Quantum impurity models of noisy qubits

D. V. Khveshchenko
Department of Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina 27599, USA
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We demonstrate that the problem of coupled two-level systems (''qubits'') which are also subject to a generic (sub-)Ohmic dissipative environment belongs to the same class of models as those describing (non)magnetic impurities embedded in strongly correlated systems. A further insight into the generalized single- and two-impurity Bose/Fermi Kondo models enables one to make specific recommendations towards a systematic engineering of highly coherent multiqubit assemblies for potential applications in quantum information processing.

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The studies of open quantum systems have long been focused on the behavior of a single two-level system (an effective spin-1/2 or, as it is nowadays often referred to, a qubit) in a dissipative environment, for this hallmark problem appears to describe a variety of physically different (yet, formally related) situations.[1]

More recently, the attention has been drawn to this problem's further extension where N coupled two-level systems would be subject to a dissipative (possibly, nonuniform) environment. This interest was largely motivated by the relevance of the problem in question for practical implementations of the ideas of quantum information processing.

However, despite the previous (mostly numerical and largely limited to weak coupling) analyses of the problem of $N=2$ noisy qubits,[2] not much of a consideration has been given to the assessment of a possibility of reducing the environmentally induced decoherence by means of properly choosing the parameters of individual qubits and/or by virtue of permanent pairwise qubit interactions which (whether desired or not) would be unavoidably present in any realistic setup.

As one step towards developing a systematic (as opposed to heuristic) approach to addressing this kind of issues, in the present work we explore a formal connection between the spin-boson model of interacting qubits coupled to a generic (multicomponent and/or (sub-)Ohmic) bosonic bath and some of the recently studied models of (non)magnetic impurities in strongly correlated electron systems.

Such analysis would be incomplete without investigating the intermediate-to-strong coupling regime where the customary Fermi's Golden rule-based estimates fail, and a more elaborate approach is needed. While, at the first sight, a strong-coupling behavior may not seem to be immediately relevant to the previously proposed designs of a practical quantum register, it should be noted that experimentally measured decoherence rates routinely exceed their best estimates obtained in the framework of the weak-coupling Bloch-Redfield and related approximations. Moreover, even in the case of a single qubit, the recent nonperturbative analyses of the strong coupling behavior as well as the effects of non-Markovian and/or structured environments have already resulted in a number of potentially interesting implications for quantum computing.[3]

Regardless of the qubits' physical makeup, the dynamics of N such species is usually described by the spin-boson Hamiltonian,

$$H_{SB}^{(N)}=\sum_{a,i} S_i^a(B^a+\gamma^a h_i^a)+\sum_{a,ij} I_{ij}^a S_i^a S_j^a+\sum_k \omega_k b_k^\dagger b_k. \quad (1)$$

The random field $h_i^a=\Sigma_k e^{i\vec{k}\vec{r}_i}\lambda_k^a(b_k^\dagger+b_{-k})/\sqrt{\omega_k}$ represents a generic multicomponent bosonic bath composed of D-dimensional propagating modes with the dispersion $\omega_k=vk$ and described by the correlation function (hereafter $R=|i-j|$ is a distance between the ith and jth qubits and Λ is an upper cutoff of order the bath's bandwidth)

$$\langle h_i^a(t)h_j^b(0)\rangle\propto\frac{\delta^{ab}\Lambda^\epsilon}{[t^2-(R/v)^2]^{1-\epsilon/2}}. \quad (2)$$

The variable parameter $0<\epsilon<1$ controls the bath's spectral density $\rho(\omega)=\Sigma_k(|\lambda_k^a|^2/\omega_k)\delta(\omega-\omega_k)\propto\Lambda^\epsilon\omega^{1-\epsilon}$, thus allowing one to study the entire range of different (sub-)Ohmic environments within the same unifying framework.

