Decoherence in a System of Many Two-Level Atoms

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I show that the decoherence in a system of N degenerate two-level atoms interacting with a bosonic heat bath is for any number of atoms N governed by a generalized Hamming distance (called ''decoherence metric'') between the superposed quantum states, with a time-dependent metric tensor that is specific for the heat bath. The decoherence metric allows for the complete characterization of the decoherence of all possible superpositions of many-particle states, and can be applied to minimize the overall decoherence in a quantum memory. For qubits which are far apart, the decoherence is given by a function describing single-qubit decoherence times the standard Hamming distance. I apply the theory to cold atoms in an optical lattice interacting with blackbody radiation.

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Decoherence is considered one of the main ingredients in the transition from quantum mechanics to classical mechanics [1]. According to experimental evidence [see, for example, [2]], ''decoherence'' can be well described within the standard framework of quantum mechanics [3]. The loss of coherence of quantum mechanical superpositions becomes increasingly rapid when the ''distance'' between the components of the superpositions gets large [4,5], such that quantum mechanical behavior like interference of wave functions is never observed for macroscopic objects. With few notable exceptions [6], most work on decoherence has focused so far on systems with only one or a few effective degrees of freedom coupled to a heat bath. Even when large numbers of particles come into play, like in superconducting qubits based on Josephson junctions or in superradiance [7], only a single effective degree of freedom is normally retained. With the rise of quantum information science, the fundamental question whether for large particle (qubit) numbers there might be new self-limitations of quantum mechanics [8], has also become of huge practical importance. Indeed, understanding and possibly suppressing decoherence of quantum superpositions in the exponentially large Hilbert space of possibly thousands of qubits is considered the most difficult problem on the way to a large scale quantum computer.

In the following I show that a generalized Hamming distance with a time-dependent metric tensor given by the heat bath and the couplings to the heat bath completely determines the decoherence process of a an arbitrarily large number of qubits. The standard Hamming distance, which counts the number of bits by which two code words differ, plays a central role in both classical and quantum error correction [9], and determines, in particular, what code words remain distinguishable in a given error model. It is therefore very satisfying that the heat bath itself determines the metric relevant for the decoherence process, as decoherence reflects to what extent the heat bath distinguishes the superposed states [4].

Starting point of the analysis are N two-level atoms at arbitrary but fixed positions $\mathbf{R}_i$ $(i = 0, \ldots, N-1)$ interacting with a common bosonic heat bath. All atoms are assumed identical with level spacing $\hbar\Omega_0$ and energy eigenstates $|-1\rangle$ and $|1\rangle$, with $\sigma_z|\pm 1\rangle = \pm|\pm 1\rangle$. The total Hamiltonian reads

$$H = \sum_k \hbar\omega_k a_k^\dagger a_k + \frac{1}{2}\hbar\Omega_0 \sum_{i=0}^{N-1} \sigma_{zi} + \hbar \sum_k \sum_{i=0}^{N-1} g_k^{(i)} \sigma_{xi} (a_k e^{i\mathbf{k}\cdot\mathbf{R}_i} + a_k^\dagger e^{-i\mathbf{k}\cdot\mathbf{R}_i}), \quad (1)$$

where σ_{xi} and σ_{zi} are Pauli matrices for atom i. While the results obtained are valid for a general bosonic heat bath, we will consider in the following as concrete example thermal blackbody (BBR) radiation dipole coupled to the atoms [10]. The index k then stands for wave vector $\mathbf{k}$ and polarization direction λ ($k_j = 2\pi n_j/L$ with integer n_j, $j = x, y, z$ for periodic boundary conditions) of the electromagnetic waves; $a_k^\dagger$ (a_k) are the creation (annihilation) operators for mode k with frequency $\omega_k = c|\mathbf{k}|$, polarization vector $\boldsymbol{\epsilon}_k$, and electric field amplitude $\mathcal{E}_k = \sqrt{\hbar\omega_k/(2\varepsilon_0 V)}$, where ε_0, c, and V are the dielectric constant of the vacuum, speed of light, and the quantization volume, respectively. The coupling constant of atom i to mode k is denoted by $g_k^{(i)} = -\frac{ed\mathcal{E}_k}{\hbar}\hat{u}^{(i)} \cdot \boldsymbol{\epsilon}_k$, where $\hat{u}^{(i)}$ stands for a unit vector in the direction of the dipole moment of atom i, $\langle -1|\mathbf{d}|1\rangle = ed\hat{u}^{(i)}$ with electron charge e and dipole length d. Hamiltonians of the form (1) have been studied before in many situations, in particular, in the context of dipole-dipole interactions in quantum optics and various forms of mode selection [see [11] and references therein]. We will restrict ourselves to atoms with degenerate energy levels, $\Omega_0 = 0$. This should set a lower limit for decoherence in quantum memories based on qubits with an allowed dipole transition. From a theoretical perspective degenerate levels are extremely attractive, as the model

