Quantum search using non-Hermitian adiabatic evolution

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We propose a non-Hermitian quantum annealing algorithm which can be useful for solving complex optimization problems. We demonstrate our approach on Grover's problem [L. K. Grover, Phys. Rev. Lett. **79**, 325 (1997)] of finding a marked item inside of an unsorted database. We show that the energy gap between the ground and excited states depends on the relaxation parameters and is not exponentially small. This allows a significant reduction of the searching time, which is proportional to the number of qubits. We discuss the relations between the probabilities of finding the ground state and the survival of a quantum computer in a dissipative environment, and we discuss alternate ways to solve NP-complete problems.

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I. INTRODUCTION

Many physical and combinatorial problems associated with complex networks of interacting degrees of freedom can be mapped to equivalent problems of finding the minimum of the cost function or the ground state of a corresponding quantum Hamiltonian, $\mathcal{H}_0$, [1–9]. One of the approaches to find the ground state of $\mathcal{H}_0$ is quantum annealing (QA) which can be formulated as follows. Consider the time-dependent Hamiltonian, $\mathcal{H}(t) = \mathcal{H}_0 + \Gamma(t)\mathcal{H}_1$, where $\mathcal{H}_0$ is the Hamiltonian to be optimized, $\mathcal{H}_1$ is an auxiliary "initial" Hamiltonian, and $[\mathcal{H}_0,\mathcal{H}_1] \neq 0$. The coefficient, $\Gamma(t)$, is a control parameter, and $\Gamma(t)$ decreases from very high value to zero during the evolution.

One starts with the ground state of $\mathcal{H}_1$ as the initial state, and if $\Gamma(t)$ is slowly decreasing, the adiabatic theorem guarantees approaching the ground state of $\mathcal{H}_0$ at the end of the computation, assuming that there are no energy level crossings between the ground and excited states. So, the quantum optimization algorithms require the presence of a gap between the ground state and first excited state. However, in typical cases the minimal gap, g_m, is exponentially small. For instance, in the commonly used quantum optimization n-qubit models, the estimation of the minimal energy gap yields $g_m \approx 2^{-n/2}$ [1,4,10–12]. This increases drastically the total computational time, and from a practical point of view the advantage of the method is lost.

Recently [13], we have proposed a non-Hermitian adiabatic quantum optimization with the non-Hermitian auxiliary Hamiltonian. We have shown that the non-Hermitian quantum annealing (NQA) provides an effective level repulsion for the total Hamiltonian. This effect enables us to develop an adiabatic theory without the usual gap condition and to determine the low-lying states of $\mathcal{H}_0$, including the ground state. Some interesting suggestions for implementation of non-Hermitian architectures by realization of the "Ising machine" based on mutually injection-locked laser systems were recently discussed in Refs. [14,15].

In this paper, we apply the NQA to Grover's problem [16], i.e., finding a marked item in an unstructured database.

II. NON-HERMITIAN QUANTUM SEARCH

Consider a set of $N = 2^n$ unsorted items among which one item is marked. The related Hilbert space is of dimension N. In this space, the basis states are written as $|i\rangle$ $(i = 1,2,\ldots,N)$, and the marked state is denoted as $|m\rangle$. The task is to find the marked item as rapidly as possible.

The Hamiltonian whose ground state is to be found can be written as $\mathcal{H}_0 = -|m\rangle\langle m|$. Its ground state, marked as $|m\rangle$, is unknown. The auxiliary Hamiltonian is given by $\mathcal{H}_1 = -|\psi_0\rangle\langle\psi_0|$, where $|\psi_0\rangle = (1/\sqrt{N})\sum_{i=1}^{N}|i\rangle$ is its ground state with energy $E_1^g = -1$. For both Hamiltonians, $\mathcal{H}_0$ and $\mathcal{H}_1$, the rest of the eigenstates have the $(N-1)$-times degenerate energy $E_r = 0$ $(r = 2,3,\ldots,N)$. (Our choice of the Hamiltonian is different from the Hamiltonian considered in Refs. [17–20] by a total shift on the unit matrix.)

Usually, the non-Hermitian Hamiltonian appears naturally when one considers a qubit based on two discrete eigenstates interacting with their continuum spectrum [21]. In this case, the non-Hermitian terms in the Hamiltonian have a structure which depends on the concrete type of a qubit and on the mechanisms of interactions between qubits and the environment.

