BQP-completeness of Scattering in Scalar Quantum Field Theory

Stephen P. Jordan[1,2], Hari Krovi[3], Keith S. M. Lee[4], and John Preskill[5]

[1]National Institute of Standards and Technology, Gaithersburg, MD, USA
[2]Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, MD, USA
[3]Quantum Information Processing Group, Raytheon BBN Technologies, Cambridge, MA, USA
[4]Centre for Quantum Information & Quantum Control and Department of Physics, University of Toronto, Toronto, ON, Canada
[5]Institute for Quantum Information and Matter, California Institute of Technology, Pasadena, CA, USA

Abstract

Recent work has shown that quantum computers can compute scattering probabilities in massive quantum field theories, with a run time that is polynomial in the number of particles, their energy, and the desired precision. Here we study a closely related quantum field-theoretical problem: estimating the vacuum-to-vacuum transition amplitude, in the presence of spacetime-dependent classical sources, for a massive scalar field theory in (1+1) dimensions. We show that this problem is BQP-hard; in other words, its solution enables one to solve any problem that is solvable in polynomial time by a quantum computer. Hence, the vacuum-to-vacuum amplitude cannot be accurately estimated by any efficient classical algorithm, even if the field theory is very weakly coupled, unless BQP=BPP. Furthermore, the corresponding decision problem can be solved by a quantum computer in a time scaling polynomially with the number of bits needed to specify the classical source fields, and this problem is therefore BQP-complete. Our construction can be regarded as an idealized architecture for a universal quantum computer in a laboratory system described by massive ϕ^4 theory coupled to classical spacetime-dependent sources.

1   Introduction

The field of computational complexity theory is the study of the resources required to solve computational problems. Problems with the same intrinsic difficulty are categorized into complexity classes, which can be either classical or quantum, and relationships between

different classes are studied. The class of computational problems that are solvable in polynomial time by quantum computers, with a small probability of error, is called BQP. The class of problems solvable in polynomial time by classical randomized computations with a small probability of error is called BPP. It is conjectured that BPP is equal to P, the class of problems solvable with certainty by deterministic classical computers (see, for example, [1]).

A BQP-hard problem $\mathcal{P}$ is one with the property that any problem in BQP can be efficiently translated into an instance of $\mathcal{P}$, so that the answer to the instance of $\mathcal{P}$ gives the answer to the original problem. The method for efficient translation is required to be a polynomial-time classical computation and is referred to as a *reduction*. A simple example of a BQP-hard problem is the following: given a bit string describing a quantum circuit C, decide whether the corresponding unitary operator U_C has an all-zeros to all-zeros transition probability $|\langle 0 \ldots 0 | U_C | 0 \ldots 0 \rangle|^2$ greater than 2/3 or smaller than 1/3, if one of these is guaranteed to be the case. We use a reduction from this problem to a problem of estimating vacuum-to-vacuum transition probabilities in a quantum field theory to show that the latter is also BQP-hard. If any BQP-hard problem were solvable in polynomial time by classical computers, then all of quantum computation would be efficiently simulable classically. (Thus, BPP would equal BQP.) It is widely believed that this is impossible and, therefore, if a problem is BQP-hard it is intractable for classical computers.

We show BQP-hardness for the problem of computing a vacuum-to-vacuum transition probability in (1+1)-dimensional ϕ^4 theory with spacetime-dependent external fields. Specifically, suppose that initially the quantum field theory is in its vacuum state and all external fields are turned off. Then, the external fields are applied with some specified variation in spacetime. Eventually, the external fields are again turned off. The computational problem is to calculate whether the final state of the system is the vacuum. More precisely, the system, being quantum mechanical, can be in a superposition of the vacuum state and other states, and the problem is to decide whether the probability (that is, squared amplitude) of being in the vacuum state is large or small.

In previous work [2–4], we showed that quantum computers can efficiently compute transition probabilities in certain interacting quantum field theories, including ϕ^4 theory. Here, we show that a slight variant of the problem solved in [2, 3] is BQP-hard. Essentially, this result implies that classical computers cannot solve the problem in polynomial time unless BQP=BPP, and thus the quantum algorithm of [2, 3] constitutes a genuine superpolynomial speedup. The scattering process used in our BQP-hardness construction differs from the process simulated in [2, 3] in that spacetime-dependent source terms are present. Nevertheless, by standard arguments [5, 6], such terms at worst induce modest efficiency penalties on the Suzuki-Trotter formulae used in [2, 3]. A second difference is that the BQP-hard problem introduced here is to estimate a vacuum-to-vacuum transition probability, whereas the simulation algorithm of [2, 3] samples from a probability distribution defined by a set of local measurements. From the methods introduced in [2, 3] for implementing the unitary time evolution and preparing the vacuum state with efficient quantum circuits, one can construct an efficient quantum algorithm estimating the vacuum-to-vacuum transition probability us-

ing the *Hadamard test*. Thus, the algorithm of [2, 3] suffices to show that the BQP-hard transition-probability decision problem discussed here is also contained in BQP. Problems such as this, which are both BQP-hard and contained in BQP, are called BQP-complete.

The quantum field theory we consider is described by the Lagrangian

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \frac{1}{4!}\lambda\phi^4 - J_2\phi^2 - J_1\phi\,, \tag{1}$$

where $J_1 = J_1(t,x)$ and $J_2 = J_2(t,x)$ are the external fields. We consider the computational problem of, given bit strings[1] specifying $J_1(t,x)$ and $J_2(t,x)$, predicting whether the system remains in the vacuum state. Specifically, at time zero the sources J_2 and J_1 are zero and the system is in the vacuum state. Then J_2 and J_1 are varied in time as specified by the given bit strings and return to zero at time T. The computational problem is to decide whether the probability of remaining in the vacuum state at time T is greater than 2/3 or smaller than 1/3, given a promise that one of these is the case. The constants 1/3 and 2/3 are conventional but arbitrary; our hardness result would be unchanged for other choices.

From the perspective of scientific computing, this formulation of the problem perhaps seems unusual. In real applications, one typically wants to compute a quantity of interest to within some precision ϵ, a task referred to here as an estimation problem. However, decision problems (namely, those whose answers are either "yes" or "no") are more convenient for complexity theory, and hardness results for decision problems automatically imply the hardness of corresponding, more natural, estimation problems. Clearly, if one could solve the estimation problem of computing the vacuum-to-vacuum transition probability p to within $\pm\epsilon$ for some $\epsilon < 1/6$, then one could use this to answer the decision problem of whether $p < 1/3$ or $p > 2/3$. Thus, our BQP-hardness result implies that neither of these problems can be solved in polynomial time by classical computers, as long as BPP $\neq$ BQP.

Previous work has investigated the computational complexity of approximating scattering amplitudes for particles hopping among the vertices of a graph [7–9]. The techniques developed in these earlier works could be relevant to BQP-hardness constructions for quantum field theories, especially if one is interested in external fields that are time-independent. However, in quantum field-theoretical scattering, one is faced with problems not encountered in scattering on graphs, in particular the encoding of the problem instance. In graph scattering, the instance is typically encoded in the graph. Here, we encode it in the spacetime dependence of an external field. Also, the graph serves to confine the particles.

The rest of this paper is organized as follows. Section 2 presents an overview of our construction and a discussion of our results. In Sec. 3, we show how a state representing an initialized array of qubits can be prepared with arbitrarily high fidelity. Then, in Sec. 4, we describe how to implement a universal set of quantum gates. The two-qubit gates we construct are subject to leakage from the computational subspace, and we explain how this issue can be addressed. Finally, in Sec. 5, we discuss the Hadamard test and particle-detector measurements, two different means of obtaining BQP-completeness results. Some technical details are relegated to appendices.

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[1] The functions $J_1(t,x)$ and $J_2(t,x)$ have bounded spatial extent and limited bandwidth, and therefore they can be specified with polynomially many bits (see Sec. 2).

2   Overview and Discussion

The essence of our BQP-hardness argument is to propose an architecture for a quantum computer in a $(1+1)$-dimensional universe governed by massive ϕ^4 theory and then to show that it is capable of scalable, universal quantum computation. This is in some ways easier and in other ways harder than designing a quantum computer architecture for the real world. On the one hand, practical experimental limitations are not a concern; operations of arbitrary precision are allowed as long as the precision scales only polynomially with the problem size. On the other hand, the set of particles and interactions from which to construct the qubits and gates is much more limited.

In our BQP-hardness construction we choose our external field $J_2(t,x)$ so that the non-relativistic limit is a collection of double-well potentials. A qubit is encoded by a double well containing one particle. The logical-zero and logical-one states of the qubit can then be represented by two states of the double well. For example, one can choose the ground and first excited states of the double well as logical zero and one, respectively. Another possible choice is particle occupation (in the ground state) of the left well for logical zero and the right well for logical one. We show that, in the nonrelativistic limit (with $J_1 = 0$), the effective n-particle Schrödinger equation has the Hamiltonian

$$H(t) = \sum_i \left(\frac{p_i^2}{2m} + \frac{J_2(t,x_i)}{m} \right) + \sum_{i<j} \left(\frac{\lambda}{4m^2}\left(1 + \frac{\lambda}{4\pi m^2}\right)\delta(x_i - x_j) - \frac{\lambda^2}{32\pi m^3} \int_0^1 dy \frac{e^{-m|x_i-x_j|/\sqrt{y(1-y)}}}{\sqrt{y(1-y)}} \right)$$
$$+ \ldots . \tag{2}$$

By varying the source term $J_2(t,x)$ as a function of time, one can move the potential wells. By moving the left and right wells of a single qubit closer together, one can implement single-qubit gates through tunneling between the wells. By moving the wells of neighboring qubits closer together, one can implement two-qubit gates through the inter-particle interactions. In this manner, we construct a universal set of quantum gates in Sec. 4.

An oscillatory $J_1(t,x)$ can create and destroy particles. This allows us to show that computing even the vacuum-to-vacuum transition probability is BQP-hard. To simulate a quantum computation, we create a state in which each double well encoding a qubit is in its logical-zero state. We show in Sec. 3 how we can prepare this state by starting with the vacuum state and then varying the source term $J_1(t,x)$ sinusoidally in time. At the end, the time-reversed version of this process annihilates the particles in the double wells. Thus, the $|0\ldots0\rangle \to |0\ldots0\rangle$ amplitude of a quantum circuit corresponds to the vacuum-to-vacuum transition amplitude, whereas other final states of the quantum circuit contribute to non-vacuum final states of the quantum field theory's dynamics.

The spatial volume used by this process is proportional to the number of qubits, up to logarithmic factors, since the coupling between wells decays exponentially with their spacing. The execution time of an individual quantum gate must scale as $\widetilde{O}(\lambda^{-2})$, so that leakage errors out of the coding subspace are adiabatically suppressed (§4.2). (The $\widetilde{O}$ suppresses logarithmic factors, which come from adiabatic theorems with exponential convergence.)

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The total duration of the process is thus $\widetilde{O}(\lambda^{-2}D)$, where D is the depth of the original quantum circuit.

It is essential that the reduction can be carried out in polynomial time by classical computers. One potential concern is that computing the function $J_2(t,x)$ corresponding to a specified quantum circuit could be intractable. We demonstrate that this is not the case by giving examples of explicit constructions for $J_2(t,x)$ in Appendices C and D. For these constructions, we assume that the coupling constant λ is $O(1/G)$, where G is the number of gates in the simulated circuit, which allows us to use low-order perturbation theory in λ to analyze our two-qubit gate to adequate accuracy. For such weak particle interactions, it takes a time scaling like G^2 to execute a single two-qubit gate adiabatically, and a time of order G^2D for the simulation of a circuit with depth D.

Let T and V be the duration and spatial volume on which J_1 and J_2 have support. Then, by the Nyquist-Shannon theorem, it suffices to use $O(T\omega V/\xi)$ real numbers to describe J_1 and J_2, where ω and ξ are the maximum frequency and minimum wavelength of J_1 and J_2. Recall that $T = \widetilde{O}(\lambda^{-2}D) = \widetilde{O}(G^2D)$. Since the interaction between particles in separate wells falls off exponentially with separation, $V = \widetilde{O}(n)$, where n is the number of qubits. The wavelength ξ is of order $1/m$, because the spacing and widths of wells that suppress unwanted tunneling are of order $1/m$. The maximum oscillation frequency ω is of order m, which occurs when an oscillatory J_1 term is used to excite particles from the vacuum. The mass m is taken to be a constant, not varying asymptotically with problem size. Thus, the total number of bits needed to specify J_1 and J_2 to adequate precision is $\widetilde{O}(nG^2D)$. This is important, because to show BQP-hardness one needs the reduction to be computable classically in polynomial time and it must induce at most a polynomial increase in the number of bits needed to describe the problem instance.

