|\downarrow\rangle\langle\downarrow|$, we get

$$\mathrm{Tr}_S\,[\rho^2(t)] = \frac{1}{2}\left[1 + e^{-2B^2(t)}\right]$$

For $\rho(0) = |\psi_0\rangle\langle\psi_0|$, the deviation from a pure state is apparent: $\rho(t>0)$ is obviously a *mixture* (integral over y) of pure-state projectors $|\psi(y,t)\rangle\langle\psi(y,t)|$, where

$$\psi(y,t) = e^{-iH_S t/2}\, e^{i[yB(t)\Lambda_S - C(t)\Lambda_S^2]}\, e^{-iH_S t/2}\, \psi_0$$

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Open Problems and Future Research Directions

	Experiment	Theory
Basic Physics	**Study spin populations coupled by 2DEG and controlled by NMR/ESR radiation and by gates**	**Derive results for couplings, relaxation, decoherence, to test our techniques for calculating spin properties at $T = 0$ and $T > 0$**
Spintronics	**Reduce the size of the polarized spin domains or regions under gates, to nanoscale**	**Effects of gates will become important to account for (break the planar symmetry, cause decoherence, etc.)**
Quantum Computing	**True single-spin control and isotope engineering**	**Aspects of measurement and the associated transport properties**

Selected Papers by Our Group, in the Field of Quantum Computing and Decoherence

Quantum computing with spin qubits in semiconductor structures

Vladimir Privman, Dima Mozyrsky, Israel D. Vagner

Department of Physics and Center for Advanced Materials Processing,
Clarkson University, Potsdam, New York 13699-5820, USA

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Abstract

We survey recent work on designing and evaluating quantum computing implementations based on nuclear or bound-electron spins in semiconductor heterostructures at low temperatures and in high magnetic fields. General overview is followed by a summary of results of our theoretical calculations of decoherence time scales and spin-spin interactions. The latter were carried out for systems for which the two-dimensional electron gas provides the dominant carrier for spin dynamics via exchange of spin-excitons in the integer quantum Hall regime.

PACS: 73.20.Dx, 71.70.Ej, 03.67.Lx, 76.60.-k

Keywords: quantum computing, semiconductor, decoherence, spin, qubit, electron gas

1. Introduction

The field of quantum computing has seem explosive growth of experimental and theoretical interest. The promise of quantum computing [1-5] has been in exponential speedup of certain calculations via quantum parallelism. In Figure 1, the top flow chart shows the "classical" computation which starts from binary input states and results in binary output states. The actual dynamics is not really that of Newtonian classical mechanics. Rather the computation involves many-body irreversible "gate" device components, made of semiconductor materials in modern computers, which evolve irreversibly, "thermodynamically" according to the laws of statistical mechanics. As the size of the modern computer components approaches atomic, the many-body quantum behavior will have to be accounted for in any case [6].

The idea of quantum computing, however, is not just to account for, but to actually utilize the quantum-mechanical dynamical behavior. This is not an easy task. Quantum mechanics allows for parallelism in evolution: one can "process" a linear superposition of

several input states at once, as illustrated in the lower flow chart in Figure 1. The price paid is that coherent processing of information, according to the law of quantum mechanics, must be accomplished in systems much larger than atomic-size (or more importantly, with many degrees of freedom). There are numerous conceptual and experimental obstacles to accomplishing this task, that have generated a lot of interest, excitement, and new results in computer science, physics, and engineering.

The functioning of a quantum computer involves initialization of the input state, then the actual dynamical evolution corresponding to computation, and finally reading off the result. Various specific requirements for implementation have been identified [2-5]; here we provide only a limited introductory overview.

Let us begin by considering the reading off of the final result. The reason for the question mark in the lower chart in Figure 1 is that quantum measurement of the final superposition state can erase the gain of the parallel dynamics, by collapsing the wave function. Therefore, a key issue in quantum computing has been to find those algorithms for which the readout of the final state, by way of projecting out a certain average property, still retains the power of the quantum parallelism. To date, only few such examples are known [1,3,4,7], the most celebrated being the Shor algorithm [1] for factoring of integers, the invention of which boosted quantum computing from an obscure theoretical field to a mainstream research topic.

The preparation of the initial state does not seem to present a problem for most quantum computing realizations [2-5], accept perhaps the ensemble liquid state NMR approach [8,9] which relies on the initial thermal distribution to produce deviation of the density matrix from the equal-probability mixture state. In most other approaches, the initial state can be produced by first fully polarizing the quantum bits (qubits), i.e., putting them in one of the two quantum levels. Note that we consider two-state qubits here, realized, for instance, by spins 1/2 of nuclei or gate- or impurity-bound electrons, in applied magnetic field. The fully polarized state is then subject to gate operations to form the desired input state. Part of a quantum-computing algorithm should be the prescription on how to choose the initial state to represent the classical information of the input, like the input integer in the factoring. In most cases, this prescription is easily accomplished by single-qubit and two-qubit gates.

The actual dynamical evolution (the process of computation) in quantum computing is fully reversible and nondissipative, unlike classical computing. Much progress has been made in resolving both the conceptual and computer-engineering “design” issues for quantum computation. Specifically, the computation can be carried out [2-5,10-13] by a universal set of gates: single-qubit rotations and nearly any two-qubit gate. The gates are not connected in space like in classical computers but are activated in succession in time, to control single-spin dynamics and also switch on and off two-spin interactions (we use “spin” and “qubit” interchangeably).

Many interesting matters have been resolved, which are not reviewed here. These include the understanding of how the finiteness of the state space (i.e., two states for spin 1/2)

replaces the "classical" digitalization in quantum computing. Also, the "classical" copying (fan-out) function is not possible in quantum mechanics. It is replaced by entanglement with ancillary qubits to accomplish redundancy needed for error correction [14-20]. Sources of errors due to interactions with environment in quantum mechanics involve not only the usual relaxation (thermalization) but also loss of coherence [21-28]. This quantum decoherence (dephasing) can be faster than relaxation because it does not require energy exchange.

A conceptually important issue has been the scalability of quantum computing: can one process macroscopically large amounts of information by utilizing quantum error correction based on redundancy via entanglement with ancillary qubits? The affirmative answer to this question has been one of the triumphs of the theory [14-20]. It provided a new paradigm for emergence of controlled/organized macroscopic behavior from microscopic dynamics, on par with the conceptual possibility of living organisms, which we observe by cannot yet "manufacture," and million-gate classical computers which are man-made.

With all these theoretical advances at hand, the next step is to ask whether a man-made quantum computer can be realized? There have been several experimental directions of exploration, most presently are still at the level of one or two qubits, or, for ensemble liquid-state NMR, which emulates quantum dynamics by evolution of the density matrix of a large collection of molecules, 5-7 qubits.

In this introductory survey, we summarize results of our work on two-spin interactions and spin decoherence in semiconductor heterostructures. In Section 2, we consider the spin-based quantum computing proposals in such systems. Time scales of relaxation and decoherence are addressed in Section 3. Finally, Section 4 reports results for models with nuclear spins as qubits.

2. Spin-Based Quantum Computing in Semiconductor Heterostructures

The general layout of a solid-state quantum computer is shown in Figure 2. Qubits are positioned with precision of few nanometers in a heterostructure. One must propose how to effect and control single-qubit interactions, two-qubit interactions, and explore how the controlled dynamics owing to these interactions compares to decoherence and relaxation. The proposal must include ideas for implementation of initialization, readout, and gate functions.

The first proposal including all these components was for qubits realized in an array of quantum dots [29] coupled by electron tunneling. The first spin-based proposal [30] utilized nuclear spins coupled by the two-dimensional electron gas, the latter in the dissipationless integer quantum Hall state [31] that requires low temperatures and high magnetic fields. An important advancement was the work of Kane [32] where gate control of nuclear-spins of donor impurities, separated less than 10 nm and coupled via the outer impurity electrons which are bound at low temperatures, was proposed. Most of

these ideas also apply to electron-spin qubits, bound at impurities, in quantum dots, or directly by gates. Several elaborate solid-state heterostructure quantum computing schemes have been proposed in the literature recently [28,33-41]. There are also other promising proposals involving surface geometries: superconducting electronics [42-46] and electrons on the surface of liquid helium [47].

There have been several planned and ongoing experimental efforts [32-36,43-45,48-54] ultimately aimed at solid-state quantum computing and other quantum information processing realizations. The final geometry is expected to be most sensitive to the implementation of readout, because it involves quantum measurement, i.e., supposedly interaction with or transfer of information to a macroscopic device. Therefore, much of the experimental effort presently has been focused on single-qubit (single-spin) measurement approaches.

The theoretical efforts can be divided into two majors tasks. The process of single-spin measurement must be understood for the readout stage of quantum computing. Several conceptual and calculations advancements have been made in understanding quantum measurement [26,32-36,46,50,55,56] as it applies to atomic-size qubit systems interacting with environment and typically "measured" directly by the effect of the spin-qubit state on transport, or first transferring the spin state to a charge state that is easier to measure, e.g., in single-electron transistors and similar devices.

In this survey, we outline results of the second evaluation task: that of understanding the processes and times scales involved in the dynamics of the actual computation. As summarized in Figure 3, this main stage of the quantum computation process involves control of spins and their interactions. It also involves processes that we do not control and are trying to minimize: relaxation and decoherence.

Control of individual qubits is usually accomplished externally. For nuclear spins, NMR radio-frequency radiation can be used, see Figure 2. For electron spins, the ESR microwave frequencies are suitable. Such radiation cannot be focused on the scale of 10-100 nm. Instead, selectivity must be accomplished by independent means. Several proposals exist, the most promising being control by gates. The applied gate voltage modifies the electronic wave function changing interactions and therefore resonant frequencies. We will denote the time scale of the external single-qubit control by T_{ext}. This can be the Rabi time of a spin flip.

The qubit-qubit interactions are typically assumed to be mediated by electrons that "visit" both qubit environments. For instance, in liquid-state ensemble NMR [8,9] with complex molecules, or in the original model [32] of phosphorous impurity donors in silicon, the wave functions of the valence, outer electrons of nearby qubits overlap. Specifically, in the P donor case, the single outer electron of the donor atom remains bound at low temperatures but has orbital radius of order 2 nm owing to the large dielectric constant of the silicon host. Therefore, it is hoped that these electrons, in nearby donors positioned as in Figure 2, will mediate nuclear-spin qubit interactions.

Our approach [27,28] allows for larger qubit separation, up to order 100 nm, by relying on the two-dimensional electron gas in the heterostructure to mediate qubit-qubit interactions. This two-dimensional electron gas is usually obtained by spontaneous or gate-induced transfer of electrons from impurities to the two-dimensional interface layer in which the qubits are positioned. The source impurities are located at some separation from this layer or in the bulk. The two-dimensional electron gas can be made nondissipative in certain ranges of large applied magnetic fields at low temperatures, when these conduction electrons in the layer are in the integer quantum Hall effect state. Owing to this property and also larger qubit separation allowed, we consider this the most promising approach and focus our present review on such systems.

The time scale of the qubit-qubit interactions will be devoted by T_{int}. This is the time it takes to accomplish a two-qubit quantum gate, such as CNOT [2-5,57]. Typically for semiconductor quantum computing proposals, $T_{int} < T_{ext}$, and in fact the case with $T_{int} \ll T_{ext}$ has some advantages because one can use several fast single-spin flips to effectively switch interactions of some qubits off over the gate cycle. Another approach to controlling (on/off) of the two-qubit interactions is by gates, see Figure 2, which affect the two-dimensional electron gas and the localized electron wavefunctions.

However, the same conduction electrons that provide the qubit-qubit interactions, also expose the qubits to the environment, causing relaxation and decoherence. Other interactions will also be present, that play no role in the useful quantum-computing dynamics but contribute to these undesirable processes. Relaxation and decoherence, and their associated time scales, are addressed in the next section.

3. Time scales of relaxation and decoherence

The processes of relaxation and decoherence considered here [21-28] are associated with the dynamics of a small, few-qubit quantum system as it interacts with the environment. Ultimately, for a large, multi-qubit system, many-body quantum chaos-like behavior must also be accounted for, and some advances in model system studies have been reported recently [5,58]. Our discussion here will be for the few-qubit case mostly because it allows more system-specific investigations for actual quantum-computing proposals.

Dynamical processes that are unwanted in quantum computing, because they result from the environmental influences rather than from the controlled radiation pulses and gate potentials, can proceed on various time scales. In fact, it is not guaranteed that processes of various types, relaxation/thermalization vs. decoherence/dephasing, can even be unambiguously distinctly identified.

At low temperatures, it is generally hoped that thermalization, which requires transfer of energy, slows down. If the fastest such processes proceed on times scales of order T_1, then this time increases at low temperatures because there are less excitations (phonons,

electron gas modes, etc.) to couple the small quantum system to the rest of the solid-state host material.

On the other hand, processes that do not require flow of energy to or from the environment, can still effect the phase of the quantum-superposition amplitudes and cause decoherence. These processes can thus proceed faster, on the time scale T_2. While these comments seem to suggest that $T_2 \leq T_1$, there is no obvious reason to have generally $T_2 \ll T_1$ at low temperatures.

However, if the spectrum of the dominant excitations mediating the qubit coupling (both to each other and to the host material) has a gap, then we expect that all the relaxation and decoherence processes will be suppressed. Furthermore, the suppression of the relaxation will be exponential, with the Boltzmann factor for that energy gap. Then, $T_2 \ll T_1$ will be satisfied but also, more importantly, the actual values of both time scales will be inordinately large. This was found, theoretically and experimentally, to be the case for the integer-quantum-Hall-state two-dimensional electron gas as mediator of the localized-spin (nuclear, electronic) coupling in semiconductor heterostructures [27,28,59-63].

It is important to emphasize that relaxation and decoherence are really many-body properties of the system plus environment. Entanglement with the environment owing to the unwanted couplings results in the small quantum system having no pure wavefunction even if initially it was prepared in a pure state. Instead, it can be described by a statistical mixture represented by a density matrix, once the environment is traced over.

This reduced density matrix of the system is expected to evolve to the thermal one at large times. The approach to the thermal density matrix, which is diagonal in the system-energy basis, defines the time scale T_1. If the temperature is low enough, then there is the expectation, see [25,26] and references therein, that for some intermediate time scales, of order T_2, the density matrix becomes nearly-diagonal in a basis which is determined not by the systems Hamiltonian (energy), but by the interaction operator with the environment. This latter process corresponds to loss of quantum coherence.

As emphasized in Figure 3, evaluation of a quantum-computing proposal requires, among other things, establishing the relation $T_{ext}, T_{int} \ll T_2, T_1$. Owing to calculational difficulties, the single-qubit times $T_{1,2}$ will usually be used, though, as mentioned earlier, some study of the multi-qubit "quantum chaos" effects may be required. For spin-qubit quantum computing in semiconductor heterostructures, the relation is typically $T_{ext} \ll T_{int} \leq T_2 \ll T_1$, so the issue is usually how small is the quality ratio $Q = T_{int} / T_2$.

The required value of Q, needed for fault-tolerant quantum error correction, depends on the physical model of error sources and can be as small as $Q = 10^{-6} - 10^{-4}$, see [15,18-20], or as large as $Q = 1/2$, see [64]. For the systems of interest to us here, spin qubits in

semiconductor structures, the value of $Q = 10^{-5}$ is a reasonable working estimate. Thus, we seek systems/conditions with $T_{int} / T_2 \leq 10^{-5}$.

4. Results for nuclear-spin qubits

In this section we outline results for models of quantum computing with nuclear spins as qubits, and with coupling mediated by the two-dimensional electron gas in the integer quantum Hall effect state [27,28,30]. In strong magnetic fields, the spatial states of the electrons confined in the two-dimensional layer in which the qubits are placed, see Figure 2, are quantized by the field to resemble free-space Landau levels. The lattice potential and the impurities actually cause formation of narrow bands instead of the sharp levels, separated by localized states. As a result, for ranges of magnetic field, the localized states fill up while the extended states resemble completely filled integer number of Landau levels. These states are further Zeeman split owing to the electron spin. At low temperatures, one can find field values such that only one Zeeman sublevel is completely filled in the ground state.

The electronic state in such systems, that show the quantum Hall effect [31] in conductivity, are highly correlated and nondissipative. If nuclear spins are used as qubits, i.e., atoms with nuclear spin 1/2 are sparsely positioned in the zero-nuclear spin host, such as the zero-nuclear-spin isotope 28 of Si, which constitutes 92% of natural silicone, then their zero-temperature relaxation will be significantly slowed down: experimentally, $T_1 \simeq 10^3$ sec [62].

Localized spins, both nuclear and electronic, interact by exchanges of spin excitons—spin waves consisting of a superposition of bound electron-hole pair states. The spectrum of these excitations [65,66], observed experimentally in [67], has a gap corresponding to the Zeeman splitting. This gap is the cause of slow relaxation and decoherence. The exchange of virtual spin excitons mediates the qubit-qubit interaction and also, via scattering of virtual excitons from impurity potentials, relaxation and decoherence of single qubits.

The original proposal to use nuclear spin qubits directly coupled by the two-dimensional electron gas [30], required positioning the qubits at distances comparable to several magnetic lengths. The latter is of order 10 nm for magnetic fields of several Tesla. The qubit-qubit interaction decays exponentially on this length scale. Recently, we proposed a new improved model [28] in which the qubit interactions are mediated via coupling of the two-dimensional electron gas to the outer impurity electrons. This applies if the atoms, whose nuclear spins are the qubits, are single-electron donors such as the isotope 31 of P. These phosphorous impurities were originally utilized in the model of Kane [32] where they must be actually positioned at separations of about 4 nm for the wavefunctions of the outer electrons, which are bound at low temperatures, to overlap significantly.

In our new improved model [28], with nuclear spins coupling to the outer bound electrons which, in turn, interact via the two-dimensional electron gas, the interaction turned out to be of a much longer range as compared to the model of [32]: the qubit separation can be of order 100 nm. Another advantage is that gate control of the individual qubits and of qubit-qubit interactions is possible. We have carried out extensive perturbative many-body calculations [27,28,30,68] allowing estimation of T_{int} and T_2 for both the original quantum-computing proposal [30] and its improved version [28], where the main improvement is in the possibility of the gate control along the lines of [32]. The "clock speed" of the improved model is also faster by about two orders of magnitude. The technical details of these rather cumbersome calculations are available in the literature and will not be detailed here.

The results are summarized in Table 1. We show estimates of all four relevant time scales for the two models introduced earlier. The "original" model [30] corresponds to nuclear spins 1/2 introduced at qubits in atoms without an outer loosely bound electron. The "improved" model corresponds to the case when the outer electron is present and its interaction with the nuclear spin and the two-dimensional electron gas dominates the dynamics.

The data shown in Table 1 were obtained assuming typical parameters for the standard heterojunctions utilized in quantum-Hall-effect experiments today, and qubit separation of 65 nm. Thus, the parameter values taken [28,30] were more appropriate for the GaAs system than for Si, even though the main isotopes of gallium and arsenic have nuclear spin 3/2 and cannot serve as spin-zero hosts. The reason for using these values has been that experimental verification of some of the numbers might be possible in the available materials before cleaner and different composition materials needed for quantum computing are produced.

Our estimates, see Table 1, indicate that the quality factor $Q = 10^{-5}$ is not obtained for the present system. Actually, no quantum computing proposal to date, scalable by other criteria, satisfies the 10^{-5} quality-factor criterion. The values range from 10^{-1} to 10^{-2}. The resolution could come from development of better error-correction algorithms or from improving the physical system to obtain a better quality factor. In our estimation of the decoherence time scale, we used parameters typical of a standard, "dirty" heterostructure with large spatial fluctuations of the impurity potential. These heterostructures have been suitable for standard experiments because they provide wider quantum-Hall plateaus, i.e., ranges of magnetic field for which all the extended states of a Zeeman sublevel are filled. Much cleaner, ultra-high mobility structures can be obtained by placing the ionized impurity layer at a larger distance from the two-dimensional gas or by injecting conduction electrons into the heterostructure by other means. Thus, our quantum-computing proposals [28,30] are unique not only in the large qubit separation allowed but also in that there is a clear direction of exploration to allow physical, rather than algorithmic, resolution of the quality factor problem. This possibility should be further explored both experimentally and theoretically.