can be solved exactly for any N. The results remain valid for small but finite Ω_0, as long as the time $t \ll 1/(N\hbar\Omega_0)$ [5]. The results are also easily extended to any model with commuting system and interaction Hamiltonian, $[H_{\rm sys}, H_{\rm int}] = 0$, such as pure dephasing models with $H_{\rm sys} \propto \sigma_{zi}$ and $H_{\rm int} \propto \sigma_{zi}$.

It is interesting to consider the decoherence process of n selected atoms ($i = 0, \ldots, n-1$) out of the N atoms. This offers the additional information how decoherence scales as function of the size of a subcluster in the quantum memory. The common heat bath can lead to entanglement between the atoms [12], such that unobserved atoms can become an important source of ''indirect'' decoherence. Besides its conceptual importance, this can be relevant, practically, if additional atoms are trapped in an optical lattice, or when information is stored in an atomic gas in a large number of atoms [13]. We therefore first trace out the bosonic modes and secondly the additional atoms $n \ldots N-1$. The reduced density matrix ρ of the remaining atoms will be expressed in the eigenbasis of the σ_{xi}, the natural basis (also called pointer basis) for studying the decoherence process [4]. The matrix elements of ρ are $\rho_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(t)$, where $\tilde{\mathbf{s}} = (s_0, \ldots, s_{n-1})$ is a subset of the code word $\mathbf{s} = (s_0, s_1, \ldots, s_{N-1})$ (with $\sigma_{xi}|s_i\rangle_x = s_i|s_i\rangle_x$, $s_i = \pm 1$, and similarly for $\tilde{\mathbf{s}}'$, i.e., $\tilde{\mathbf{s}}$ and $\tilde{\mathbf{s}}'$ are binary representations of the matrix indices). We assume that the heat bath is initially in thermal equilibrium at temperature T, and all unobserved atoms are initially in a product state with equal probability in state $|1>_x$ or $|-1>_x$, and uncorrelated with the selected atoms.

Using the method of shifted harmonic oscillators [14] one shows that the time evolution of ρ is given by

$$\rho_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(t) = \rho_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(0) \exp\Big\{ -\sum_{i,j=0}^{n-1} (s_i - s_i')(s_j - s_j') f_{ij}(t, \mathbf{R}_i - \mathbf{R}_j) + i \sum_{j=1}^{n-1} \sum_{i=0}^{j-1} (s_i s_j - s_i' s_j') \varphi_{ij}(t, \mathbf{R}_i - \mathbf{R}_j) \Big\} \times \prod_{l=n}^{N-1} \cos\Big[\sum_{i=0}^{n-1} (s_i - s_i') \varphi_{il}(t, \mathbf{R}_i - \mathbf{R}_l) \Big]. \quad (2)$$

The functions f_{ij} and φ_{ij} are given by

$$f_{ij}(t, \mathbf{R}) = \sum_k \frac{g_k^{(i)} g_k^{(j)}}{\omega_k^2} \cos(\mathbf{k}\cdot\mathbf{R})(1 - \cos\omega_k t) \coth\frac{\beta\hbar\omega_k}{2}$$

$$\varphi_{ij}(t, \mathbf{R}) = 2\sum_k \frac{g_k^{(i)} g_k^{(j)}}{\omega_k^2} \cos(\mathbf{k}\cdot\mathbf{R})(\omega_k t - \sin\omega_k t). \quad (3)$$