There are potentially many different computational problems arising in quantum field theory whose hardness one might wish to study. In choosing a problem to establish the BQP-hardness of, we have been guided by the criterion that the problem should be physically natural. In other words, it should be as close as possible to familiar problems one is interested in solving in practice. Specifically, the choice entails the selection of a particular field theory and the set of allowed inputs and observables. These must have sufficient richness to allow the encoding of a quantum circuit whose output is to be "simulated" by the dynamics of the quantum field theory. From the computational perspective, of course, the more economical the choice is, the stronger and more interesting an associated BQP-hardness result will be. With these factors in mind, we consider the problem of computing a vacuum-to-vacuum transition amplitude in a theory with spacetime-dependent external fields, where the description of the external fields constitutes the input to the problem. Such a calculation is the evaluation of a generating functional $Z[J]$. The formal computational problem that we have proposed and analyzed in this paper is physically and computationally well-motivated. However, other reasonable BQP-hardness statements can be proposed, not all of which are manifestly equivalent to ours.

In particular, we have defined scattering to be purely unitary dynamics without any measurements performed during the scattering process. This is in keeping with the standard

notion of scattering in quantum field theory. If intermediate measurements and feedforward are allowed, then simpler BQP-hardness constructions may be possible along the lines of the KLM construction [10]. In architectures for real quantum computers, intermediate measurements and active error correction are used to achieve a constant success probability in quantum computations of polynomially many gates, even though each gate is implemented with only constant precision. In our BQP-hardness construction, we instead achieve a constant success probability by implementing each of the G quantum gates with an infidelity scaling as $O(1/G)$ and preparing each of the n qubits with an infidelity scaling as $O(1/n)$.

Our definition of the scattering problem allows spacetime-dependent source terms, which break translational invariance, in the Lagrangian of the quantum field theory. Physically, such source terms correspond to externally applied classical fields. In other words, although the laws of physics are invariant under translations in time and space, the presence of an experimental apparatus in a particular location breaks this symmetry. Our formulation of the scattering problem considers the experimental apparatus that applies the fields that manipulate the qubits to be external. We do not demand quantum field-theoretical simulation of the particles making up this apparatus.

Lastly, in our BQP-hardness construction, we have demanded that the initial state be the vacuum. The creation of the particles to be scattered is considered part of the dynamics. This makes our construction more complicated, as we must design a state-preparation scheme and analyze its fidelity (§3). Our construction implies as an immediate corollary that, if one allows the initial state in the scattering problem to consist of particles bound in the potential wells, then the associated scattering problem is BQP-hard. By showing that BQP-hardness still holds when the initial state is restricted to be the vacuum, we achieve a meaningful strengthening of our result. In a high-energy scattering problem, one is typically interested in situations where there are initial-state particles, but these are propagating relativistically, rather than already bound in potential wells.

One can heuristically obtain a BQP-hardness result for the Standard Model of particle physics by noting that the physics accessible in today's laboratories is described by the Standard Model. Some of these laboratories contain prototype quantum computers, and therefore the computational problem of simulating the dynamics of these laboratories (and their many-qubit successors) must be BQP-hard. Moreover, one might make the argument that since nonrelativistic quantum mechanics is a limiting case of quantum field theory and, in principle, the laws of quantum mechanics permit the efficient solution of the problems in BQP, it must be true that the problem of simulating dynamics of quantum field theories is BQP-hard. What, then, can be learned from a derivation of BQP-hardness?

First, within a given quantum field theory, BQP-hardness depends on the computational problem, which in physical terms corresponds to the set of observables and phenomena implementing the computation. Furthermore, a bigger goal is to study the whole space of quantum field theories in terms of their computational power. In other words, it is interesting to investigate which quantum field theories (in arbitrary spacetime dimensions) give rise to classically tractable problems and which ones give rise to intractable problems. In particular, we aim to discover what features of a field theory determine this division. For example, we

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wish to know if this property is affected by integrability or quantum chaos. This paper takes a first step towards addressing some of these issues. In particular, we find that, with a sufficiently complex variation in the external fields, it is already hard to simulate a weakly-coupled quantum field theory that is in only one spatial dimension and is purely bosonic.

One of the central goals of computer science is to understand the ultimate capabilities and limitations of computers. Since the seminal works on quantum computation by Feynman and Deutsch in the 1980s, we have known that this understanding cannot be achieved in isolation from physics. The question thus becomes: What is the class of computational problems solvable using polynomial resources within the laws of physics that govern our universe? In essence, this work, together with [3], places matching upper and lower bounds on the computational power of a universe described by ϕ^4 theory. This represents a step in a larger program of characterizing the computational power of the Standard Model, which is the quantum field theory describing all known physical phenomena other than gravity. Characterizing the computational power of quantum gravity is a more distant goal.

3 State Preparation

For the decision problem defined in the previous section, our starting point is the vacuum state of the weakly interacting ϕ^4 theory with $J_2(x) = J_1(x) = 0$. First, we adiabatically turn on the static double-well potential (by turning on $J_2(x)$) to prepare the corresponding vacuum state. Next, we turn on an oscillatory $J_1(t, x)$ to create a particle in the logical-zero state of each double well. The ground and first excited states of the double-well potential, which are symmetric and antisymmetric superpositions over the two wells, can serve as these logical states. It is also possible to choose a localized particle in the left or right well, although these states are not eigenstates, as long as the two wells are sufficiently separated; the energy splitting between the two states is then exponentially suppressed and, apart from accumulating a global phase, these states evolve only exponentially slowly.

From the adiabatic theorem given in [11], it follows that one can prepare the vacuum state of the static potential in a time of $\widetilde{O}(1/(m - \mathcal{B})^2)$, where m is the physical mass of the particles in the interacting theory and $\mathcal{B}$ is the binding energy of the well. Note that we cannot choose the binding energy of the well to be larger than the particle mass, because in this case the vacuum becomes unstable: it becomes energetically favorable to create a particle occupying the well.

After creating the vacuum state for the system with nonzero J_2, we wish to create exactly one particle in each double well. We do this by applying an oscillating source term in the full interacting theory. The idea is to ensure that the creation of one particle is on resonance, while the creation of more than one particle is off resonance. Perhaps the simplest version of this procedure is to use Rabi oscillation, in which we drive a transition to the single-particle state using a $J_1(t, x)$ that oscillates on resonance with the energy difference between this state and the vacuum.

Because of the interaction term $\lambda \phi^4$ in the Lagrangian, the system is anharmonic. While the energy to create one particle in the ground state of a well is $m - \mathcal{B}$, the energy to create

two particles in the ground state is $2(m - \mathcal{B}) - \delta$, where δ is a binding energy arising from the inter-particle potential. Suppose we choose $J_1(t, x)$ to have the form

$$J_1(t, x) = g \cos(\omega t) h(x) \,, \tag{3}$$

where $h(x)$ is a function localized in the well (for example, a Gaussian), and g is a constant quantifying the strength of the source. If we choose $\omega = m - \mathcal{B}$, then the source is on resonance for the transition from vacuum to the single-particle bound state, but off resonance for the transition from the single-particle bound state to the two-particle bound state.

Standard analysis of Rabi oscillation shows that, for sufficiently weak g, the source $J_1(t, x)$ described in Eq. (3) will drive oscillations between the vacuum and the single-particle ground state $|\psi_0\rangle$ of the well with frequency

$$\Omega = g \langle \psi_0 | \int dx h(x) \phi(x) |\text{vac}\rangle \,. \tag{4}$$

Thus, by applying the oscillating source for a time $\tau = \pi / 2\Omega$, one can drive a near-perfect transition to the state $|\psi_0\rangle$. In principle, errors (that is, excitations to higher-energy states) can be arbitrarily suppressed by making g smaller and τ correspondingly larger. Because we assume no intermediate measurements in our scattering process, we cannot invoke fault-tolerance constructions. Thus, each of the n qubits must be prepared with infidelity of $O(1/n)$.

The disadvantage of this construction is that, to prepare the state $|\psi_0\rangle$ with arbitrarily high fidelity, one needs arbitrarily precise knowledge of both the resonance frequency $\omega = m - \mathcal{B}$ and the Rabi oscillation frequency Ω determined by the matrix element (4). Thus, we instead apply a related scheme called adiabatic passage, which requires only approximate knowledge of these quantities.

In Sec. 3.1, we provide an overview of adiabatic passage. Specifically, we present the theoretical description in the case of a two-level system. In the following subsections, we analyze the effect of source terms and the application of adiabatic passage to our problem. In the familiar case of the free ($\lambda = 0$) scalar theory without any sources, one can simply go to Fourier space, express the Hamiltonian in terms of creation and annihilation operators for the Fourier modes, and thus obtain its spectrum. The addition of a linearly coupled classical source of finite duration ($J_1(x) \neq 0$ for a finite time) can also be treated straightforwardly. In Sec. 3.2, we present the analogous equations when there is a quadratically coupled source ($J_2(x) \neq 0$). The expressions make clear that $J_2(x)$ acts like a potential, with the spectrum now having a discrete part as well as a continuum. One can furthermore see that the choice of $J_1(x)$ determines the probabilities of various particle types being created. Next, in Sec. 3.3, we examine the interacting ϕ^4 theory with both sources. In particular, we consider $J_1(x)$ with a time dependence that implements adiabatic passage. Calculation of the Fourier spectrum of such a function of time reveals that one can suppress transitions to states that are not in resonance with the desired transition and whose transition frequency is not a multiple of the desired transition frequency. Hence, one can suppress the production of multiple particles in the discrete part of the spectrum, since it is anharmonic. We show that the

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production of unwanted unbound particles can also be suppressed. Thus, we obtain a set of necessary conditions for successful state preparation. The parameter scalings that satisfy these conditions determine the time required.

3.1 Adiabatic Passage

Adiabatic passage is an experimental technique for driving transitions between eigenstates. Instead of applying a sinusoidal driving term tuned precisely to the desired transition frequency, as in Rabi oscillation, one applies a driving term whose frequency sweeps across this resonance. For our purposes, the advantage of this technique is that excited-state preparation of arbitrarily high fidelity is achievable with only limited knowledge of the relevant transition frequency and matrix element. The theoretical description of such a coupled system is summarized below.

3.1.1 Effective Hamiltonian in the Rotating Frame

Consider a two-level system with energy splitting $\omega_0 > 0$, where the transition between the ground and excited states is being driven by a source with frequency $\omega = \omega_0 + \Delta$; we say that the driving field is "detuned" from resonance by Δ. This system satisfies the Schrödinger equation

$$\frac{d}{dt}|\psi\rangle = -iH(t)|\psi\rangle, \tag{5}$$

with the time-dependent Hamiltonian

$$H(t) = \begin{bmatrix} 0 & e^{i\omega t}\Omega/2 \\ e^{-i\omega t}\Omega/2 & \omega_0 \end{bmatrix}. \tag{6}$$

When expressed in terms of a "rotating frame", Eq. (6) becomes

$$\frac{d}{dt}|\varphi\rangle = -iH_{\text{eff}}|\varphi\rangle. \tag{7}$$

Here,

$$|\psi\rangle = \begin{bmatrix} 1 & 0 \\ 0 & e^{-i\omega t} \end{bmatrix}|\varphi\rangle, \tag{8}$$

and the effective Hamiltonian is

$$H_{\text{eff}} = \begin{bmatrix} 0 & \Omega/2 \\ \Omega/2 & -\Delta \end{bmatrix} = \begin{bmatrix} -\Delta/2 & 0 \\ 0 & -\Delta/2 \end{bmatrix} + \frac{1}{2}\sqrt{\Omega^2 + \Delta^2}\begin{bmatrix} -\cos 2\theta & \sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{bmatrix}, \tag{9}$$

where $\tan 2\theta = -\Omega/\Delta$ and $0 \leq \theta \leq \pi/2$. The eigenstates of this effective Hamiltonian are

$$|+\rangle = \sin\theta|g\rangle + \cos\theta|e\rangle, \tag{10}$$

$$|-\rangle = \cos\theta|g\rangle - \sin\theta|e\rangle, \tag{11}$$

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with eigenvalues $-\frac{1}{2}\Delta \pm \frac{1}{2}\sqrt{\Omega^2 + \Delta^2}$, respectively. Here, $|g\rangle$ and $|e\rangle$ are the ground and excited states of the undriven Hamiltonian with $\Omega = 0$ and $\omega = 0$.

In adiabatic passage, the detuning Δ sweeps through zero. Well below resonance (large negative detuning Δ, $\theta \approx 0$), the lower-energy eigenstate of H_{eff} is $|-\rangle \approx |g\rangle$, whereas well above resonance (large positive Δ, $\theta \approx \pi/2$) we have $|-\rangle \approx -|e\rangle$. If the sweep is slow enough, the system is unlikely to be excited across the minimal energy gap Ω of the effective Hamiltonian, and it evolves adiabatically from the ground state $|g\rangle$ to the excited state $|e\rangle$. (See Fig. 1.)
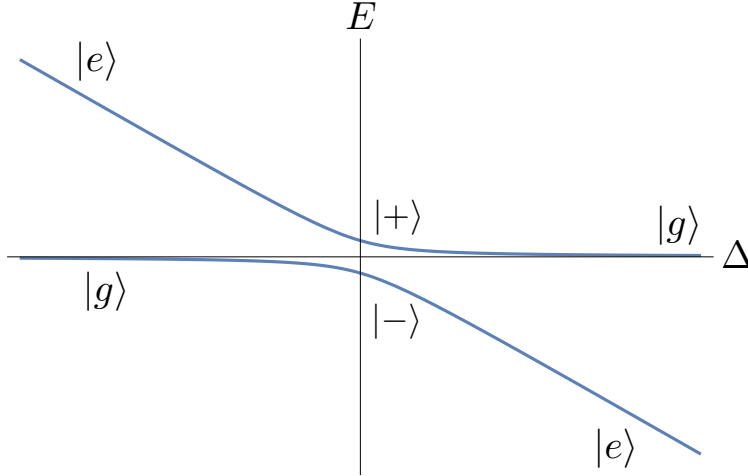

Figure 1: Avoided crossing of energy levels. As the detuning Δ sweeps adiabatically through zero, the eigenstate $|-\rangle$ changes from the uncoupled ground state $|g\rangle$ to the uncoupled excited state $|e\rangle$.