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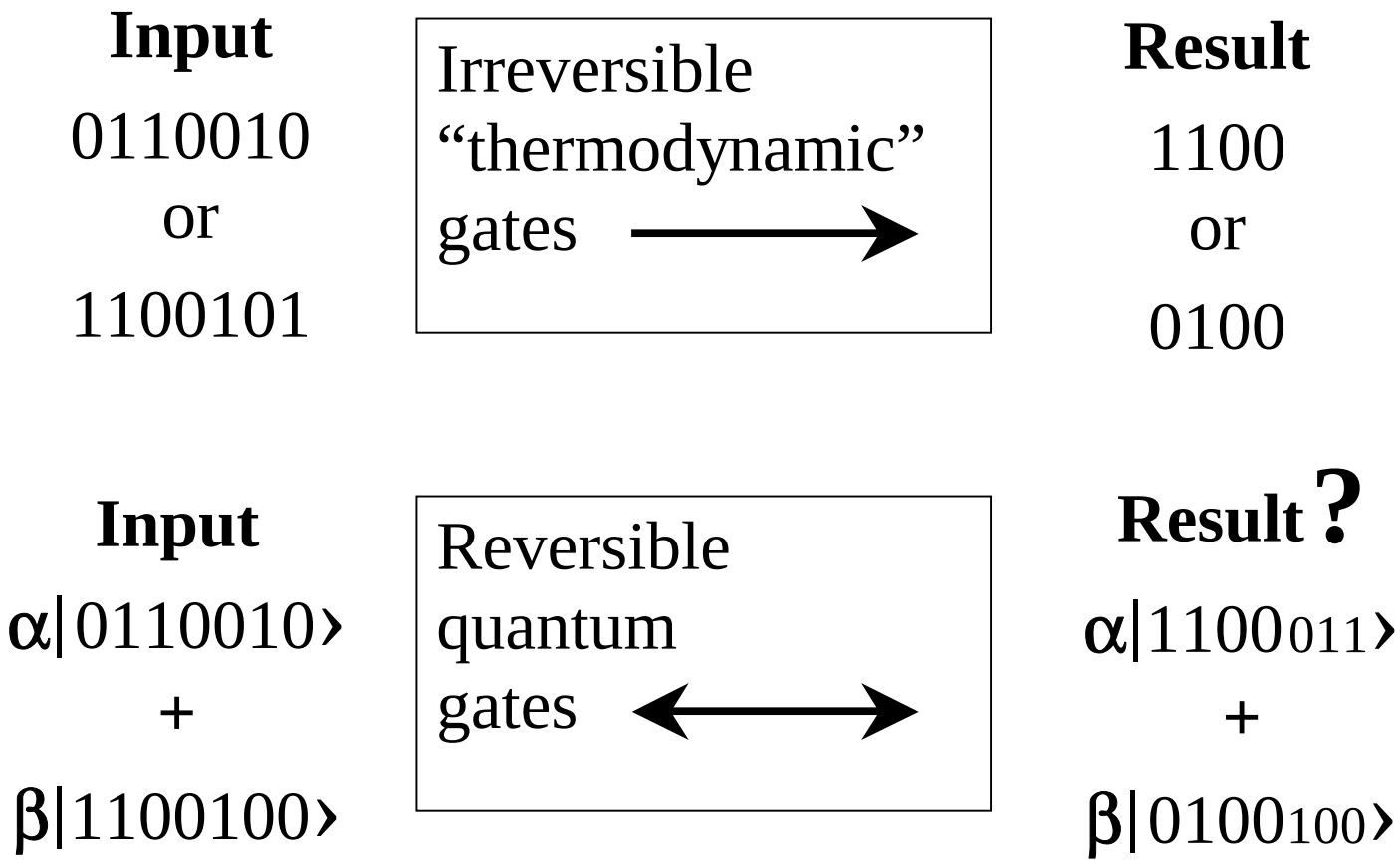

Figure 1. Comparison of the classical and quantum approaches to computing. The upper flow chart schematically represents implementation of a traditional irreversible “classical” computation process, where transformation of the input set of bits into the result is accompanied by a succession of irreversible gates. Owing to their irreversibility, the gates can be connected in space rather than switched on and off at different times. The lower flow chart shows quantum processing of information, where the input and the final result are both in superposition states, yielding quantum parallelism. The dynamics is reversible: there is a one-to-one correspondence between the initial and final states. Therefore, number of the input and output quantum bit (qubits) is the same even though some of the output qubits (set in a smaller font) might not be used in the final extraction of the classical result by measurement. The quantum gates are applied in succession by being switched on and of at different times during the computation. The question mark signifies the difficulty of finding quantum algorithms that retain the power of quantum parallelism after measurement needed to read off the final result as classical information.

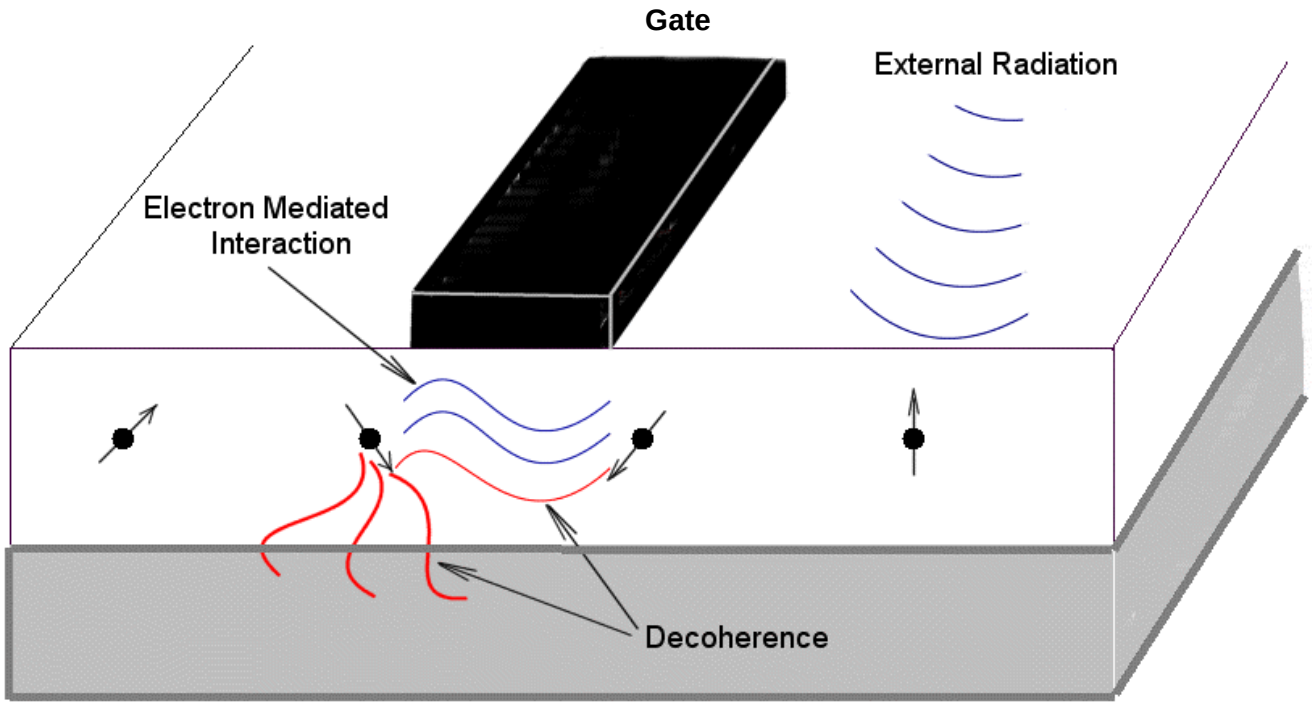

Figure 2. Schematic illustration of a semiconductor heterostructure quantum information processor. The qubits, represented by the arrows overlaying heavy dots, are spins 1/2 of nuclei or localized electrons. Individual control of the temporal evolution of the spins can be achieved with the use of external electromagnetic radiation, i.e., NMR or ESR pulses. The spins are also coupled with each other via interaction mediated by the two-dimensional electron gas in the heterostructure, or by other means. The external and internal interactions can be controlled by gates formed on top of the heterostructure. The external environment, that includes crystal lattice, electron gas, defects, impurity potentials, causes relaxation and decoherence of the qubits.

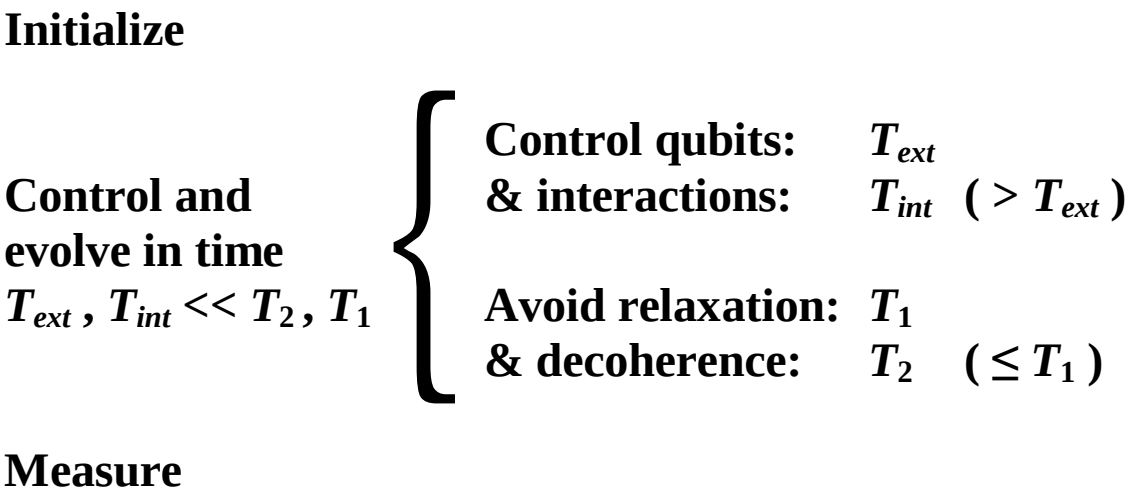

Figure 3. Evaluation of quantum computing models. One of the criteria for feasibility of quantum computing in a given physical system is the possibility of initialization of the qubits in the desired superposition state. Another important design consideration is control of qubit states and of their interactions. In order to implement quantum computing effectively, the time scales for realization of single and two-qubit logic gates, T_{ext} and T_{int}, respectively, should be several orders of magnitude smaller than the time scales of relaxation and decoherence, T_1 and T_2. The relationships between these time scales are further explained in the text. Finally, efficient and reliable measurement of the output state of the qubits is required for reading off the result of the computation and presently represents a formidable experimental challenge.

Table 1. Time scales of the qubit dynamics for the original [30] and improved [28] versions of the nuclear spin quantum computer with interactions mediated by the two-dimensional electron gas.

	The original model	The improved model
T_{ext}	$O(10^{-5})$ sec	$O(10^{-5})$ sec
T_{int}	$O(1)$ sec	$O(10^{-2})$ sec
T_1	$O(10^{3})$ sec	$O(10)$ sec
T_2	$O(10)$ sec	$O(10^{-1})$ sec

Indirect Interaction of Solid-State Qubits via Two-Dimensional Electron Gas

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We propose a mechanism of long-range coherent coupling between nuclear spin qubits in semiconductor-heterojunction quantum information processing devices. The coupling is via localized donor electrons which interact with the two-dimensional electron gas. An effective interaction Hamiltonian is derived and the coupling strength is evaluated. We also discuss mechanisms of decoherence and consider gate control of the interaction between qubits. The resulting quantum computing scheme retains all the control and measurement aspects of earlier approaches, but allows qubit spacing at distances of the order of 100 nm, attainable with the present-day semiconductor device technologies.

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Recent technological advances in electronics related to spin polarization [1,2] have boosted experimental and theoretical interest in quantum information science in condensed matter systems, specifically, in semiconductor heterostructures at low temperatures and in high magnetic fields. The solid-state implementations of quantum information devices seem to be among the most promising ones, due to possible scalability of the elementary logic gates into more complicated integrated circuits. Several designs for solid state and related spin-based quantum information processors have been suggested [3–8]. Preliminary experiments, involving several quantum bits (qubits), have been carried out or are being contemplated [9,10].

Our work stems from the proposals that utilize nuclear or electronic spins as qubits for information processing [3–7]. These are natural choices for qubits because at low temperatures spin states in semiconductors have relatively long decoherence times, sometimes milliseconds or even longer for electronic spins, and seconds for nuclear spins [11–14]. We propose a new mechanism for coupling between two nuclear-spin qubits, combining aspects of two models of quantum information processors, one based on nuclear spins in quantum-Hall effect systems [4], and another utilizing the nuclear spins of phosphorous donors in a silicon heterostructure [5].

An appealing aspect of Kane's model [5] is a possibly experimentally feasible scheme for reading out the state of the quantum register, i.e., measurement of a nuclear spin, achieved by transferring the nuclear-spin polarization to the electronic state, while the latter is measured with the use of a single electron transistor. The model proposed in [4] has a different advantage: Unlike [5], the interaction between the nuclear spins is mediated by the two-dimensional (2D) electron gas, and thus is longer ranged due to the highly correlated state of the 2D electron gas in the quantum-Hall regime. This opens up possibilities for experimental realization of such quantum information processors, because large separation between spin qubits means greater lithographic dimensions in manufacturing the device. The price paid is that the coupling is weak, and therefore the time scales of the "gate function" can be as large as 1 s.

In this work we combine the two proposals, thus retaining the measurement and control scheme proposed in [5,7,9] and at the same time allowing larger separations, of the order of 100 nm, between interacting qubits. The resulting system is thus realizable with the present-day semiconductor technologies. We propose a model where sparsely positioned phosphorous donors are imbedded in a 2D electron gas in the quantum-Hall regime. The localized donor electrons interact via the delocalized 2D electrons and thus indirectly mediate nuclear-spin interactions. In 3D, spin coupling mechanisms via conduction electrons have been well studied [15]. Here, we estimate the range of this induced nuclear-spin interaction for the 2D case and find it to be of the order of 100 nm. This is large compared to atomic dimensions, donor-electron bound state radii, and even the electronic magnetic length which is typically of the order of 10 nm. We find that this interaction is also stronger, thus corresponding to faster gate function times, than in [4].

We assume that the coupling between the electronic and the nuclear donor spins is given by the Fermi contact interaction, $H_{e-n} = A\sigma_n \cdot \sigma_e$. Here, $A = (8\pi/3)\mu_B g_n \mu_n |\Psi_0(0)|^2$, where μ_n and g_n are the nuclear magnetron and nuclear g factor, respectively, $|\Psi_0(0)|^2$ is the donor-electron probability density at the nucleus, μ_B denotes the Bohr magnetron, and σ's are Pauli matrices. Coupling of the delocalized electrons to the nuclear spin is considerably weaker than that of the localized donor electron. Therefore, we assume that the nuclear spin interacts with conduction electrons indirectly via the donor electron.

As a prototype system, we consider ^{31}P donors positioned in Si, so all the spins involved are $\frac{1}{2}$. The donor electronic and nuclear spins form a four-level system. The spectrum of this two-spin system can be obtained to O(A) with H_{e-n} treated as perturbation. The energy levels are $E_0 = -(\gamma_n + \Delta)/2 + A$, $E_1 = (\gamma_n - \Delta)/2 - A$, $E_2 = (-\gamma_n + \Delta)/2 - A$, and $E_3 = (\gamma_n + \Delta)/2 + A$, where $\gamma_n = g_n \mu_n H$ is the nuclear-spin splitting. Here, H is the

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magnetic field, and the expression for Δ, the electronic Zeeman gap, will be given shortly. The eigenstates associated with these energy levels are $|0\rangle = |\downarrow e \downarrow n\rangle$, $|1\rangle = |\downarrow e \uparrow n\rangle + (2A/\Delta)|\uparrow e \downarrow n\rangle$, $|2\rangle = |\uparrow e \downarrow n\rangle + (2A/\Delta)|\downarrow e \uparrow n\rangle$, and $|3\rangle = |\uparrow e \uparrow n\rangle$, where $|\downarrow e \downarrow n\rangle$ represents the electronic and nuclear-spin down state, etc. Here we propose to consider the states $|0\rangle$ and $|1\rangle$ as qubit states of a quantum computer. By altering the hyperfine coupling constant A by distorting the spatial state Ψ_0 of the donor electron with an electrostatic gate [5,7], one can selectively control the state of an individual qubit by means of the NMR technique.

In order to calculate the interaction Hamiltonian between two qubits, we first consider the coupling between the donor electron and conduction electrons. The ground state of the donor electron is bound (localized) and will typically lie in the energy gap, several meV below the conduction band edge. For temperatures of order mK, electronic transitions from this localized state to the conduction band are highly improbable. The dominant interaction between the localized electron and conduction electrons is their Coulomb interaction. We are interested only in the exchange part of this interaction, i.e., the spin-dependent part. The spin-independent part causes screening, but it is weak in 2D [16] and, especially in the presence of the magnetic field, cannot ionize the donor.

In a large magnetic field, the delocalized 2D electrons occupy highly degenerate Landau energy levels [16]. It is convenient to introduce electron bound state creation and annihilation operators $b_{ns}^\dagger$ and b_{ns}, where n represents the donor spatial state, and s is the spin z component, $\uparrow$ or $\downarrow$. Let $a_{mk_xs}^\dagger$, a_{mk_xs} denote the creation and annihilation operators for the delocalized 2D electrons, where m labels the Landau level, while $\hbar k_x$ is the x momentum (we use the asymmetric gauge). Then the exchange coupling between the bound and delocalized electrons can be written as

$$H_{\rm ex} = \frac{1}{2}\sum G^{n,n'}_{m,m',k_x,k_x'} b_{ns}^\dagger a_{mk_xs'}^\dagger b_{n's'} a_{m'k_x's}\,, \qquad (1)$$

where the sum is over all the indices. Here, we have neglected the spin-orbit interaction. In what follows, we will retain only the lowest donor-electron spatial state, i.e., account only for the transitions between the two Zeeman levels of the ground state.

The 2D electrons are assumed to be in a nondissipative quantum-Hall state with filling factor $\nu = 1$; i.e., the lower Zeeman sublevel of the Landau ground state is completely filled [4]. This choice ensures reduced decoherence and relaxation effects [14], owing to the energy gap in the spectrum of the lowest-energy spin-wave excitations which are well studied [17,18]; their spectrum is given by $\mathcal{E}_{\mathbf{k}} = \Delta + E_c[1 - I_0(\ell^2k^2/4)\exp(-\ell^2k^2/4)]$, where I_0 is the modified Bessel function. Here, $\Delta = g\mu_B H$ is the Zeeman gap, $E_c = (\pi/2)^{1/2}(e^2/\epsilon\ell)$ is the characteristic Coulomb energy, and g is the effective g factor in the potential well that holds the 2D electron gas, while ϵ is the dielectric constant of the material, and $\ell = (\hbar c/eH)^{1/2}$ is the magnetic length. Extension to larger integer filling factors is possible [14,17,18]. One can also introduce [18] normalized creation and annihilation operators for the spin waves, quadratic in electronic operators,

$$S_{\mathbf{k}}^\dagger = \left(\frac{2\pi\ell^2}{L_xL_y}\right)^{1/2}\sum_p e^{i\ell^2k_yp} a_{p+(k_x/2),\downarrow}^\dagger a_{p-(k_x/2),\uparrow}\,, \qquad (2)$$

Here, $L_{x,y}$ are the transverse dimensions, taken to infinity in the final calculation. The summation over p is taken in such a way [18] that the wave number subscripts are quantized in multiples of $2\pi/L_x$. The spectrum of these spin waves has been experimentally verified in GaAs heterostructures [19].

We will include only these lowest excitations in the sum (1); our goal is to rewrite (1) in terms of the spin-wave operators (2). The exchange coupling is thus truncated to $G^{n,n'}_{m,m',k_x,k_x'} = G_{k_x,k_x'}\delta_{n,0}\delta_{n',0}\delta_{m,0}\delta_{m',0}$, where

$$G_{k_x,k_x'} = \int d^3\mathbf{R}_1\, d^3\mathbf{R}_2\, \Psi_0^*(\mathbf{R}_1)\Psi_0(\mathbf{R}_2) \times U(\mathbf{R}_1 - \mathbf{R}_2)\Phi_{0,k_x}^*(\mathbf{R}_2)\Phi_{0,k_x'}(\mathbf{R}_1)\,, \qquad (3)$$

$U(\mathbf{R}_1 - \mathbf{R}_2) = e^2/\epsilon|\mathbf{R}_1 - \mathbf{R}_2|$ is the Coulomb interaction, and $\Psi_0(\mathbf{R})$ is the donor-electron ground state. The states of the conduction electrons confined in the 2D well are $\Phi_{0,k_x'}(\mathbf{R}) = \phi_{0,k_x'}(\mathbf{r})\chi(z)$, where $\phi_{0,k_x'}(\mathbf{r})$ are the standard 2D Landau states [16]; $\chi(z)$ describes the confinement of the conduction electron wave function in the z direction and depends on the nature of the confinement potential. Here and in the following $\mathbf{R} = (\mathbf{r}, z)$, with $\mathbf{R}$ and $\mathbf{r} = (x, y)$ being 3D and 2D coordinates, respectively, while z is the direction perpendicular to the heterostructure, in which the applied magnetic field is pointing.

With the use of the expressions for Landau ground state wave functions, $\phi_{0,k_x'}(\mathbf{r}) = \ell^{-1}(\pi L_x)^{-1/2}e^{ik_xx} \times \exp[-(y - \ell^2k_x)^2/2\ell^2]$, and (2), after a lengthy calculation, we get

$$H_{\rm ex} = \frac{1}{2}\sum_{\mathbf{k}}[W_{\mathbf{k}}|\uparrow_e\rangle\langle\downarrow_e|S_{\mathbf{k}} + W_{\mathbf{k}}^*|\downarrow_e\rangle\langle\uparrow_e|S_{\mathbf{k}}^\dagger], \quad (4)$$

where $|\uparrow_e\rangle\langle\downarrow_e| = b_\uparrow^\dagger b_\downarrow$ in the appropriate subspace, and

$$W_{\mathbf{k}} = \frac{1}{\ell(2\pi L_xL_y)^{1/2}}\int d^3\mathbf{R}_1\, d^3\mathbf{R}_2\, \Psi_0^*(\mathbf{R}_1)\Psi_0(\mathbf{R}_2) \times U(\mathbf{R}_1 - \mathbf{R}_2)\chi^*(z_2)\chi(z_1)C_{\mathbf{k}}(\mathbf{r}_1,\mathbf{r}_2)\,, \qquad (5)$$

$$C_{\mathbf{k}}(\mathbf{r}_1,\mathbf{r}_2) \equiv \exp\left\{-\frac{1}{4\ell^2}[(x_1 - x_2)^2 + (y_1 - y_2)^2 - 2i(x_1 - x_2)(y_1 + y_2)]\right\} \times \exp\left[-\frac{\ell^2}{4}(k_x^2 + k_y^2) - \frac{k_y}{2}(iy_1 + iy_2 - x_1 + x_2) - \frac{k_x}{2}(ix_1 + ix_2 + y_1 - y_2)\right]. \qquad (6)$$

Note that since all the position vectors $\mathbf{R}$, $\mathbf{r}$ are measured from the origin at the donor atom, the quantity $W_{\mathbf{k}}$ depends also on the donor coordinates. To the leading order, (4) gives the interaction of the donor electron spin with excitations of the 2D electron gas in the $\nu = 1$ integer quantum-Hall state.