Recently, a new reincarnation of the Hamiltonian (1) has emerged under the name of the Bose Kondo model in the theory of (non)magnetic impurities in strongly correlated systems, such as heavy fermions, Mott insulators, and high-T_c cuprates.[4]

In the case of a single qubit ($N=1$), the Hamiltonian (1) gives rise to the renormalization group (RG) equations which, to the first order in the dimensional regularization parameter $\epsilon=3-D\ll 1$, read

$$\frac{dg_\parallel}{dl}=\left(\epsilon-\sum_{a=1,2} g_{\perp,a}\right)g_\parallel,$$

$$\frac{dg_{\perp,a}}{dl}=\left(\epsilon-\sum_{b\neq a} g_{\perp,b}-g_\parallel-\vec{B}^2\right)g_{\perp,a},$$

$$\frac{dB_a}{dl}=\left(1-\sum_{a=1,2} g_{\perp,a}\right)B_a. \quad (3)$$

In these equations which generalize the analysis of Ref. 4 to the case of a finite uniform field $\vec{B}\neq 0$, $l=\ln\Lambda/\omega$ is the energy-dependent renormalization scale. The longitudinal

$g_{\parallel}=(\vec{\gamma}\vec{B})^2/B^2$ and the transverse $g_{\perp,a}$ $[\Sigma_{a=1,2}g_{\perp,a}=\vec{\gamma}^2-(\vec{\gamma}\vec{B})^2/B^2]$ qubit-bath couplings are defined with respect to the direction of $\vec{B}=(0,0,\tilde{\Delta})$.

Equations (3) feature a variety of fixed points that can be classified according to the number of effectively equal components of the vector $\vec{g}$. Namely, we find unstable SU(2)- ($g_{\perp,a}=g_{\parallel}$) and XY- ($g_{\perp,a}=g$, $g_{\parallel}=0$) invariant fixed points, while the only stable one is a pair of Ising fixed points ($g_{\parallel}=g_{\perp,1}=0$ or $g_{\parallel}=g_{\perp,2}=0$). Thus, in a striking contrast with the conventional (Fermi) Kondo model,[1] an anisotropy of the bosonic couplings does not renormalize away, but instead tends to increase.

In the Ising case, the coupling to a one-component Ohmic bath gives rise to the conventional Kosterlitz-Thouless (KT) transition that occurs at $g_I=1$, $\tilde{\Delta}_I=0$ and separates the regime where a sufficiently small initial $\tilde{\Delta}$ continues to decrease ($g>1$) from that where it instead grows ($g<1$). In the language of the Fermi Kondo model (see below), these two regimes correspond to the ferromagnetic (FM) Kondo effect and the usual antiferromagnetic (AFM) Kondo screening, respectively.

The behavior of the running RG variable $\tilde{\Delta}(l)$ should not, of course, be confused with that of the renormalized splitting between the qubit's energy levels $\Delta(l)=\tilde{\Delta}(l)e^{-l}$ which still decreases (albeit, in different ways) in both cases. In the extensively studied AFM regime of the Ohmic problem, the latter is given by the well-known solution

$$\Delta_{*}\sim\Lambda(\Delta_0/\Lambda)^{1/1-g} \qquad (4)$$

of the self-consistent equation, $\Delta_{*}=\Delta(l=\ln\Lambda/\Delta_{*})$.[1]

In the case of a sub-Ohmic ($\epsilon>0$) bath and in the vicinity of the Ising fixed point, the RG flow decribed by Eqs. (3) is characterized by a constantly increasing effective coupling $g(l)$ and a vanishing (possibly, after some temporary increase) $\tilde{\Delta}(l)$, provided that its bare value Δ_0 falls below the separatrix which connects the unstable fixed point at $g_I=1$, $\tilde{\Delta}_I=\epsilon^{1/2}$ to the trivial one at the origin of the $g-\tilde{\Delta}$ plane.

Such a behavior signals a total loss of coherence and a complete qubit's localization in one of the two degenerate states (overdamped regime), in agreement with the customary expectations.[1] However, for $\Delta_0\gtrsim\Lambda[2ge^{1/2-g}]^{1/\epsilon}$ the solution of Eqs. (3) shows that coherent damped oscillations with a frequency $\Delta_{*}\sim\Lambda(2g)^{1/\epsilon}$ might still be possible, thus supporting the earlier prediction made in Ref. 5.