We emphasize that, even if the off-diagonal term in $H(t)$ is small, we cannot analyze adiabatic passage by treating this term in time-dependent perturbation theory; for adiabatic passage to succeed, the off-diagonal driving term must be turned on for long enough that its effects are not perturbatively small. Correspondingly, in a field-theory setting, the probability of successful particle creation by adiabatic passage cannot be computed by summing a finite number of Feynman diagrams: instead, resummation of an infinite class of diagrams is required. Our strategy will be to justify approximating the field theory problem by the two-level system just described, and then to compute the success probability within that two-level approximation. What must be shown is that terms in the Hamiltonian coupling these two energy levels to other energy levels can be safely neglected. This issue arises in any treatment of adiabatic passage between two energy levels of a multilevel system.

3.1.2 Rotating-Wave Approximation

In Eq. (3), the source term $J_1(t, x)$ is proportional to $\cos(\omega t)$, whereas in Eq. (6) we included only off-diagonal terms with small detuning, neglecting counter-rotating terms, which are far from resonance. Intuitively, these terms, which oscillate rapidly in the rotating frame, have

effects that nearly average away. Ignoring the counter-rotating terms in the Hamiltonian is called the *rotating-wave approximation.*

In the rotating frame, the counter-rotating part of the Hamiltonian is

$$H'_{\text{eff}}(t) = \begin{bmatrix} 0 & e^{-2i\omega t}\Omega/2 \\ e^{2i\omega t}\Omega/2 & 0 \end{bmatrix}. \tag{12}$$

To justify the rotating wave approximation, we first express the Schrödinger equation as an integral equation, namely,

$$|\varphi(T)\rangle = |\varphi(0)\rangle - i \int_0^T dt H_{\text{eff}}(t)|\varphi(t)\rangle, \tag{13}$$

and note that the error ignoring the counter-rotating term introduces is

$$|\epsilon\rangle = i \int_0^T dt H'_{\text{eff}}(t)|\varphi(t)\rangle, \tag{14}$$

which after an integration by parts becomes

$$|\epsilon\rangle = \frac{\Omega}{4\omega}\left(\begin{bmatrix} 0 & -e^{-2i\omega t} \\ e^{2i\omega t} & 0 \end{bmatrix}|\varphi(t)\rangle\right)_0^T + i\frac{\Omega}{4\omega}\int_0^T dt \begin{bmatrix} 0 & -e^{-2i\omega t} \\ e^{2i\omega t} & 0 \end{bmatrix} H_{\text{eff}}(t)|\varphi(t)\rangle. \tag{15}$$

We can therefore bound the error using

$$\epsilon := \||\epsilon\rangle\| \le \frac{\Omega}{2\omega} + \frac{\Omega T}{4\omega}\max_{t\in[0,t]}\|H_{\text{eff}}(t)\| \le \frac{\Omega}{2\omega} + \frac{\Omega T}{4\omega}(\Delta + \Omega). \tag{16}$$

We can use a similar argument to bound the contribution from rapidly oscillating on-diagonal terms in the Hamiltonian (which are also rapidly oscillating in the rotating frame).

3.1.3 Conditions for Successful Adiabatic Passage

To be concrete, consider the two-level Hamiltonian

$$H(t) = \begin{bmatrix} 0 & h(t) \\ h(t) & \omega \end{bmatrix}, \tag{17}$$

where the off-diagonal driving term has the time dependence

$$h(t) = \begin{cases} \Omega\cos(\tilde{\omega}(t)t), & -T/2 \le t \le T/2, \\ 0, & \text{otherwise}, \end{cases} \tag{18}$$

and

$$\tilde{\omega}(t) = \omega_0 + \Delta(t), \quad \Delta(t) = Bt/T. \tag{19}$$

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In other words, this source term is turned on for a total time T, during which the detuning ramps linearly in time from $-B/2$ to $B/2$. We refer to B as the (circular) frequency bandwidth of the time-dependent source. In the rotating-wave approximation, the effective Hamiltonian has the form of Eq. (9), with Δ given by Eq. (19). We wish to find sufficient conditions for passage from the initial state $|g\rangle$ to the final state $|e\rangle$ to occur with a small error ϵ.

First, when the source turns on suddenly at $t = -T/2$, we want the initial state $|g\rangle$ to be close to the eigenstate $|-\rangle$ in Eq. (10), and when the source turns off at $t = T/2$ we want $|-\rangle$ to be close to $|e\rangle$. To ensure that the error due to misalignment of $|-\rangle$ with the initial and target states is sufficiently small, we impose the condition

$$\Omega/B = O(\epsilon). \tag{20}$$

Second, we need the sweep of the detuning to be slow enough for the evolution to be adiabatic. The effective Hamiltonian (in the rotating-wave approximation) obeys

$$\left\| \frac{d}{ds} H_{\text{eff}}(s) \right\| = \left| \frac{d}{ds} \Delta(s) \right| = B, \tag{21}$$

where $s = t/T$, and its minimum gap is $\gamma = \Omega$; therefore, by the adiabatic theorem [12], the error due to a diabatic transition will be $O(\epsilon)$ provided

$$\frac{1}{T\gamma^3} \left\| \frac{d}{ds} H_{\text{eff}}(s) \right\|^2 = \frac{B^2}{T\Omega^3} = O(\epsilon). \tag{22}$$

Third, for the corrections to the rotating-wave approximation bounded in Eq. (16) to be small, we impose the conditions

$$\Omega/\omega_0 = O(\epsilon), \quad \Omega B T/\omega_0 = O(\epsilon). \tag{23}$$

Note that, while we require T to be small enough to justify the rotating-wave approximation, it must also be large enough to ensure adiabaticity during the sweep.

The conditions listed so far already arise in the analysis of the two-level system, Eq. (17). We need to impose further conditions to ensure that the amplitude is small for transitions from these two levels to other states and thereby justify the two-level approximation. With that purpose in mind, we now discuss particle creation by a time-dependent source in a field-theory context, first in a free theory and then in an interacting theory.

3.2 Free Theory with Sources

Consider first the free theory with a static quadratically coupled source. One can analyze the effect of the source through a straightforward generalization of standard sourceless free-theory calculations. The Hamiltonian can be expressed in terms of creation and annihilation operators $a_l^\dagger$ and a_l as

$$H = \oint_l \omega_l \left(a_l^\dagger a_l + \frac{1}{2} [a_l, a_l^\dagger] \right), \tag{24}$$

where

$$(-\partial_x^2 + m^2 + 2J_2(x))\psi_l(x) = \omega_l^2 \psi_l(x) \tag{25}$$

and

$$\phi(t,x) = \oint_l \frac{1}{\sqrt{2\omega_l}} \left(a_l \psi_l^*(x) e^{-i\omega_l t} + a_l^\dagger(x) \psi_l(x) e^{i\omega_l t} \right). \tag{26}$$

In other words, $\psi_l(x)$ and ω_l^2 are the energy eigenfunctions and eigenvalues of a Schrödinger equation with potential $m^2(x) = m^2 + 2J_2(x)$. Here, $\oint$ indicates a sum over the discrete part plus an integral over the continuous part of the spectrum.

Thus, the spectrum consists of particles associated with the solution of the Schrödinger equation with a potential determined by the source term $J_2(x)\phi^2$.

Now consider turning on a linearly coupled source $J_1(t,x)\phi(t,x)$ for a finite time. Let

$$\tilde{J}_1(\omega_l, l) = \int d^2y \, \psi_l(y^1) e^{i\omega_l y^0} J(y^0, y^1). \tag{27}$$

(In the special case $J_2 = 0$, the ψ_l are simply plane-wave solutions with $\omega_p^2 = p^2 + m^2$, and $\tilde{J}_1$ is then the Fourier transform of $J_1(x)$.) Using the equation of motion and the retarded Green's function, one finds that

$$H = \oint_l \omega_l \left(b_l^\dagger b_l + \frac{1}{2} [b_l, b_l^\dagger] \right), \tag{28}$$

where

$$b_l = a_l + \frac{i}{\sqrt{2\omega_l}} \tilde{J}_1(\omega_l, l). \tag{29}$$

The probabilities of no particles being created, $P(0)$, and a single k-type particle being produced, $P(k)$, are

$$P(0) = |A(0)|^2 = \exp\left[-\oint_l \frac{1}{2\omega_l} |\tilde{J}_1(\omega_l, l)|^2 \right], \tag{30}$$

$$P(k) = |A(k)|^2 = |\tilde{J}_1(\omega_k, k)|^2 \exp\left[-\oint_l \frac{1}{2\omega_l} |\tilde{J}_1(\omega_l, l)|^2 \right]. \tag{31}$$

Production of n particles can also occur, with the probability given by the Poisson distribution. Thus, the non-interacting theory does not allow one adequately to suppress creation of more than one particle from the vacuum state.

3.3 Interacting Theory with Sources

Suppose that the time-dependent source term in the Hamiltonian density is $J_1(t,x)\phi(t,x)$, where

$$J_1(t,x) = f(t)h(x) \tag{32}$$

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and

$$f(t) = \begin{cases} g\cos(\omega_0 t + Bt^2/T), & -T/2 \le t \le T/2, \\ 0, & \text{otherwise}. \end{cases} \tag{33}$$

If the two-level approximation is justified, then the analysis of adiabatic passage in Sec. 3.1 applies, with the Rabi frequency Ω given by Eq. (4).

In Appendix B, we analyze the properties of $\mathcal{F}(\omega)$, the Fourier transform of $f(t)$. There, it is shown that $\mathcal{F}(\omega)$ is approximately constant for frequencies in a band of width B centered at ω_0:

$$\mathcal{F}(\omega) \approx g\sqrt{T/B}, \quad \omega_0 - B/2 < \omega < \omega_0 + B/2. \tag{34}$$

Outside this band, $\mathcal{F}(\omega)$ is much smaller: for δ scaling like $\sqrt{B/T}$, we have

$$\mathcal{F}(\omega) = O(g/B), \quad |\omega - \omega_0| \ge B/2 + \delta. \tag{35}$$

Thus, for $BT \gg 1$, $\mathcal{F}$ is well approximated by a rectangular function in frequency space, supported on the interval $|\omega - \omega_0| \le B/2$.

Now consider the effect of the $\lambda\phi^4$ interaction. Recall that we cannot use perturbation theory to analyze the production of a single bound particle by adiabatic passage, instead needing the nonperturbative analysis of the two-level effective Hamiltonian described in Sec. 3.1. Nevertheless, we can use perturbation theory to bound the error arising from unwanted transitions.

One process arising in the free theory that we need to consider is the production of more than one particle in the potential well. In the interacting theory, the energy of a two-particle state is shifted from twice the energy of a one-particle state by $O(\lambda)$, because of the interaction between particles. The amplitude for a transition that changes the energy by ω scales like $\mathcal{F}(\omega)$. To suppress production of multiple particles, we need the coupling λ to be large enough to shift the energy of the transition from one particle to two particles outside the band where $\mathcal{F}(\omega)$ is large. We therefore require

$$B = O(\lambda). \tag{36}$$

There is still a contribution to the error from the amplitude for the $1 \to 2$ transition driven by the source outside that frequency window; we therefore impose

$$g/B = O(\epsilon), \tag{37}$$

where ϵ is the error.

In contrast with the two-particle bound state (whose energy is shifted away from 2ω), there is a single-particle unbound state with momentum $p_{2\omega}$ such that the total energy is exactly 2ω. The transition to this state from the single-particle state of energy ω is on resonance, that is, it is not suppressed by the decaying tail of $\mathcal{F}(\omega)$. However, one can suppress this unwanted excitation by judiciously choosing the spatial profile $h(x)$ so that the matrix element of the term $\int dx\, h(x)\phi(x)$ coupling the single-particle bound state to

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the single-particle momentum-$p_{2\omega}$ unbound state is small. By computing the spatial profile $\psi_0(x)$ of the mode corresponding to the single-particle bound state, one can in fact ensure that this matrix element is precisely zero. For $\lambda = 0$, one can solve for $\psi_0(x)$ exactly if the double wells defined by $J_2(x)$ are chosen from among the double-well potentials with known exact solutions. Then, as $\lambda \to 0$ this approximation becomes parametrically more precise.