One can rewrite the interaction (4)–(6), with (4) multiplied by the unit operator in the nuclear-spin Hilbert space, in terms of the eigenstates of the electron-nucleus system. With the use of the expressions derived earlier for these eigenstates in terms of direct products of electronic and nuclear spin states, we obtain

$$H_{\mathrm{ex}} = \frac{1}{2}\sum_{\mathbf{k}} W_{\mathbf{k}}\Big(\frac{2A}{\Delta}\,|1\rangle\langle 0| + |2\rangle\langle 0| + |3\rangle\langle 1| - \frac{2A}{\Delta}\,|3\rangle\langle 2|\Big)S_{\mathbf{k}} + \mathrm{H.c.} \qquad (7)$$

Now one can calculate an effective Hamiltonian for the interaction of two qubits. Since the electronic Zeeman gap is much larger than the nuclear one, we can truncate the Hilbert space of the combined electron-nucleus spins to the two lowest lying states. Thus, we retain only the $|0\rangle\langle 1|$ and conjugate transitions in the exchange interaction (7).

An effective interaction between two qubits can be obtained within the standard framework of second order perturbation theory by tracing out the states of the spin waves; see [15,20,21] for similar calculations. The result can be written as

$$H_{1,2} = J|0_1 1_2\rangle\langle 1_1 0_2| + J^*|1_1 0_2\rangle\langle 0_1 1_2|\,. \qquad (8)$$

Here, the coupling constant between the two qubits is

$$J = \Big(\frac{A}{\Delta}\Big)^2 \sum_{\mathbf{k}\neq 0} \frac{W_{\mathbf{k},1} W^*_{\mathbf{k},2}}{\mathcal{E}_{\mathbf{k}} + E_1 - E_0}\,. \qquad (9)$$

The subscripts 1 and 2 in (8) and (9) label the two donor qubits, while $W_{\mathbf{k},1}$ and $W_{\mathbf{k},2}$ are the coupling constants of each donor electron spin to spin waves, given by (5), and $\mathcal{E}_{\mathbf{k}}$ is the spin-wave energy.

The nuclear-spin energy gap is much smaller than the electronic spin-wave excitation energies. Therefore, we can ignore $E_1 - E_0$ in the denominator in (9). Furthermore, due to the large value of the spin-wave spectral gap at $\mathbf{k} = 0$, $\mathcal{E}_0 = \Delta$, we do not have the "small denominator" problem encountered in other calculations of this sort, e.g., [20]. Physically, this means that the spin excitations in the 2D electron gas mediating the effective qubit-qubit interaction are virtual, and so this interaction does not cause appreciable relaxation or decoherence on the gate function time scale $\hbar/J$.

It is important to note that one can construct a universal CNOT logic gate from the controlled dynamics governed by Hamiltonians of the form of $H_{1,2}$ and single qubit rotations [6]. The coupling strength J between the qubits can be externally controlled by the electrostatic gates built above the 2D inversion layer. By applying gate voltages, one can locally vary the density of the 2D electrons, thus changing coupling between the delocalized and donor electrons. This results in control over the effective coupling constant J in (9). The precise effect of gates on interactions between the qubits, as well as on decoherence of their states, should be further studied in order to establish the feasibility of the quantum-computing approach proposed here. Most other semiconductor solid-state quantum-computing approaches [3–7] utilize gates.

Let us explicitly calculate the coupling constant J in (8) and (9). Because the spatial ground state of the donor is localized on a scale smaller than the magnetic length ℓ, the overlap integrand in (5) is vanishingly small for $|\mathbf{r}_1 - \mathbf{r}_2| > \ell$. At the same time, for $|\mathbf{k}| > 1/\ell$, the value of $C_{\mathbf{k}}$ decreases exponentially. Thus, $C_{\mathbf{k}}$ can be simplified by neglecting the $x_1 - x_2$ and $y_1 - y_2$ terms in (6). Moreover, for two donors at separation larger than ℓ, we can put $(\mathbf{r}_1 + \mathbf{r}_2)/2 \simeq \mathbf{r}_j$, with $\mathbf{r}_j$ being the location of either one of them. Then (5) can be approximated by $W_{\mathbf{k},j} = Z(L_x L_y)^{-1/2}\exp(-\frac{\ell^2 k^2}{4} - i\mathbf{k}\cdot\mathbf{r}_j)$, with $Z = (1/2\pi\ell^2)^{1/2}\int d^3\mathbf{R}_1\, d^3\mathbf{R}_2\, \Psi_0^*(\mathbf{R}_1)\Psi_0(\mathbf{R}_2)U(\mathbf{R}_1 - \mathbf{R}_2) \times \chi^*(z_2)\chi(z_1)$.

Finally, the coupling constant J of the effective interaction (8) can be obtained by transforming the summation in (9) to integration in the limit $L_{x,y} \to \infty$,

$$J = \Big(\frac{A}{\Delta}\Big)^2 \frac{|Z|^2}{(2\pi)^{1/2} E_c \ell^2}\Big(\frac{d}{r}\Big)^{1/2}\exp\Big(-\frac{r}{d}\Big), \quad (r > \ell)\,, \qquad (10)$$

where $d = (E_c/2\Delta)^{1/2}\ell$. A similar dependence of the coupling on the donor separation r was obtained in a study of nuclear polarization diffusion in the quantum-Hall regime [21]. Interaction (8) between the spins has finite range d, which, however, is very large compared to the effective Bohr radius of the donor ground state. Thus, the indirect exchange at large distances dominates the direct exchange interaction resulting from the overlap of the two atomic wave functions. For magnetic field $H = 6$ T and $\epsilon = 12$, we get $d \simeq 65$ nm, which is indeed much greater than the characteristic Bohr radius for a donor electron in silicon.

In order to estimate J, we have to evaluate the overlap integral Z. For an order-of-magnitude estimate, we will assume that $\chi(z)$ is constant inside the well and zero outside. Then $Z \simeq (2\pi)^{-1/2}(\delta\ell)^{-1}\int d^3\mathbf{R}_1\, d^3\mathbf{R}_2 \times \Psi_0^*(\mathbf{R}_1)\Psi_0(\mathbf{R}_2)U(\mathbf{R}_1 - \mathbf{R}_2)$, where δ is the width of the well. We put $\delta \simeq 4$ nm. For $\Psi_0(\mathbf{R})$, the donor ground state, we choose a spherically symmetric hydrogenlike ground state with the effective Bohr radius $a_B \simeq 2$ nm. This is, of course, not the case in a realistic situation [22]. The ground state of the donor will be influenced by the band structure, by the magnetic field, and by the confining 2D well potential, while the states of the conducting electrons will be distorted by the impurity potentials. We are not aware of a thorough study of these effects for our system. For the purposes of an order of magnitude estimate, however, a spherical state should be sufficient.

Evaluating the integral for the Coulomb potential U, we obtain $Z \simeq (5a_B^2/16\delta)E_c$. Assuming that the two donors are separated by the distance $r = 100$ nm and using the value $2A/h = 58$ MHz from [4], we obtain the estimate $J/\hbar \sim 10^2\ \mathrm{s}^{-1}$.

The clock speed of the information processor just described appears to be a fraction of kHz and should be compared with the time scales for relaxation and decoherence. The leading mechanism for these at low temperatures is through interaction with impurities. It has been found theoretically [12,23] and confirmed experimentally [2] that nuclear-spin relaxation in the quantum-Hall regime is slow and strongly dependent on the impurity potentials; typically, the relaxation time T_1 is of order 10^3 s. In our case, the interaction of a qubit with the 2D gas is stronger, and, as a result, the relaxation is expected to be faster. An estimate from formulas in [12,23] gives $T_1 \simeq 1$ s. There is, however, another important issue—decoherence, on time scales T_2. Recently, this quantity has been calculated in the same framework, that is, when the interaction of the conduction electrons with impurities is taken into account [14]. The results of [14] can be adjusted for the present case and yield the estimate $T_2 \simeq 10^{-1}$ s.

The existing quantum error correction protocols require the quality factor, equal the ratio of the gate-function clock time to decoherence time, not to exceed 10^{-5} [24]. Our estimates indicate that this is not the case for the present system. Actually, no quantum-computing proposal to date, scalable by other criteria, satisfies this 10^{-5} quality-factor criterion. The values range from 10^{-1} to 10^{-3}. The resolution could come from development of better error-correction algorithms or from improving the physical system to obtain a better quality factor. In our estimate of the decoherence time scale, we used parameters typical of a standard, "dirty" heterostructure with large spatial fluctuations of the impurity potential. These heterostructures have been suitable for standard experiments because they provide wider quantum-Hall plateaus. Much cleaner, ultrahigh mobility structures can be obtained by placing the ionized impurity layer at a larger distance from the 2D gas or by injecting conduction electrons into the heterostructure by other means.

Thus, our present quantum-computing proposal offers a clear direction for exploring a physical, rather than algorithmic, resolution to the quality-factor problem. This possibility should be further examined both experimentally and theoretically. Our new quantum-computing paradigm suggests several interesting avenues for research. The effect of gates on the switching of qubit interactions and on decoherence requires further investigation. The first experimental realizations will probably involve only a few qubits. The interactions of these may be significantly affected by the geometry, specifically, the edges, of the heterostructure.

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Nuclear-spin qubit dephasing time in the integer quantum Hall effect regime

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We report a theoretical estimate of the nuclear-spin dephasing time T_2 owing to the spin interaction with the two-dimensional electron gas, when the latter is in the integer quantum Hall state, in a two-dimensional heterojunction or quantum well at low temperature, and in large applied magnetic field. We argue that the leading mechanism of dephasing is due to the impurity potentials that influence the dynamics of the spin via virtual magnetic spin-exciton scattering. Implications of our results for implementation of nuclear spins as quantum bits (qubits) for quantum computing are discussed.

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I. INTRODUCTION

Recent ideas[1–3] for utilizing nuclear spins in semiconductor quantum wells and heterojunctions as quantum bits (qubits) for quantum computation have generated an emphasis on the studies of nuclear-spin relaxation and, especially, quantum decoherence, in such systems. In this paper we consider the case of the integer $\nu=1$ quantum Hall state.[4] The two-dimensional electron gas is then in a nondissipative state. Since the electrons mediate the dominant interaction[1,5,6] between nuclear spins, it is reasonable to expect that relaxation times of the latter, as well as decoherence/dephasing effects, will occur on large time scales.

Solid-state proposals for quantum computation[1–3] with nuclear spins are all presently theoretical. Related proposals to utilize quantum dots[7–15] are also, at present, all in the theory stage. Usually, nonzero nuclear-spin atoms will be considered placed[1] by modern ''atomic engineering'' techniques in a host material of zero nuclear-spin isotope. In order to allow positioning with respect to other features of the system, such as gate electrodes,[2] and making replicas,[1] etc., the nuclear-spin separation will be larger than the atomic size, typically, of the order of 20 to 100 Å. At these separations, the direct magnetic dipole-dipole interaction of the nuclear spins is negligible.

The dynamics of the nuclear spins is governed by their interactions with each other and with their environment. In the regime of interest, these interactions are mediated by the two-dimensional electron gas. Various time scales are associated with this dynamics. The relaxation time T_1 is related to the energy exchange and thermalization of the spins. Quantum-mechanical decoherence and dephasing will occur on the time scale T_2. The latter processes correspond to the demolition of the quantum-mechanical superposition of states and erasure of phase information, due to interactions with the environment. Generally, there are many dynamical processes in the system, so the times T_1 and T_2 may not be uniquely, separately defined.[16,17] Theoretically and experimentally, it has been established that processes of energy exchange are slow at low temperatures, so T_1 is very large, but there still might be some decoherence owing to quantum fluctuations. Generally, for various systems, there are extreme examples of theoretical prediction, ranging from no decoherence to finite decoherence[18-20] at zero temperature, depending on the model assumptions.

In order to consider control (''programming'') of a quantum computer, we have to identify the time scale $T_{\rm ext}$ of the single-spin rotations owing to the interactions with an external NMR magnetic field. We also identify the time scale $T_{\rm int}$ associated with evolution owing to the pairwise spin-spin interactions. The preferred relation of the time scales is T_1, $T_2 \gg T_{\rm ext}$, and $T_{\rm int}$, which is obviously required for coherent quantum-mechanical dynamics.

The aim of this paper is to advance theoretical understanding of the time scales of interest for the quantum computer proposal[1] based on nuclear spins in a two-dimensional electron gas, with the latter in the integer quantum Hall effect state obtained at low temperatures, of order 1 K, and in high magnetic fields, of several Tesla, in two-dimensional semiconductor structures.[4] This system is a promising candidate for quantum computing because the nuclear spin relaxation time T_1 can be as large as 10^3 sec. In the summarizing discussion, Sec. V, we discuss and compare the values of all the relevant time scales.

Our main result, presented in Secs. II through IV, is a theoretical calculation of the nuclear-spin dephasing/decoherence time scale T_2 for such systems. We note that the recent study[21–23] of the nuclear-spin relaxation time T_1 has relied heavily on the accepted theoretical and experimental views of the properties and behavior of the *electronic state* of the two-dimensional electron gas in the quantum Hall regime. These electronic properties have been a subject of several studies.[4–6,21–29] We utilize these results in our calculation as well.

II. THE MODEL

We consider a single nuclear spin coupled to a two-dimensional electron gas in a strong magnetic field B along the z axis that is perpendicular to the two-dimensional structure. Assuming nuclear spin-1/2, for simplicity, we write the Hamiltonian as

$$H = H_n + H_e + H_{ne} + H_{\rm imp}. \tag{1}$$

Here, the first term is the nuclear-spin interaction with the external magnetic field, $H_n=-1/2\gamma_n B\sigma_z$, where γ_n includes $\hbar$ and the nuclear g factor, and σ_z is a Pauli matrix.

The second term is the electronic component of the total Hamiltonian (1). Within the free-electron nomenclature, the Fermi level lies in between the two Zeeman sublevels of the lowest Landau level. The spin-up sublevel is then completely occupied, so the filling factor is $\nu=1$, while the spin-down sublevel is completely empty; note that the relevant effective electronic g factor in typically negative. In fact, the calculation need not be limited to the lowest Landau level. Here, however, to avoid unilluminating mathematical complications, we restrict our attention to the lowest level, as has been uniformly done in the literature.[24,25]

The last two terms in Eq. (1) correspond to the nuclear-spin electron interactions and to the effects of impurities. These will be addressed shortly. The magnetic sublevels are actually broadened by impurities. At low temperatures, the $\nu=1$ system is in the quantum Hall state. The interactions of the two-dimensional electron gas with the underlying material are not shown in Eq. (1). They are accounted for phenomenologically, as described later.

The electron-electron interactions are treated within an approximate quasiparticle theory that only retains transition amplitudes between Zeeman sublevels. The elementary excitations of the electron gas are then well described as magnetic spin excitons, or spin waves.[24–27] The spin excitons are quasiparticles arising as a result of the interplay between the Coulomb repulsion of the electrons and their exchange interaction. A creation operator of a spin exciton with a two-dimensional wave vector $\mathbf{k}$ can be written in terms of the electronic creation operators $a^\dagger$ in the spin-down Zeeman sublevel and annihilation operators b in the spin-up sublevel as

$$A_{\mathbf{k}}^\dagger=\sqrt{\frac{2\pi l^2}{L_xL_y}}\sum_p\ e^{il^2k_xp}a_{p+k_y/2}^\dagger b_{p-ky/2}. \tag{2}$$

Here, $l=\sqrt{c\hbar/eB}$ is the magnetic length, and the p summation is taken in such a way that the wave number subscripts are quantized in multiples of $2\pi/L_y$. Note that expression (2) assumes the Landau gauge, which is not symmetric under $x\leftrightarrow y$.

For our purposes, the following parabolic approximation for the dispersion relation of the excitons[24–27] provides an adequate approximation,

$$E_{\mathbf{k}}=\Delta+\left(\frac{\pi}{2}\right)^{1/2}\left(\frac{e^2}{\epsilon l}\right)\frac{l^2k^2}{2}. \tag{3}$$

Here, $\Delta=|g|\mu_BB$, where μ_B is the Bohr magneton, and g is the electronic g factor, and ϵ is the dielectric constant of the material. It has been pointed out[6,23] that the gap Δ in the excitonic spectrum suppresses nuclear-spin relaxation at low temperatures. The dispersion relation for spin excitons actually levels out at large wave vectors. However, its precise form is only known within a single-Landau-level approximation,[24,25] which is not valid, for instance, for Si, a material that is a likely candidate for quantum computer realizations. Calculations beyond this approximation[27] are not definitive. Therefore, in order to avoid introduction of an arbitrary cutoff parameter, we stick with the parabolic form, which allows an analytical calculation, even though some of our expressions require the dispersion relation for wave-vector values that are not technically small.

The electronic Hamiltonian can be written in terms of the spin exciton operators as

$$H_e=\mathcal{E}_0+\sum_{\mathbf{k}}\ E_{\mathbf{k}}A_{\mathbf{k}}^\dagger A_{\mathbf{k}}, \tag{4}$$

where the c-number $\mathcal{E}_0$ is the spin-independent ground-state energy of the electron gas. This description of the electronic gas is appropriate only for low density of excitons, which is the case in our calculation, as will be seen later.

We now turn to the third term in Eq. (1), the interaction between the electrons and nuclear spins. It can be adequately approximated by the hyperfine Fermi contact term

$$H_{ne}=\frac{8\pi}{3}\gamma_ng\mu_B\mathbf{I}_n\cdot\sum_e\ \mathbf{S}_e\delta^{(3)}(\mathbf{r}_e-\mathbf{R}_n). \tag{5}$$

Here, $\hbar\mathbf{I}_n$ and $\hbar\mathbf{S}_e$ are nuclear- and electronic spin operators, respectively, and $\mathbf{r}_e$ are the electron coordinates. The nuclear coordinate $\mathbf{R}_n$ can be put equal to zero. Such an interaction can be split into two parts

$$H_{ne}=H_{\mathrm{diag}}+H_{\mathrm{offdiag}}, \tag{6}$$

where H_{diag} corresponds to the coupling of the electrons to the diagonal part of nuclear-spin operator I_n, and H_{offdiag}—to its off-diagonal part.

The diagonal and off-diagonal contributions can be rewritten in terms of electronic creation and annihilation operators as

$$H_{\mathrm{diag}}=\frac{(8\pi/3)\gamma_ng\mu_B|w_0(0)|^2}{\sqrt{\pi}L_yld}\times\sum_{k,q}\ e^{-l^2/2(k^2+q^2)}\sigma_z(a_k^\dagger a_q-b_k^\dagger b_q), \tag{7}$$

$$H_{\mathrm{offdiag}}=\frac{(8\pi/3)\gamma_ng\mu_B|w_0(0)|^2}{\sqrt{\pi}L_yld}\times\sum_{k,q}\ e^{-l^2/2(k^2+q^2)}(\sigma^+b_k^\dagger a_q+\sigma^-a_k^\dagger b_q). \tag{8}$$

Here, $\sigma^\pm=1/2(\sigma_x\pm i\sigma_y)$. The interactions of the electrons of the two-dimensional gas with the underlying material are incorporated phenomenologically through the dielectric constant and g factor, see Eq. (3), *et seq.*, and via $|w_0(0)|^2$ and d in Eq. (8) above. The latter is the transverse dimension of the effectively two-dimensional region (heterojunction, quantum well) in which the electrons are confined. The quantity $w_0(0)$ represents phenomenologically the enhancement of the amplitude of the electron wave function at the nuclear position owing to the effective potential it experi-

ences as it moves in the solid-state material. It is loosely related[5,6] to the zero-momentum lattice Bloch wave function at the origin.

For the purposes of the calculations performed here, with the relevant states being the ground state and the single-exciton states of the electron gas, one can show that the terms in Eq. (7) that correspond to different k and q do not contribute, while the remaining sum over k becomes a c number, representing the Knight shift of the polarized electrons. Thus, $H_{\rm diag}$ can be incorporated into the nuclear-spin energy splitting, redefining the Hamiltonian of the nuclear spin as $H_n = 1/2\Gamma\sigma_z$, where $\Gamma = \gamma_n(B + B_{\rm Knight})$. Note that the Knight shift can be used to estimate the value of the phenomenological parameter $|w_0(0)|$ from experimental data. The off-diagonal coupling (8) can be expressed in terms of the excitonic operators (2) as follows:[5,6,23]

$$H_{\rm offdiag} = \frac{C}{\sqrt{L_x L_y}} \sum_{\mathbf{k}} e^{-l^2k^2/4}(A_{\mathbf{k}}^{\dagger}\sigma^- + A_{\mathbf{k}}\sigma^+), \tag{9}$$

where

$$C = \frac{(8\pi/3)\gamma_n g \mu_B |w_0(0)|^2}{\sqrt{2\pi} l d}. \tag{10}$$

The summations over k_x and k_y are taken over all the integer multiples of $2\pi/L_x$ and $2\pi/L_y$, respectively.

The last term in Eq. (1) describes the interaction of the electrons with impurities and plays a crucial role in nuclear relaxation in the systems of interest. This interaction can be written in the spin-exciton representation as[23,26]

$$H_{\rm imp} = (2i/L_x L_y) \sum_{\mathbf{k},\mathbf{q}} U(\mathbf{q}) \sin[l^2(k_x q_y - k_y q_x)/2] A_{\mathbf{k}}^{\dagger} A_{\mathbf{k}+\mathbf{q}}, \tag{11}$$

where $U(\mathbf{q}) = \int U_{\rm imp}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^2\mathbf{r}$ is the Fourier component of the impurity potential for electrons in the two-dimensional plane. We will assume[23,26] that the impurity potential has a zero average and can be modeled by the Gaussian white noise completely described by its correlator, $\langle U_{\rm imp}(\mathbf{r}) U_{\rm imp}(\mathbf{r}')\rangle = Q\delta^{(2)}(\mathbf{r} - \mathbf{r}')$.