In contrast to the Ising case, the coupling to a multicomponent ("nonabelian") Ohmic bath may give rise to a markedly different behavior. In both cases of the XY- and SU(2)-symmetrical couplings, our solution of Eqs. (3) shows that the standard KT fixed point is absent, and the renormalized level splitting continues to grow [although it may temporarily descrease at $g(l)\sim 1$], thus enabling the qubit to avoid localization.

Furthermore, in the "weakly sub-Ohmic" ($0<\epsilon\ll 1$) case a new unstable fixed point emerges at $g_{XY}=\epsilon$ ($g_{SU(2)}=\epsilon/2$) for the XY- [SU(2)-] symmetrical couplings and $\tilde{\Delta}_{XY,SU(2)}=0$. Notably, this nontrivial fixed point governs the regime of small $g(l)$ and $\tilde{\Delta}(l)$ which is of primary importance for quantum computing-related applications of Eq. (1).

In the latter case, contrary to the naive expectation drawn from the weak-coupling analysis, the coupling $g(l)$ may first increase, before succumbing to the continuing growth of $\tilde{\Delta}(l)$ and reverting to the opposite, decreasing, behavior, provided that the initial values of the RG variables satisfy the condition $\max[g_0,\tilde{\Delta}_0^2]\lesssim\epsilon$.

Besides, Eqs. (3) indicate that for a strongly sub-Ohmic bath ($\epsilon>\epsilon_{*}=1/2$) yet another unstable XY-symmetrical fixed point can emerge at $g_{XY,II}=1/2$ and $\tilde{\Delta}_{XY,II}=(\epsilon-\epsilon_{*})^{1/2}$, while the fixed point at $g_{XY,I}=\epsilon$ and $\tilde{\Delta}_{XY,I}=0$ would then become stable. Considering the fact that the corresponding threshold value ϵ_{*} is quite large, this prediction may turn out to be spurious. Nevertheless, from a general viewpoint, it is conceivable that even a multicomponent (yet, sufficiently strongly sub-Ohmic) bath could still be capable of causing a complete localization of the qubit for small $\tilde{\Delta}_0$.

The above predictions for the RG flow of the couplings and the effective level splitting have a direct bearing on the properties of such observables as the qubits' correlation functions $\langle\{S_i^a(t),S_j^a(0)\}\rangle$ and the corresponding dynamical spectral functions

$$\chi_{ij}(\omega)=\mathrm{Im}\sum_{n,m}(\rho_{nn}-\rho_{mm})\frac{\langle n|S_i^a|m\rangle\langle m|S_j^a|n\rangle}{\omega-E_n+E_m+i\Gamma_{nm}} \qquad (5)$$

given by the sums over renormalized and broadened energy levels $|n\rangle$ of the interacting noiseless qubits which are weighted with the diagonal elements of the equilibrium density matrix $\rho_{nn}=|n\rangle\langle n|$.

The analysis of Eq. (5) reveals that for noninteracting qubits the coherent (single-qubit) behavior manifests itself through the presence of inelastic peaks at $\omega=\pm\Delta_{*}/2$ in the normalized spectral density $\chi_{ij}(\omega)/\omega^{1-\epsilon}\propto\delta_{ij}$.[3,5] The width of these peaks is controlled by the decoherence rate

$$\Gamma\propto g_{*}\rho(\Delta_{*})\coth(\Delta_{*}/2T), \qquad (6)$$

which increases as $\Gamma\sim g_{*}T(\Lambda/\Delta_{*})^{\epsilon}$ with increasing g_{*} and decreasing $\Delta_{*}\lesssim T$. As the qubits lose their coherence, the spectral weight gets transferred from the inelastic peaks to the small energies ($\omega\approx 0$), this behavior constitutes the decohering effect of the environment. The onset of complete localization is usually preceeded by exponential relaxation which separates the former regime from that of the partly coherent damped oscillations.[1]