We are interested in the initial stages of the decay of the off-diagonal matrix elements (the ''coherences''), when f_{ij} and φ_{ij} are both much smaller than 1, as later basically no coherences are left anyway. I define the ''decoherences'' $d_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(t)$ through

$$\frac{|\rho_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(t)|}{|\rho_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(0)|} \equiv 1 - d_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(t). \quad (4)$$

Expanding Eq. (2) to lowest order in f_{ij} and φ_{ij} we find

$$d_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(t) \simeq \tfrac{1}{4}(\tilde{\mathbf{s}} - \tilde{\mathbf{s}}')\mathbf{M}(t)(\tilde{\mathbf{s}} - \tilde{\mathbf{s}}')^T, \quad (5)$$

where ^{T} denotes the transpose, and $\mathbf{M}(t)$ is a real, symmetric, and non-negative matrix with elements ($i, j = 0, \ldots, n-1$)

$$M_{ij} = 4f_{ij}(t, \mathbf{R}_i - \mathbf{R}_j) + 2\Phi_{ij}(t, \mathbf{R}_i, \mathbf{R}_j),$$
$$\Phi_{ij}(t, \mathbf{R}_i, \mathbf{R}_j) = \sum_{l=n}^{N-1} \varphi_{il}(t, \mathbf{R}_i - \mathbf{R}_l)\varphi_{jl}(t, \mathbf{R}_j - \mathbf{R}_l). \quad (6)$$

The properties of $\mathbf{M}$ allow us to consider $\mathbf{M}(t)$ as a time-dependent metric tensor, and to define a metric in the vector space $\mathbb{R}^n$ containing all code words. The heat bath itself therefore induces a natural distance defined as

$$\|\tilde{\mathbf{s}} - \tilde{\mathbf{s}}'\|_{M(t)} = \tfrac{1}{2}\sqrt{(\tilde{\mathbf{s}} - \tilde{\mathbf{s}}')\mathbf{M}(t)(\tilde{\mathbf{s}} - \tilde{\mathbf{s}}')^T}. \quad (7)$$

We will call $\|\tilde{\mathbf{s}} - \tilde{\mathbf{s}}'\|_{M(t)}$ with $\mathbf{M}(t)$ given by Eq. (6) ''decoherence metric'' and $\mathbf{M}$ ''decoherence metric tensor'' (DMT). Equation (5) shows that the decoherence process of a superposition of code words $\tilde{\mathbf{s}}$ and $\tilde{\mathbf{s}}'$ is governed by the decoherence metric,

$$d_{\tilde{\mathbf{s}}\tilde{\mathbf{s}}'}(t) \simeq \|\tilde{\mathbf{s}} - \tilde{\mathbf{s}}'\|^2_{M(t)}, \quad (8)$$

with a DMT $\mathbf{M}(t)$ defined by the heat bath itself and the couplings to the heat bath. Equation (8) constitutes the central result of this Letter.

The distance $\|\tilde{\mathbf{s}} - \tilde{\mathbf{s}}'\|_{M(t)}$ generalizes the well-known Hamming distance $D^H(\tilde{\mathbf{s}}, \tilde{\mathbf{s}}')$, i.e., the number of digits in which $\tilde{\mathbf{s}}$ and $\tilde{\mathbf{s}}'$ differ. The Hamming distance $D^H(\tilde{\mathbf{s}}, \tilde{\mathbf{s}}')$ is recovered from Eq. (7) for the trivial metric tensor $\mathbf{M} = \mathbf{I}$, where $\mathbf{I}$ is the identity matrix in n dimensions, as $D^H(\tilde{\mathbf{s}}, \tilde{\mathbf{s}}') = \|\tilde{\mathbf{s}} - \tilde{\mathbf{s}}'\|_I^2$. As an immediate consequence we find that the entanglement of a quantum state does not (or at least not fully) determine the decoherence between its components. Indeed, all states related by qubit flips in the components [such as, e.g., $(|000\rangle + |111\rangle)/\sqrt{3}$ and $(|100\rangle + |011\rangle)/\sqrt{3}$] have the same entanglement and the same Hamming distance, but the off-diagonal elements of $\mathbf{M}$ lead to different time-dependent decoherences for these states.