In summary, the relevant terms in the full Hamiltonian (1) can be expressed solely in terms of the nuclear-spin operators and spin-exciton operators as

$$H = -\frac{1}{2}\Gamma\sigma_z + \sum_{\mathbf{k}} E_{\mathbf{k}} A_{\mathbf{k}}^{\dagger} A_{\mathbf{k}} + \sum_{\mathbf{k}} g_{\mathbf{k}}(A_{\mathbf{k}}^{\dagger}\sigma^- + A_{\mathbf{k}}\sigma^+) + \sum_{\mathbf{k},\mathbf{q}} \phi_{\mathbf{k},\mathbf{q}} A_{\mathbf{k}}^{\dagger} A_{\mathbf{k}+\mathbf{q}}, \tag{12}$$

where the explicit expressions for $E_{\mathbf{k}}$, $g_{\mathbf{k}}$ and $\phi_{\mathbf{k},\mathbf{q}}$ can be read off Eqs. (3), (9), and (10), respectively, and the quantity Γ was introduced in the text preceding Eq. (9).

III. ENERGY RELAXATION

In order to set the stage for the calculation of T_2, let us first briefly summarize in this section aspects of the calculation of the nuclear-spin relaxation time T_1, along the lines of.[22,23] The dominant mechanism for both processes at low temperatures is the interactions with impurities. Thus, both calculations are effectively zero temperature, single spin; these assumptions will be further discussed in Sec. V.

We assume that initially at time $t=0$ the nuclear spin is polarized, while the excitons are in the ground state, $|\Psi(0)\rangle = |-\rangle \otimes |\mathbf{0}\rangle$, where $|-\rangle$ is the polarized-down (excited) state of the nuclear spin and $|\mathbf{0}\rangle$ is the ground state of spin excitons. Since the Hamiltonian (12) conserves the z component of the total spin in the system, the most general wave function evolving from $|\Psi(0)\rangle$ can be written as

$$|\Psi(t)\rangle = \alpha(t)|-\rangle \otimes |\mathbf{0}\rangle + \sum_{\mathbf{k}} \beta_{\mathbf{k}}(t)|+\rangle \otimes |\mathbf{1}_{\mathbf{k}}\rangle, \tag{13}$$

with $|+\rangle$ corresponding to the nuclear spin in the ground state and $|\mathbf{1}_{\mathbf{k}}\rangle$ describing the single-exciton state with the wave vector $\mathbf{k}$. Equations of motion for the coefficients α and $\beta_{\mathbf{k}}$ can be easily derived from the Schrödinger equation:

$$i\hbar\dot{\alpha} = \frac{1}{2}\Gamma\alpha + \sum_{\mathbf{k}} g_{\mathbf{k}}\beta_{\mathbf{k}}, \tag{14}$$

$$i\hbar\dot{\beta}_{\mathbf{k}} = -\frac{1}{2}\Gamma\beta_{\mathbf{k}} + E_{\mathbf{k}}\beta_{\mathbf{k}} + \sum_{\mathbf{q}} \phi_{\mathbf{k},\mathbf{q}}\beta_{\mathbf{q}} + g_{\mathbf{k}}\alpha. \tag{15}$$

In order to solve the system of Eqs. (14) and (15), we introduce Laplace transforms, $\tilde{f}(S) = \int_0^{\infty} f(t) e^{-St} dt$, which satisfy

$$iS\hbar\tilde{\alpha} - i\hbar = \frac{1}{2}\Gamma\tilde{\alpha} + \sum_{\mathbf{k}} g_{\mathbf{k}}\tilde{\beta}_{\mathbf{k}}, \tag{16}$$

$$iS\hbar\tilde{\beta}_{\mathbf{k}} = -\frac{1}{2}\Gamma\tilde{\beta}_{\mathbf{k}} + E_{\mathbf{k}}\tilde{\beta}_{\mathbf{k}} + \sum_{\mathbf{q}} \phi_{\mathbf{kq}}\tilde{\beta}_{\mathbf{q}} + g_{\mathbf{k}}\tilde{\alpha}. \tag{17}$$

Let us first solve Eqs. (16) and (17) for the case when the interaction of spin excitons with impurities is switched off, i.e., $\phi_{\mathbf{k},\mathbf{q}} = 0$. After some algebra we obtain

$$\frac{1}{\tilde{\alpha}(s)} = s + \frac{i}{\hbar}\sum_{\mathbf{k}} \frac{g_{\mathbf{k}}^2}{is\hbar + \Gamma - E_{\mathbf{k}}}, \tag{18}$$

where we have shifted the variable: $s = S + i\Gamma/(2\hbar)$, which only introduces an noninteresting phase factor.

In the absence of the hyperfine interaction, i.e., for $g_{\mathbf{k}} = 0$, $\tilde{\alpha}(s)$ in Eq. (18) has only the pole at $s=0$. When the interaction is switched on, the pole shifts from zero. This shift can be calculated in a standard way, within the leading order perturbative approach, by taking the limit $s \to 0$, so that $1/(i\hbar s^+ + \Gamma - E_{\mathbf{k}}) \to \mathcal{P}[1/(\Gamma - E_{\mathbf{k}})] - i\pi\delta(\Gamma - E_{\mathbf{k}})$, where $\mathcal{P}$ denotes the principal value. This type of approximation is encountered in quantum optics.[30] The relaxation rate and the added phase shift of the nuclear-spin excited-state probability amplitude $\alpha(t)$ are given by the real and imaginary parts of the pole, $1/T_1 = (2\pi/\hbar)\Sigma_{\mathbf{k}} g_{\mathbf{k}}^2 \delta(\Gamma - E_{\mathbf{k}})$ and $\omega = \mathcal{P}\Sigma_{\mathbf{k}}[g_{\mathbf{k}}^2/(\Gamma - E_{\mathbf{k}})]$, respectively, so that $\alpha(t) \propto e^{-t/2(T_1) + i\omega t}$. It is obvious that due to the large gap in the spin-exciton spectrum (3) $\Gamma \ll \Delta$ the energy conservation re-

quired by the delta function above can never be satisfied, and so in the absence of interaction with impurities, $T_1=\infty$. It also transpires that T_2 is infinite,[30] as will become apparent later.

Interactions with impurities, described by the last term in Eq. (12), will modify the solution of Eqs. (16) and (17), and, as a consequence, the energy conservation condition. In particular, if the impurity potential is strong enough, it can provide additional energy to spin excitons, so that their energy can fluctuate on the scale of order Γ, thus making nuclear-spin relaxation possible. This mechanism[22,23] corresponds to large fluctuations of the impurity potential $U(\mathbf{r})$, which usually occur with a rather small probability, so T_1 is very large for such systems.

In order to carry out the above program quantitatively, one has to solve the system of Eqs. (16) and (17) with nonzero $\phi_{\mathbf{k},\mathbf{q}}$. Such a solution is only possible within an approximation. One can introduce the effective spin-exciton self-energy $\Sigma_{\mathbf{k}}$ in Eq. (18), so that $1/(i\hbar s+\Gamma-E_{\mathbf{k}}) \to 1/(i\hbar s+\Gamma-E_{\mathbf{k}}+\Sigma_{\mathbf{k}})$. An integral equation for $\Sigma_{\mathbf{k}}$ can then be derived, taking the continuum limit in Eqs. (16) and (17). Solving this equation would allow one to calculate the relaxation rate from Eq. (18). However, in order to satisfy the energy conservation, we require $\Gamma-E_{\mathbf{k}}+\Sigma_{\mathbf{k}}=0$, so the self-energy should be rather large, of order $E_{\mathbf{k}}$. Therefore, as a result of the spectral gap of the excitons, the perturbative approach is inadequate as it automatically assumes that $|\Sigma_{\mathbf{k}}| \ll |E_{\mathbf{k}}|$. Instead, a certain variational approach[23,31,32] has been adapted to evaluate T_1, consistent with the experimental values[33,34] of order 10^3 sec; for further discussion, see Sec. V.

IV. DEPHASING MECHANISM

We argue that in order to calculate the phase shift due to the impurity potential, one can indeed use the perturbative solution of Eqs. (16) and (17). Indeed, phase shifts result in virtual processes that do not require energy conservation and therefore are dominated by relatively small fluctuations of the impurity potential simply because large fluctuations are very rare. Moreover, the terms of the sum in Eq. (18) that contribute to the relaxation rate do not contribute to the phase shift, see the discussion above. This consideration also applies when the self-energy is introduced.

One can show that the contribution to dephasing linear in $\phi_{\mathbf{k},\mathbf{p}}$ vanishes due to symmetry. Thus, let us solve Eqs. (16) and (17) perturbatively up to the second order in $\phi_{\mathbf{k},\mathbf{p}}$ and perform the inverse Laplace transform of $\tilde{\alpha}(s)$. Within this approximation, the pole of $\tilde{\alpha}(s)$ in the complex-s plane is imaginary, so that $|\alpha(t)|=1$. We conclude that $\alpha(t) \propto e^{i\omega_U t}$ and $\beta_{\mathbf{k}}(t)=0$, where the part of the phase shift responsible for dephasing is

$$\omega_U=-\frac{1}{\hbar}\sum_{\mathbf{k}}\frac{g_{\mathbf{k}}}{E_{\mathbf{k}}}\sum_{\mathbf{q}}\frac{\phi_{\mathbf{k},\mathbf{q}}}{E_{\mathbf{k}-\mathbf{q}}}\sum_{\mathbf{p}}\frac{\phi_{\mathbf{k}-\mathbf{q},\mathbf{p}}g_{\mathbf{k}-\mathbf{q}-\mathbf{p}}}{E_{\mathbf{k}-\mathbf{q}-\mathbf{p}}}. \quad (19)$$

The zeroth-order term in Eq. (19) was dropped as irrelevant for our calculation of the dephasing time. Since Γ is much smaller than $E_{\mathbf{k}}$, it was also omitted.

As expected, the perturbative solution does not describe the energy relaxation (T_1), but it does yield the additional phase shift due to the impurity potential. We will see shortly that this phase shift, when averaged over configurations of the impurity potential, produces a finite dephasing time, T_2.

Let us consider the reduced density matrix of the nuclear spin, given by

$$\rho_n(t)=[\mathrm{Tr}_e|\Psi(t)\rangle\langle\Psi(t)|]_U, \quad (20)$$

recall Eq. (13). Here the trace is partial, taken over the states of the spin excitons, while the outer brackets denote averaging over the impurity potential. The trace over the spin excitons can be carried out straightforwardly because, within the leading-order perturbative approximation used here, they remain in the ground state; all excitations are virtual and contribute only to the phase shift. The diagonal elements of $\rho_n(t)$ are not influenced by virtual excitations and remain constant.

The off-diagonal elements of $\rho_n(t)$ contain the factors $e^{\pm i\omega_U t}$. It is the averaging of these quantities over the white-noise impurity potential $U(\mathbf{r})$ that yields dephasing of the nuclear spin. In order to proceed, let us rewrite Eq. (19) more explicitly. From Eqs. (9)–(11), after changing the summation index $(\mathbf{k}\to\mathbf{k}-(\mathbf{q}+\mathbf{p})/2)$ in the first sum in Eq. (19) we obtain

$$\omega_U=\frac{4C^2}{\hbar(L_xL_y)^3}\sum_{\mathbf{q},\mathbf{p}}U(\mathbf{q})U(\mathbf{p})e^{-(l^2/8)(\mathbf{p}+\mathbf{q})^2} \times\sum_{\mathbf{k}}\frac{e^{-(l^2/2)\mathbf{k}^2}\sin\frac{l^2}{2}\left[\mathbf{k}+\frac{\mathbf{p}}{2},\mathbf{q}\right]_z\sin\frac{l^2}{2}\left[\mathbf{k}-\frac{\mathbf{q}}{2},\mathbf{p}\right]_z}{E_{\mathbf{k}+\mathbf{q}+\mathbf{p}/2}E_{\mathbf{k}+\mathbf{q}-\mathbf{p}/2}E_{\mathbf{k}-\mathbf{q}+\mathbf{p}/2}}. \quad (21)$$

Here we use the following shorthand notation for the z component of a vector product

$$[\mathbf{k},\mathbf{q}]_z=k_xq_y-k_yq_x.$$

It is appropriate to assume that impurity potentials are short ranged, i.e., $a \ll l$, where a is the scale of variation of $U_{\mathrm{imp}}(\mathbf{r})$. This assumption and the white-noise property of the impurity potentials, are required to make the problem amenable to analytical calculation. Thus, the main contribution to the Fourier transform $U(\mathbf{p})$, dominating the summation in Eq. (21), comes from large wave vectors $\mathbf{p}$ (and $\mathbf{q}$), of the order $a^{-1} \gg l^{-1}$. Therefore, one can replace the exponent $e^{-(l^2/8)(\mathbf{p}+\mathbf{q})^2}$ by the Kronecker symbol $\delta_{\mathbf{q},-\mathbf{p}}$, to obtain a simplified expression for ω_U

$$\omega_U=\frac{4C^2}{\hbar(L_xL_y)^3}\sum_{\mathbf{p}}U(\mathbf{p})U(-\mathbf{p})\sum_{\mathbf{k}}\frac{e^{-(l^2/2)\mathbf{k}^2}\sin^2\frac{l^2}{2}[\mathbf{k},\mathbf{p}]_z}{E_{\mathbf{k}}^2E_{\mathbf{k}+\mathbf{p}}}. \quad (22)$$

Now the sum over $\mathbf{k}$ can be carried out because for $\mathbf{p} \gg \mathbf{k}$, we can assume that $E_{\mathbf{k}+\mathbf{p}} \simeq E_{\mathbf{p}} \simeq E_c(l^2/2)\mathbf{p}^2$, where $E_c=(\pi/2)^{1/2}[e^2/(\epsilon l)]$.

Moreover, for large $\mathbf{p}$, the factor $\sin^2\{(l^2/2)[\mathbf{k},\mathbf{p}]_z\}$ can be replaced by its average, 1/2. Finally, we get

$$\frac{1}{L_xL_y}\sum_{\mathbf{k}}\frac{e^{-(l^2/8)\mathbf{k}^2}\sin^2\frac{l^2}{2}[\mathbf{k},\mathbf{p}]_z}{E_{\mathbf{k}}^2E_{\mathbf{k}+\mathbf{p}}} \simeq \frac{1}{E_cl^2\mathbf{p}^2}\frac{1}{2\pi}\int kdk\frac{e^{-l^2/8k^2}}{\left(\Delta+E_c\frac{l^2}{2}k^2\right)^2}. \quad (23)$$

The integral can be evaluated explicitly; specifically, for $\Delta/E_c \ll 1$ we get

$$\int_0^\infty kdk\frac{e^{-l^2/8k^2}}{\left(\Delta+E_c\frac{l^2}{2}k^2\right)^2}\simeq\frac{1}{l^2E_c\Delta}, \quad (24)$$

so that

$$\omega_U=\frac{2C^2}{\hbar\pi E_c^2l^4\Delta}\frac{1}{(L_xL_y)^2}\sum_{\mathbf{p}}\frac{U(\mathbf{p})U(-\mathbf{p})}{\mathbf{p}^2}. \quad (25)$$

Recall that we have assumed the white-noise distribution for the impurity potential, $\langle U_{\rm imp}(\mathbf{r})U_{\rm imp}(\mathbf{r}')\rangle = Q\delta^{(2)}(\mathbf{r}-\mathbf{r}')$. This corresponds to the following probability distribution functional for the Fourier transformed potential:

$$P[U(p)]=N\exp\left[-\frac{1}{2QL_xL_y}\sum_{\mathbf{p}}U(\mathbf{p})U(-\mathbf{p})\right]. \quad (26)$$

The latter expression, and other approximations assumed earlier, allow us to reduce the averaging of $e^{i\omega_U t}$ to a product of Gaussian integrations. The off-diagonal elements of the nuclear-spin density matrix are, thus,

$$\rho_{01}\sim\prod_{\mathbf{p}}\left(1-\frac{i\tau}{L_xL_y\mathbf{p}^2}\right)^{-1/2} =\exp\left[-\frac{1}{2}\sum_{\mathbf{p}}\ln\left(1-\frac{i\tau}{L_xL_y\mathbf{p}^2}\right)\right], \quad (27)$$

where $\tau=4QC^2t/(\hbar\pi E_c^2l^4\Delta)$.

We are interested in the real part of the sum in Eq. (27), which represents decoherence/dephasing of the nuclear spin. The off-diagonal elements decay exponentially as

$$\rho_{01}\sim\exp\left[-\frac{1}{4}\sum_{\mathbf{p}}\ln\left(1+\frac{\tau^2}{(L_xL_y)^2\mathbf{p}^4}\right)\right]. \quad (28)$$

The summation over $\mathbf{p}$ can be converted into integration

$$\sum_{\mathbf{p}}\ln\left(1+\frac{\tau^2}{(L_xL_y)^2\mathbf{p}^4}\right)=\frac{L_xL_y}{(2\pi)^2}\int d^2\mathbf{p}\ln\left(1+\frac{\tau^2}{(L_xL_y)^2\mathbf{p}^4}\right). \quad (29)$$

Explicit calculation then yields the result that $\rho_{01}\sim e^{-\tau/16}$ or $\rho_{01}\sim e^{-t/T_2}$, where

$$T_2=\frac{2\hbar l^2\Delta}{U_2C^2} \quad (30)$$

with $U_2=Q/(2\pi l^2E_c^2)$.

V. RESULTS AND DISCUSSION

The quantity U_2 characterizes the strength of the impurity potential with respect to the Coulomb interactions.[26] Let us summarize typical parameter values[26] for a GaAs heterojunction, which is the system best studied in the literature. For magnetic field value $B=10\,\mathrm{T}$, we have the following values of parameters: $l=0.8\times10^{-8}\,\mathrm{m}$, $E_c=3\times10^{-21}\,\mathrm{J}$, $C=2.5\times10^{-36}\,\mathrm{Jm}$, $\Delta=4.6\times10^{-23}\,\mathrm{J}$. From the experimental data for electronic mobility, one then estimates[26] $U_2\simeq0.0025$, yielding $T_2\simeq40\,\mathrm{sec}$. We emphasize that this is an order of magnitude estimate only, because of the uncertainty in various parameter values assumed and the fact that the parameters, especially the strength of the disorder, may vary significantly from sample to sample. For instance, there is another estimate of the disorder strength Q available in the literature,[23] obtained by fitting the value of T_1 to the experimentally measured $10^3\,\mathrm{sec}$,[33,34] as cited earlier. This yields an estimate for T_2 that is smaller, $T_2\simeq0.5\,\mathrm{sec}$. Generally, we expect that with typical-quality samples, T_2 may be a fraction of a second or somewhat larger.

In ordinary semiconductors, even at low temperatures, the decoherence times would be expected to be 2–3 orders of magnitude shorter than our values. The reason that the decoherence is that slow here is that we consider the case when the spectrum of the electron-gas excitations has a gap, which slows down both relaxation and decoherence. The main indication that there are no other mechanisms operational comes from the success of the relaxation time T_1 calculations,[21–23] which were confronted with experiment.[33,34] However, we emphasize that at close nuclear-spin separations, their direct dipolar interaction does provide an alternative, at least as an effective mechanism.[35] Thus, our results are limited to the case of large nuclear spin separations, appropriate for quantum computing architectures, for which the host material will have to be isotope engineered with zero nuclear spins, e.g., Si.[2] To date, there are no direct experimental probes of dephasing by the disorder-dominated mechanism identified here for dilute nuclear-spin positioning. For those materials whose atoms have nonzero nuclear-spin-isotope nuclei, specifically, for GaAs (spins 3/2), we are aware only of one experiment[35] where indirect information on dephasing can be obtained from the linewidth. Indeed, in that case the dipolar interaction likely provides the dominant dephasing mechanism. We also point out that the assumption of low temperature assures that indirect decoherence and relaxation mechanisms via the electrons are not operational.

Let us now compare various time scales relevant for quantum computing applications. The relaxation time T_1 is of order $10^3\,\mathrm{sec}$.[23,33,34] For the spin-spin interaction time scale $T_{\rm int}$, values as short as $10^{-11}\,\mathrm{sec}$ have been proposed.[1,5] These estimates are definitely overly optimistic and require further work. Since such calculations require

considerations beyond the single spin interactions, they are outside the scope of the present paper. For T_{ext}, modern experiments have used NMR field intensities corresponding to the spin-flip times of 10^{-5} sec. This can be reduced to 10^{-7} sec, and with substantial experimental effort, perhaps even shorter times, the main limitation being heating up of the sample by the radiation.

Thus, the present information on the relevant time scales does not show a violation of the condition T_1, $T_2 \gg T_{ext}$, T_{int}, stated in the introduction, required for quantum computing. To firmly establish the feasibility of quantum computing, reliable theoretical evaluation of T_{int} is needed, as well as experimental realizations of few-qubit systems engineered with nuclear spins positioned as separations of order 30–100 Å.

We also note that typical lab samples, for which the parameter values used were estimated, have been prepared to observe the quantum Hall effect plateaus in the resistance. The latter requires a finite density of impurities. However, for the quantum-computer applications, a much cleaner sample would suffice. Indeed, as suggested by our calculations, T_2 is mostly due to dephasing owing to virtual spin-exciton scattering from impurities. Therefore, the value of T_2 can be increased by using cleaner samples.

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Quantum computation in quantum-Hall systems

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Abstract

We describe a quantum information processor (quantum computer) based on the hyperfine interactions between the conduction electrons and nuclear spins embedded in a two-dimensional electron system in the quantum-Hall regime. Nuclear spins can be controlled individually by electromagnetic pulses. Their interactions, which are of the spin-exchange type, can be possibly switched on and off pair-wise dynamically, for nearest neighbors, by controlling impurities. We also propose the way to feed in the initial data and explore ideas for reading off the final results. © 1998 Elsevier Science B.V.

The field of quantum computing has seen an explosive growth of theoretical development [1–7]. It has been realized that quantum computers can be faster than classical computers for some problems [1–3,8–13]. The analog nature of errors and possible error correction schemes have been explored [6,7,9,13–21]. There have also been several proposals for actual realizations of quantum information processing [4,5,13,22–31]. Two of these proposals, the ion-trap system [5,22,25,27,28] and the ensemble-of-molecules liquid-state NMR approach [29–31] have been studied extensively as possible experimental realizations of quantum computing. However, all experimental results to date only accomplish the simplest quantum-logic functions such as single-spin rotations or two-spin controlled-NOT [1–7].