It is worth reminding that different probes may signal the loss of coherence at different critical couplings. In the extensively studied Ohmic case, such a difference is exemplified by the juxtaposition of the single-qubit average $\langle S_i^a(t)\rangle$ and the autocorrelation function $\chi_{ii}(w)\coth\omega/2T$ whose coherent peaks get washed out at, respectively, $g=1/2$ (Toulouse point)[1] and $g=1/3$,[6] both critical values being lower than the beforementioned estimate $g_I=1$.

In light of the above mentioned possibility of a nonmonotonic behavior of $g(l)$ near the SU(2)- and XY-symmetrical fixed points at small g_0 and $\tilde{\Delta}_0$, the initial increase of the coupling strength may give rise to the situation where the inelastic peaks in the spectral function (5) might temporarily become rather broad before they can narrow down at still lower energies.

The above findings strongly suggest that by operating a noisy qubit in the vicinity of one of the XY- and SU(2)-symmetrical fixed points one can better retain its quantum coherence.

One could argue, however, that for noninteracting qubits the intrinsic instability of the model (1) towards developing the Ising-like anisotropy may hinder any possibility of taking advantage of the greater robustness of quantum coherence found at the high-symmetry fixed points. To this end, below we show that the loss of coherence caused by the outward flow of the single-qubit RG trajectory away from a desired operating point can be thwarted by interqubit couplings which provide for an extra protection against decoherence.

In fact, some exchangelike interaction between the qubits is necessarily generated by the qubit-bath couplings themselves. The instantaneous part of this (generally, retarded and FM-like) interaction which arises in the course of integrating over the bosonic modes down to the energy scale $\omega \sim v/R$,

$$I_B^a = -\sum_k \frac{\lambda_k^a \lambda_{-k}^b}{\omega_k^2} e^{i\vec{k}(\vec{r}_i - \vec{r}_j)} \propto -\delta^{ab} g \Lambda^{\epsilon}/R^{1-\epsilon}, \qquad (7)$$

combines together with the direct interqubit coupling into the effective parameters I_{ij}^a introduced in Eq. (1).

It can be easily seen that a sufficiently strong FM exchange ($I \to -\infty$) forces a pair of qubits into a triplet state which then follows an effective, $S=1$, Bose Kondo scenario. In the opposite, strongly AFM, limit ($I \to +\infty$) the two qubits get locked into a singlet state, which prevents them from any unwanted entanglement with the environment. According to Eq. (7), however, the latter regime cannot be attained in the absence of a sufficiently strong AFM direct coupling between the qubits.

At intermediate values, I provides a cutoff for the RG flow which now terminates at $l_I = \ln \Lambda/|I|$ before reaching the strong coupling limit, thereby resulting in a larger effective $\Delta_* = \Delta(l_I)$ that determines the position and the width of the coherent peaks.

In the case of the 3D Ohmic bath, a further insight can be gained from the previously established correspondence between the $N=2$ Hamitonian (1) and the anisotropic two-impurity (Fermi) Kondo (TIKM) model

$$H_{TIFK}^{(2)} = -iv \sum_{i=1,2} \int_{-\infty}^{\infty} dx c_i^\dagger \partial_x c_i + \sum_a I^a S_1^a S_2^a + \sum_a [J_+^a S_+^a (c_1^\dagger \sigma^a c_1 + c_2^\dagger \sigma^a c_2) + J_-^a S_-^a (c_1^\dagger \sigma^a c_1 - c_2^\dagger \sigma^a c_2) + J_m^a S_+^a (c_1^\dagger \sigma^a c_2 + c_2^\dagger \sigma^a c_1)], \qquad (8)$$

where the autocorrelation function of the 1D spin-1/2 fermions with the Fermi momentum k_F is $\langle c_i^\dagger(t) c_j(0) \rangle \propto \delta_{ij}/t$, while the Kondo couplings