The decoherence metric is in the strict sense a pseudometric. It is symmetric, non-negative, and obeys the triangle inequality, but there can be code words $\tilde{\mathbf{s}}$ and $\tilde{\mathbf{s}}'$ with $\tilde{\mathbf{s}} \neq \tilde{\mathbf{s}}'$ such that $\|\tilde{\mathbf{s}} - \tilde{\mathbf{s}}'\|_{M(t)} = 0$. Such code words constitute a decoherence free subspace (DFS), which plays an important role in quantum information processing [15]. For the ease of language, I will continue to use the word ''metric,'' however. The desire to keep the triangle inequality motivates the choice of the square root in Eq. (7), whereas the Hamming distance is defined without it. The latter still obeys the triangle inequality for binary code words, but the triangle inequality can be broken if the metric tensor has nondiagonal matrix elements and the metric is defined without the square root. The decoherence

metric has the form of a Mahalanobis distance used in statistical analysis [16].

The first part of the DMT, $4f_{ij}(t, \mathbf{R}_i - \mathbf{R}_j)$ in Eq. (6), depends on the n selected atoms only. It describes the direct decoherence of the atoms due to their exposure to the heat bath. The second part, $2\Phi_{ij}(t, \mathbf{R}_i, \mathbf{R}_j)$, however, depends on all atoms, even the nonselected ones, such that this contribution is not translationally invariant. Φ_{ij} describes the ''indirect decoherence'' which arises due to the effective interaction and subsequent correlations or even entanglement that the heat bath induces between the atoms [12]. Remarkably, the total decoherence $d_{\mathrm{tot}}(t)$, as defined by $\sum_{\mathbf{s}\neq\mathbf{s}'}|\rho_{\mathbf{ss}'}(t)|/\sum_{\mathbf{s}\neq\mathbf{s}'}|\rho_{\mathbf{ss}'}(0)| \equiv 1 - d_{\mathrm{tot}}(t)$, involves only the trace of the DMT, $d_{\mathrm{tot}}(t) = \frac{1}{2-2^{-n+1}}\,\mathrm{tr}\mathbf{M}(t)$. In situations where Φ_{ii} is absent (e.g., for $n = N$), the total decoherence scales for large n proportional to n, as f_{ii} is independent of n; otherwise, the scaling of Φ_{ii} with n and N has to be taken into account.

The DMT can be evaluated explicitly for the present physical model. Here, we will limit ourselves to direct decoherence of $n = N$ two-level atoms interacting with BBR. We express all lengths in terms of the dipole length d and times in units of d/c, $t \to ct/d$, and define $r_{ij} = |\mathbf{R}_i - \mathbf{R}_j|/d$. To simplify the presentation we will assume that all dipoles are oriented in the same direction. This means that $g_k^{(i)}$ is independent of i, and $f_{ij}(t, \mathbf{R}_i - \mathbf{R}_j)$ depends on i and j in the frame aligned with $\mathbf{R}_i - \mathbf{R}_j$ only through r_{ij} and the angle ϑ between the $\hat{u}_k^{(i)}$ and $\mathbf{R}_i - \mathbf{R}_j$. The azimuthal angle is irrelevant, and we can write $f_{ij}(t, \mathbf{R}_i - \mathbf{R}_j) = \hat{f}(t, r_{ij}, \vartheta)$. In the continuum limit $V \to \infty$, the sums in Eq. (3) become integrals over $\mathbf{k}$ which can be done analytically for $T = 0$. The result reads $\hat{f}(t, r, \vartheta) = \frac{\alpha}{2\pi}\frac{1}{r^2} \times [s(t, r)\sin^2\vartheta + c(t, r)\cos^2\vartheta]$ with