Below we use a simplified model (similar to that in Ref. [22]) for a non-Hermitian term in the Hamiltonian, because our main goal in this paper is to demonstrate the principal effects related to non-Hermitian effects. The total time-dependent non-Hermitian Hamiltonian is chosen as follows: $\mathcal{H}_\tau(t) = \mathcal{H}_0 + h(t)\mathcal{H}_1$, where

$$h(t) = \begin{cases} \gamma(\tau - t), & 0 \leqslant t \leqslant \tau, \\ 0, & t \geqslant \tau. \end{cases} \tag{1}$$

We denote $\gamma = (g + i\delta)/\tau$, where g (an effective field) and δ (a damping parameter) are real. In what follows we assume that $\delta \ll g$.

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The adiabatic quantum search algorithm consists of (i) preparing the system in the initial state, $|\psi(0)\rangle = |\psi_0\rangle$, and (ii) performing an evolution by applying the non-Hermitian Hamiltonian, $\mathcal{H}_\tau(t)$, during a time, τ. At the end of evolution, the non-Hermitian part of the total Hamiltonian disappears. Then, if the evolution is sufficiently slow, the system remains in its ground state, which will be the ground state of the Hermitian Hamiltonian, $\mathcal{H}_0$.

We start with the solution of the eigenvalue problem for $\mathcal{H}_\tau(t)$. This yields an $(N-2)$-times degenerate highest eigenvalue, $E_2 = 0$, and two lowest eigenvalues, E_0 and E_1, which are given by

$$E_0(t) = -\frac{\varepsilon(t)}{2} - \frac{\Omega(t)}{2}, \tag{2}$$

$$E_1(t) = -\frac{\varepsilon(t)}{2} + \frac{\Omega(t)}{2}, \tag{3}$$

where $\Omega(t) = \sqrt{h^2(t) - 2h(t)\cos\alpha + 1}$ and $\varepsilon(t) = h(t) + 1$. We set $\sin(\alpha/2) = 1/\sqrt{N}$.

The energy gap between the ground state and the first excited state is given by $|\Delta E(t)| = |\sqrt{h^2(t) - 2h(t)\cos\alpha + 1}|$. For $N \gg 1/\delta$ one can show that the minimum of the energy gap is given by $|\Delta E|_{\min} = \delta/\sqrt{g^2 + \delta^2} + O(1/N)$.

In the two-dimensional subspace spanned by the vectors, $|\psi_0\rangle$ and $|m\rangle$, we choose an orthonormal basis as $|\psi_0\rangle$ and $|\psi_1\rangle = (\sin(\alpha/2)|\psi_0\rangle - |m\rangle)/\cos(\alpha/2)$. We complement it to the basis of the N-dimensional Hilbert space by adding $(N-2)$ vectors, $|\psi_k\rangle$ $(k = 2, \ldots, N-1)$, which form the orthonormal basis of the orthogonal $(N-2)$-dimensional Hilbert subspace. Then, an arbitrary state, $|\Psi(t)\rangle$, can be expanded as $|\Psi(t)\rangle = c_0(t)|\psi_0\rangle + c_1(t)|\psi_1\rangle + \sum_{k=2}^{N-1} c_k(t)|\psi_k\rangle$.

Inserting this expansion into the Shrödinger equation, $i\partial/\partial t|\Psi\rangle = \mathcal{H}_\tau|\Psi(t)\rangle$, we find that the differential equations for the coefficients $c_0(t)$ and $c_1(t)$ do not involve the coefficients $c_k(t)$ $(k = 2, \ldots, N-1)$. Then, effectively the N-dimensional problem is exactly reduced to the two-dimensional one. So, it suffices to confine our attention to the two-dimensional subspace.

Choosing the orthonormal basis as $\{|\psi_0\rangle = \binom{0}{1}, |\psi_1\rangle = \binom{1}{0}\}$, one can write the corresponding effective (non-Hermitian) Hamiltonian as

$$\mathcal{H}_{\rm ef}(t) = -\frac{\varepsilon(t)}{2} + \frac{\mathbf{\Omega}(t)}{2}\cdot\boldsymbol{\sigma}, \tag{4}$$

where $\mathbf{\Omega}(t) = (\sin\alpha, 0, h(t) - \cos\alpha)$ is a complex vector and $\boldsymbol{\sigma}$ denotes the Pauli matrices.