$$J_+^a = J^a, \quad J_m^a = J^a \frac{\sin(k_F R)}{(k_F R)}, \quad J_-^a = J^a \sqrt{1 - \frac{\sin^2(k_F R)}{(k_F R)^2}} \qquad (9)$$

between $S_\pm^a = S_1^a \pm S_2^a$ and the even, odd, and mixed bilinear combinations of the fermion fields $c_{1,2} = (c_e \pm c_o)/\sqrt{2}$ at the two qubits' locations are given in terms of the exchange constants of the single-impurity anisotropic Fermi Kondo model[7] which, in turn, are related to the parameters of the $N=1$, $\epsilon=0$ Hamiltonian (1): $g = [1 - (2/\pi)\tan^{-1}(\pi J^{\parallel}/4\Lambda)]^2$ and $\tilde{\Delta} = J^{\perp}$.[1]

In contrast to its bosonic counterpart (7), the Ruderman-Kittel-Kasuya-Yosida like interqubit coupling mediated by the fermionic bath behaves as $I_F \propto (J^2/\Lambda) \times [(2k_F R)\cos(2k_F R) - \sin(2k_F R)]/(2k_F R)^4$. Therefore, unless one chooses to neglect any environmentally induced contributions to the exchange coupling I altogether, the strict correspondence between TIKM and the $N=1$ model (1) can only hold for small interqubit separations, $R \ll 1/k_F$ (see below).

In the presence of the particle-hole symmetry, the two-channel TIKM (8) possesses an unstable fixed point at a critical (AFM) value I_* which is set by the single-qubit Kondo scale $T_K^{(S=1/2)}$. This critical point, which in the SU(2)-symmetrical case $[T_K^{(S=1/2)} = \Lambda \exp(-\Lambda/J)]$ occurs at $I_* \approx 2.5 T_K^{(S=1/2)}$, gets replaced by a crossover, if the particle-hole symmetry is broken.[7]

In the FM regime ($I \lesssim -T_K^{(S=1/2)}$), the Kondo screening of the composite spin $S=1$ is characterized by the scale $T_K(I) \sim T_K^{(S=1/2)} (T_K^{(S=1/2)}/|I|)^{\eta}$ which interpolates between $T_K^{(S=1/2)}$ and $T_K^{S=1} = T_K(I \lesssim -\Lambda)$. The nonuniversal exponent η depends on the exchange anisotropy and assumes the value $\eta = 2$ in the SU(2)-invariant case $[T_K^{(S=1)} = \Lambda \exp(-2\Lambda/J)]$.

The above behavior pertains to the two-channel model which describes a pair of well separated qubits ($R \gg 1/k_F$), whereas at small separations the term in Eq. (8) proportional to $J_-^a \ll J_+^a \approx J_m^a$ can be disregarded, and Eq. (8) reduces to the single-channel TIKM model formulated solely in terms of the even combination c_e of the fermion orbitals which is coupled to the total spin $\vec{S}_+$. Remarkably, the two- and single-channel TIKM models appear to describe the two opposite limits which correspond to independent and collective decoherence, respectively.

For a pair of identical qubits ($J_1 = J_2$), the single-channel TIKM undergoes a simple first order transition (level crossing), as I is tuned past its critical value I_*, from the underscreened $S=1$ model at $I < I_*$ to the two-qubit singlet state which is completely decoupled from the bath at $I > I_*$.[8]

If, however, the qubits are different ($J_1 \neq J_2$), then, as I increases past I_*, the more strongly coupled qubit first gets screened at $T_K^{(I)} = \Lambda \exp(-\Lambda/\max[J_1, J_2])$, followed by the KT-type transition (which now occurs regardless of the presence of the particle-hole symmetry) at $T_K^{(II)} = \max[I - I_*, T_K^{(I)} \exp(-T_K^{(I)}/I - I_*)]$.