$$
\begin{aligned}
s(t, r) = {} & \frac{2}{1-(t/r)^2}\left[\cos(\kappa r)\cos(\kappa t) + \frac{t}{r}\sin(\kappa r)\sin(\kappa t)\right. \\
& \left. - \left(\frac{t}{r}\right)^2\right] + 2\left[\frac{\sin\kappa r}{\kappa r}[1-\cos(\kappa t)] - \cos(\kappa r)\right] \\
& + \frac{t}{r}\left[\ln\left|\frac{t-r}{t+r}\right| - \mathrm{Ci}\,(\kappa|t-r|) + \mathrm{Ci}\,(\kappa|t+r|)\right]
\end{aligned}
$$

$$
\begin{aligned}
c(t, r) = {} & 2\frac{t}{r}\left[\mathrm{Ci}\,(\kappa|t-r|) - \mathrm{Ci}\,(\kappa|t+r|) - \ln\left|\frac{t-r}{t+r}\right|\right] \\
& + \frac{4}{\kappa r}\sin(\kappa r)[\cos(\kappa t) - 1], \qquad (9)
\end{aligned}
$$

where $\alpha = e^2/(4\pi\varepsilon_0\hbar c) \simeq 1/137.06$ is the fine-structure constant, and $\kappa = k_{\max}d$ a UV cutoff of the integral over $\mathbf{k}$. A cutoff is only needed for the diagonal part f_{ii} which corresponds to $r_{ij} = 0$, but in order to assure the positivity of the decoherence metric, the same cutoff should be used for both diagonal and off-diagonal parts. The off-diagonal terms f_{ij} arise due to interference effects between two qubits. They decay as functions of r on a length scale of the order $1/\kappa$ (see Fig. 1). There can also be regions in the t, r plane where f_{ij} becomes negative (not withstanding the fact that the decoherence metric is always non-negative). One such zone is a ridge along the light cone $t = r$. Another one exists for fixed r almost independently of t, for distances of the order $1/\kappa$. The function $\hat{f}(t, r, \vartheta)$ is continuous in the limit $r \to 0$, and leads to diagonal matrix elements f_{ii} independent of ϑ and i, $f_{ii}(t, \mathbf{0}) = \hat{f}(t, 0, \vartheta) \equiv f_{ii}(t)$, which describe single-qubit decoherence (i.e., $n = N = 1$).

$$
f_{ii}(t) = \frac{2}{3\pi}\alpha\left(\frac{\kappa^2}{2} + \frac{1-\cos(\kappa t) - \kappa t\sin(\kappa t)}{t^2}\right). \qquad (10)
$$

The expressions (9) and (10) are exact in the limit $T \to 0$. Corrections due to finite temperature are of order $k_BT/(\hbar\omega_{\max})$ with $\omega_{\max} = ck_{\max}$, and will be neglected in the following. The divergence of f_{ii} for $\kappa \to \infty$ makes the cutoff a relevant physical quantity. A cutoff always arises, at the latest at $\kappa \sim 1$ when the dipole approximation breaks down. Much smaller values of κ are expected for realistic atoms when transitions to excited levels come into play.

In the limit of large qubit distances ($r \gg 1/\kappa$) the decoherence between two code words is just given by the Hamming distance times the single-qubit decoherence, $d_{\mathbf{ss}'}(t) = 4f_{00}(t)D^H(\mathbf{s}, \mathbf{s}')$, as the qubits are then independent and each qubit contributes to decoherence if and only if it is in a superposition of $|-1\rangle$ and $|1\rangle$. This is shown in Fig. 2 for the example of 3×3 qubits arranged on a 2D square optical lattice with lattice constant a. The larger a the smaller the spread of the decoherences around the value given by the Hamming distance and single-qubit decoherence.