We denote the (right) instantaneous eigenvectors, corresponding to the eigenvalues, $E_a(t)$, as $|u_a(t)\rangle$ $(a = 0, 1)$. One can show that $|u_0(0)\rangle = |\psi_0\rangle + O(1/N)$ and $|u_0(t)\rangle \to |\psi_1\rangle + O(1/N)$, as $t \to \tau$.

For the two-level system (TLS) governed by the effective non-Hermitian Hamiltonian (4), the wave function can be written as $|\psi(t)\rangle = c_0(t)|\psi_0\rangle + c_1(t)|\psi_1\rangle$. Writing $c_a = u_a(t)\exp[\frac{i}{2}\int_0^t \varepsilon(t)dt]$, and employing the Schrödinger equation for the TLS governed by the effective Hamiltonian of Eq. (4), we obtain

$$i\dot{u}_0 = \tfrac{1}{2}\{\sin\alpha u_1 - [h(t) - \cos\alpha)]u_0\}, \tag{5}$$

$$i\dot{u}_1 = \tfrac{1}{2}\{[h(t) - \cos\alpha]u_1 + \sin\alpha\, u_0\}. \tag{6}$$

Further, it is convenient to introduce a new variable, $z(t) = e^{i\pi/4}[\gamma(\tau - t) - \cos\alpha]/\sqrt{\gamma}$. Then, for new functions, $u_a(t) = U_a(z)$, we rewrite Eqs. (5) and (6) in the standard Landau-Zener form [23,24],

$$\frac{d}{dz}U_0 = -\frac{z}{2}U_0 + \sqrt{i\nu_k}U_1, \tag{7}$$

$$\frac{d}{dz_k}U_1 = \frac{z}{2}U_1 + \sqrt{i\nu_k}U_0, \tag{8}$$

where $\nu = \sin^2\alpha/4\gamma$. From Eqs. (7) and (8) we obtain the second-order Weber equation [25,26]

$$\frac{d^2}{dz^2}U_{0,1} + \left(\pm\frac{1}{2} - \frac{z^2}{4} - i\nu\right)U_{0,1} = 0. \tag{9}$$

Solutions of Weber's equation are given by the parabolic cylinder functions, $D_{-i\nu}(\pm z)$:

$$U_0(z) = AD_{-i\nu}(z) + BD_{-i\nu}(-z), \tag{10}$$

$$U_1(z) = \sqrt{i\nu}[BD_{-i\nu-1}(-z) - AD_{-i\nu-1}(z)]. \tag{11}$$

The constants, A and B, should be determined from the initial conditions. We assume that the evolution of the TLS starts at $t_0 = 0$ in the state $|\psi(0)\rangle = |\psi_0\rangle$. This implies the following initial conditions: $c_0(0) = 1$ and $c_1(0) = 0$. From here we obtain $A = D_{-i\nu-1}(-z_0)\Gamma(1 + i\nu)/\sqrt{2\pi\nu}$ and $B = D_{-i\nu-1}(z_0)\Gamma(1 + i\nu)/\sqrt{2\pi\nu}$, where we set $z_0 = z(0)$.

It is assumed that the quantum measurement will determine the state of the quantum system at $t > \tau$, when the external field $h(t) = 0$ [see Eq. (1)]. We denote the final state of the system as $|\psi_\tau\rangle$. Then, the probability, P_n, of finding the system in a given state, $|n\rangle$, can be written as

$$P_n = \frac{|\langle n|\psi_\tau\rangle|^2}{|\langle\psi_\tau|\psi_\tau\rangle|^2}. \tag{12}$$

Since for non-Hermitian systems the norm of the wave function is not conserved, we define the (intrinsic) probability of transition $|\psi_0(t)\rangle \to |\psi_1(t)\rangle$ as

$$P_\tau(t) = \frac{|c_1(t)|^2}{|c_0(t)|^2 + |c_1(t)|^2}. \tag{13}$$

Using the functions, $U_{0,1}(z)$, we recast Eq. (13) as

$$P_\tau(t) = \frac{1}{1 + \frac{|U_0(z)|^2}{|U_1(z)|^2}}. \tag{14}$$

To estimate P_τ at the end of evolution $(t = \tau)$, we use asymptotic formulas for the parabolic functions [27]. The leading term is

$$\frac{U_0(z_\tau)}{U_1(z_\tau)} \approx -\frac{e^{-\pi\nu/2}e^{-z_\tau^2/2}\Gamma(1 + i\nu)}{\sqrt{2\pi\nu i}}, \tag{15}$$

where $z_\tau = z(\tau) = -e^{\pi i/4}\cos\alpha/\sqrt{\gamma}$. Using Eq. (15), we obtain

$$P_\tau = \frac{1}{1 + \frac{|\Gamma(1+i\nu)|^2}{2\pi|\nu|}e^{-\pi{\rm Re}\nu - {\rm Re}z_\tau^2}}. \tag{16}$$