A major challenge faced by both experiment and theory has involved scaling up from one to many quantum gates and actual "programming," i.e., conducting calculations by coherent quantum unitary evolution, in a controlled fashion. Experimentally, quantum computation requires switching on and off pair-wise interactions between various two-state systems, e.g., spins $\frac{1}{2}$, termed "qubits." Initialization and reading off the final results are also nontrivial parts of the process. Ideally, the latter should involve efficient measurement of a single qubit. The NMR variant [29–31] measures instead ensemble averages (expectation values). Certain "fault-tolerant" error correction schemes [7,13,17,19–21] actually also require measurements of some of the qubits *during* the computation.

Theoretically, the most striking recent development has been the formulation of the fault-tolerant error correction schemes [7,13,17,19–21]. Correction of analog errors inherent in quantum computation due to the superposition-of-states property (which in turn is central to the speed-up of some calculations) means an uphill battle against the second law of thermodynamics. These error correction schemes [7,13,17,19–21] aim at calculations that can go on indefinitely

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provided the overall error rate at each qubit is small enough.

It is not our goal here to review these issues: We will adopt the point of view that modern error correction schemes will allow calculations long enough to be useful provided a working quantum information processor can be devised. It is the latter aspect that we address in this work. Thus, we propose a quantum computer realization based on hyperfine interactions [32] between the conduction electrons and nuclear spins embedded in a two-dimensional electron system in which the electron gas is in the quantum-Hall effect (QHE) regime [33,34]. Such systems have been made at the interfaces between semiconductor materials and in superlattices (layered semiconductor structures) [35].

In these systems, at temperatures of order 1 K and applied magnetic fields of several teslas, there are intervals of magnetic field values for which the electrons fill up an integer number of Landau levels [36]. The electron gas then forms a nondissipative QHE fluid [35]; the Hall resistance exhibits a plateau at a value that is a multiple of e^2/h, while the dissipativity of the conduction electron gas (the magnetoresistance) approaches zero. Nuclear-spin thermalization/relaxation processes occur on the time scale denoted T_1 [32], which, experimentally, ranges from several minutes to half an hour [37–39]. It is then expected that the nuclear spin dynamics is dominated by coherent spin exchanges mediated by electrons [40,41]. Owing to rapid advances in the experimental facilities, the hyperfine interactions in QHE systems have recently attracted growing theoretical [41,42] and experimental [37–39] interest; this progress makes it feasible to handle the electron spin–nuclear spin interactions with almost atomic precision.

Similar to the ion-trap system [5,22,25,27,28], we consider a chain of spin-$\frac{1}{2}$ nuclei, of atoms positioned by the molecular-beam epitaxy techniques [35] in an effectively two-dimensional system subjected to a strong magnetic field. The typical separation should be comparable to the magnetic length $\ell_H = (\hbar c/eH)^{1/2}$, where H is the applied magnetic field, perpendicular to the two-dimensional layer. This length is of the order of 100 Å. We propose to control individual nuclear spins by electromagnetic-radiation pulses in the nuclear magnetic resonance (NMR) frequency range [32].

An important question is how to control nuclear spins individually. Use of a magnetic field gradient could be contemplated to achieve differentiation, but there are severe limitations on the field variation owing to the need to maintain the QHE electronic state. Instead, one can use *different nuclei*. Theoretically, there is no apparent limit on how many different spins can be arranged in a chain. However, practically the number of suitable spin-$\frac{1}{2}$ isotopes may be limited. Thus, achieving sufficient chemical-shift dispersion for systems of more than few qubits may require additional ideas; the following ones are tentative because presently it is not known how realistic these proposals are from the point of view of actual experimental realizations. Specifically, one can position nuclear spins in different crystalline environments. The latter can be controlled by implanting atoms and complexes into the host material [32]. It may also be possible to utilize small clusters of nuclear spins, rather than individual spins. These can be made coherent [43] by lowering the temperature to a value of order of several μK, as compared to order 1 K needed to achieve the QHE state.

Under the typical conditions of QHE the direct dipole–dipole interaction of the nuclear spins is negligibly small [41]. The dominant interaction will be mediated by the contact hyperfine interactions between nuclear spins and conduction electrons [40]. Similarly, electron-mediated interactions leading to the scalar coupling have been utilized in the liquid-state NMR realization of quantum computation [29–31]. In ordinary metals, the electron-mediated nuclear spin interactions exhibit Friedel oscillations [32] because of the existence of a sharp Fermi surface.

In the quantum-Hall regime, however, the energy spectrum of the two-dimensional electron gas is discretized by the magnetic field. As a result, the interaction is no longer oscillatory but rather monotonic, exponentially decaying [40] on the length scale ℓ_H. The following terms in the effective phenomenological two-spin interaction Hamiltonian correspond to the second-order perturbative calculation (carried out for two identical nuclei) of Ref. [40], where for different nuclei we replaced Z^2 by the product of the two atomic numbers (which is basically a guess),

$$-VZ^{(1)}Z^{(2)}H^{-1}\sqrt{\frac{c\ell_H}{r}}e^{-cr/\ell_H}(\sigma_-^{(1)}\sigma_+^{(2)}+\sigma_+^{(1)}\sigma_-^{(2)}), \tag{1}$$

where c is a dimensionless quantity [40] of order 1, $Z^{(j)}$ are the atomic numbers of the nuclei, while V is some constant. Note that

$$r/\ell_H \propto r\sqrt{H}. \tag{2}$$

Here H is the applied field, r is the spin–spin separation, while $\sigma^{(j)}$ are the Pauli matrices corresponding to the spin-$\frac{1}{2}$ operators of the two nuclei labeled by the superscripts $j = 1, 2$. Each nuclear spin also interacts with the applied field via the magnetic coupling of the form $-\gamma^{(j)}\hbar H\sigma_z^{(j)}$. Determination of the precise effective spin–spin interaction Hamiltonian will likely be accomplished to a large extent by direct experimental probe. The strength of the interaction in Eq. (1) can be roughly estimated to be of order 10^{-16} erg, which corresponds to a frequency of order 10^{11} Hz.

For quantum computation, one has to devise the means to control the spin–spin interactions. Ideally, one would like to be able to switch interactions on and off at will, for varying time intervals Δt. Switching on a pair-wise interaction would allow one to carry out a unitary transformation on a pair of spins independently of the other spins. It has been established [13,23,44–47] that nearly any such transformation, combined with single-spin transformations which can be accomplished by radiation pulses form a universal set in the sense that an arbitrary "computer program" can be built from them. There are NMR "refocusing" methods that allow for such control, as utilized, for instance, in the liquid-state NMR formulation [29–31] of quantum computing. However, until the full form of the spin–spin interaction Hamiltonian is established for our case, it is useful to consider other ideas as well.

Geometry constraints would limit the pairs of spins for which the two-spin interactions are nonnegligible typically to nearest-neighbor pairs. Furthermore, other interactions cannot be really *fully* eliminated, but only reduced. Still, control of the spin–spin interactions would allow for added flexibility in "programming" the unitary evolution of a computational device. Even when the control is possible, in practice it would be unrealistic to expect the form of the interaction, such as Eq. (1) above, to be known exactly from theoretical calculations alone. Thus, Eq. (1) is a leading-

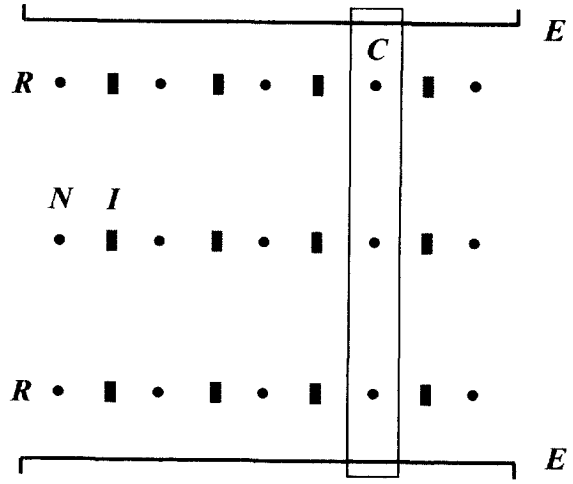

Fig. 1. The schematics of the proposed two-dimensional nuclear spin system: N denotes atoms with spin-$\frac{1}{2}$ nuclei; I denotes impurity atoms or complexes that can be ionized to disrupt the spin-exchange interactions mediated by conduction electrons (the impurity placement may be different, see text); R represents replicas (actually there will be many of them); E and C represent conducting electrodes and the connecting strip for measurement (see text).

approximation/guess phenomenological form. Input from experiments will be required to fine-tune the computer functions that depend on such internal interactions.

One possibility not based on the NMR methods is to disrupt (ideally, switch off), for the duration of some time interval Δt, the interaction for one (nearest-neighbor) pair of spins by placing impurities between the spins, see Fig. 1. The impurities can be ionized by external electromagnetic pulses to electronic configurations that capture electrons and locally destroy the coherence of the electron gas. Differentiation can be achieved by using different impurity species. Admittedly, this is a rather speculative idea. Specifically, it may be more appropriate to place the impurities near or surrounding the nuclear spins, instead of the geometry of Fig. 1.

It is important to emphasize that the pair-wise interactions are "on" most of the time, for each pair of spins. Therefore, the "idle" unitary transformations in the latter approach will not be simple phase changes as for noninteracting spins. The ability to change the interactions locally, pair-wise, will only allow one to

change the *relative* unitary transformations to which nearest-neighbor spin pairs are subject. In addition, one has the single-spin rotations that can be done by external electromagnetic pulses. Programming of such a computer is therefore less straightforward than usually expected in the theoretical approaches that assume *noninteracting* idling elements [1–7,13,23,44–47]; however, this is only a matter of new mathematical developments being called for.

We now turn to the process of "feeding in" the initial data into the computer. This can be accomplished as follows. Initially, all the nuclear spins in the system are pumped in one direction. This can be achieved by shining a polarized light at the system [49] that creates electron–hole pairs. These pairs annihilate, forcing on a fixed nuclear spin polarization, corresponding to that of the incident light [49]. After the initial alignment, the nuclear spins can be rotated to the desired quantum states needed for computation by electromagnetic pulses at their respective frequencies.

In all the proposals for quantum computation [1–7,13,22–31], reading off the final spin states by measuring, and also the measurement processes that are required for error correction [7,13,17,19–21] are most challenging to realize. This is because direct interaction of a microscopic system with any macroscopic system for the purpose of measurement is disruptive and difficult to carry out in an orderly fashion for all the individual spins in the system.

We note that as for the liquid-NMR proposal [29–31], we could read off averages by NMR techniques by producing replicas of the spin chain, see Fig. 1, and letting them evolve in parallel. The electromagnetic pulses that control the computation can be applied to all the replicas at once. However, some quantum error correction protocols [7,13,17,19–21] require actual measurements rather than averages. Furthermore, unlike the liquid-state NMR, there may be uncontrollable differences between the replicas. The only thing that might save the situation is the fact that our spins are located at distances much larger than atomic dimensions. Therefore, some averaging of the "atomic" scale influences may be expected in the spin–spin interactions controlling the actual computation in each chain. The latter observation suggests that measurement methods other than NMR based must be explored. We propose three measuring processes below: The first and second may be more appropriate for final-state readout while the second and third for error correction schemes.

First, let us assume that the final state is one of the direct-product states of the n-spin system. It is possible to generate by holographic and other methods [48–51] a narrow strip of conductance at each spin in turn, see Fig. 1, and send a current of spin-polarized electrons through it. The observed current can be pre-calibrated to enable high certainty determination of whether there was a spin-exchange scattering event, thus determining the nuclear spin's direction, resembling the spin-diode [38,52] techniques. Furthermore, one can extend the strip of conductance over several replicas of the spin chain, separated an order of magnitude more than the spins, e.g., 1000 Å. One can probably have enough of them to significantly reduce any uncertainty in the spin direction determination.

Second, if the final or intermediate state (the latter case is relevant for error correction) can be entangled, so that one cannot simply measure each spin in turn, then the situation is more complicated. One can generate a "mask" of conducting strips, for all or a group of spins. However, "calibration" to derive data pertinent to the multispin quantum state may be a challenge.

Third, some error correction schemes [7,13,17,19–21] require measurement of the difference of the components of nearby spins. This might be contemplated by having two conducting strips with the spin-polarized electron current, and adding a time-dependent component to the applied magnetic field for the duration of the measurement. The difference in the nuclear spin states will then affect the Aharonov–Bohm oscillatory structure of the observed current; see Ref. [53] for a survey of such effects.

In summary, we have proposed a model of a quantum computer based on the hyperfine interactions between the electron and nuclear spins in quantum Hall effect systems. This brings to two the number of proposals that have been formulated theoretically for realizations of quantum computing which can be potentially done in *solid-state systems*; the other is the quantum-dot proposal [26]. The possibility of quantum computing in solid state is exciting. Indeed, the intricacies of modern technology, especially as far as nanoscale "engineering" is concerned, are much more geared for solid-state systems than any other medium. All modern electronic devices, presently, with components on submicron scales, are solid state.

However, unlike the more "established" quantum computing proposals such as ion traps and liquid-state NMR, the two solid-state proposals are presently theoretical. There are several investigations needed of the form and strength of the spin–spin interactions, of the time scales of interaction versus decoherence, and other topics, before initial experimental attempts to build few-qubit QHE quantum computing systems can be deemed realistic. Specifically, no estimates are available of the time scales of decoherence which may be orders of magnitude shorter than T_1.

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Initial Decoherence of Open Quantum Systems

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Abstract

We present a new short-time approximation scheme for evaluation of decoherence. At low temperatures, the approximation is argued to apply at intermediate times as well. It then provides a tractable approach complementary to Markovian-type approximations, and appropriate for evaluation of deviations from pure states in quantum computing models.

Key Words: decoherence, thermalization, relaxation, open quantum systems

1. Introduction

Consider a microscopic quantum system with the Hamiltonian H_S. We will refer to the quantum-computing single quantum bit (qubit) or multi-qubit paradigm to help define the questions and set up the challenges, in describing how the system, S, interacts with the surrounding macroscopic world. However, in principle S can be any quantum system.

Interactions with the surroundings can be quite different depending on the setting. For example, in quantum measurement, which is presently not fully understood, the wavefunction of the system is probed, so part of the process would involve a strong interaction with the measuring device, such that the system's own Hamiltonian plays no role in the process. However, in most applications, the external interactions are actually quite weak. Furthermore, the aim is to minimize their effect, especially in quantum computing.

Traditionally, interactions with the surrounding world have been modeled by the modes of a bath, B, with each mode described by its Hamiltonian M_K, so that the bath of modes is represented by

$$H_B = \sum_K M_K \ . \tag{1.1}$$

The interaction, I, of the bath modes with the system S, will be modeled by

$$H_I = \Lambda_S P_B = \Lambda_S \sum_K J_K \ , \tag{1.2}$$

where Λ_S is some Hermitean operator of S, coupled to the operator P_B of the bath.

The bath, or "heat bath", can be a collection of modes, such as photons, phonons, spins, excitons, etc. For a bosonic bath of oscillators, [1-6], which we use for derivation

of specific results, we take

$$M_K = \omega_K a_K^\dagger a_K \ , \tag{1.3}$$

$$J_K = g_K^* a_K + g_K a_K^\dagger \ . \tag{1.4}$$

Here we have assumed that the energy of the ground state is shifted to zero for each oscillator, and we work in units such that $\hbar = 1$.

The total Hamiltonian of the system and bath is

$$H = H_S + H_B + H_I \ . \tag{1.5}$$

More generally, the interaction, (1.2), can involve several system operators, each coupling differently to the bath modes, or even to different baths. The bath modes, in turn, can be coupled to specified external objects, such as impurities.

Let $\rho(t)$ represent the reduced density matrix of the system at time $t \geq 0$, after the bath modes have been traced over. For large times, the effect of the environment on a quantum system that is not otherwise externally controlled, is expected to be thermalization: the density matrix should approach

$$\rho(t \to \infty) = \frac{\exp\left(-\beta H_S\right)}{\mathrm{Tr}_S\left[\exp\left(-\beta H_S\right)\right]} \ , \tag{1.6}$$

where $\beta \equiv 1/kT$. At all times, we can consider the degree to which the system has departed from coherent pure-quantum-state evolution. This departure is due to the interactions and entanglement with the bath. We also expect that the temperature, T, and other external parameters that might be needed to characterize the system's density

matrix, are determined by the properties of the bath, which in turn might interact with the rest of the universe.

Let us introduce the eigenstates of H_S,

$$H_S|n\rangle = E_n|n\rangle \ , \tag{1.7}$$

and have ΔE denote the characteristic energy gap values of S. We also consider the matrix elements of $\rho(t)$,

$$\rho_{mn}(t) = \langle m|\rho(t)|n\rangle \ . \tag{1.8}$$

For large times, we expect the diagonal elements ρ_{nn} to approach values proportional to $e^{-\beta E_n}$, while the off-diagonal elements, $\rho_{m\neq n}$, to vanish. These properties are referred to as thermalization and decoherence in the energy basis.

To establish these thermalization and decoherence properties, several assumptions are made regarding the system and bath dynamics [1-11]. At time $t = 0$, it is usually assumed that the bath modes, K, are thermalized, i.e., have density matrices

$$\theta_K = e^{-\beta M_K} \Big/ \mathrm{Tr}_K \left(e^{-\beta M_K}\right) \ . \tag{1.9}$$

The density matrix R of the system plus bath at time $t = 0$ is then the direct product

$$R(0) = \rho(0) \prod_K \theta_K \ , \tag{1.10}$$

and the system and bath modes are not entangled with each other.

Now, a series of assumptions are made, e.g., the Markovian and secular approximations. The most important is the Markovian approximation, which, even though it

can be stated and introduced in various ways, essentially assumes that the density matrices of the bath modes are reset externally to the thermal ones, on time scales shorter than any dynamical times of the system interacting with the bath. This is a natural assumption, because each bath mode is coupled only weakly to the system, whereas it is "monitored" by the rest of the universe and kept at temperature T. In its straightforward version, this amounts to using (1.10) for times $t > 0$. Ultimately, such approaches aim at master equations for the evolution of $\rho_{mn}(t)$ at large times, consistent with the Golden Rule and with the expected thermalization and decoherence properties.

In variants of these formalisms, several time scales are identified. One is the inverse of the upper cutoff, Debye frequency of the bath modes, $1/\omega_D$. Another is the thermal time $\hbar/kT = \beta$ (in units of $\hbar = 1$). The system S has its own characteristic time, $1/\Delta E$, as well as the system-bath dynamical times of thermalization and decoherence, etc., $T_{1,2,...}$, corresponding to the "intrinsic" NMR/ESR times T_1, T_2, etc. Heuristically, bath modes of frequencies ω comparable to ΔE are needed to drive thermalization and decoherence. Initial decoherence can be also mediated by the modes near $\omega = 0$. At low temperatures, we can assume that $1/\omega_D < 1/\Delta E < \beta$.

There is evidence [7,11,12] that at low temperatures, the Markovian-type and other approximations used in the derivation of equations for thermalization and decoherence, are only valid for times larger than the thermal time scale β. For quantum computing applications, in solid-state semiconductor-heterostructure architectures [13-19], we expect temperatures of several tens of μK. The thermal time scale then becomes dangerously close to the external single-qubit control, Rabi-flip time even for slower qubits, those based on nuclear spins. We emphasize that not all the approximation schemes have this problem [11].

In Section 2, we offer additional comments on decoherence and quantum computing. Then, in Section 3, we develop a short-time-decoherence approximation. In a

discussion at the end of Section 3, we offer arguments that, at low temperatures, our approximation is actually valid for intermediate times, larger than $1/\omega_D$, hopefully up to times comparable or larger than $1/\Delta E$. Specific results for the bosonic heat bath are presented in Section 4. Section 5 comments on the case of adiabatic decoherence, when the short-time approximation becomes exact.

2. Decoherence and quantum computing

Quantum computing architectures usually emphasize systems, both the qubits and the modes that couple them (and at the same time act as a bath mediating unwanted coupling to the rest of the universe), that have large spectral gaps. It is believed that, especially at low temperatures, spectral gaps slow down relaxation processes. Therefore, quantum computing architectures usually assume [13-19] qubits in quantum dots, or in atoms, or subject to large magnetic fields, and coupled by highly nondissipative quantum media [14,19].

The spectral gaps are expected to slow down exponentially, by the Boltzmann factor, the processes of thermalization, involving energy exchange. Off-shell virtual exchanges, will be also slowed down, but less profoundly. The latter processes contribute to decoherence. Therefore, at low temperatures, we might expect separation of time scales of the initial decoherence vs. later-stage thermalization and further decoherence. The latter two processes are described by the traditional NMR/ESR intrinsic T_1 and T_2, respectively.

Since only thermalization is clearly associated with the energy eigenbasis, one can also ask whether the energy basis is the appropriate one to describe decoherence for short and intermediate times, before the thermalizing processes, that also further drive decoherence, take over. The issue of the appropriate basis for studying decoherence, has also come up in models of quantum measurement. It has been argued [20-24] that the eigenbasis of the interaction operator, Λ_S, may be more appropriate for intermediate times than the energy eigenbasis.

Yet another aspect of decoherence in quantum computing, involves the observation that we really want to retain a *pure state* in the quantum computation process [25-30]. Decay of off-diagonal matrix elements, in whatever basis, might not be the best

measure of deviations from the pure-state density matrix. For instance, the deviation of $\mathrm{Tr}_S\left[\rho^2(t)\right]$ from 1, may be more appropriate. Therefore, it is desirable to have basis-independent expressions for the reduced density operator $\rho(t)$.