The minimum and maximum decoherence, and the width of the decoherence distribution, show a substantial dependence on the lattice spacing (see Fig. 3). Notably, for small lattice spacing ($r \ll 1/\kappa$) the minimum decoherence tends to zero. A DFS arises, as the atoms then couple in a symmetric way to the heat bath (the latter does not contain sufficiently short waves for distinguishing the positions of the atoms). The decoherence metric allows to generalize

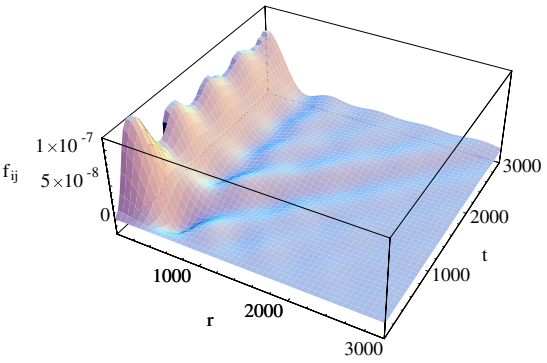

FIG. 1 (color online). The function $\hat{f}(t, r_{ij}, \vartheta)$, for $\kappa = 0.01$ and $\vartheta = \pi/2$ at $T = 0$. The limit $r \to 0$ represents the single-qubit decoherence, $f_{ii}(t)$.

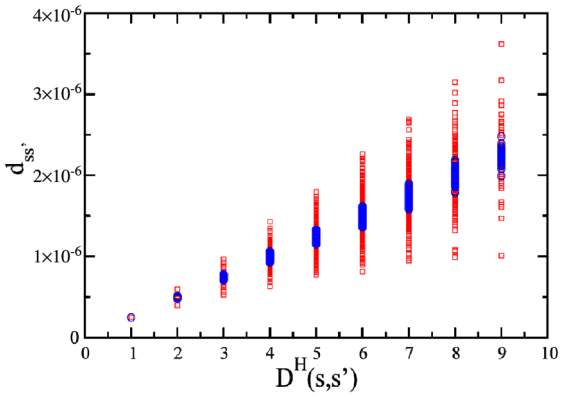

FIG. 2 (color online). Decoherences $d_{s,s'}(t)$ of 9 qubits in a 3×3 square optical lattice at $t = 200.0$ as function of the Hamming distances $D^H(\mathbf{s}, \mathbf{s}')$. Small red squares are for $a = 580d$, large blue circles for $a = 1000d$. Same parameters as in Fig. 1.

the DFS concept in the sense that even for nonsymmetric coupling one may optimize now the performance of the quantum computer by encoding in the states with *smallest* decoherence, which can be explicitly found using the decoherence metric. In [17] a method was introduced that allows us to quantum compute within a DFS, based on a strong coupling to the environment and corresponding broadening of non-DFS states. It is expected that this method can be generalized to the current approach.

As a summary, I have derived a ''decoherence metric'' that induces a natural distance between binary quantum code words. The decoherence metric generalizes the well-known Hamming distance and determines directly the time-dependent decoherence in an arbitrarily large system of qubits with degenerate energy levels coupled to a heat bath of harmonic osciallators.

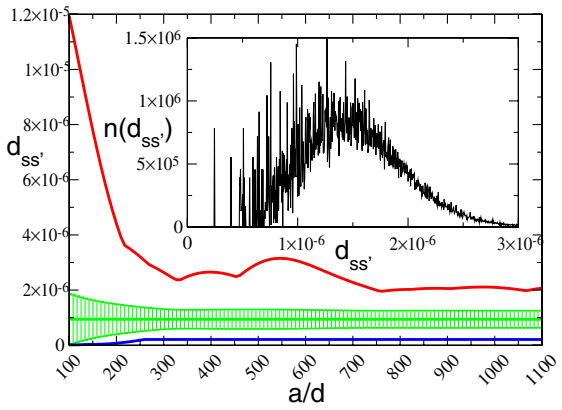

FIG. 3 (color online). Statistical analysis of all 2^{23} independent decoherences of 3×4 qubits in a 2D square lattice for $a = 100d \ldots 1100d$ (parameters as in Fig. 2). The average decoherence, given by the trace of the DMT, is independent of the lattice spacings (central green curve, error bars represent $\pm$ 1 standard deviation). The minimum decoherence (bottom curve, blue) indicates a DFS at small spacings; the top curve (red) is the maximum decoherence. The inset shows a histogram of all decoherences for $a = 580d$.

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