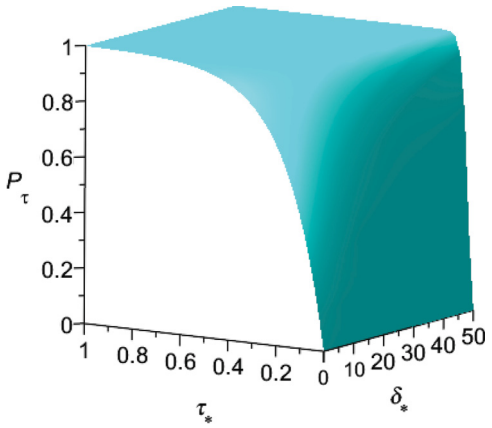

FIG. 1. (Color online) The transition probability, P_τ, as a function of a scaled decay rate, $\delta_* = \delta\tau_0/g^2$, and scaled annealing time, $\tau_* = \tau/\tau_0$, where $\tau_0 = gN$.

For $\delta \ll g$ we can approximate

$$\mathrm{Re}\nu \approx (\tau/4g)\sin^2\alpha, \tag{17}$$

$$\mathrm{Re}z_\tau^2 \approx (\delta\tau/g^2)\cos^2\alpha, \tag{18}$$

$$\Gamma(1+i\nu) \approx \Gamma(1+i\mathrm{Re}\nu). \tag{19}$$

Inserting Eqs. (17)–(19) into Eq. (16) and using the relation [26]

$$|\Gamma(iy)|^2 = \frac{\pi}{y\sinh\pi y}, \tag{20}$$

for real y, we obtain

$$P_\tau = \frac{1-e^{-2\pi\mathrm{Re}\nu}}{1-e^{-2\pi\mathrm{Re}\nu}+e^{-2\pi\mathrm{Re}\nu-\mathrm{Re}z_\tau^2}}. \tag{21}$$

In Fig. 1, the transition probability, P_τ, as a function of a scaled decay rate, $\delta_* = \delta\tau_0/g^2$, and a scaled annealing time, $\tau_* = \tau/\tau_0$, is demonstrated, where $\tau_0 = gN$ denotes the characteristic time scale of the QA. As one can see, even for $\delta \ll 1$ and small $\tau \ll \tau_0$, the probability, P_τ, is close to 1.

For the Hermitian QA ($\delta = 0$) Eq. (21) yields the Landau-Zener formula [23,24]

$$P_\tau = 1 - e^{-2\pi\nu}, \tag{22}$$

where for $N \gg 1$ we obtain $\nu = (\tau/\tau_0)$. We conclude that $P_\tau \approx 1$, if $\tau \geqslant \tau_0 = gN$. Thus, to obtain the probability close to 1 to remain in the ground state at the end of evolution, the computational time should be of order N. In fact, this result is equivalent to the well-known result on the complexity of order N provided by the quantum adiabatic evolution approach [18], which is the same as in the classical search algorithm.

For the NQA with $N \gg 1$, we can approximate $\mathrm{Re}\nu \approx \tau/\tau_0$ and $\mathrm{Re}z_\tau^2 \approx \delta\tau/g^2$. Assuming $\tau \ll \tau_0$, we obtain

$$P_\tau \approx \frac{1}{1+\frac{\tau_0}{2\pi\tau}e^{-\delta\tau/g^2}}. \tag{23}$$

