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Quantum computing for quantum tunneling

Steven Abel*

*Institute for Particle Physics Phenomenology, and Department of Mathematical Sciences,
Durham University, Durham DH1 3LE, United Kingdom*

Nicholas Chancellor[†]

*Department of Physics and Durham Newcastle Joint Quantum Centre Durham University,
South Road, Durham DH1 3LE, United Kingdom*

Michael Spannowsky[‡]

*Institute for Particle Physics Phenomenology, Department of Physics, Durham University,
Durham DH1 3LE, United Kingdom*



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We demonstrate how quantum field theory problems can be practically encoded by using a discretization of the field theory problem into a general Ising model, with the continuous field values being encoded into Ising spin chains. To illustrate the method, and as a simple proof of principle, we use a (hybrid) quantum annealer to recover the correct profile of the thin-wall tunnelling solution. This method is applicable to many nonperturbative problems.

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I. INTRODUCTION

There has been increasing interest in the possibility of simulating quantum field theory (QFT) on quantum computers [1], with the development of efficient algorithms to compute scattering probabilities in simple theories of scalars and fermions [2–17]. In particular it is known that by latticizing field theories, quantum computers should be able to compute scattering probabilities in QFTs with a run time that is polynomial in the desired precision, and in principle to a precision that is not bounded by the limits of perturbation theory. However a particularly difficult aspect of this programme is the preparation of scattering states [4–6,8,9,14–17], with several works having proposed a hybrid classical/quantum approach to solving this problem [11,17–19]. A complementary approach is to map field theory equations to discrete quantum walks [20–23] which can be simulated on a universal quantum computer.

Certain nonperturbative quantum processes do not suffer from this difficulty, and lend themselves much more readily to study on quantum computers in the short term.

These include the tunneling and related processes, which are of fundamental importance for the explanation of quantum mechanical and quantum field theoretical phenomena, for example transmission rates of electron microscopes, first-order phase transitions during baryogenesis, or the potential initiation of stochastic gravitational wave spectra in the early Universe and many more.

Typically in tunneling, the system begins in a false vacuum state that is nondynamical and virtually trivial. The initial state can be very long lived, with tunneling to a lower “true” vacuum state taking place via nonperturbative instanton configurations. The objective of this work is to demonstrate how a field theory problem can be successfully encoded on a quantum spin device, by studying the classic problem of obtaining such tunneling instanton solution for a system stuck in a metastable minimum (a.k.a. false vacuum).

II. SETUP OF A SIMPLE PROBLEM

A useful potential to focus on is the following quartic one:

$$V(\phi) = \frac{\lambda}{8}(\phi^2 - a^2)^2 + \frac{\epsilon}{2a}(\phi - a). \quad (1)$$

It is convenient to henceforth remove the extraneous constant term by working with $U(\phi) = V(\phi) - V(\phi_+)$, which has $U(\phi_+) = 0$. The resulting potential is shown in Fig. 1. On the left we show the “thick-wall” regime where ϵ is large. This limit is when the barrier is close to

*s.a.abel@durham.ac.uk

†nicholas.chancellor@gmail.com

‡michael.spannowsky@durham.ac.uk

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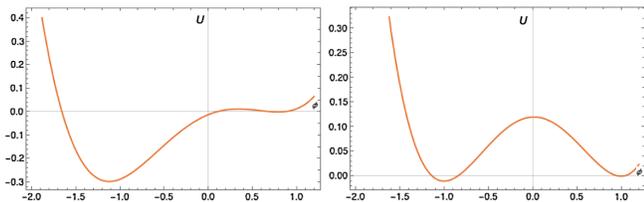


FIG. 1. The thick-wall potential in the left panel (with $\epsilon = 0.3$, and true and false minima at $\phi_- = -1.12542$ and $\phi_+ = 0.786483$ respectively), and the thin-wall potential in the right panel (with $\epsilon = 0.01$).

disappearing (or has disappeared altogether) and the walls become comparable in size to the bubble itself. For numerics we choose $a = \lambda = 1$ and $\epsilon = 0.3$. The opposite “thin-wall” regime (for which we choose $\epsilon = 0.01$) is the limit in which ϵ is small and is approximately the difference in vacuum energy density between the false and true minima.