We also need to take into account the production of unwanted states that are on resonance with multiples of the source frequency, including the production of unbound particles in the continuum. There are connected Feynman diagrams, higher order in λ, in which k J_1 insertions, each with frequency in the band where $\mathcal{F}(\omega)$ is large, combine to produce one or more particles with total energy of approximately $k\omega_0$. An example is shown in Fig. 2. There are also additional tree-level diagrams suppressed by more powers of $(\lambda/m^2)(J_1/m^2)^2$, as well as $O(\lambda)$ loop corrections. The most dangerous diagram, the one shown in Fig. 2, scales like $\lambda \mathcal{F}(\omega)^3$; to ensure that it is adequately small, we impose

$$\lambda \left(g\sqrt{T/B} \right)^3 \sim \frac{\left(g\sqrt{T} \right)^3}{\sqrt{B}} = O(\epsilon), \tag{38}$$
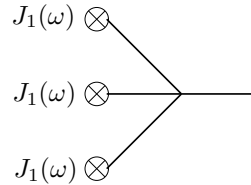
where we have used $\lambda \sim B$.

Figure 2: Example of a connected diagram, suppressed by $(\lambda/m^2)(J_1/m^2)^3$, in which three insertions of the source each with frequency ω produce a single particle with frequency 3ω.

In Eqs. (20), (22), (23), (36), (37), and (38), we have now enumerated a set of sufficient conditions to ensure that our state preparation by adiabatic passage succeeds with a small error ϵ (where we recall that $\Omega \sim g$). We just need to check that all of these conditions can be satisfied simultaneously. One can verify that all conditions are satisfied by choosing parameters to scale with ϵ as follows:

$$g \sim \epsilon^5, \quad \lambda \sim B \sim \epsilon^4, \quad T \sim 1/\epsilon^8. \tag{39}$$

If we wish to simulate an n-qubit circuit accurately, the error ϵ in the preparation of each qubit should scale like $1/n$. We conclude that the state preparation can be achieved in a time of order n^8, if all the qubits are prepared in parallel.

However, as we discuss in Sec. 4, in the simulation of a circuit with G gates, we choose $\lambda \sim 1/G$ to ensure that the action of our entangling two-qubit gate can be computed classically both accurately and efficiently. For a deep circuit, the requirement $\lambda \sim 1/G$ is more stringent than the condition $\lambda \sim 1/n^4$ implied by Eq. (39), and therefore g must be correspondingly

smaller as well, and T correspondingly larger. We conclude that the state preparation can be achieved in the time

$$T \sim \max(n^8, G^2) \,. \tag{40}$$

If G is much larger than n^4, the corresponding state-preparation error of order $G^{-1/4}$ is actually much smaller than is needed for an accurate simulation.

4   Quantum Gates

In this section, we describe how one can perform universal quantum computation. We first discuss how what is perhaps the most obvious attempt does not work and then explain how one can overcome this difficulty. One might naively try to choose the encoding and then implement each gate from a particular universal gate set. This set must include a two-qubit gate, which one would try to realize by bringing the qubit double wells closer to each other. For instance, to implement a controlled-phase gate with a dual-rail encoding, one would decrease the separation of the logical-one wells, with the intention that the interactions between the particles would implement the operation. The problem with this idea is that tunneling of particles between double wells can occur. Tunneling leads to states not in the computational subspace; in short, the qubit encoding is destroyed. In Sec. 4.1, we demonstrate that there is no regime in which the particle interaction is parametrically larger than the tunneling between double wells.

Instead, we can achieve universality by using unitary operations within the larger space of all six configurations in which four wells are occupied by two particles without double occupations. (Transitions to doubly occupied states are suppressed by adiabaticity.) In Sec. 4.2, we describe how to realize unitary transformations within this larger space that closely approximate entangling two-qubit gates acting on the computational subspace. Our analysis uses adiabatic theorems, which show how slowly one must perform the operations in order to implement a gate with a specified precision.

Before we present the details, let us examine quantitatively the effects of the static source and particle interactions. Consider the Lagrangian after J_1 has been used for state preparation and turned off:

$$\mathcal{L} = \frac{1}{2}\partial_\mu \phi \partial^\mu \phi - \frac{1}{2}m^2\phi^2 - \frac{1}{4!}\lambda\phi^4 - J_2\phi^2 \,. \tag{41}$$

One can obtain the tree-level (lowest-order in λ) nonrelativistic Lagrangian as follows. Let

$$\phi \equiv \frac{1}{\sqrt{2m}}\left(e^{-imt}\psi + e^{imt}\psi^*\right) \,. \tag{42}$$

Then,

$$\mathcal{L}_{NR} = i\dot{\psi}\psi^* + \frac{1}{2m}\psi^*\nabla^2\psi - \frac{J_2}{m}\psi^*\psi - \frac{\lambda}{16m^2}(\psi^*\psi)^2 \,. \tag{43}$$

Thus, $\pi = \partial \mathcal{L}_{NR}/\partial \dot{\psi} = i\psi^*$, and the nonrelativistic Hamiltonian $\mathcal{H}_{NR} = \pi \dot{\psi} - \mathcal{L}_{NR}$ is

$$\mathcal{H}_{NR} = -\frac{1}{2m}\psi^* \nabla^2 \psi + \frac{J_2}{m}\psi^* \psi + \frac{\lambda}{16m^2}(\psi^*\psi)^2 \,. \tag{44}$$

Since $p = -i\nabla$, the lowest-order Schrödinger-picture Hamiltonian is

$$\mathcal{H}_{NR} = \sum_i \frac{p_i^2}{2m} + \sum_i \frac{J_2(x_i)}{m} + \frac{\lambda}{4m^2}\sum_{i<j}\delta(x_i - x_j)\,, \tag{45}$$

where x_i denotes the position of particle i. Including the $\mathcal{O}(\lambda^2)$ term (see [3]), we obtain

$$\mathcal{H}_{NR} = \sum_i \frac{p_i^2}{2m} + \sum_i \frac{J_2(x_i)}{m} + \frac{\lambda}{4m^2}\Big(1 + \frac{\lambda}{4\pi m^2}\Big)\sum_{i<j}\delta(x_i - x_j) - \frac{\lambda^2}{32\pi m^3}\sum_{i<j}\int_0^1 dy \frac{e^{-m r_{ij}/\sqrt{y(1-y)}}}{\sqrt{y(1-y)}}\,, \tag{46}$$

where r_{ij} is the distance between particles i and j. We see that the static source J_2 induces a nonrelativistic effective potential $V(x) = J_2(x)/m$. Equation (46) shows only the lowest-order terms in p^2 and J_2; higher-order terms can also be efficiently computed.

We choose $J_2 \sim \lambda$, which ensures that both the binding energy and the kinetic energy of a particle in a potential well scales like λ. As we shall explain in Sec. 4.2, it takes a time of order λ^{-2} to execute our two-qubit entangling gate. Therefore, by including all terms up to order λ^2 in the effective Hamiltonian, we can compute the action of the gate up to an $O(\lambda)$ error. For this purpose, there are some contributions we need to include beyond what is shown in Eq. (46). One is the first relativistic correction to the kinetic energy, namely $-\sum_i p_i^4/8m^3$. In addition, there are $O(\lambda J_2)$ terms arising from Feynman diagrams with a single point interaction and also a J_2 insertion on one of the four external legs. For a specific choice of J_2, these diagrams can be computed numerically.

To justify using perturbation theory up to $O(\lambda^2)$ for the purpose of computing the action of the gate, we recall that perturbation theory is provably asymptotic in ϕ^4 theory (without sources) in two spacetime dimensions (and, more generally, in two-dimensional theories in which the interaction is a polynomial in ϕ) [13–15]: when scattering matrix elements are computed in perturbation theory to N^{th} order in λ, the error is $O(\lambda^{N+1})$ as $\lambda \to 0$.

4.1   Gate Times

The inter-particle potential is created by the scattering of two particles. For ϕ^4 theory, in which there is only one type of particle (a massive scalar), the potential has an $O(\lambda)$ repulsive contact term (that is, a term proportional to the delta function) and an $O(\lambda^2)$ exponentially decaying attractive term arising from the exchange of two massive particles.

To analyze the entangling gate between a pair of dual-rail-encoded qubits, we consider the interaction between two particles, each confined to a potential well, where the wells are widely separated. The leading contribution to the phase shift comes from the contact interaction and can be efficiently computed. In a circuit with G gates, to ensure a small error, we wish to specify the action of each gate to infidelity $O(1/G)$. For this reason, we

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choose $\lambda = O(1/G)$, so that corrections to the phase shift that are higher order in λ can be neglected.

In addition to this phase shift, which occurs when both potential wells are occupied by particles, we need to consider the tunneling between wells that occurs when one of the two wells is unoccupied, which can also be efficiently computed. For a potential barrier with height V and width ℓ, the tunneling matrix element for a particle with energy E scales like $\mathcal{W} = \exp(-\ell\sqrt{2m(V - E)})$. The interaction energy of two particles of energy E separated by the barrier, due to the overlap of their wave functions and the contact interaction, scales like $(\lambda/m^2) \times \mathcal{W}^2$ and is therefore parametrically small compared with the tunneling matrix element when λ is small. Thus, the time needed to generate a large phase shift is large compared with the tunneling time, and tunneling cannot be ignored during the execution of a two-qubit entangling gate.

Let us verify that the contributions to the interaction energy that are higher order in λ can be safely neglected. Feynman diagrams corresponding to the leading contributions to $2 \to 2$ scattering from particle exchange are shown in Fig. 3, for both ϕ^3 and ϕ^4 interaction terms. In Fig. 3a a single particle is exchanged; the internal line in the diagram is the dressed propagator

$$\bar{\Delta}_{x_1,x_2} = -\left(\frac{1}{-\frac{d^2}{dx^2} + m^2 + 2J_2(x)}\right)_{x_1,x_2}, \tag{47}$$
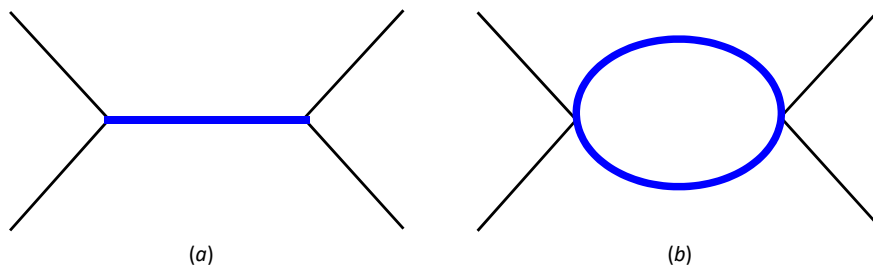
which includes the effects of the $J_2\phi^2$ source term.

(a)   (b)

Figure 3: Feynman diagrams contributing to two-particle scattering at order λ^2 for (a) a $\lambda\phi^3$ interaction and (b) a $\lambda\phi^4$ interaction. The heavy internal lines are dressed propagators.

To be concrete, consider the exactly solvable case in which J_2 is a static square barrier of width ℓ and height mV. We wish to compute the Green's function

$$G(x_1, x_2; z) = (H - z)^{-1}_{x_1,x_2}, \tag{48}$$

where

$$H = -\frac{1}{2m}\frac{d^2}{dx^2} + V(x), \tag{49}$$

$J_2 = mV$, and $z = -m/2$. We can evaluate $G(x_1, x_2; z)$ in terms of the Wronskian (see [16]).

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Let $u_L(x; z)$ and $u_R(x; z)$ be solutions to the eigenvalue equation

$$Hu(x; z) = zu(x; z),\tag{50}$$

which approach zero as $x \to -\infty$ and $x \to +\infty$ respectively. The Wronskian is then

$$W(z) = u_L'(x; z)u_R(x; z) - u_L(x; z)u_R'(x; z).\tag{51}$$

It can be shown that $dW/dx = 0$, so the Wronskian is independent of x and depends only on the eigenvalue z. The Green's function can be written in terms of the Wronskian as

$$G(x_1, x_2; z) = \frac{2m}{W(z)}[u_L(x_1; z)u_R(x_2; z)\theta(x_2 - x_1) - u_L(x_2; z)u_R(x_1; z)\theta(x_1 - x_2)],\tag{52}$$

where $\theta(x)$ is the Heaviside step function.