The above conclusions, which were drawn in the case of the SU(2)-invariant couplings, apply not only to qubits represented by physical (electron or nuclear) spins but also to the effective qubit operators which represent, e.g., electron states in two-level single or lateral/vertical double quantum dots. Such operators have been routinely introduced in the Anderson or resonant level models where the genuinely SU(2)-invariant exchange couplings are generated from the electron tunneling amplitudes by the Schrieffer-Wolff transformation.

A comparison between several different kinds of the Ising-type qubit interactions studied in the context of the $N=2$ problem[2] indicates that a pair of qubits can better retain their coherence if the interaction term commutes with the qubit-bath coupling operator. In this regard, the Heisenberg exchange, which not only commutes with the overall qubit-bath coupling in the case of collective decoherence but also provides for the strongest lifting of the singlet-triplet degeneracy, might offer the best available option for reducing decoherence.

We note, in passing, that spin-rotationally invariant couplings may not be easily realizable for some of the pseudospin qubits. Among such examples are the Josephson junction qubits whose Hamiltonians, while being potentially well controllable, generally would have no particular symmetries at all. Therefore, it is conceivable that future designs of practical solid-state qubits will need to optimize between the somewhat contradictory requirements of efficient control and robust coherence.

The formal analogy between the problems of noisy qubits and quantum impurities established in this work can be pursued even further. In particular, the $\vec{B}\neq 0$ counterpart of the previously studied Fermi-Bose Kondo model[4] can describe a system of qubits coupled to one Ohmic (represented by a fermionic) and the other sub-Ohmic (bosonic) bath. Such a situation occurs, e.g., in the Josephson qubits where the effects of both the Nyquist ($\epsilon=0$) and $1/f$ ($\epsilon=1$, if treated as approximately Gaussian) noises which are caused, respectively, by fluctuating currents and background charges often need to be considered on equal footing.

The fact that the only stable fixed points of the mixed Fermi-Bose model are the pure Fermi and pure Bose ones[4] suggests a possibility of effectively blocking off a more harmful type of coupling, while tackling the remaining one with, e.g., error-correction techniques.

To summarize, in the present work we exploited a formal similarity between the problem of interacting qubits in (sub-)Ohmic dissipative environments and the recently studied models of quantum impurities in strongly correlated systems. This insight enabled us to formulate a number of concrete recommendations for achieving the optimal (coherence-wise) regime for operating a noisy multiqubit quantum register.

Firstly, we investigated the RG properties of the (sub-)Ohmic single-qubit model (1) in the vicinity of its fixed points of different symmetries. In the course of this analysis, we discovered that for non-interacting qubits and a "weakly-sub-Ohmic" bath ($0\leq\epsilon<\epsilon_*$), the best possible conditions for preserving coherence would require the most spin rotationally symmetrical qubit-bath couplings γ^a.

Secondly, we ascertained the possible benefits of permanent interactions I_{ij}^a between the elements of a multiqubit array for attaining the most coherence-friendly regime and protecting the qubits' quantum memory during the idling periods between consecutive gate operations. Specifically, we found that it would be advantageous to tune the [preferably, SU(2)-symmetrical] pair-wise interqubit coupling I close to (yet, smaller than) the critical value I_* of the TIKM model, thereby causing an incipient singlet formation and concomitant quenching of the Kondo screening.

Lastly, the Kondo physics-conscious approach to the engineering of robust qubit Hamiltonians might prove instrumental in solid-state implementations of quantum information processing where, unlike in liquid-state NMR or trapped-ion designs, such active noise suppression techniques as dynamical decoupling/recoupling schemes may not be readily available. Therefore, we believe that this work will further spur the ongoing cross-fertilization between the developing theory of quantum information and such well-established topics in materials theory as Kondo physics of heavy fermions and quantum dots.

Note added in proof. In the case $n=1$ and $\epsilon>0$, Eq. (2) of this work (first made available in Ref. 10) and the conclusions regarding the possibility of a delocalization transition for a sufficiently large Δ were recently confirmed in Ref. 9.

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