From here, in the limit of $\delta \to 0$, we obtain

$$P_\tau \to \frac{1}{1+\frac{\tau_0}{2\pi\tau}} \ll 1. \tag{24}$$

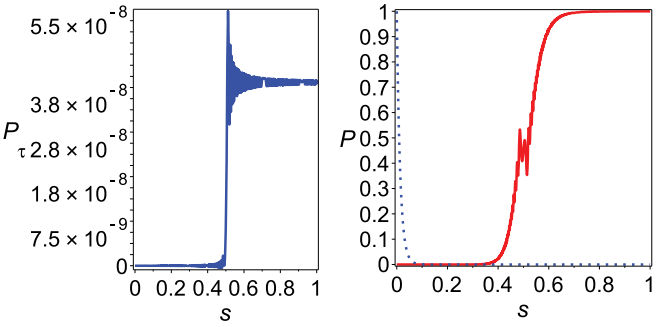

FIG. 2. (Color online) Left panel: The transition probability, P_τ, as a function of the scaled time, $s = t/\tau$ ($\delta = 0$). Right panel: The survival probability, P_s (dotted blue line), and the transition probability, P_τ (red line), as functions of the scaled time, $s = t/\tau$ ($\delta = 0.0025$). In all cases $g = 2$, $\tau = 1.5\times10^4$, and $N = 2^{40}$.

This result is expected, because in this case, the time of the Hermitian annealing, τ, is small with respect to the characteristic time, τ_0: $\tau \ll \tau_0$.

Next, assuming

$$\frac{\delta\tau}{g^2} - \ln\frac{\tau_0}{2\pi\tau} \gg 1. \tag{25}$$

we obtain

$$P_\tau \approx 1 - \frac{\tau_0}{2\pi\tau}e^{-\delta\tau/g^2}, \tag{26}$$

As one can see $P_\tau \approx 1$, if conditions of Eq. (25) are satisfied.

From Eq. (25) we obtain the following rough estimate of the computational time: $\tau \approx (g^2/\delta)\ln N$. Recognizing that $\tau \ll \tau_0$, this can be recast as $\delta \gg (g/N)\ln N$. The obtained results mean that the characteristic time of non-Hermitian annealing, even for small but finite $\delta \neq 0$, is defined not by N (as in Hermitian annealing), but mainly by the dissipation rate, δ [see Fig. 1 and Eq. (26)]. Thus, the non-Hermitian quantum search has complexity of order $\ln N$, which is much better than the quantum Hermitian (global) adiabatic algorithm. Also, this complexity is certainly better than that of the adiabatic local search algorithm which has a total running time of order $\sqrt{N}$ [17].

In Fig. 2 we present the results of our numerical simulation. For the Hermitian QA ($\delta = 0$) the transition probability (to remain in the ground state) at the end of evolution is $P_\tau \approx 3\times10^{-8}$; and for the NQA with weak dissipation, $\delta = 0.0025$, the transition probability is $P_\tau = 1$ ($\tau = 1.5\times10^4$).

III. NONLINEAR NQA

We define the survival probability of the lossy system as the trace of the density matrix, $P_s(t) = \mathrm{Tr}\rho(t)$. Using the asymptotic formulas for the Weber functions, one can show that for $N \gg 1$ the asymptotic behavior of the survival probability is given by $P_s(t) \approx e^{-\delta t}$ (see Fig. 2, dotted blue line). Then, one can see that the conditions to obtain high probabilities for (i) finding the ground state, leading to inequality, $\tau \geqslant (g^2/\delta)\ln N$, and (ii) survival of qubits, $\delta t \leqslant 1$, are not compatible. A compromise can be found by using a local adiabatic evolution approach [17].

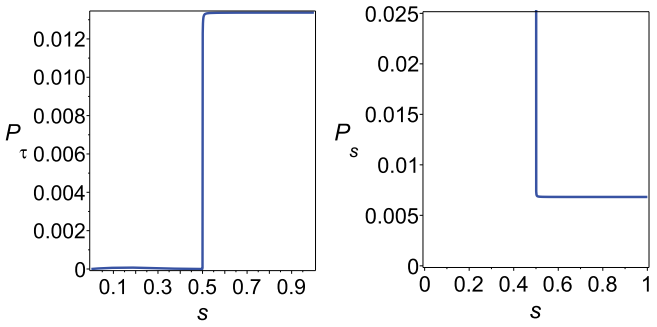

FIG. 3. (Color online) Nonlinear NQA. The transition probability (left panel) and the survival probability (right panel) as the functions of the scaled time, $s = t/\tau$ ($g = 2, \delta = 10^{-4}, \tau = 5 \times 10^4, N = 2^{40}$).