For the square well considered here, we have [16]

$$\bar{\Delta}_{-\ell/2,\ell/2} = -\left(\frac{1}{-\frac{d^2}{dx^2} + m^2 + 2J_2(x)}\right)_{-\ell/2,\ell/2} = \frac{2}{W},\tag{53}$$

where

$$W = -4m\left(\cosh(\ell\sqrt{m^2 + 2mV}) + \frac{m^2 + mV}{m(\sqrt{m^2 + 2mV})}\sinh(\ell\sqrt{m^2 + 2mV})\right).\tag{54}$$

For large ℓ, this expression becomes

$$\bar{\Delta}_{-\ell/2,\ell/2} \approx \frac{-\exp\left(-\ell\sqrt{m^2 + 2mV}\right)}{m\left(1 + \frac{m^2+mV}{m\sqrt{m^2+2mV}}\right)}.\tag{55}$$

We can interpret the result by noting that $\bar{\Delta}_{-l/2,l/2}$ scales like $\exp\left(-m_{\text{eff}}\ell\right)$, where the effective mass of the exchanged particle is

$$m_{\text{eff}} = \sqrt{m^2 + 2mV}.\tag{56}$$

As well as being suppressed by an additional factor of λ, this contribution to the interaction energy falls off more rapidly with ℓ than the contribution from the contact term. In $\lambda\phi^4$ theory, two particles are exchanged at order λ^2. (see Fig. 3b). Therefore, the interaction energy is suppressed by a further factor of $\exp\left(-m_{\text{eff}}\ell\right)$.

4.2 Gate Universality

As we saw in the previous subsection, if we attempt to perform operations on two qubits by bringing one well from each qubit close together, the particle is more likely to tunnel than to interact. If the particle tunnels, then the state will leave the computational subspace.

However, as we show in this subsection, by rotating through a larger space we can implement a universal gate set on the computational subspace. Specifically, we show how one can perform an arbitrary two-qubit gate, corresponding to a 4×4 unitary matrix, to polynomial precision by smoothly varying the well depths and separations.

As we wish to show BQP-hardness of scattering, in our BQP-hardness construction we do not allow access to measurements during the execution of the quantum circuit. (Allowing measurements would change the BQP-hardness question substantially. By the KLM construction [10], one can achieve computational universality using adaptive measurements on a free field theory.) Furthermore, we do not assume any reservoir of cleanly prepared ancilla qubits. Thus we cannot simply invoke fault-tolerance threshold theorems such as that in [17]. In the absence of error correction, it suffices to perform each gate in a quantum circuit of G gates with $O(1/G)$ infidelity (see, for example, [18]).

For a pair of double wells containing two particles, there are six nearly degenerate states corresponding to the $\binom{4}{2}$ combinations of two identical particles in four wells without double occupation. Let us call the subspace spanned by these six states $\mathcal{S}$. States involving double occupation of a well are not degenerate with those in $\mathcal{S}$, since their energy is altered by the interparticle potential induced by the ϕ^4 term. Excited bound states of the wells, states in which the particles are unbound from the wells, and states involving additional particles all have higher energy than those in $\mathcal{S}$. Thus, by varying the depths and separations of the wells slowly enough we can keep the system in the adiabatic regime, with transitions out of $\mathcal{S}$ suppressed by the energy gaps separating $\mathcal{S}$ from the rest of the spectrum above and below.

The adiabatic theorem proven in [19] shows that the probability of leakage out of the subspace $\mathcal{S}$ can be made exponentially small as a function of how slowly we vary the Hamiltonian, as long as the time variation of the Hamiltonian is sufficiently smooth.[2] Let $H(s)$ be a parameterized family of Hamiltonians, and consider the time evolution induced by the time-dependent Hamiltonian $H(t/\tau)$. If $H(s)$ belongs to the Gevrey class of order α, then the diabatic error scales as

$$\epsilon \sim \exp\left[-\tau^{\frac{1}{1+\alpha}}\right]. \tag{57}$$

A function $g(s)$ in the Gevrey class of order α is a smooth function on $\mathbb{R}$ such that on any interval $I = [a, b] \subset \mathbb{R}$ there are constants C and R for which

$$\left|\frac{d^k g}{ds^k}\right| \leq CR^k k^{\alpha k}, \quad \text{for } k = 1, 2, 3, \ldots. \tag{58}$$

For $\alpha = 1$ this is the class of analytic functions. For larger α the condition is less restrictive. In particular, for $\alpha > 1$ there exist smooth, compactly supported "bump" functions not identically equal to zero. By varying the well depths and well separations according to such bump functions, we can limit leakage errors out of $\mathcal{S}$ to ϵ at a cost of $\tau = \text{poly}(\log \epsilon)$. Thus, the requirement $\epsilon \sim 1/G$ contributes only a polylogarithmic factor to the time needed to execute G gates.

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[2]See also [11, 20].

Given that the total amplitude to be outside of the subspace $\mathcal{S}$ is limited to $\epsilon \sim 1/G$, we can neglect this amplitude and solve for the dynamics within $\mathcal{S}$ with the approximation $|\psi(t)\rangle \in \mathcal{S}(t)$ for all t. We do so in the adiabatic frame, that is, the instantaneous eigenbasis of $H(t)$, writing $\mathcal{S} = \mathrm{span}\{|L_1(t)\rangle, \ldots, |L_6(t)\rangle\}$, with $H(t)|L_j(t)\rangle = E_j(t)|L_j(t)\rangle$. In Appendix A, we obtain the following effective Schrödinger equation for the dynamics within $\mathcal{S}(t)$:

$$\frac{d|\psi\rangle}{dt} = -iH_A(t)|\psi\rangle + O(1/G), \tag{59}$$

$$\langle L_j(t)|H_A(t)|L_k(t)\rangle = \begin{cases} E_j(t), & \text{if } j = k, \\ i\frac{\langle L_j(t)|\frac{dH}{dt}|L_k(t)\rangle}{E_j(t)-E_k(t)}, & \text{otherwise.} \end{cases} \tag{60}$$

We now consider in more detail how one can implement a universal set of quantum gates using these dynamics. First, consider single-qubit gates. Recall that, if we choose dual-rail encoding, logical zero and one are encoded by occupation of the ground state of the left and right wells, respectively. The ground and first excited eigenstates of the double-well Hamiltonian are to a very good approximation the symmetric and antisymmetric linear combinations of these states, respectively. Their energy separation is exponentially small as a function of the separation of the wells. Thus, the left and right occupied states are exponentially long-lived and form a convenient basis in which to work.

One can perform logical Z rotations[3] on a qubit by varying the depths of the wells (see Fig. 4). This procedure implements the rotation $e^{-iZ\theta}$ in the logical basis such that the angle θ is proportional to the product of the depth and duration of the variation of the wells. To prevent the accumulation of error, one is required by the adiabatic theorem to perform the variation of the wells logarithmically slower as the number of gates in the circuit is increased. To achieve a fixed target rotation angle, one can decrease the depth of the well variation by the same factor by which the duration of the variation is increased. For a concrete realization of a Z gate in this scheme, see Appendix D.

On can implement an X rotation by temporarily lowering the barrier between wells (see Fig. 4). From Eq. (60) one sees that, in the limit where the two wells are completely isolated from all others, the off-diagonal elements of H_A in the eigenbasis are zero because dH/dt and the ground state have exact left-right symmetry, whereas the first excited state is antisymmetric. Thus, H_A implements a pure Z rotation in the eigenbasis. This corresponds to a pure X rotation in the logical basis, as this is related to the eigenbasis by the Hadamard transform

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{61}$$

One can accommodate the limits on gate speed imposed by adiabaticity while still implementing the desired rotation angle by correspondingly adjusting the degree of lowering of the barrier. For a concrete quantitative realization of an X gate in this manner, see Appendix C.

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[3]Following quantum information conventions, we use X, Y, Z rather than $\sigma_x, \sigma_y, \sigma_z$ to denote the Pauli matrices.
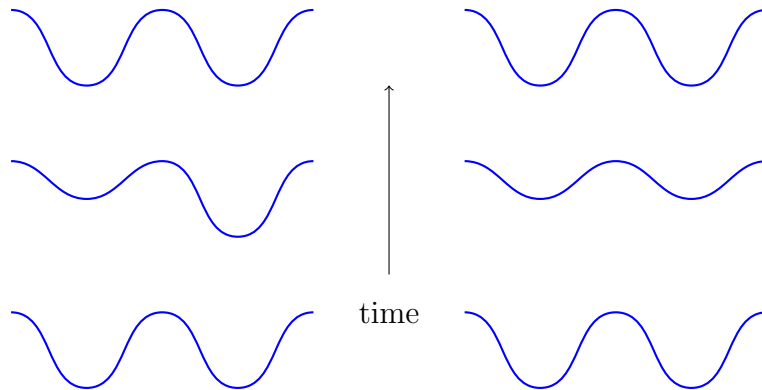
Figure 4: The variation of well depths implements a Z rotation (left-hand side), while lowering the barrier height implements an X rotation (right-hand side).

From X and Z rotations, one can construct an arbitrary single-qubit gate using Euler angles. Any entangling two-qubit gate yields a universal quantum gate set when supplemented by arbitrary single-qubit gates [21]. Thus the final task of this subsection is to construct an entangling two-qubit gate through the use of the inter-particle interaction. We perform the analysis in the occupation-number basis for $\mathcal{S}$ (Fig. 5).

We perform a two-qubit gate by temporarily decreasing the separation between the two center wells in the quadruple-well system (Fig. 6). The induced Hamiltonian on $\mathcal{S}$ in the occupation-number basis takes the form

$$
H_A(t) \simeq
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & b(t) \\
0 & c(t) & 0 & 0 & 0 & 0 \\
0 & 0 & d(t) & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & b(t) & 0 \\
0 & 0 & 0 & b(t) & 0 & 0 \\
b(t) & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{matrix}
0101 \\
0110 \\
1001 \\
1010 \\
1100 \\
0011
\end{matrix}
\tag{62}
$$

for some time-dependent coefficients $b(t)$, $c(t)$ and $d(t)$, which depend on the choice of the shapes of the wells and their trajectories and can be determined numerically from Eq. (60). Here, exponentially suppressed tunneling matrix elements between distant wells have been neglected. The off-diagonal $b(t)$ entries describe the tunneling transition $|01\rangle \leftrightarrow |10\rangle$ for the two wells that approach each other. In addition, there are on-diagonal contributions because the energy changes slightly as the wells get closer together. We have defined our (time-dependent) zero of energy so that this energy shift vanishes when one of the two wells is occupied and the other is empty. Therefore, the only nonzero diagonal entries in $H_A(t)$ are those where both wells are occupied or both are empty, denoted $c(t)$ and $d(t)$, respectively.

Recall that we encode a qubit by placing a single particle in either one of two adjacent potential wells. Thus, the two-qubit Hilbert space is spanned by the four states $\{|0101\rangle, |0110\rangle, |1001\rangle, |1010\rangle\}$, while the two states $\{|1100\rangle, |0011\rangle\}$ are not valid encodings. We want to execute an entangling gate that preserves the valid two-qubit subspace. We
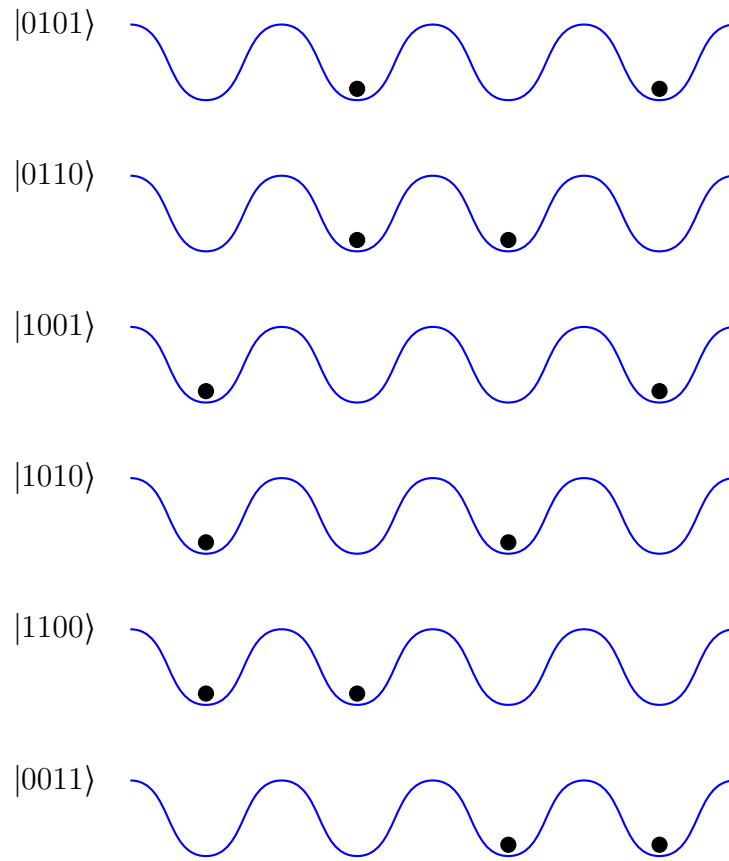
Figure 5: The occupation-number basis for the four wells associated with a pair of logical qubits. In dual-rail encoding, the occupation-number states $|0101\rangle$, $|0110\rangle$, $|1001\rangle$, and $|1010\rangle$ encode the logical qubit states $|11\rangle$, $|10\rangle$, $|01\rangle$, and $|00\rangle$, respectively. The occupation-number states $|1100\rangle$ and $|0011\rangle$ lie outside the coding subspace but are unavoidable because of tunnelling.
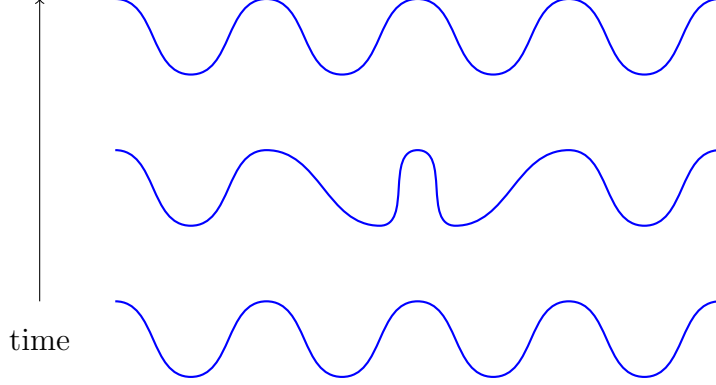
Figure 6: Our implementation of an entangling two-qubit gate. If the center two wells are occupied (corresponding to the logical $|10\rangle$ state), the attraction between particles induces a phase rotation. In the case that exactly one of the two center wells is occupied, there is a tunneling amplitude into the noncoding subspace.