Recently, several groups have reported [12,19,24,31-41] results for spin decoherence in solid state systems appropriate for quantum computing architectures. Some of these works have not invoked the full battery of the traditional approximations, Markovian and secular, etc., or have utilized the spectral gap of the bath modes, to achieve better reliability of the short-time results. In [41], interaction of the spin-exciton bath modes with impurities was accounted for, as the main mechanism of decoherence. In the present work, we limit ourselves to the bath modes only interacting with the system. Experimental efforts are picking up momentum, with the first limited results available [42,43] by traditional NMR/ESR techniques, with the quantum-computing emphasis.

An approach, termed adiabatic decoherence, have been developed by us [24], expanding the earlier works [12,31-33], with the goal of avoiding the ambiguity of the basis selection and achieving exact solvability. The price paid was the assumption that H_S is conserved (a particular version of the quantum nondemolition processes), which is equivalent to requiring that

$$[H_S, H] = [H_S, \Lambda_S] = 0 \qquad \text{(adiabatic case)} \; . \tag{2.1}$$

This makes the eigenbasis of H_S and Λ_S the same, but precludes energy relaxation, thus artificially leaving only energy-conserving relaxation pathways that contribute to decoherence. We will comment on the results of this approach in Section 5.

Most of the results referred to earlier, have involved approximations of one sort or another. The most popular and widely used approximation has been the second-order perturbative expansion in the interaction strength, H_I, though some nonperturbative

results have also been reported. In Section 3, we describe a novel approximation scheme [44] that is valid for short times. It has several advantages, such as becoming exact in the adiabatic case, allowing derivation of several explicit results, and, at least in principle, permitting derivation of higher-order approximations. Certain models of quantum measurement evaluate decoherence by effectively setting $H_S = 0$. Our approximation then becomes exact, and our results are consistent with these studies [45,46].

Our formulation in Section 3, will be quite general, and we will not use the specific bath or thermalization assumptions. However, we do utilize the factorization property (1.10) at time $t = 0$. Thus, we do have to assume that, at least initially, the system and the bath modes are not entangled. In fact, the present formulation also relies on that the Hamiltonians at hand are all time-independent. Therefore, we have excluded the possibility of controlled dynamics, in the quantum computing sense, when gate functions are accomplished by external couplings to individual qubits and by external control of their pairwise interactions. Our formulation, therefore, applies to "idling" qubits or systems of (possibly interacting) qubits. It is reasonable to assume that a lower limit on decoherence rate can be evaluated in such an idling state, even though for quantum error correction, qubits otherwise idling, might be frequently probed (measured) and entangled with ancillary qubits [25-30].

The $t = 0$ factorization assumption (1.10), shared by all the recent spin-decoherence studies, then represents the expectation that external control by short-duration but large externally applied potentials, measurement, etc., will "reset" the qubits, disentangling them from the environment modes to which the affected qubits are only weakly coupled. Thus, we assert that it is the qubit system that gets approximately reset and disentangled from the bath towards time $t = 0$, rather than the bath is thermalized by the rest of the universe, as assumed in Markovian approximation schemes.

3. Short-time decoherence

In addition to the energy basis, (1.7), we also define the eigenstates of the interaction operator Λ_S, by

$$\Lambda_S|\gamma\rangle = \lambda_\gamma|\gamma\rangle \ , \tag{3.1}$$

where the Greek index labels the eigenstates of Λ_S, with eigenvalues λ_γ, while the Roman indices will be used for the energy basis, and, when capitalized, for the bath modes, (1.2)-(1.4).

The time dependence of the density matrix $R(t)$ of the system and bath, is formally given by

$$R(t) = e^{-i(H_S+H_B+H_I)t} R(0)\, e^{i(H_S+H_B+H_I)t} \ . \tag{3.2}$$

We will utilize the following approximate relation for the exponential factors, as our short-time approximation,

$$e^{i(H_S+H_B+H_I)t+O(t^3)} = e^{iH_St/2}\, e^{i(H_B+H_I)t}\, e^{iH_St/2} \ . \tag{3.3}$$

This relation has the following appealing properties. It becomes exact for the adiabatic case, (2.1). Furthermore, if we use the right-hand side and its inverse to replace $e^{\pm iHt}$, then we are imposing three time-evolution-type transformations on $R(0)$. Therefore, the approximate expression for $R(t)$ will have all the desired properties of a density operator. Finally, extensions to higher-order approximations in powers of t are possible, by using relations derived in [47], where various expressions valid to $O(t^4)$ and $O(t^5)$ were considered.

Our goal is to evaluate the resulting approximation to the matrix element,

$$\rho_{mn}(t) = \mathrm{Tr}_B \langle m| e^{-iH_S t/2}\, e^{-i(H_B+H_I)t}\, e^{-iH_S t/2} R(0)\, e^{iH_S t/2}\, e^{i(H_B+H_I)t}\, e^{iH_S t/2} |n\rangle \,. \tag{3.4}$$

First, we apply the operators H_S in the outer exponentials, acting to the left on $\langle m|$, and to the right on $|n\rangle$, replacing H_S by, respectively, E_m and E_n. We then note that the second exponential operator in (3.4) contains Λ_S, see (1.2). Therefore, we insert the decomposition of the unit operator in the system space, in terms of the eigenbasis of Λ_S, before the second exponential, and one in terms of the eigenbasis of H_S after it. This allows us to apply Λ_S in the second exponential and also H_S in the third exponential. The same substitution is carried out on the other side of $R(0)$, with the result

$$\rho_{mn}(t) = \sum_{\gamma\, p\, q\, \delta} \mathrm{Tr}_B \Big[e^{-iE_m t/2} \langle m|\gamma\rangle\langle\gamma|p\rangle e^{-i(H_B+\lambda_\gamma P_B)t}\, e^{-iE_p t/2} \rho_{pq}(0)$$

$$\times \Big(\prod_K \theta_K \Big) e^{iE_q t/2}\, e^{i(H_B+\lambda_\delta P_B)t} \langle q|\delta\rangle\langle\delta|n\rangle e^{iE_n t/2} \Big] \,. \tag{3.5}$$

The next step is to collect all the terms, and also identify that the trace over the bath can be now carried out for each mode separately. We use (1.1)-(1.2) to write

$$\rho_{mn}(t) = \sum_{\gamma\, p\, q\, \delta} \Big\{ e^{i(E_q+E_n-E_p-E_m)t/2} \langle m|\gamma\rangle\langle\gamma|p\rangle\, \rho_{pq}(0)\, \langle q|\delta\rangle\langle\delta|n\rangle$$

$$\times \prod_K \mathrm{Tr}_K \Big[e^{-i(M_K+\lambda_\gamma J_K)t}\, \theta_K\, e^{i(M_K+\lambda_\delta J_K)t} \Big] \Big\} \,. \tag{3.6}$$

While this expression looks formidable, it actually allows rather straightforward calculations in some cases. Specifically, the simplest quantum-computing applications involve

two-state systems. Therefore, the sums in (3.6) are over two terms each. The calculations involving the overlap Dirac brackets between the eigenstates of H_S (labeled by m, n, p and q) and of Λ_S (labeled by γ and δ), as well as the energy-basis matrix elements of $\rho(0)$, cf. (1.8), involve at most diagonalization of two-by-two Hermitean matrices. Of course, the approximation (3.6) can be used for evaluation of short-time density matrices for systems more general than two-state.

The challenging part of the calculation involves the trace over each mode of the bath. Since these modes have identical structure, e.g., (1.3)-(1.4) for the bosonic bath case, but with K-dependent coupling constants, the calculation needs only be done once, in the space of *one mode*. Furthermore, results for the bath models ordinarily used, such as the bosonic and spin baths, are either already available in the literature or can be calculated without much difficulty. For the thermalized initial bath-mode density matrix θ_K, we give the exact bosonic-model expression in the next section.

In the remainder of this section, we first further analyze the trace over one bath mode entering (3.6). We then comment on the limits of validity of the present approximation.

In an obvious shorthand notation, we write the single-mode trace in (3.6) as

$$\mathrm{Tr}\left[e^{-i(M+\gamma J)t}\,\theta\,e^{i(M+\delta J)t}\right] = \mathrm{Tr}\left[\theta\,e^{i(M+\delta J)t}\,e^{-i(M+\gamma J)t}\right]. \tag{3.7}$$

Now, to the same order of approximation as used in (3.3), we can write

$$e^{i(M+\delta J)t+O(t^3)} = e^{iMt/2}\,e^{i\delta Jt}\,e^{iMt/2}\,. \tag{3.8}$$

The resulting approximation for the trace (3.7) reads

$$\mathrm{Tr}\left[\left(e^{-iMt/2}\,\theta\,e^{iMt/2}\right)e^{i(\delta-\gamma)Jt}\right], \tag{3.9}$$

which illustrates that, within this approximation, the product of traces in (3.6) is a function of the difference $\lambda_\gamma - \lambda_\delta$. In fact, this product is exactly 1 for $\lambda_\gamma = \lambda_\delta$ and, in most applications, the following form is likely to emerge,

$$\prod_K \mathrm{Tr}_K[\ldots] = e^{-\,\mathrm{const}\,(\lambda_\gamma-\lambda_\delta)^2 t^2 + O\left(t^3\right)}\,, \tag{3.10}$$

though we caution the reader that (3.10) is somewhat speculative and suggested by the exact result for the bosonic heat bath, reported in the next section.

Finally, we point out that in most cases of interest, the initial single-mode density matrix θ will commute with the bath-mode energy operator M. In fact, the thermalized θ is a function of M. Therefore, (3.9) can be further simplified to

$$\mathrm{Tr}\left[\,\theta\,e^{i(\delta-\gamma)Jt}\right]. \tag{3.11}$$

However, let us emphasize that the approximate relations (3.9)-(3.11) are likely of value only as far as they help to derive basis-independent (operator) approximations to $\rho(t)$, by a technique illustrated in the next section. Indeed, for most bath models it is advisable to calculate the single-mode trace exactly first, according to (3.6), and then attempt various approximations.

The latter statement reflects our expectation that the approximation developed here is valid, for low temperatures, not only for short times, defined by $t < 1/\omega_D$, but also for intermediate times, exceeding $1/\omega_D$. This is suggested by the result of an illustrative calculation in the next section, but mainly by the fact that (3.11) only includes the bath-mode energy scales via θ, and, therefore, at low temperatures, is

dominated by the lowest bath-mode excitations, and is not sensitive to frequencies of order ω_D. Thus, we expect our approximation to be applicable complementary to the Markovian-type approximations and definitely break down in the regime of fully developed thermalization, for $t \geq O(\beta)$. Additional supporting observations are offered in Section 5, when we consider the adiabatic case (2.1).

4. The bosonic heat bath

In this section, we consider the bosonic heat bath [6], see (1.3)-(1.4), in the initially thermalized state,

$$\theta_K = e^{-\beta M_K} / \operatorname{Tr}_K \left(e^{-\beta M_K} \right) = \left(1 - e^{-\beta \omega_K} \right) e^{-\beta \omega_K a_K^\dagger a_K} \ . \tag{4.1}$$

The product of the single-mode traces in (3.6), is then available in the literature [12,24,31],

$$\rho_{mn}(t) = \sum_{\gamma\, p\, q\, \delta} \Big\{ e^{i(E_q + E_n - E_p - E_m)t/2} \langle m|\gamma\rangle\langle\gamma|p\rangle\langle q|\delta\rangle\langle\delta|n\rangle \rho_{pq}(0)$$

$$\times \exp\Big(-\sum_K \frac{|g_K|^2}{\omega_K^2} \Big[2\left(\lambda_\gamma - \lambda_\delta\right)^2 \sin^2 \frac{\omega_K t}{2} \coth \frac{\beta\omega_K}{2} + i\left(\lambda_\gamma^2 - \lambda_\delta^2\right)\left(\sin \omega_K t - \omega_K t\right) \Big] \Big) \Big\} \ . \tag{4.2}$$

The last term in the exponent, linear in t, is usually viewed as "renormalization" of the system energy levels due to its interaction with the bath modes. It can be removed by adding the term,

$$H_R = \Lambda_S^2 \sum_K |g_K|^2 / \omega_K \ , \tag{4.3}$$

to the total Hamiltonian. However, the usefulness of this identification for short times is not clear, and we will not use it. One can check that, *unmodified*, (4.2) is consistent with the expectation (3.10).

Let us now define two non-negative real spectral sums, $B(t)$ and $C(t)$, over the bath modes,

$$B^2(t) = 8 \sum_K \frac{|g_K|^2}{\omega_K^2} \sin^2 \frac{\omega_K t}{2} \coth \frac{\beta \omega_K}{2} \ , \tag{4.4}$$

$$C(t) = \sum_K \frac{|g_K|^2}{\omega_K^2} \left(\omega_K t - \sin \omega_K t \right) \ . \tag{4.5}$$

When converted to integrals over the bath mode frequencies, with the cutoff at ω_D, these sums have been discussed extensively in the literature [6,12,31], for several choices of the bath mode density of states and coupling strength g as functions of the mode frequency.

The final expression is,

$$\rho_{mn}(t) = \sum_{\gamma\, p\, q\, \delta} \left\{ e^{i(E_q + E_n - E_p - E_m)t/2} \langle m|\gamma\rangle\langle\gamma|p\rangle\langle q|\delta\rangle\langle\delta|n\rangle \rho_{pq}(0) \right.$$

$$\left. \times \exp\left[-\frac{1}{4} B^2(t) \left(\lambda_\gamma - \lambda_\delta\right)^2 \ - \ iC(t) \left(\lambda_\gamma^2 - \lambda_\delta^2 \right) \right] \right\} . \tag{4.6}$$

When the spectral functions are expanded in powers of t, this result confirms all the conclusions and conjectures discussed in Section 3, in connection with relations (3.9)-(3.11).

Let us now turn to the derivation of the basis-independent representation for $\rho(t)$, by utilizing the integral identity

$$\sqrt{\pi} \exp[-B^2(\Delta\lambda)^2/4] = \int_{-\infty}^{\infty} dy\, e^{-y^2} \exp[iyB(\Delta\lambda)] \ . \tag{4.7}$$

Exponential factors in (4.6) can then be reproduced by applying operators on the wave-functions entering the overlap Dirac brackets, with the result

$$\sqrt{\pi}\,\rho(t) = \int dy\, e^{-y^2}\, e^{-iH_S t/2}\, e^{i[yB(t)\Lambda_S - C(t)\Lambda_S^2]}\, e^{-iH_S t/2}\, \rho(0)\, e^{iH_S t/2}\, e^{-i[yB(t)\Lambda_S - C(t)\Lambda_S^2]}\, e^{iH_S t/2}\ . \tag{4.8}$$

Within the $O(t^2)$ approximation (3.3), given that B and C are of order linear or higher in t, we can combine the exponential operators to get an alternative approximation,

$$\sqrt{\pi}\,\rho(t) = \int dy\, e^{-y^2}\, e^{-i[tH_S - yB(t)\Lambda_S + C(t)\Lambda_S^2]}\, \rho(0)\, e^{i[tH_S - yB(t)\Lambda_S + C(t)\Lambda_S^2]}\ , \tag{4.9}$$

though (4.6) and (4.8) are in fact easier to handle in actual calculations.

As an application, let us consider the case of H_S proportional to the Pauli matrix σ_z, e.g., a spin-1/2 particle in magnetic field, and $\Lambda_S = \sigma_x$, with the proportionality constant in the latter relation absorbed in the definition of the coupling constants g_K in (1.4). Let us study the deviation of the state of a spin-1/2 qubit, initially in the energy eigenstate $|\uparrow\rangle$ or $|\downarrow\rangle$, from pure state, by calculating $\mathrm{Tr}_S\,[\rho^2(t)]$ according to (4.8). We note that for a two-by-two density matrix, this trace can vary from 1 for pure quantum states to the lowest value of 1/2 for maximally mixed states.

A straightforward calculation with $\rho(0) = |\uparrow\rangle\langle\uparrow|$ or $|\downarrow\rangle\langle\downarrow|$, yields

$$\mathrm{Tr}_S\,[\rho^2(t)] = \frac{1}{2}\left[1 + e^{-2B^2(t)}\right]\ . \tag{4.10}$$

As the time increases, the function $B^2(t)$ grows monotonically from zero [6,12,24,31]. Specifically, for Ohmic dissipation, $B^2(t)$ increases quadratically for short times $t < O(1/\omega_D)$, then logarithmically for $O(1/\omega_D) < t < O(\hbar/kT)$, and linearly for $t > O(\hbar/kT)$. (For other bath models, it need not diverge to infinity at large times.) This

calculation thus illustrates the fact that the present approximation can yield reasonable results for short and even intermediate times.

Both approximations, (4.8)-(4.9), make the deviation from a pure state $\rho(0) = |\psi_0\rangle\langle\psi_0|$ apparent: $\rho(t > 0)$ is obviously a *mixture* (integral over y) of pure-state projectors $|\psi(y,t)\rangle\langle\psi(y,t)|$, where, for instance for (4.9),

$$\psi(y,t) = e^{-i[tH_S - yB(t)\Lambda_S + C(t)\Lambda_S^2]}\,\psi_0 \ , \tag{4.11}$$

with a somewhat different expression for (4.8).

5. The adiabatic case

Relation (2.1) corresponds to the system's energy conservation. Therefore, energy flow in and out of the system is not possible, and normal thermalization mechanisms are blocked. The fact that our approximation becomes exact in this case, provides support to the expectation that, at low temperatures, it is generally valid beyond the cutoff time scale $1/\omega_D$, providing a reasonable evaluation of decoherence and deviation from a pure state, as exemplified by the calculation yielding (4.10), in Section 4.

With (2.1), we can select a common eigenbasis for H_S and Λ_S. Then the distinction between the lower-case Roman and Greek indices in (3.6) becomes irrelevant, and the sums can all be evaluated to yield

$$\rho_{mn}(t) = e^{i(E_n - E_m)t}\, \rho_{mn}(0) \prod_K \mathrm{Tr}_K \left[e^{-i(M_K + \lambda_m J_K)t}\, \theta_K\, e^{i(M_K + \lambda_n J_K)t} \right] . \tag{5.1}$$

This expression was discussed in detail in our work on adiabatic decoherence [24]. Specifically, for the initially thermalized bosonic heat bath case, we have, for the absolute values of the density matrix elements,

$$\left|\rho_{mn}(t)\right| = \left|\rho_{mn}(0)\right| e^{-B^2(t)(\lambda_m - \lambda_n)^2/4} . \tag{5.2}$$

The decay of the off-diagonal matrix elements thus depends of the properties of the spectral function $B^2(t)$ as the time increases. Such explicit results [12,24,31-33] illustrate that for true irreversibility, the number of bath modes must be infinite, with the spectral function evaluated in the continuum limit.

In summary, we have derived short-time approximations for the density matrix and its energy-basis matrix elements. Our expressions are quite easy to work with, because

for few-qubit systems they only involve manipulation of finite-dimensional matrices, and they will be useful in estimating decoherence and deviation from pure states in quantum computing models, including results for low temperatures.

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MEASUREMENT OF A QUANTUM SYSTEM COUPLED TO INDEPENDENT HEAT-BATH AND POINTER MODES

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We present an exact derivation of a process in which a microscopic measured system interacts with the heat-bath and pointer modes of a measuring device, via a coupling involving a general Hermitian operator Λ of the system. In the limit of strong interaction with these modes, over a small time interval, we derive the exact effective many-body density matrix of the measured system plus pointer. We then discuss the interpretation of the dynamics considered as the first stage in the process of quantum measurement, eventually involving the wave-function collapse due to interactions with "the rest of the universe". We establish that the effective density matrix represents the required framework for the measured system and the pointer part of the measuring device to evolve into a statistical mixture described by direct-product states such that the system is in each eigenstate of Λ with the correct quantum-mechanical probability, whereas the expectation values of the pointer-space operators retain amplified information of the system's eigenstate.

1. Introduction

The problem of quantum measurement has fascinated scientists for a long time.[1,2] It has been argued that a large "bath" is an essential ingredient of the measurement process. Interaction with the bath, which might be a heat-bath in thermal equilibrium, causes decoherence which is needed to form a statistical mixture of eigenstates out of the initially fully or partially coherent quantum state of the measured system. An "external" bath ("the rest of the universe") may also play a role in the selection of those quantum states of the pointer that manifest themselves in classical observations.[2–7] In this work, we propose a model in which the pointer retains information on the measurement result because of its coupling to the measured system, without the need to also couple it to the internal bath. The measured system is still coupled to the internal bath.

In an exactly solvable model of a quantum oscillator coupled to a heat bath of oscillators, it has been shown[4] that the reduced density matrix of the system, with the bath traced over, decoheres, i.e. it loses its off-diagonal elements in the eigenbasis of the interaction Hamiltonian. Recent work on decoherence[8–11] has explored the latter effect for rather general cases, for bosonic (oscillator) and spin baths.

Applications for various physical systems have been reported.[12–18] Fermionic heat bath has also been used in the literature.[19]

It is clear, however, that the full function of a large, multimode measuring device, interacting with a small (microscopic) quantum system, must be different from thermal equilibration or similar averaging effect. The device must store and amplify the measurement outcome information. In this work, we propose a solvable model that shows how this is accomplished.

It must be stressed that for a complete description of the measurement process, one needs to interpret the transfer of the information stored after the system-pointer and system-internal bath interaction to the macroscopic level.[2] Our attention here is ~~not~~ on the process which corresponds to the first stage of the measurement, in which the pointer acquires amplified information by entanglement with the state of the system. Thus, we do not claim to resolve the foundation-of-quantum mechanics issue of how that information is passed on to the classical world, involving the collapse of the wave functions of the system and each pointer mode. Indeed, it is unlikely that the wave-function collapse can be fully described within the quantum-mechanical description of the three subsystems involved. Presumably, it would require consideration of an external bath with which the pointer and the internal bath interact. This problem is not presently solved,[1–3] and we first sidestep it by assuming separation of time scales (see below). However, we later argue that our results provide useful hints on how to view the larger problem of quantum measurement.