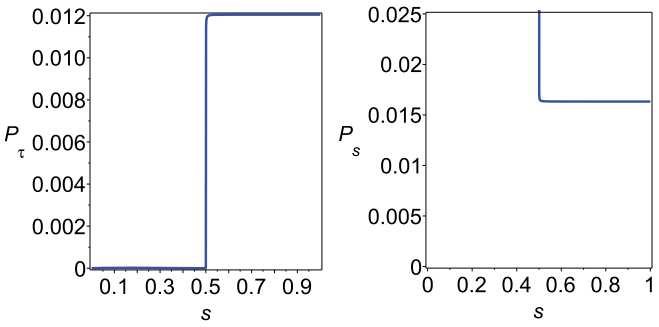

FIG. 4. (Color online) Nonlinear NQA. The transition probability (left panel) and the survival probability (right panel) as functions of the scaled time, $s = t/\tau$ ($g = 2, \delta = 7.5 \times 10^{-5}, \tau = 5.5 \times 10^4, N = 2^{40}$).

We rewrite the total time-dependent non-Hermitian Hamiltonian as

$$\mathcal{H}_\tau(t) = \mathcal{H}_0 + h_0[1 - f(t)]\mathcal{H}_1, \tag{27}$$

where $h_0 = (g + i\delta)$ and $f(t)$ is a monotonic function of t. For concreteness, we choose $g = 2$ and impose the following boundary conditions: $f(0) = 0$ and $f(\tau) = 1$, where τ denotes the computational time.

We choose $f(t)$ as a solution of

$$\frac{df}{dt} = \frac{\beta\delta}{\tau}\left[1 + \left(\frac{(1-2f)}{\delta}\right)^2\right], \tag{28}$$

where $\beta = \arctan(1/\delta)$. Performing the integration, we find

$$t = \frac{\tau}{2} + \frac{\tau}{2\beta}\arctan\frac{(2f-1)}{\delta}. \tag{29}$$

By inverting this function we obtain

$$f(t) = \frac{1}{2} + \frac{\delta}{2}\tan\left[\beta\left(\frac{2t}{\tau} - 1\right)\right]. \tag{30}$$

From here it follows that $f(\tau) = 1$, and the computation time is τ.

In Figs. 3 and 4 we present the results of numerical calculations for different choices of parameters, δ and τ. Our results show that the nonlinear NQA can be realized with the transition probabilities $P_\tau \approx 1.2 \times 10^{-2}$ and $P_s \approx 1.6 \times 10^{-2}$. The computational time $\tau \approx 5.5 \times 10^4$ is better than the time of quantum search predicted by the Grover algorithm, $\tau = \sqrt{N} \approx 10^6$ (for $n = 40$).

IV. CONCLUSION

The field of quantum adiabatic computation is well established, and many useful results are discussed in the literature. One of the main problems of this approach is that the energy gap between the ground state to be found and the excited states is generally exponentially small. This requires exponentially large computational times, $\tau \sim \sqrt{N}$, in the best case. On the other hand, in the dissipative (non-Hermitian) regime, the energy gap is defined by the relaxation parameters and may not be exponentially small (see also Refs. [14,15]). In this case, the computational time can be significantly reduced, $\tau \sim (g^2/\delta)\ln N$. This means that the characteristic time of non-Hermitian annealing, even for a small but finite dissipation parameter δ, is defined mainly not by N, but by a dissipation rate, $\sim\delta$.

At the same time, another problem appears—the quantum computer has a finite probability to be destroyed (which happens anyway). One way to overcome this problem is discussed in Refs. [14,15], where both dissipation and external pumping in the locked laser system were used to model the Ising system in its stationary ground state. But still many theoretical and experimental issues must be resolved in order to build this type of "Ising machine."

The results presented in our paper demonstrate that non-Hermitian quantum computations can be used for two purposes. One is to use non-Hermitian quantum algorithms together with the use of classical computers to significantly reduce computational time, which, we expect, would help in solving NP-complete problems. We are in the process of demonstrating this option for some classes of Ising models [28]. Another purpose is to build a real "non-Hermitian quantum computer" (NHQC) to solve specific complex problems rapidly. As was demonstrated in this paper, in the later case there will be a tradeoff between the probability of finding the desired outcome and the probability of survival of the computer. As our results show, there are useful ways to improve the performance of a NHQC.

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