note that the unitary time evolution induced by the time-dependent Hamiltonian $H_A(t)$ is a direct sum of a diagonal transformation acting on $\{|0110\rangle, |1001\rangle\}$ and two identical X rotations $e^{iX\theta_x}$ in span$\{|0101\rangle, |0011\rangle\}$ and span$\{|1010\rangle, |1100\rangle\}$. If we replace $H_A(t)$ with $H_A(t/z)$, thus increasing the duration of the execution of the gate by the factor z, then the rotation angle θ_x also increases by the factor z. We choose z sufficiently large that our adiabaticity constraint is satisfied and tune its value so that $\theta_x/2\pi$ is an integer. The resulting unitary transformation U preserves the four-dimensional subspace spanned by our two encoded qubits; acting on span$\{|0101\rangle, |0110\rangle, |1001\rangle, |1010\rangle\}$, it is the diagonal gate

$$U = \operatorname{diag}\left(1, e^{i\alpha}, e^{i\beta}, 1\right), \tag{63}$$

where we evaluate the phases α and β by integrating $c(t)$ and $d(t)$, respectively. This U is an entangling gate unless $e^{i(\alpha+\beta)} = 1$, which will not be satisfied for a generic choice of the shapes and trajectories of the wells.

Because the interaction strength is $O(\lambda)$, the time taken to execute a single entangling gate with an $O(1)$ phase shift is at least $O(1/\lambda)$. Adiabatic protection against leakage from the coding subspace imposes a stronger lower bound on the gate duration. The energy gap γ separating the doubly occupied states is of order λ, and hence the runtime must scale as $\widetilde{O}(\gamma^{-2}) = \widetilde{O}(\lambda^{-2})$. In a circuit with G gates, we need to choose $\lambda = O(1/G)$ to justify neglecting corrections that are higher order in λ when computing the form of the source term J_2 needed to implement a given gate with infidelity $O(1/G)$. Therefore, the simulation time is $O(G^2)$ for a single gate and $O(G^2 D)$ for the complete circuit, where D is the circuit depth (not including the state-preparation step analyzed in Sec. 3.3).

Furthermore, we note that our two-qubit gates are geometrically local in one dimension: only neighboring qubits interact. To perform our entangling two-qubit gate on two distantly separated qubits A and B, we would perform a series of swap gates to bring A and B into neighboring positions, execute the entangling gate, and then use swap gates to return A and

B to their original positions. The swap gate can be well approximated via our universal gate repertoire with only polylogarithmic overhead, but the swaps would increase the circuit depth by a factor $O(n)$, where n is the number of qubits, compared with a circuit with nonlocal two-qubit gates.

5 Measurements and BQP-completeness

The main line of reasoning in this paper establishes a BQP-hardness argument for the problem of determining transition probabilities in $(1 + 1)$-dimensional ϕ^4 theory to polynomial precision. To obtain a BQP-completeness result we need to establish that (the decision version of) this problem is also contained in BQP, that is, that it can be solved by a polynomial-time quantum algorithm. Essentially, the quantum algorithm achieving this is given in [2, 3]. However, there are some small differences between the BQP-hard problem given in this paper and the problem solved by the quantum algorithm of [2, 3]. Here, we address several ways to bridge this gap, that is, several problems that one can show to be BQP-complete by technical variations of the algorithms of [2, 3] and the argument of the preceding sections.

In our main BQP-hardness argument, given a quantum circuit, we construct $J_1(t, x)$ and $J_2(t, x)$ so that the vacuum-to-vacuum transition amplitude approximates the $|0\dots0\rangle$ to $|0\dots0\rangle$ amplitude of the quantum circuit. The problem of deciding whether the magnitude of the amplitude $|0\dots0\rangle \to |0\dots0\rangle$ of a quantum circuit is smaller than $1/3$ or larger than $2/3$, given the promise that one of these is the case, is BQP-complete. As an immediate corollary, it is BQP-hard to estimate the corresponding vacuum-to-vacuum transition probability to within $\pm\epsilon$, for a sufficiently small constant ϵ.

The existence of a polynomial-time quantum algorithm that estimates the vacuum-to-vacuum transition amplitude to adequate precision would imply that the decision problem is not only BQP-hard but also BQP-complete. One can devise such an algorithm using the methods of [2, 3], which described quantum algorithms for preparing the vacuum state and implementing the unitary time evolution in ϕ^4 theory. This procedure can be applied without modification in the presence of the spacetime-dependent source terms $J_1(t, x)$ and $J_2(t, x)$, at the cost of modest performance penalties, by the analysis of [5, 6]. With these tools from [2, 3], we can construct the algorithm for estimating the amplitude $\langle \text{vac}|U|\text{vac}\rangle$ using a standard technique, called the *Hadamard test*, which is illustrated in Fig. 7. The probability of measuring $|0\rangle$ is $p_0 = [1 + \text{Re}(\langle\psi|U|\psi\rangle)]/2$. Thus, one can obtain the real part of $\langle\psi|U|\psi\rangle$ to within ϵ by making $O(1/\epsilon^2)$ measurements. Similarly, by initializing the control qubit to $\frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$, one can estimate the imaginary part of $\langle\psi|U|\psi\rangle$.

If we can prepare the state $|\psi\rangle$, execute the conditional unitary transformation U controlled by a single qubit, namely,

$$\text{controlled}-U = |0\rangle\langle0| \otimes I + |1\rangle\langle1| \otimes U, \tag{64}$$

and measure the control qubit, then we can estimate $\langle\psi|U|\psi\rangle$ using the Hadamard test. We can promote the circuit described in [2, 3] for implementing the unitary time-evolution operator U to a circuit for controlled-U by replacing each gate G in the circuit with controlled-G.
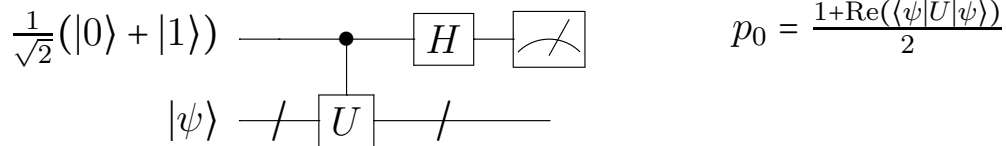
Figure 7: Circuit implementing the Hadamard test. The boxed H and U denote Hadamard and controlled-U gates, and the slashed line indicates multiple qubits. The probability of measuring $|0\rangle$ is denoted p_0.

(If G is a two-qubit gate, then controlled-G is a three-qubit gate, which can be efficiently decomposed into the original gate set through standard techniques.) Therefore, the methods described in [2, 3] for preparing the vacuum and for implementing time evolution, together with the Hadamard test, provide a procedure for estimating the vacuum-to-vacuum amplitude in the presence of sources that vary in space and time. This procedure, combined with the result obtained in this paper that the problem is BQP-hard, shows that the corresponding decision problem is BQP-complete.

This scheme for demonstrating the BQP-completeness of a quantum field theory problem has the advantage that only a single-qubit measurement is required to read out the result, but also the disadvantage that each gate needs to be replaced by its controlled version. There are other ways to bridge the gap between the BQP-hardness result presented in this paper and the simulation algorithms formulated in [2, 3], in which we avoid the nuisance of replacing each G by controlled-G at the cost of executing a more complicated measurement at the end of the algorithm. For example, we could omit the final step of the BQP-hardness construction, in which particles in the logical-zero states are annihilated through adiabatic passage. In that case, the transition probability that is BQP-hard to estimate is the probability to start in the vacuum and end with all of the double wells in the logical-zero state. The algorithm that estimates this transition probability includes a final step that simulates, through phase estimation, a particle detector measuring the energy in a spatially localized region. This detector simulation was described in [3]. Another motivation for discussing particle-detecting measurements is that our BQP-hardness construction can be regarded as an idealized architecture for constructing a universal quantum computer from laboratory systems, namely, condensed-matter or atomic-physics experimental platforms that are described by ϕ^4 theory. With these motivations in mind, we briefly explain, following [3], how to measure the energy in a local region.

At the end of our scattering process, the Hamiltonian is

$$H = \int dx \mathcal{H}(x), \tag{65}$$

where

$$\mathcal{H}(x) = \frac{1}{2}\pi^2(x) + \frac{1}{2}\phi(x)\frac{d^2}{dx^2}\phi(x) + \frac{1}{2}m^2\phi^2(x) + J_2(x)\phi^2(x) + \frac{\lambda}{4!}\phi^4(x). \tag{66}$$

Measuring the observable H would yield the total energy of the system. Correspondingly,

consider the operator

$$H_f = \int dx f(x) \mathcal{H}(x), \tag{67}$$

where f is some envelope function that is localized in some spatial region R. Then, measuring the observable H_f yields an approximation to the energy within R. If a particle is present within R, then the measured energy will be detectably larger than if H_f is measured for vacuum.

The envelope function f must be chosen with care. The naive choice

$$f(x) = \begin{cases} 1, & x \in R, \\ 0, & \text{otherwise} \end{cases} \tag{68}$$

is unsuitable because of the $\phi(x)\frac{d^2}{dx^2}\phi(x)$ term and the discontinuity in f. More quantitatively, one can introduce a lattice cutoff, as is done in [3], and compute the variance of H_f in the vacuum state. For the functional form (68), this diverges as the lattice spacing is taken to zero. In one spatial dimension, one can obtain a convergent variance by instead choosing f to be a Gaussian envelope.

With the aim of interpreting H_f, it is helpful to consider the free theory ($\lambda = 0$), which can be exactly solved. Associated with each potential well created by $J_2(x)$ there is at least one localized mode representing a particle bound in this well. The creation and annihilation operators associated with this mode can be expanded in the form

$$a^\dagger = \int dx \left[c_\phi(x)\phi(x) + c_\pi(x)\pi(x) \right]. \tag{69}$$

The magnitudes of c_ϕ and c_π decay exponentially with characteristic decay length $1/m$ outside the well. Hence, if the Gaussian envelope is centered on the well and has a large width relative to the width of the well plus $1/m$, then $[a^\dagger, H_f] \simeq [a^\dagger, H]$ and $[a, H_f] \simeq [a, H]$. This in turn implies that the presence of a particle in the well raises the expectation value of H_f by approximately the same amount that the expectation of H is raised, that is, by the energy of the particle. In the $\lambda \neq 0$ case, the qualitative behavior will be similar.

A   Dynamics within an Adiabatic Subspace

Suppose that we have a time-dependent Hamiltonian in which some subset of eigen-energies are at all times well separated from the rest of the spectrum. Then, using adiabatic theorems, one can prove that the amplitude to escape the isolated subspace is always less than

some bound ϵ. In this appendix, we adapt fairly standard arguments to prove that, in this circumstance, the dynamics within the isolated subspace induced by an adiabatic process of duration t is given by Eq. (60), up to errors of order ϵt.