We are interested in the situation where the system starts in the false vacuum, and our objective is to determine the rate per unit volume of tunneling out of it. Using the well-known technique of [24–27], the bubble profile is given by finding a “bounce solution” to the following differential equation:

$$\frac{d^2\phi}{d\rho^2} + \frac{c}{\rho} \frac{d\phi}{d\rho} = \frac{\partial U}{\partial \phi}, \quad (2)$$

where in four dimensions, c takes the value 2 or 3 for a finite temperature $O(3)$ symmetric bubble, or a purely quantum tunneling $O(4)$ symmetric instanton, respectively, and where ρ is the radial coordinate of the solution. The required “bounce” is subject to the boundary condition that $d\phi/d\rho = 0$ as $\rho \rightarrow 0, \infty$, which determines the starting value $\phi(0)$, which is the field-value at the centre of the radially symmetric bubble or instanton (also called the escape-point). The resulting $\phi(\rho)$ profile for our particular choice of parameters is shown in Fig. 2.

Once such a solution is determined, the tunneling rate per unit volume can be estimated from its classical action:

$$\Gamma_4 \sim e^{-S_4[\phi]}; \quad \Gamma_3 \sim T e^{-S_3[\phi]/T}, \quad (3)$$

respectively.

The action can be expressed in simple analytic terms in the two limits. In the thick wall limit the bounce action can be accurately approximated by expanding around the value $\epsilon = \epsilon_0$, above which the barrier disappears (i.e., when the discriminant vanishes), which gives a cubic potential about the false vacuum. This critical value corresponds to $\epsilon_0 = 2\lambda a^4/3\sqrt{3}$. Then following the rescaling procedure of [27], the tunneling actions for the $O(4)$ and $O(3)$ symmetric solutions can be written in terms of standard actions $S_4^0 = 91$ and $S_3^0 = 19.4$:

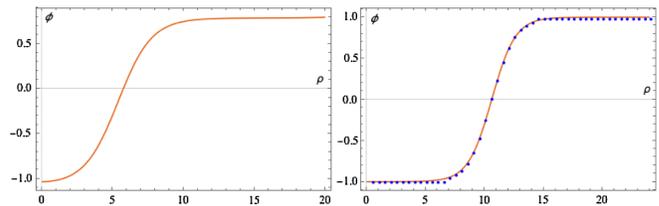


FIG. 2. Solutions for the thick- and thin-wall potentials. Note that in the thick-wall case the solution has to start away from the minimum due to the friction term (in this case $\phi_e = -1.03488$). The thin-wall solution computed using the hybrid quantum-classical techniques as discussed later is overlaid on the right panel.

$$S_4 = \frac{3\rho}{\lambda} S_4^0; \quad S_3 = \frac{3a\rho^{3/2}}{\lambda^{1/2}} S_3^0. \quad (4)$$

The thin-wall regime is somewhat easier to study numerically, and semianalytically the actions can be expressed in terms of the action S_1 for the one-dimensional $c = 0$ problem¹:

$$S_4 = \frac{27\pi^2 S_1^4}{2\epsilon^3}; \quad S_3 = \frac{16\pi^3 S_1^3}{3\epsilon^2}. \quad (5)$$

As we stated in the Introduction, the point of our study is not to find these classical instanton solutions for the tunneling *per se*, which are well known, but rather to demonstrate that the corresponding field-theory configuration can be suitably encoded onto a quantum spin system, for example a quantum annealer. Once we have established this as a working principle, one could even envisage testing for the above behavior directly. Therefore we will in what follows focus on using a quantum device to recover the simple $c = 0$ solution required for the thin-wall regime, as a proof of principle. We will therefore set ourselves the task of minimizing the corresponding action integral,

$$S_1 = \int_0^\infty d\rho \frac{1}{2} \dot{\phi}^2 + U(\phi), \quad (6)$$

which should yield a solution of the form shown in Fig. 2(b).