We now identify the three quantum systems involved. First, the measured system, S, is a microscopic system with the Hamiltonian which will also be denoted by S. Second, the measuring device must have the "bath" or "body" part, B, containing many individual modes. The kth mode will have the Hamiltonian B_k. The bath part of the device is not observed, i.e. it can be traced over. Finally, the device must also have modes that are not traced over. These modes constitute the pointer, P, that amplifies the information obtained in the measurement process and can later pass it on for further amplification or directly to macroscopic (classical) systems. The mth pointer mode has the Hamiltonian P_m. It is expected that expectation values of some quantities in the pointer undergo a large change during the measurement process.

It turns out, *a posteriori*, that the device modes involved in the measurement process can be quite simple and they need not interact with each other. This assumption allows us to focus on the evolution of the system S and its effect on the pointer P. However, it is the pointer's interaction with the external bath (some external modes, "the rest of the universe") that is presumed to select those quantum states of P that manifest themselves classically. For now, let us avoid the discussion of this matter, see Refs. 2–6, by assuming that the added evolution of the pointer due to such external interactions occurs on time scales larger than the measurement time, t. Similarly, when we state that the internal bath modes can be "traced over", we really mean that their interactions with the rest of the universe are such that

these modes play no role in the wave-function-collapse stage of the measurement process.

Furthermore, the measurement process probes the wave function of the measured system at the initial time, $t = 0$, rather than its time evolution under S alone. It is ideally instantaneous. In practice, it is faster than the time scales associated with the dynamics under S. Such a process can be obtained as the limit of a system in which very strong interactions between S and B, and also between S and P, are switched on at $t = 0$ and switched off at $t > 0$, with small time interval t. At later times, the pointer can interact with other external systems to pass on the result of the measurement.

Thus, we assume that the Hamiltonian of the system itself, S, can be ignored in the process. The total Hamiltonian of the system plus device will be taken as

$$H = \sum_k B_k + \sum_m P_m + b\Lambda \sum_k L_k + p\Lambda \sum_m C_m \,. \tag{1}$$

Here, Λ is some Hermitian operator of the system that couples to certain operators of the modes, L_k and C_m. The parameters b and p are introduced to measure the coupling strength for the bath and pointer modes, respectively. They are assumed to be very large; the ideal measurement process corresponds to $b, p \to \infty$.

We note that the modes of P and B can be similar. The only difference between the bath and pointer modes is in how they interact with the "rest of the universe": the bath is traced over (unobserved), whereas the pointer modes have their wave functions collapsed in a later step of the measurement process. Thus, we actually took the same coupling operator Λ for the bath and pointer. In fact, all the exact calculations reported in this work can also be carried out for different coupling operators Λ_b and Λ_p, for the bath and pointer modes, provided they commute, $[\Lambda_b, \Lambda_p] = 0$, so that they share a common set of eigenfunctions. The final wave function of the measured system, after the measurement, is in this set. Analytical calculation can even be extended to the case when the system's Hamiltonian S is retained in (1), provided all three operators, S, Λ_b, Λ_p, commute pairwise. The essential physical ingredients of the model are captured by the simpler choice (1).

We will later specify all the operators in (1) as the modes of the bosonic heat bath of the Caldeira–Leggett type.[17,19–26] For now, however, let us keep our discussion general. We will assume that the system operator Λ has nondegenerate, discrete spectrum of eigenstates:

$$\Lambda|\lambda\rangle = \lambda|\lambda\rangle \,. \tag{2}$$

Some additional assumptions on the spectrum of Λ and S will be encountered later. We also note that the requirement that the coupling parameters b and p are large may in practice be satisfied because, at the time of the measurement, the system's Hamiltonian S corresponds to slow or trivial dynamics.

Initially, at $t = 0$, the quantum systems (S, B, P) and their modes are not correlated with each other. We assume that ρ is the initial density matrix of the

measured system. The initial state of each bath and pointer mode will be assumed thermalized, with $\beta = 1/(kT)$ and the density matrices

$$\theta_k = \frac{e^{-\beta B_k}}{\mathrm{Tr}_k(e^{-\beta B_k})} \qquad \sigma_m = \frac{e^{-\beta P_m}}{\mathrm{Tr}_m(e^{-\beta P_m})}\,. \tag{3}$$

We cannot offer any fundamental physical reason for having the initial bath and pointer mode states thermalized, especially for the pointer; this choice is made to allow exact solvability.

The density matrix of the system at time t is

$$R = e^{-iHt/\hbar}\rho\left(\prod_k \theta_k\right)\left(\prod_m \sigma_m\right)e^{iHt/\hbar}\,. \tag{4}$$

The bath is not probed and it can be traced over. The resulting reduced density matrix r of the combined system $S + P$ will be represented by its matrix elements in the eigenbasis of Λ. These quantities are each an operator in the space of P:

$$r_{\lambda\lambda'} = \langle\lambda|\mathrm{Tr}_B(R)|\lambda'\rangle\,. \tag{5}$$

We now assume that operators in different spaces and of different modes commute. Then, one can show that

$$r_{\lambda\lambda'} = \rho_{\lambda\lambda'}\left[\prod_m e^{-it(P_m+p\lambda C_m)/\hbar}\sigma_m e^{it(P_m+p\lambda' C_m)/\hbar}\right] \times\left[\prod_k \mathrm{Tr}_k\left\{e^{-it(B_k+b\lambda L_k)/\hbar}\theta_k e^{it(B_k+b\lambda' L_k)/\hbar}\right\}\right] \tag{6}$$

where $\rho_{\lambda\lambda'} = \langle\lambda|\rho|\lambda'\rangle$. This result involves products of P-space operators and traces over B-space operators which are all single mode. Therefore, analytical calculations are possible for some choices of the Hamiltonian (1). The observable Λ can be kept general.

The role of the product of traces over the modes of the bath in (6) is to induce decoherence which is recognized as essential for the measurement process, e.g. Refs. 1 and 2. At time t, the absolute value of this product should approach $\delta_{\lambda\lambda'}$ in the limit of large b. Let us now assume that the bath is bosonic. The Hamiltonian of each mode is then $\hbar\omega_k a_k^\dagger a_k$, where for simplicity, we shifted the zero of the oscillator energy to the ground state. The coupling operator L_k is usually selected as $L_k = g_k^* a_k + g_k a_k^\dagger$. For simplicity, though, we will assume that the coefficients g_k are real:

$$B_k = \hbar\omega_k a_k^\dagger a_k \qquad L_k = g_k(a_k + a_k^\dagger). \tag{7}$$

For example, for radiation field in a unit volume, coupled to an atom,[27] the coupling is via a linear combination of the operators $(a_k + a_k^\dagger)/\sqrt{\omega_k}$ and $i(a_k - a_k^\dagger)/\sqrt{\omega_k}$. For a spatial oscillator, these are proportional to position and momentum, respectively. Our calculations can be extended to have an imaginary part of g_k which adds interaction with momentum.

The product of traces in (6) can be calculated by coherent-state or operator-identity techniques.[8–10] Here and below, we only list the results of such calculations which are usually quite cumbersome:

$$\prod_k \mathrm{Tr}_k\{\cdots\} = \exp\left\{-2b^2(\lambda-\lambda')^2\Gamma(t) + ib^2[\lambda^2-(\lambda')^2]\gamma(t)\right\} \tag{8}$$

$$\Gamma(t) = \sum_k (\hbar\omega_k)^{-2} g_k^2 \sin^2\frac{\omega_k t}{2}\coth\frac{\hbar\beta\omega_k}{2}\,. \tag{9}$$

The explicit form of $\gamma(t)$ is also known.[8]

In the continuum limit of many modes, the density of the bosonic bath states in unit volume, $D(\omega)$, and the Debye cutoff with frequency, ω_{D}, are introduced[22] to get

$$\Gamma(t) = \int_0^\infty d\omega\,\frac{D(\omega)g^2(\omega)}{(\hbar\omega)^2}\,e^{-\omega/\omega_{\mathrm{D}}}\,\sin^2\frac{\omega t}{2}\coth\frac{\hbar\beta\omega}{2}\,. \tag{10}$$

Let us consider the popular choice termed Ohmic dissipation,[22] motivated by atomic-physics[27] and solid-state applications,[22] corresponding to

$$D(\omega)g^2(\omega) = \Omega\,\omega\,, \tag{11}$$

where Ω is a constant. Other powers of ω have also been considered, e.g. Ref. 11. In studies of decoherence[8–11] for large times t, for models without strong coupling, not all the choices of $D(\omega)g^2(\omega)$ lead to complete decoherence[11] because $\Gamma(t)$ must actually diverge to $+\infty$ for $t \gg \hbar\beta$, as it happens for the choice (11).

Let us assume that the energy gaps of S are bounded so that there exists a well-defined time scale $\hbar/\Delta S$ of the evolution of the system under S. There is also the time scale $1/\omega_{\mathrm{D}}$ set by the frequency cutoff assumed for the interactions. The thermal time scale is $\hbar\beta$. The only real limitation on the duration of measurement is that t must be less then $\hbar/\Delta S$. In applications, typically[22] one can assume that $1/\omega_{\mathrm{D}} \ll \hbar/\Delta S$. Furthermore, it is customary to assume that the temperature is low,[22]

$$t \text{ and } 1/\omega_{\mathrm{D}} \ll \hbar/\Delta S \ll \hbar\beta\,. \tag{12}$$

In the limit of large $\hbar\beta$, the absolute value of (8) reduces to

$$\mathrm{Abs}\left(\prod_k \mathrm{Tr}_k\{\cdots\}\right) \simeq \exp\left\{-\frac{\Omega}{2\hbar^2}b^2(\lambda-\lambda')^2\ln[1+(\omega_{\mathrm{D}}t)^2]\right\}\,. \tag{13}$$

In order to achieve effective decoherence, the product $(\Delta\lambda)^2\,b^2\ln[1+(\omega_{\mathrm{D}}t)^2]$ must be large. The present approach only applies to operators Λ with nonzero scale of the smallest spectral gaps, $\Delta\lambda$.

We note that the decoherence property needed for the measurement process will be obtained for nearly any well-behaved choice of $D(\omega)g^2(\omega)$ because we can rely on the value of b being large rather than on the properties of the function $\Gamma(t)$. If b can be large enough, very short measurement times are possible. However, it may

be advisable to use measurement times $1/\omega_{\rm D} \ll t \ll \hbar/\Delta S$ to get the extra amplification factor $\sim \ln(\omega_{\rm D} t)$ and allow for fuller decoherence and less sensitivity to the value of t in the pointer part of the dynamics, which is to be addressed shortly. We notice, furthermore, that the assumption of a large number of modes is important for monotonic decay of the absolute value of (8) in decoherence studies,[8–11] where irreversibility is obtained only in the limit of infinite number of modes. In our case, it can be shown that such a continuum limit allows us to extend the possible measurement times from $t \ll 1/\omega_{\rm D}$ to $1/\omega_{\rm D} \ll t \ll \hbar/\Delta S$.

For consideration of the reduced density matrix r of $S+P$, see (6). It becomes diagonal in $|\lambda\rangle$, at time t, because all the nondiagonal elements are small,

$$r = \sum_{\lambda} |\lambda\rangle\langle\lambda|\, \rho_{\lambda\lambda} \prod_{m} e^{-it(P_m + p\lambda C_m)/\hbar} \sigma_m e^{it(P_m + p\lambda C_m)/\hbar}\,. \tag{14}$$

Thus, the described stage of the measurement process yields the density matrix that can be interpreted as describing a statistically distributed system, without quantum correlations. This, however, is only meaningful within the ensemble interpretation of quantum mechanics.

For a single system plus device, coupling to the rest of the universe is presumably needed (this problem is not fully understood in our opinion, see Ref. 2) for that system to be left in one of the eigenstates $|\lambda\rangle$, with probability $\rho_{\lambda\lambda}$. After the measurement interaction is switched off at t, the pointer coupled to that system will carry information on the value of λ. This information is "amplified", owing to the large parameter p in the interaction.

We note that one of the roles of the pointer having many modes, many of which can be identical and noninteracting, is to allow it (the pointer only) to be still treated in the ensemble, density matrix description, even if we focus on the later stages of the measurement when the wave functions of a single measured system and of each pointer mode are already collapsed. This pointer density matrix can be read off (14). This aspect is new and it may provide a useful hint on how to set up the treatment of the full quantum-measurement process description.

Another such hint is provided by the fact that, as will be shown shortly, the changes in the expectation values of some observables of the pointer retain amplified information on the system's eigenstate. So, coupling to the rest of the universe that leads to the completion of the measurement process should involve such an observable of the pointer. Eventually, the information in the pointer, perhaps after several steps of amplification, should be available for probe by interactions with classical devices.

At time $t = 0$, expectation values of various operators of the pointer will have their initial values. These values will be different at time t of the measurement owing to the interaction with the measured system. It is expected that the large coupling parameter p will yield large changes in the expectation values of the pointer

quantities. This does not apply equally to all operators in the P-space. Let us begin with the simplest choice: the Hamiltonian $\sum_m P_m$ of the pointer.

We will assume that the pointer is described by the bosonic heat bath and, for simplicity, use the same notation for the pointer modes as that used for the bath modes. The assumption that the pointer modes are initially thermalized, see (3), was not used thus far. While it allows exact analytical calculations, it is not essential: the effective density matrix describing the pointer modes at time t, for the system's state λ, will retain amplified information on the value of λ for general initial states of the pointer.

This effective density matrix is the product over the P modes in (14). For the "thermal" σ_m from (3), the expectation value of the pointer energy E_P can be calculated from

$$\begin{aligned}\langle E_P\rangle_\lambda \,\mathrm{Tr}_P(e^{-\hbar\beta\sum_s \omega_s a_s^\dagger a_s})\\ = \mathrm{Tr}_P\Bigg\{\left(\sum_m \hbar\omega_m a_m^\dagger a_m\right)\prod_n \Big[e^{-it[\omega_n a_n^\dagger a_n + p\lambda g_n(a_n+a_n^\dagger)]/\hbar}(e^{-\hbar\beta\sum_k \omega_k a_k^\dagger a_k})\\ \times\, e^{it[\omega_n a_n^\dagger a_n + p\lambda g_n(a_n+a_n^\dagger)]/\hbar}\Big]\Bigg\}. \end{aligned} \tag{15}$$

The right-hand side can be reduced to calculations for individual modes. Operator identities can then be utilized to obtain the results

$$\langle E_P\rangle_\lambda(t) = \langle E_P\rangle(0) + \langle \Delta E_P\rangle_\lambda(t) \tag{16}$$

$$\langle E_P\rangle(0) = \hbar\sum_m \omega_m e^{-\hbar\beta\omega_m}(1-e^{-\hbar\beta\omega_m})^{-2} \tag{17}$$

$$\langle \Delta E_P\rangle_\lambda(t) = \frac{4p^2\lambda^2}{\hbar}\sum_m \frac{g_m^2}{\omega_m}\sin^2\left(\frac{\omega_m t}{2}\right). \tag{18}$$

For a model with Ohmic dissipation, the resulting integral in the continuum limit can be calculated to yield

$$\langle \Delta E_P\rangle_\lambda(t) = \frac{2\,\Omega\,\omega_\mathrm{D}\lambda^2 p^2}{\hbar}\frac{(\omega_\mathrm{D}t)^2}{1+(\omega_\mathrm{D}t)^2} \tag{19}$$

which should be compared to the exponent in (13). The energy will be an indicator of the amplified value of the square of λ, provided p is large. Furthermore, we see here the advantage of larger measurement times, $t \gg 1/\omega_\mathrm{D}$. The change in the energy then reaches saturation. After the time t, when the interaction is switched off, the energy of the pointer will be conserved.

Let us consider the expectation value of the following Hermitian operator of the pointer:

$$X = \sum_m C_m = \sum_m g_m(a_m + a_m^\dagger). \tag{20}$$

For an atom in a field, X is related to the electromagnetic field operators.[24] One can show that $\langle X_P \rangle(0) = 0$ and

$$\langle \Delta X_P \rangle_\lambda(t) = \langle X_P \rangle_\lambda(t) = -\frac{4p\lambda}{\hbar} \sum_m \frac{g_m^2}{\omega_m} \sin^2\left(\frac{\omega_m t}{2}\right)$$

$$= -\frac{2\,\Omega\,\omega_{\rm D}\lambda p}{\hbar} \frac{(\omega_{\rm D} t)^2}{1+(\omega_{\rm D} t)^2}\,. \tag{21}$$

The change in the expectation value of X is linear in λ. However, this operator is not conserved. One can show that after the time t, its expectation value decays to zero for times $t + \mathcal{O}(1/\omega_{\rm D})$.

We note that by referring to "unit volume", we have avoided the discussion of the "extensivity" of various quantities. For example, the initial energy $\langle E_P \rangle(0)$ is obviously proportional to the system volume, V. However, the change $\langle \Delta E_P \rangle_\lambda(t)$ will not be extensive; typically, $g^2(\omega) \propto 1/V$, $D(\omega) \propto V$. Thus, while the amplification in our measurement process can involve a numerically large factor, the changes in the quantities of the pointer will be multiples of microscopic values. Multistage amplification, or huge coupling parameter p, would be needed for the information in the pointer to become truly "extensive" macroscopically.

In practice, there will probably be two types of pointer involved in a multistage measurement process. Some pointers will consist of many *noninteracting* modes. These pointers carry the information stored in a density matrix rather than a wave function of a single system. The latter transference hopefully makes the wave function collapse and transfer of the stored information to the macroscopic level less "mysterious and traumatic". The second type of pointer will involve strongly interacting modes and play the role of an amplifier by utilizing the many-body collective behavior of the coupled modes (phase-transition style). Its role will be to alleviate the artificial requirement for large mode-to-system coupling parameters encountered in our model.

In summary, we described the first stage of a measurement process. It involves decoherence due to a bath and transfer of information to a large system (pointer) via strong interaction over a short period of time. The pointer itself need not be coupled to the internal bath. While we do not offer a solution to the foundation-of-quantum-mechanics wave-function collapse problem,[2] our results do provide two interesting observations.

Firstly, the pointer operator "probed" by the rest of the universe during the wave-function collapse stage may in part be determined not only by how the pointer modes are coupled to the external bath,[3–7] but also by the amplification capacity of that operator in the first stage of the process, as illustrated by our calculations.

Secondly, for a single system (rather than an ensemble), the multiplicity of the (noninteracting) pointer modes might allow the pointer to be treated within the density matrix formalism even after the system and each pointer-mode wave functions were collapsed. Since it is the information in the pointer that is passed on,

this observation might seem to resolve part of the measurement puzzle. Specifically, it might suggest why only those density matrices entering (14) are selected for the pointer: they carry classical (large, different from other values) information in expectation values, rather than quantum-mechanical superposition. However, presumably[2] only a full description of the interaction of the external world with the system $S + P$ can explain the wave-function collapse of S.

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ADIABATIC DECOHERENCE

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ABSTRACT

We study a general quantum system interacting with environment modeled by the bosonic heat bath of Caldeira and Leggett type. General interaction Hamiltonians are considered that commute with the system's Hamiltonian so that there is no energy exchange between the system and bath. We argue that this model provides an appropriate description of adiabatic quantum decoherence, i.e., loss of entanglement on time scales short compared to those of thermal relaxation processes associated with energy exchange with the bath. The interaction Hamiltonian is then proportional to a conserved "pointer observable." Calculation of the elements of the reduced density matrix of the system is carried out exactly, and time-dependence of decoherence is identified, similar to recent results for related models. Our key finding is that the decoherence process is controlled by spectral properties of the interaction rather than system's Hamiltonian.

1. Introduction

Quantum decoherence, dissipation, and thermalization due to interactions with environment have long been important fundamental issues theoretically and experimentally.[1−11] Decoherence and related topics have attracted much interest recently due to rapid development of new fields such as quantum computing and quantum information theory.[12−18] Decoherence due to external interactions is a major obstacle in the way of implementation of devices such as quantum computers. Thus in addition to studies of the physics of decoherence processes there emerged a new field of quantum error correction[19−25] aiming at effective stabilization of quantum states against decoherence essentially by involving many additional quantum systems and utilizing redundancy. The present work contributes to the former topic: the physics of decoherence.

Decoherence is a result of the coupling of the quantum system under consideration to the environment which, generally, is the rest of the universe. In various experimentally relevant situations the interaction of the quantum system with environment is dominated by the system's microscopic surroundings. For example, the dominant source of such interaction for an atom in an electromagnetic cavity is the electromagnetic field itself coupled to the dipole moment of the atom.[26] In case of Josephson

junction in a magnetic flux[27] or defect propagation in solids, the interaction can be dominated by acoustic phonons or delocalized electrons.[28] Magnetic macromolecules interact with the surrounding spin environment such as nuclear spins.[18] Numerous other specific examples could be cited.

In this work we aim at a general phenomenological description that models the physically important effects of external interactions as far as adiabatic decoherence, to be defined later, is concerned. We note that generally thermalization and decoherence are associated with the interaction of the quantum system, described in isolation by the Hamiltonian H_S, with another, large system which we will term the "bath" and which internally has the Hamiltonian H_B. The actual interaction will be represented by the Hamiltonian H_I so that the total Hamiltonian of the system, H, is

$$H = H_S + H_B + H_I \,. \tag{1.1}$$

It is important to realize that typically the bath is a large, macroscopic system. Truly irreversible interactions of a quantum system with its environment, such as thermal equilibration or decoherence associated with measurement processes, can only be obtained in the Hamiltonian description (1.1) when it is supplemented by taking the limit of the number of

particles or degrees or freedom of the bath going to infinity.

Interactions of a quantum system with macroscopic systems can lead to different outcomes. For instance, interaction with a true "heat bath" leads to thermalization: the reduced density matrix of the system approaches $\exp(-\beta H_S)$ for large times. Here

$$\beta = 1/(kT) \tag{1.2}$$

as usual, and by "reduced" we mean the density matrix traced over the states of the bath. On the other hand for decoherence we expect the reduced density matrix to approach a diagonal form in the "preferred basis" somehow selected by the "pointer observable" Hermitian operator[1–6,29,30] which is thereby "measured" by the macroscopic system (bath).