Let $H(t)$ be a differentiable time-dependent Hamiltonian. Let $|L_1(t)\rangle$, $|L_2(t)\rangle$, ... be a normalized eigenbasis with corresponding eigenvalues $E_1(t)$, $E_2(t)$, ..., so that, for all j and all t,

$$H(t)|L_j(t)\rangle = E_j(t)|L_j(t)\rangle, \tag{70}$$

with

$$\langle L_j(t)|L_j(t)\rangle = 1. \tag{71}$$

The normalization condition Eq. (71) leaves us free to choose the phase. If $|L'_k(t)\rangle$ is a normalized eigenvector of $H(t)$, then so is

$$|L_k(t)\rangle = e^{i\vartheta(t)}|L'_k(t)\rangle \tag{72}$$

for any real-valued function $\vartheta(t)$. Henceforth, we shall generally leave the time dependence implicit in $|L'_k\rangle$. Differentiating the normalization condition $\langle L'_k|L'_k\rangle = 1$ yields

$$\frac{d\langle L'_k|}{dt}|L'_k\rangle + \langle L'_k|\frac{d|L'_k\rangle}{dt} = 0. \tag{73}$$

Thus, for all k and t,

$$\mathrm{Re}\left[\langle L'_k|\frac{d|L'_k\rangle}{dt}\right] = 0. \tag{74}$$

By Eq. (74), we can let

$$\vartheta(t) = i\int_0^t ds \langle L'_k(s)|\frac{d|L'_k(s)\rangle}{ds}ds, \tag{75}$$

which is purely real and hence gives a normalized $|L_k(t)\rangle$ via Eq. (72). This choice of $\vartheta(t)$ yields

$$\langle L_k(t)|\frac{d|L_k\rangle}{dt} = \langle L'_k|e^{-i\vartheta(t)}\frac{d}{dt}e^{i\vartheta(t)}|L'_k\rangle \tag{76}$$

$$= i\frac{d\vartheta}{dt} + \langle L'_k|\frac{d|L'_k\rangle}{dt} \tag{77}$$

$$= 0. \tag{78}$$

Thus we are free to choose

$$\langle L_k|\frac{d|L_k\rangle}{dt} = 0, \quad \forall k, t, \tag{79}$$

as this is ultimately a phase convention. We shall adopt this convention for the remainder of this section.

Next, following standard treatments (see, for example, [22]) we express the dynamics in the instantaneous eigenbasis[4] of $H(t)$, that is,

$$|\psi(t)\rangle = \sum_j \alpha_j(t)|L_j(t)\rangle. \tag{80}$$

By Eq. (80) and Schrödinger's equation,

$$\frac{d\alpha_j}{dt} = \frac{d}{dt}\langle L_j|\psi\rangle \tag{81}$$

$$= \frac{d\langle L_j|}{dt}|\psi\rangle - i\langle L_j|H|\psi\rangle. \tag{82}$$

By Eqs. (70 and (80), this simplifies to

$$\frac{d\alpha_j}{dt} = \frac{d\langle L_j|}{dt}|\psi\rangle - iE_j\alpha_j. \tag{83}$$

Differentiating Eq. (70) yields

$$\frac{dH}{dt}|L_j\rangle + H\frac{d|L_j\rangle}{dt} = \frac{dE}{dt}|L_j\rangle + E_j\frac{d|L_j\rangle}{dt}. \tag{84}$$

Thus,

$$(H - E_j)\frac{d|L_j\rangle}{dt} = \left(\frac{dE_j}{dt} - \frac{dH}{dt}\right)|L_j\rangle. \tag{85}$$

Let

$$G_j = \sum_{k \neq j} \frac{P_k}{E_k - E_j}, \tag{86}$$

where $P_k = |L_k\rangle\langle L_k|$ is the projector on to the kth eigenspace. Then

$$G_j(H - E_j) = \mathbb{1} - P_j. \tag{87}$$

Thus, multiplying Eq. (85) by G_j yields

$$(\mathbb{1} - P_j)\frac{d|L_j\rangle}{dt} = G_j\left(\frac{dE_j}{dt} - \frac{dH}{dt}\right)|L_j\rangle. \tag{88}$$

By our phase convention Eq. (79), this simplifies to

$$\frac{d|L_j\rangle}{dt} = G_j\left(\frac{dE_j}{dt} - \frac{dH}{dt}\right)|L_j\rangle. \tag{89}$$

The first term on the right-hand side vanishes because G_j commutes with dE_j/dt (which is just a c-number) and projects out $|L_j\rangle$. Thus

$$\frac{d|L_j\rangle}{dt} = -G_j\frac{dH}{dt}|L_j\rangle. \tag{90}$$

---

[4]We shall refer to this as the adiabatic frame. Some older references such as [22] refer to this as the rotating-axis representation.

Substituting Eq. (90) into Eq. (83) yields

$$\frac{d\alpha_j}{dt} = -\langle L_j | \frac{dH}{dt} G_j | \psi \rangle - i\alpha_j E_j. \tag{91}$$

By Eqs. (80) and (86),

$$G_j | \psi \rangle = \sum_{k \neq j} \frac{\alpha_k}{E_k - E_j} | L_k \rangle, \tag{92}$$

Therefore Eq. (91) yields

$$\frac{d\alpha_j}{dt} = -i\alpha_j E_j - \sum_{k \neq j} \frac{\langle L_j | \frac{dH}{dt} | L_k \rangle}{E_k - E_j} \alpha_k + O(\epsilon). \tag{93}$$

We thus have a Schrödinger-like equation for the coefficients $\alpha_1, \alpha_2, \ldots$, namely,

$$\frac{d}{dt} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{bmatrix} = -iM \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{bmatrix}, \tag{94}$$

where M is the Hermitian matrix

$$M_{jk} = \begin{cases} E_j, & \text{if } j = k, \\ i\frac{\langle L_j | \frac{dH}{dt} | L_k \rangle}{E_j - E_k}, & \text{if } j \neq k. \end{cases} \tag{95}$$

So far, our analysis has been only a change of frame, maintaining both exactness and a high degree of generality.[5] Now, assume that the eigenstates $|L_1(t)\rangle, \ldots, |L_d(t)\rangle$ are separated from the rest of the spectrum by an energy gap sufficiently large that, by an adiabatic theorem (for example, [19]), a state initially within the span of $|L_1(t)\rangle, \ldots, |L_d(t)\rangle$ remains within this subspace for all time, up to corrections of order ϵ. The dynamics in the adiabatic frame is then of the form

$$\frac{d}{dt} \begin{bmatrix} \alpha_- \\ \alpha_+ \end{bmatrix} = -i \begin{bmatrix} M_{--} & M_{-+} \\ M_{+-} & M_{++} \end{bmatrix} \begin{bmatrix} \alpha_- \\ \alpha_+ \end{bmatrix}, \tag{96}$$

where M_{--} is a $d \times d$ matrix, α_- is a d-dimensional column vector, etc.

Next, we make an approximation: we suppose that α_+ can be neglected, because the adiabatic theorem guarantees that the magnitude of the vector $|\alpha_+\rangle = \sum_{j>d} \alpha_j |L_j(t)\rangle$ is at most ϵ. In other words, we approximate the full dynamics on $\mathcal{H}$ by a self-contained dynamics within $\mathcal{H}_-(t)$, namely,

$$|\bar{\psi}\rangle = \sum_{j=1}^{d} \bar{\alpha}(t) |L_j\rangle, \tag{97}$$

---

[5]We have not maintained full generality in Eqs. (94) and (95) in that it has been convenient to make the technical assumption that the spectrum of $H(t)$ is fully discrete and nondegenerate. This is generally not true of quantum field theories, but it suffices for our analysis in Sec. 4.2 because the relevant low-lying spectrum is discrete and nondegenerate.

where $\bar{\alpha}_j(0) = \alpha_j(0)$ and

$$\frac{d}{dt}|\bar{\psi}\rangle = -iM_{--}|\bar{\psi}\rangle. \tag{98}$$

Thus $|\bar{\psi}(t)\rangle$ is an approximation to the exact state $|\psi(t)\rangle$ with corrections of order ϵ. More quantitatively, if $|\psi(0)\rangle \in \mathcal{H}_-$ then

$$\langle\bar{\psi}(0)|\psi(0)\rangle = 1 \tag{99}$$

and

$$\begin{aligned}
\frac{d}{dt}\langle\bar{\psi}|\psi\rangle &= \frac{d\langle\bar{\psi}|}{dt}|\psi\rangle + \langle\bar{\psi}|\frac{d|\psi\rangle}{dt} \tag{100} \\
&= i\langle\bar{\psi}|M_{--}^\dagger|\psi\rangle - i\langle\bar{\psi}|\left(M_{--}|\psi_-\rangle + M_{-+}|\psi_+\rangle\right) \tag{101} \\
&= -i\langle\bar{\psi}|M_{-+}|\psi_+\rangle, \tag{102}
\end{aligned}$$

where we have used Eq. (98) and the fact that M_{--} is Hermitian. Combined with Eq. (99), this yields

$$\langle\bar{\psi}(t)|\psi(t)\rangle = 1 - i\int_0^t d\tau \langle\bar{\psi}|M_{-+}|\psi_+\rangle. \tag{103}$$

Thus,

$$|\langle\bar{\psi}(t)|\psi(t)\rangle| \geq 1 - \int_0^t \left\|M_{-+}|\psi_+\rangle\right\|. \tag{104}$$

By assumption, an adiabatic theorem tells us that $\||\psi_+\rangle\| \leq \epsilon$ for all t, and therefore the above inequality implies

$$|\langle\bar{\psi}(t)|\psi(t)\rangle| = 1 - O(\epsilon t). \tag{105}$$

If M_{-+} is a bounded operator, then Eq. (104) yields

$$|\langle\bar{\psi}(t)|\psi(t)\rangle| \geq 1 - \epsilon t \|M_{-+}\|. \tag{106}$$

Examining Eq. (95), one sees that if dH/dt is a bounded operator (as is the case if it is finite-dimensional), one obtains from Eq. (106) the following:

$$|\langle\bar{\psi}(t)|\psi(t)\rangle| \geq 1 - \frac{\left\|\frac{dH}{dt}\right\|}{\gamma}\epsilon t, \tag{107}$$

where

$$\begin{aligned}
\gamma(t) &= E_{d+1}(t) - E_d(t), \tag{108} \\
\gamma &= \min_t \gamma(t). \tag{109}
\end{aligned}$$

31

B Fourier Transform of the Source

Here we verify the properties, stated in Sec. 3.3, of the Fourier transform of the source used in adiabatic passage. For convenience, we choose the normalization

$$f(t) = \frac{2}{\sqrt{T}}\mathrm{rect}\Big(\frac{t}{T}\Big)\cos(\omega_0 t + \kappa t^2/2)\,, \tag{110}$$

for which the integral of $|f(t)|^2$ is O(1), independent of T. The Fourier transform of $f(t)$ is then

$$\mathcal{F}(\omega) = \mathcal{G}_+(\omega - \omega_0) + \mathcal{G}_-(\omega + \omega_0)\,, \tag{111}$$

where $\mathcal{G}_\pm(\omega)$ is the Fourier transform of

$$g_\pm(t) = \frac{1}{\sqrt{T}}\mathrm{rect}\Big(\frac{t}{T}\Big)e^{\pm i\kappa t^2/2}\,. \tag{112}$$

Integration gives

$$\mathcal{G}_\pm(\omega) = \sqrt{\frac{\pi}{\kappa T}}\,e^{\mp i\omega^2/2\kappa}\big\{C(x^\pm) + C(x^\mp) \pm i\,[S(x^\pm) + S(x^\mp)]\big\}\,, \tag{113}$$

where

$$x^\pm = \sqrt{\frac{\kappa}{\pi}}\Big(\frac{T}{2} \mp \frac{\omega}{\kappa}\Big)\,. \tag{114}$$

The special functions $C(z)$ and $S(z)$ are the Fresnel integrals, defined as

$$C(z) = \int_0^z \cos\Big(\frac{1}{2}\pi t^2\Big)dt\,, \tag{115}$$

$$S(z) = \int_0^z \sin\Big(\frac{1}{2}\pi t^2\Big)dt\,. \tag{116}$$

Thus, with $B = \kappa T$, the magnitude of $G_\pm$ is

$$\frac{B}{\pi}|\mathcal{G}_\pm(\omega)|^2 = \Big\{C\Big[\Big(\frac{BT}{\pi}\Big)^{1/2}\Big(\frac{1}{2} - \frac{\omega}{B}\Big)\Big] + C\Big[\Big(\frac{BT}{\pi}\Big)^{1/2}\Big(\frac{1}{2} + \frac{\omega}{B}\Big)\Big]\Big\}^2 \tag{117}$$
$$+ \Big\{S\Big[\Big(\frac{BT}{\pi}\Big)^{1/2}\Big(\frac{1}{2} - \frac{\omega}{B}\Big)\Big] + S\Big[\Big(\frac{BT}{\pi}\Big)^{1/2}\Big(\frac{1}{2} + \frac{\omega}{B}\Big)\Big]\Big\}^2\,.$$

We now consider the behavior of Eq. (117) for large but finite values of T, with B fixed. For small arguments of the Fresnel integrals, we can use the series expansions

$$C(z) = \sum_{n=0}^{\infty} \frac{(-1)^n(\pi/2)^{2n}}{(2n)!(4n + 1)}z^{4n+1}\,, \tag{118}$$

$$S(z) = \sum_{n=0}^{\infty} \frac{(-1)^n(\pi/2)^{2n+1}}{(2n + 1)!(4n + 3)}z^{4n+3}\,, \tag{119}$$

which converge for all finite values of z. From Eqs. (118) and (119), we see the following: if z is real with $z^4 < (8/\pi^2)m(2m-1)(4m+1)/(4m-3)$ and $z^4 < (8/\pi^2)m(2m+1)(4m+3)/(4m-1)$, respectively, then keeping only the first m terms gives an error with the same sign as and bounded in magnitude by the mth term.