It is important to realize that study of decoherence in the present context does not fully resolve the problem of understanding quantum measurement and other fundamental issues at the borderline of quantum and classical behaviors, such as, for instance, the absence of macroscopic manifestations of Schrödinger-cat type quantum superposition of states. The more optimistic recent literature[4–6] considers description of entanglement and decoherence the key to such understanding. However, these fundamental problems have remained open thus far.

The most explored and probably most tractable approach to modeling the environmental interactions has involved representing their effects by coupling the original quantum system to a set of noninteracting harmonic oscillators (bosonic heat bath).[1,2,8–11,14,31–33] Fermionic heat bath can be also considered, e.g., Ref. 34. We will use the term "heat bath" for such systems even when they are used for other than thermalization studies because they have the temperature parameter defined via initial conditions, as described later.

Rigorous formulation of the bosonic heat bath approach was initiated by Ford, Kac and Mazur[32] and more recently by Caldeira and Leggett.[11,29] It has been established, for harmonic quantum systems, that the influence of the heat bath described by the oscillators is effectively identical to the external uncorrelated random force acting on a quantum system under consideration. In order for the system to satisfy equation of motion with a linear dissipation term in the classical limit the coupling was chosen to be linear in coordinates while the coupling constants entered lumped in a spectral function which was assumed to be of a power-law form in the oscillator frequency, with the appropriate Debye cutoff. We will make this concept more explicit later.

This model of a heat bath was applied to studying effects of dissipation on the probability of quantum tunneling from a metastable

state.[8,29] It was found that coupling a quantum system to the heat bath actually decreases the quantum tunneling rate. The problem of a particle in a double well potential was also considered.[9,33] In this case the interaction with the bath leads to quantum coherence loss and complete localization at zero temperature. This study has lead to the spin-boson Hamiltonian[9,10] which found numerous other applications. The Hilbert space of the quantum systems studied was effectively restricted to the two-dimensional space corresponding to the two lowest energy levels.

Another possible application of the bosonic heat bath model concerns aspects of quantum measurement. It is believed that the bath is an intrinsic part of a measuring device. In other words, it continuously monitors the physical quantity whose operator is coupled to it.[4−6] It has been shown in the exactly solvable model of the quantum oscillator coupled to a heat bath[5] that the reduced density matrix of the quantum system decoheres, i.e., looses its off-diagonal elements representing the quantum correlations in the system, in the eigenbasis of the interaction Hamiltonian. It has also been argued that the time scale on which this "measurement" occurs is much less than the characteristic time for thermal relaxation of the system.

It is natural to assume that if such a "bath" description of the process of measurement of a Hermitian operator Λ_S exists, then the inter-

action Hamiltonian H_I in (1.1) will involve Λ_S as well as some bath-Hilbert-space operators. No general description of this process exists. Furthermore, when we are limited to specific models in order to obtain tractable, e.g., analytically solvable, examples, then there is no general way to separate decoherence and thermalization effects. We note that thermalization is naturally associated with exchange of energy between the quantum system and heat bath. Model system results and general expectations mentioned earlier suggest that at least in some cases decoherence involves its own time scales which are shorter than those of approach to thermal equilibrium.

In this work we propose to study adiabatic decoherence, i.e., a special case of no energy exchange between the system and bath. Thus we assume that H_S is conserved, i.e., $[H_S, H] = 0$. This assumption is a special case of "quantum nondemolition measurement" concept[2,30] exemplified by the Kerr effect, for instance. Since H_S and H_B is (1.1) operate in different Hilbert spaces, this is equivalent to requiring

$$[H_S, H_I] = 0\,. \tag{1.3}$$

Furthermore, we will assume that H_I is linear in Λ_S:

$$H_I = \Lambda_S P_B\,, \tag{1.4}$$

where P_B acts in the Hilbert space of the bath. Then we have

$$[\Lambda_S, H_S] = 0\,. \tag{1.5}$$

Thus, we consider cases in which the measured, "pointer" observable Λ_S is one of the conserved quantities of the quantum system when it is isolated. Interaction with the bath will then correspond to measurement of such an observable, which can be the energy itself. Specifically, the model of Ref. 14 corresponds to $\Lambda_S = H_S$ for the case of the spin-$\frac{1}{2}$ two-state system, motivated by quantum-computing applications; see also Refs. 2, 12-15. The models of Refs. 1 and 2 correspond to the choices of $\Lambda_S = H_S$ and $\Lambda_S = f(H_S)$, respectively, for a system coupled to a bosonic spin bath, where f is an arbitrary well-behaved function.

Here we derive exact results for adiabatic decoherence due to coupling to the bosonic heat bath, assuming general Λ_S that commutes with H_S. While technically this represents an extension of the results of Refs. 1 and 2, we demonstrate that the general case reveals certain new aspects of the decoherence process. Our new exact-solution method utilizes coherent states and may be of interest in other applications as well. In Section 2, we define the system. Specifically, we choose the bosonic heat bath form for H_B and P_B in (1.1) and (1.4), but we keep H_S and Λ_S general. However, we also analyze the mechanism leading to exact solvability of

general models of this type. Section 3 reports our derivation of the exact expression for the reduced density matrix of the system. Discussion of the results and definition of the continuum limit are given in Section 4.

2. Models of Adiabatic Decoherence

We will be mainly interested in the following Hamiltonian for the quantum system coupled to a bath of bosons (harmonic oscillators) labeled by the subscript k:

$$H = H_S + \sum_k \omega_k a_k^\dagger a_k + \Lambda_S \sum_k \left(g_k^* a_k + g_k a_k^\dagger \right) . \tag{2.1}$$

Here $a_k^\dagger$ and a_k are bosonic creation and annihilation operators, respectively, so that their commutation relation is $[a_k, a_k^\dagger] = 1$. The second term in (2.1) represents the free field or Hamiltonian of the heat bath H_B. The last term is the interaction Hamiltonian H_I. The coupling constants will be specified later; exact results obtained in Section 3 apply for general ω_k and g_k. Here and in the following we use the convention

$$\hbar = 1 \tag{2.2}$$

and we also assume that the energy levels of each oscillator are shifted by $\frac{1}{2}\omega_k$ so that the ground state of each oscillator has zero energy.

Since we assume that H_S and Λ_S commute, we can select a common set $|i\rangle$ of eigenstates:

$$H_S|i\rangle = E_i|i\rangle\,, \tag{2.3}$$

$$\Lambda_S|i\rangle = \lambda_i|i\rangle\,. \tag{2.4}$$

One of the simplifications here, due to the fact that H_S and Λ_S commute, is that these eigenstates automatically constitute the "preferred basis" mentioned earlier.

We will assume that initially the quantum system is in a pure or mixed state described by the density matrix $\rho(0)$, not entangled with the bath. For the bath, we assume that each oscillator is independently thermalized (possibly by prior contact with a "true" heat bath) at temperature T, with the density matrix θ_k. The total system-plus-bath density matrix will then be the product

$$\rho(0)\prod_k \theta_k\,. \tag{2.5}$$

Here

$$\theta_k = Z_k^{-1} e^{-\beta\omega_k a_k^\dagger a_k}\,, \tag{2.6}$$

$$Z_k \equiv (1 - e^{-\beta\omega_k})^{-1}\,, \tag{2.7}$$

where Z_k is the partition function for the oscillator k. The quantity β was defined in (1.2). Introduction of the temperature parameter via the initial state of the bath is common in the literature.[1,2,8–11,14–17,29,32,33] While it may seem artificial, we recall that the bath is supposed to be a large system presumably remaining thermalized on the time scales of interest. Specific results indicating that the bosonic heat bath can be viewed as a source of thermalizing noise have been mentioned earlier; see also Ref. 35.

Our objective is to study the reduced density matrix of the system at time $t \geq 0$; it has the following matrix elements in the preferred basis:

$$\rho_{mn}(t) = \mathrm{Tr}_B \left[\langle m|e^{-iHt} \left(\rho(0) \prod_k \theta_k \right) e^{iHt}|n\rangle \right] . \tag{2.8}$$

Here the outer trace is taken over the states of the heat bath, i.e., the bosonic modes. The inner matrix element is in the space of the quantum system. Note that for no coupling to the bath, i.e., for $g_k = 0$, the density matrix of the system is simply

$$[\rho_{mn}(t)]_{g_k=0} = \rho_{mn}(0)e^{i(E_n - E_m)t}\,. \tag{2.9}$$

For the interacting system, the heat-bath states must be summed over in the trace in (2.8). It is instructive to consider a more general case with the bath consisting of independent "modes" with the Hamiltonians M_k, so that

$$H_B = \sum_k M_k \,, \tag{2.10}$$

where for the bosonic bath we have $M_k = \omega_k a_k^\dagger a_k$. Similarly, for the interaction term we assume coupling to each mode independently,

$$H_I = \Lambda_S \sum_k J_k \,, \tag{2.11}$$

where for the bosonic bath we have $J_k = g_k^* a_k + g a_k^\dagger$. Relation (2.5) remains unchanged, with the definitions (2.6) and (2.7) replaced by

$$\theta_k = Z_k^{-1} e^{-\beta M_k} \,, \tag{2.12}$$

$$Z_k = \mathrm{Tr}_k \left[e^{-\beta M_k} \right] \,, \tag{2.13}$$

where the trace is over a single mode k.

Owing to the fact that H_S and Λ_S share common eigenfunctions,

the inner matrix element calculation in (2.8), in the system space, can be expressed in terms of the eigenvalues defined in (2.3)-(2.4). Specifically, we define the bath-space operators

$$h_i = E_i + \sum_k M_k + \lambda_i \sum_k J_k \,, \tag{2.14}$$

which follow from the form of the Hamiltonian. The calculation in (2.8) then reduces to

$$\rho_{mn}(t) = \mathrm{Tr}_B \left[\langle m| e^{-ih_m t} \left(\rho(0) \prod_k \theta_k \right) e^{ih_n t} |n\rangle \right] \,, \tag{2.15}$$

which yields the expression

$$\rho_{mn}(t) = \rho_{mn}(0) \mathrm{Tr}_B \left[e^{-ih_m t} \left(\prod_k \theta_k \right) e^{ih_n t} \right] \,. \tag{2.16}$$

We will now assume that the operators of different modes k commute. This is obvious for the bosonic or spin baths and must be checked explicitly if one uses the present formulation for a fermionic bath. Then we can factor the expression (2.16) as follows:

$$\rho_{mn}(t) = \rho_{mn}(0) e^{i(E_n - E_m)t} \prod_k \left\{ \mathrm{Tr}_k \left[e^{-i(M_k + \lambda_m J_k)t} \theta_k e^{i(M_k + \lambda_n J_k)t} \right] \right\} \,. \tag{2.17}$$

This expression, or variants derived in earlier works,[1,2,14] suggests that the problem is exactly solvable in some cases. Indeed, the inner trace in over a single mode of the bath. For a spin bath of spin-$\frac{1}{2}$ "modes" the calculation involves only (2×2)-matrix manipulations and is therefore straightforward.[2,14] However, in this case the only nontrivial choice of the "pointer observable" corresponds, in our notation, to $\Lambda_S = H_S$, with both operators usually chosen equal to the Pauli matrix σ_z. There is also hope for obtaining analytical results for other baths with modes in finite-dimensional spaces, such as spins other than $\frac{1}{2}$; we have not explored this possibility.

For the bosonic spin bath, the calculation is in the space of a single harmonic oscillator. It can be carried out by using operator identities.[1,2] We have used instead a method based on the coherent-state formalism which is detailed in the next section.

3. Exact Solution for the Density Matrix

We utilize the coherent-state formalism, e.g., Refs. 35, 36. The coherent states $|z\rangle$ are the eigenstates of the annihilation operator a with complex eigenvalues z. Note that from now on we omit the oscillator index k whenever this leads to no confusion. These states are not orthogonal:

$$\langle z_1|z_2\rangle = \exp\left(z_1^* z_2 - \frac{1}{2}|z_1|^2 - \frac{1}{2}|z_2|^2\right). \tag{3.1}$$

They form an over-complete set, and one can show that the identity operator in a single-oscillator space can be obtained as the integral

$$\int d^2z\, |z\rangle\langle z| = 1\,. \tag{3.2}$$

Here the integration by definition corresponds to

$$d^2z \equiv \frac{1}{\pi} d\,(\mathrm{Re}z)\, d\,(\mathrm{Im}z)\ . \tag{3.3}$$

Furthermore, for an arbitrary operator A, we have, in a single-oscillator space,

$$\mathrm{Tr}A = \int d^2z \, \langle z|A|z\rangle \, . \tag{3.4}$$

Finally, we note the following identity,[35] which will be used later,

$$e^{\Omega a^\dagger a} = \mathcal{N}\left[e^{a^\dagger (e^\Omega - 1)a}\right] \, . \tag{3.5}$$

In this relation Ω is an arbitrary c-number, while $\mathcal{N}$ denotes normal ordering.

The result (2.17) for the reduced density matrix, assuming the bosonic spin bath, can be written as

$$\rho_{mn}(t) = \rho_{mn}(0)e^{i(E_n - E_m)t}\prod_k S_{mn,k} \equiv [\rho_{mn}(t)]_{g_k=0}\prod_k S_{mn,k} \, , \tag{3.6}$$

where we used (2.9). Omitting the mode index k for simplicity, the expression for S_{mn} for each mode in the product is

$$S_{mn} = Z^{-1}\mathrm{Tr}\left[e^{-it\gamma_m}e^{-\beta\omega a^\dagger a}e^{it\gamma_n}\right] \, , \tag{3.7}$$

where the trace is in the space of that mode, and we defined

$$\gamma_m = \omega a^\dagger a + \lambda_m\left(g^* a + g a^\dagger\right) \, . \tag{3.8}$$

The partition function Z is given in (2.7). Relations (3.6)-(3.8) already illustrate one of our main results: apart from the phase factor which would be present in the noninteracting case anyway, the system energy eigenvalues E_n do not enter in the expression for $\rho_{mn}(t)$. The interesting time dependence is controlled by the eigenvalues λ_n of the "pointer observable" operator Λ_S (and by the heat-bath coupling parameters ω_k and g_k).

In order to evaluate the trace in (3.7), we use the coherent-state approach. We have

$$ZS_{mn} = \int d^2z_0\, d^2z_1\; d^2z_2\; \langle z_0|e^{-it\gamma_m}|z_1\rangle\langle z_1|e^{-\beta\omega {a^\dagger}^a}|z_2\rangle\langle z_2|e^{it\gamma_n}|z_0\rangle\,. \tag{3.9}$$

The normal-ordering formula (3.5) then yields for the middle term,

$$\langle z_1|e^{-\beta\omega {a^\dagger}^a}|z_2\rangle = \langle z_1|z_2\rangle e^{z_1^*(e^{-\beta\omega}-1)z_2} =$$

$$\exp\left[z_1^* z_2 - \frac{1}{2}|z_1|^2 - \frac{1}{2}|z_2|^2 + z_1^*(e^{-\beta\omega}-1)z_2\right]. \tag{3.10}$$

In order to evaluate the first and last factors in (3.9) we define shifted operators

$$\eta = a + \lambda_m \omega^{-1} g \,, \tag{3.11}$$

in terms of which we have

$$\gamma_m = \omega \eta^\dagger \eta - \lambda_m^2 \omega^{-1} |g|^2 \,. \tag{3.12}$$

Since η and $\eta^\dagger$ still satisfy the bosonic commutation relation $[\eta, \eta^\dagger] = 1$, the normal-ordering formula applies. Thus, for the first factor in (3.9), for instance, we get

$$\langle z_0 | e^{-it\gamma_m} | z_1 \rangle = e^{it\lambda_m^2 \frac{|g|^2}{\omega}} \langle z_0 | z_1 \rangle e^{\left(e^{-i\omega t}-1\right)\left(z_0^* + \lambda_m \frac{g^*}{\omega}\right)\left(z_1 + \lambda_m \frac{g}{\omega}\right)} \,. \tag{3.13}$$

Collecting all these expressions, one concludes that the calculation of S_{mn} involves six Gaussian integrations over the real and imaginary parts of the variables z_0, z_1, z_2. This is a rather lengthy calculation but it can be carried out in closed form. The result, with indices k restored, is

$$S_{mn,k} = \exp\left(-\omega_k^{-2} |g_k|^2 P_{mn,k}\right) , \tag{3.14}$$

where

$$P_{mn,k} = 2\left(\lambda_m - \lambda_n\right)^2 \sin^2 \frac{\omega_k t}{2} \coth \frac{\beta\omega_k}{2} + i\left(\lambda_m^2 - \lambda_n^2\right)\left(\sin\omega_k t - \omega_k t\right) . \tag{3.15}$$

The expression (3.15), with (3.14), when inserted in (3.6), is the principal result of this section. It will be discussed in the next section. Here we note that in the studies of systems involving the bosonic heat bath one frequently adds the "renormalization" term[2,29] in the Hamiltonian,

$$H = H_S + H_B + H_I + H_R\,, \tag{3.16}$$

where in our case

$$H_R = \Lambda_S^2 \sum_k \omega_k^{-1} |g_k|^2\,. \tag{3.17}$$

The role of this renormalization has been reviewed in Ref. 29. Here we only notice that the sole effect of adding this term in our calculation is to modify the imaginary part of $P_{mn,k}$ which plays no role in our subsequent discussion. The modified expression is

$$P_{mn,k} = 2\left(\lambda_m - \lambda_n\right)^2 \sin^2 \frac{\omega_k t}{2} \coth \frac{\beta\omega_k}{2} + i\left(\lambda_m^2 - \lambda_n^2\right)\sin\omega_k t\,. \tag{3.18}$$

4. Continuum Limit and Discussion

The results of the preceding section, (3.6), (3.14), (3.15), can be conveniently discussed if we consider magnitudes of the matrix elements of the reduced density matrix $\rho(t)$. We have

$$|\rho_{mn}(t)| = |\rho_{mn}(0)| \exp\left[-\frac{1}{4}\left(\lambda_m - \lambda_n\right)^2 \Gamma(t)\right] , \tag{4.1}$$

where we introduced the factor $\frac{1}{4}$ to have the expression identical to that obtained in Ref. 14:

$$\Gamma(t) = 8 \sum_k \omega_k^{-2} |g_k|^2 \sin^2 \frac{\omega_k t}{2} \coth \frac{\beta\omega_k}{2} . \tag{4.2}$$

These results suggest several interesting conclusions. First, the decoherence is clearly controlled by the interaction with the heat bath rather than by the system's Hamiltonian. The eigenvalues of the "pointer observable" Λ_S determine the rate of decoherence, while the type of the bath and coupling controls the form of the function $\Gamma(t)$. It is interesting to note that states with equal eigenvalues λ_m will remain entangled even if their energies E_m are different. As expected, the magnitude of the diagonal matrix elements remains unchanged.

Secondly, we note that $\Gamma(t)$ is a sum of positive terms. However, for

true decoherence, i.e., in order for this sum to diverge for large times, one needs a continuum of frequencies and interactions with the bath modes that are strong enough at low frequencies; see below. From this point on, our discussion of the function $\Gamma(t)$ is basically identical to that in Ref. 14 (see also Ref. 1); we only outline the main points. In the continuum limit, exemplified for instance by phonon modes in solid state, we introduce the density of states $G(\omega)$ and sum over frequencies rather than modes characterized by their wave vectors. The latter change of the integration variable introduces the factor which we will loosely write as $\frac{dk}{d\omega}$; it must be calculated from the dispersion relation of the bosonic modes. Thus we have

$$\Gamma(t) \propto \int d\omega \, \frac{dk}{d\omega} G(\omega) |g(\omega)|^2 \, \omega^{-2} \sin^2 \frac{\omega t}{2} \coth \frac{\beta\omega}{2} \, . \tag{4.3}$$

In Ref. 14, the following choice was considered, motivated by properties of the phonon field in solids; see also Refs. 8-11, 12-18, 29:

$$\frac{dk}{d\omega} G(\omega) |g(\omega)|^2 \propto \omega^n e^{-\frac{\omega}{\omega_c}} \, . \tag{4.4}$$

This combination of the coupling constants and frequencies has been termed the spectral function. Here ω_c is the Debye cutoff frequency.

Specifically, the authors of Ref. 14 have analyzed the cases $n = 1$ and

$n = 3$. For $n = 1$, three regimes were identified, defined by the time scale for thermal decoherence, β, which is large for low temperatures, see (1.2), and the time scale for quantum-fluctuation effects, ω_c^{-1}. Recall that we use the units $\hbar = 1$. The present treatment only makes sense provided $\omega_c^{-1} \ll \beta$. According to Ref. 14, the first, "quiet" regime $t \ll \omega_c^{-1}$ corresponds to no significant decoherence and $\Gamma \propto (\omega_c t)^2$. The next, "quantum" regime, $\omega_c^{-1} \ll t \ll \beta$, corresponds to decoherence driven by quantum fluctuations and $\Gamma \propto \ln(\omega_c t)$. Finally, for $t \gg \beta$, in the "thermal" regime, thermal fluctuations play major role in decoherence and $\Gamma \propto t/\beta$.

For $n = 3$, decoherence is incomplete.[14] Indeed, while n must be positive for the integral in (4.3) to converge, only for $n < 2$ we have divergent $\Gamma(t)$ growing according to a power law for large times (in fact, $\propto t^{2-n}$) in the "thermal" regime. Thus, strong enough coupling $|g(\omega)|$ to the low-frequency modes of the heat bath is crucial for full decoherence.

In summary, we derived exact results for the model of decoherence due to energy-conserving interactions with the bosonic heat bath. We find that the spectrum of the "pointer observable" that enters the interaction with the bath controls the rate of decoherence. The precise functional form of the time dependence is determined both by the choice of heat-bath and system-bath coupling. However, for the case studied, it is universal

for all pointer observables and for all the matrix elements of the reduced density matrix.

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