For large arguments, we use

$$C(z) = \frac{1}{2} + f(z)\sin\left(\frac{1}{2}\pi z^2\right) - g(z)\cos\left(\frac{1}{2}\pi z^2\right),\tag{120}$$

$$S(z) = \frac{1}{2} - f(z)\cos\left(\frac{1}{2}\pi z^2\right) - g(z)\sin\left(\frac{1}{2}\pi z^2\right),\tag{121}$$

with the asymptotic expansions

$$f(z) \sim \frac{1}{\pi z} \sum_{m=0}^{\infty} (-1)^m \frac{\left(\frac{1}{2}\right)_{2m}}{(\pi z^2/2)^{2m}},\tag{122}$$

$$g(z) \sim \frac{1}{\pi z} \sum_{m=0}^{\infty} (-1)^m \frac{\left(\frac{1}{2}\right)_{2m+1}}{(\pi z^2/2)^{2m+1}},\tag{123}$$

as $z \to \infty$. Here, $(\alpha)_0 = 1$ and $(\alpha)_n = \alpha(\alpha + 1)(\alpha + 2)\cdots(\alpha + n - 1)$, $n = 1, 2, 3, \ldots$. When z is a positive real number, truncation of Eqs. (122) and (123) gives an error with the same sign as and bounded in magnitude by the first neglected terms [23]. This property of the remainder terms is used below.

Now, $\mathcal{G}_{\pm}(\omega) = \mathcal{G}_{\pm}(-\omega)$, so consider the region $\omega/B \geq 0$. If $1/2 - \omega/B \gg \sqrt{\pi/BT}$ for some large, finite value of T, then

$$\frac{B}{2\pi}|\mathcal{G}_{\pm}(\omega)|^2 = \frac{c_{-3}}{(BT)^3} + \frac{c_{-2}}{(BT)^2} + \frac{c_{-3/2}}{(BT)^{3/2}} + \frac{c_{-1}}{BT} + \frac{c_{-1/2}}{(BT)^{1/2}} + 1,\tag{124}$$

where the coefficients $c_i = c_i(B, T, \omega)$ are

$$c_{-3} = \frac{64\eta_2^2}{\pi(1 - 4\hat{\omega}^2)^6}\left(1 + 60\hat{\omega}^2 + 240\hat{\omega}^4 + 64\hat{\omega}^6 + (1 - 4\hat{\omega}^2)^3\cos(\omega T)\right),\tag{125}$$

$$c_{-2} = -\frac{128\eta_1\eta_2}{\pi(1 - 4\hat{\omega}^2)^3}\hat{\omega}\sin(\omega T),\tag{126}$$

$$c_{-3/2} = -\frac{\eta_2}{\sqrt{\pi}\hat{\omega}_-^3}\left(\cos(BT\hat{\omega}_-^2/2) + \sin(BT\hat{\omega}_-^2/2)\right)$$
$$-\frac{\eta_2}{\sqrt{\pi}\hat{\omega}_+^3}\left(\cos(BT\hat{\omega}_+^2/2) + \sin(BT\hat{\omega}_+^2/2)\right),\tag{127}$$

$$c_{-1} = \frac{4\eta_1^2}{\pi(1 - 4\hat{\omega}^2)^2}\left(1 + 4\hat{\omega}^2 + (1 - 4\hat{\omega}^2)\cos(\omega T)\right),\tag{128}$$

$$c_{-1/2} = -\frac{\eta_1}{\sqrt{\pi}\hat{\omega}_-}\left(\sin(BT\hat{\omega}_-^2/2) - \cos(BT\hat{\omega}_-^2/2)\right)$$
$$-\frac{\eta_1}{\sqrt{\pi}\hat{\omega}_+}\left(\sin(BT\hat{\omega}_+^2/2) - \sin(BT\hat{\omega}_+^2/2)\right).\tag{129}$$

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Here and below, $\hat\omega = \omega/B$, $\hat\omega_+ = \omega/B + 1/2$, $\hat\omega_- = 1/2 - \omega/B$, and $0 \le \eta_1, \eta_2, \xi_1, \xi_2 < 1$.

If ω/B is in the neighborhood of $1/2$, namely, $|\omega/B - 1/2| \ll \sqrt{\pi/BT}$, then

$$\frac{B}{2\pi}|\mathcal{G}_\pm(\omega)|^2 = \frac{c_{-3}}{(BT)^3} + \frac{c_{-3/2}}{(BT)^{3/2}} + \frac{c_{-1}}{BT} + \frac{c_{-1/2}}{(BT)^{1/2}} + c_0 \,, \tag{130}$$

where the coefficients are

$$c_{-3} = \frac{32\eta_2^2}{\pi(1 + 2\hat\omega)^6} \,, \tag{131}$$

$$c_{-3/2} = -\frac{\eta_2}{6\sqrt{\pi}\hat\omega_+^3}\left(3(1 + 2\xi_1\sqrt{BT/\pi}\hat\omega_-)\cos(BT\hat\omega_+^2/2)\right.$$
$$\left. + (3 + \pi\xi_2(\sqrt{BT/\pi}\hat\omega_-)^3)\sin(BT\hat\omega_+^2/2)\right) \,, \tag{132}$$

$$c_{-1} = \frac{32\eta_1^2}{\pi(1 + 2\hat\omega)^2} \,, \tag{133}$$

$$c_{-1/2} = \frac{\eta_1}{6\sqrt{\pi}\hat\omega_+}\left(3(1 + 2\xi_1\sqrt{BT/2}\hat\omega_-)\sin(BT\hat\omega_+^2/2)\right.$$
$$\left. - (3 + \pi\xi_2(\sqrt{BT/2}\hat\omega_-)^3)\cos(BT\hat\omega_+^2/2)\right) \,, \tag{134}$$

$$c_0 = \frac{1}{4} + \frac{\xi_1\sqrt{BT}\hat\omega_-}{2\sqrt{\pi}}(1 + \xi_1\sqrt{BT/\pi}\hat\omega_-) + \frac{\pi\xi_2}{72}(\sqrt{BT/\pi}\hat\omega_-)^3(6 + \pi\xi_2(\sqrt{BT/\pi}\hat\omega_-)^3) \,. \tag{135}$$

Here, the observation following Eq. (119) has been used.

In the region $\omega/B \ge 1/2$, if $\omega/B - 1/2 \gg \sqrt{\pi/BT}$, then

$$\frac{B}{2\pi}|\mathcal{G}_\pm(\omega)|^2 = \frac{c_{-3}}{(BT)^3} + \frac{c_{-2}}{(BT)^2} + \frac{c_{-1}}{BT} \,, \tag{136}$$

where

$$c_{-3} = \frac{64\eta_2^2}{\pi(1 - 4\hat\omega^2)^6}\left(1 + 60\hat\omega^2 + 240\hat\omega^4 + 64\hat\omega^6 + (1 - 4\hat\omega^2)^3\cos(\omega T)\right), \tag{137}$$

$$c_{-2} = -\frac{128\eta_1\eta_2}{\pi(1 - 4\hat\omega^2)^3}\hat\omega\sin(\omega T) \,, \tag{138}$$

$$c_{-1} = \frac{4\eta_1^2}{\pi(1 - 4\hat\omega^2)^2}\left(1 + 4\hat\omega^2 + (1 - 4\hat\omega^2)\cos(\omega T)\right) \,. \tag{139}$$

Eqs. (124)–(139) show that $|\mathcal{G}_\pm(\omega)|$ converges to the low-pass filter $\sqrt{2\pi}\text{rect}(\omega/B)/\sqrt{B}$ as $T \to \infty$, with rigorously bounded corrections scaling as $1/\sqrt{T}$ and $1/\omega$. In more detail, Eq. (124) shows that at low frequencies the magnitude is constant, up to corrections given explicitly in Eqs. (125)–(129). Likewise, the behaviour in the transition region is given by Eqs. (130)–(135). Finally, Eq. (136) shows that in the tail the magnitude is zero, up to corrections given explicitly in Eqs. (137)–(139).

C Example X Gate

Section 4.2 describes methods for implementing X rotations, Z rotations, and controlled-phase gates through the variation of the configuration of the potential wells. In this appendix, we give a concrete example showing how one can implement an X rotation by π (that is, a Pauli X gate) by varying the barrier height of a double-well potential.

Specifically, we use the potential

$$V(x) = \frac{V_1}{\cosh^2(x)} + \frac{V_2}{1 + g\cosh^2(x)} + \frac{V_3}{(1 + g\cosh^2(x))^2}, \tag{140}$$

where

$$V_1 = \frac{g(g+2)}{4(1+g)^2}, \quad V_2 = -4b^2(g+2), \quad V_3 = 4b(b+1)(1+g). \tag{141}$$

If $b > 0$ and $b > \frac{g}{2(1+g)} + 1$, then this is *quasi-exactly solvable* [24], a term meaning that a subset of the spectrum is exactly solvable. The ground and first excited energies are then (in units where $\hbar = 2m = 1$)

$$E_1 = -\frac{(2 + g - 4b(1+g))^2}{4(1+g)^2}, \tag{142}$$

$$E_2 = -\frac{(2 + 3g - 4b(1+g))^2}{4(1+g)^2}. \tag{143}$$

If we lower the barrier and raise it back to its original height with a time dependence that is in a Gevrey class of some finite order, then we can invoke the adiabatic theorem of [19], which guarantees exponential convergence to perfect adiabaticity as a function of the slowness of the variation (§ 4.2). In this case, up to exponentially small errors, the dynamics induced by the variation is described by the 2×2 adiabatic-frame Hamiltonian H_A given in Eq. (60). The off-diagonal matrix elements of H_A are precisely zero here because the ground state is an even function of x, the first excited state is an odd function of x, and $\frac{dH}{dt}$ has $x \to -x$ symmetry. Thus the unitary transformation induced is

$$U = \exp\left(\int dt \begin{bmatrix} E_1(t) & 0 \\ 0 & E_2(t) \end{bmatrix}\right) = e^{i\alpha} \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}, \tag{144}$$

where

$$\alpha = \int_0^\tau dt\, E_1(t), \tag{145}$$

$$\phi = \int_0^\tau dt\, (E_2(t) - E_1(t)). \tag{146}$$

Thus, up to an irrelevant global phase α, U is a Z gate if $\phi = \pi$.

Concretely, we can achieve this as follows. Let $B(s)$ be the bump function

$$B(s) = \begin{cases} \exp\left(-\frac{1}{s(1-s)}\right), & 0 < s < 1, \\ 0, & \text{otherwise.} \end{cases} \tag{147}$$

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This is in the Gevrey class of order 2. One can vary the barrier height in time by setting

$$b(t/\tau) = 1 + \beta B(t/\tau) \tag{148}$$

for some choices of β and τ. For example, one numerically finds that by choosing $g = 0.01$, $\beta = 50$, and $\tau = 96.1602$, one obtains $\phi = \pi$. Thus, this choice of parameters achieves a Z gate in the eigenbasis of the double well, which is an X gate, if we interpret occupation of the left (right) well as logical zero (one).

D   Example Z Gate

The Z gate can be analyzed in the limit in which the double-well potential becomes two separate wells. Consider the convenient exactly solvable example in which each well is a special case of the hyperbolic Poschl-Teller potential [25] (and the Rosen-Morse potential [26]), namely,

$$V(x) = -\alpha^2 \frac{\lambda(\lambda - 1)}{\cosh^2(\alpha x)}, \tag{149}$$

in units where $\hbar = m = 1$. For $\lambda > 1$ this is an attractive potential well, and its ground-state energy is

$$E_0 = -\alpha^2(\lambda - 1)^2. \tag{150}$$

If we temporarily increase the well depth α^2 for the logical-one well, then this induces a Pauli Z rotation $e^{iZ\theta}$, for some angle θ. In particular, $\theta = \pi$ corresponds to a standard Z gate.

Concretely, we can vary α^2 according to

$$\alpha^2(t) = \alpha_0^2(1 + \beta B(t/\tau)), \tag{151}$$

where B is the bump function given in Eq. (147), α_0^2 is the initial well depth, and β is a parameter we choose. As we make the process slower by increasing τ, the diabatic error amplitudes vanish as $\exp\left[-\tau^{1/3}\right]$ (§ 4.2). To achieve a fixed target phase θ as we increase τ, we must correspondingly decrease β. Specifically, a brief calculation yields

$$\beta = -\frac{\theta}{(\lambda - 1)^2 \tau \alpha_0^2 \eta}, \tag{152}$$

where

$$\eta = \int_0^1 ds \exp\left[-\frac{1}{s(1-s)}\right] \simeq 7.0299 \times 10^{-3}. \tag{153}$$

In reality, the wells will not be infinitely separated. The corrections to the above analysis, in which we have assumed the wells to be perfectly isolated, are of the order of the inner product between the ground states of the two wells. The Poschl-Teller potential well is well localized: for $|x| \gg 1/\alpha$, $V(x) \simeq 0$. Consequently, in the outer region $|x| \gg 1/\alpha$, the ground-state wavefunction decays as $\exp[-\sqrt{-2mE_0}x]$ (where we have now included explicit dependence on m but kept $\hbar = 1$). Thus the above approximation becomes exponentially good as the separation between wells is increased.

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