III. ENCODING THE FIELD THEORY

Let us start with the central problem, which is how to formulate a continuous scalar field theory on a quantum spin system. For this study we will make use of quantum annealers which are a convenient device that is available at the time of writing. But the same method can be used on

¹This is also the energy of the physical “domain wall” solution, but for reasons that will become apparent it would be confusing to use this terminology.

any device that can encode and optimize a generalized Ising model.

A quantum annealer in particular is based on the adiabatic theorem of quantum mechanics, which implies that a physical system will remain in the ground state if a given perturbation acts slowly enough, and if there is a gap between the ground state and the rest of the system's energy spectrum [28].

The crucial form of the Hamiltonian that we are interested in, and that is represented on a quantum annealer is that of a general Ising model, in addition to a time-dependent transverse field:

$$\mathcal{H}_{\text{QA}}(t) = \sum_i \sum_j J_{ij} \sigma_i^Z \sigma_j^Z + \sum_i h_i \sigma_i^Z + \Delta(t) \sum_i \sigma_i^X, \quad (7)$$

where $\sigma_i^Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ ($\sigma^Z|0\rangle = |0\rangle$, $\sigma^Z|1\rangle = -|1\rangle$) is the Pauli Z operator, with the subscript indicating which spin it acts upon, and σ^X is its friend pointing in the X -direction. The gradual decrease of $\Delta(t) \rightarrow 0$ from a large value should drive the system into the ground state of the time-independent part of the Hamiltonian, and this is where we will put the field theory:

$$\mathcal{H} = \sum_i \sum_j J_{ij} \sigma_i^Z \sigma_j^Z + \sum_i h_i \sigma_i^Z. \quad (8)$$

For the annealer to provide a solution to a mathematical problem, e.g., the calculation of $\phi(\rho)$ for Eq. (6), we have to find a mapping such that the expectation value of its Hamiltonian can be identified with its solution, i.e., that it allows in this example to draw a material equivalence:

$$\phi(\rho) \Leftrightarrow \lim_{\Delta(t) \rightarrow 0} \langle \mathcal{H}_{\text{QA}}(t) \rangle, \quad (9)$$

namely that minimizing the Hamiltonian of the quantum annealer, \mathcal{H} , is the same as extremizing the field theory action in ϕ .

It is worth noting that the couplings J_{ij} and h_i could also be adiabatically adjusted in the annealing process, and this could ultimately be used to adjust the potential $U(\phi)$ of a system in the quantum annealer so as to observe tunneling, assuming it can be encoded. We will further split the Hamiltonian into three generic pieces, as

$$\mathcal{H} = \mathcal{H}^{(\text{chain})} + \mathcal{H}^{(\text{QFT})} + \mathcal{H}^{(\text{BC})}. \quad (10)$$

Here, $\mathcal{H}^{(\text{QFT})}$ is the Hamiltonian corresponding to the minimization of the action in Eq. (6) and $\mathcal{H}^{(\text{BC})}$ is a Hamiltonian that we add to enforce the boundary conditions.²

²For a classical neural network-based approach to solving Eq. (2) by treating it as an optimization problem see [29].

However our first task is to encode continuous field values over a continuous domain, with only the discrete Ising model to hand: this is what $\mathcal{H}^{(\text{chain})}$ is for. We begin by splitting the radius variable ρ into $M \gg 1$ discrete values and the field value at the ℓ 'th position into $N \gg 1$ discrete values:

$$\begin{aligned} \rho_\ell &= \ell\nu = \nu \dots M\nu \\ \phi(\rho_\ell) &= \phi_0 + \alpha_\ell \xi = \phi_0 + \xi \dots \phi_0 + N\xi, \end{aligned}$$

where in the present context one might for example take a fiducial value $\phi_0 \approx -a$ and $\xi = 2a/N$, with $M\nu = \Delta\rho$. Thus our Ising interaction J_{ij} is an $(MN) \times (MN)$ matrix, while h_i is an (NM) -vector.

We must now separate those spins in the annealer that correspond to fields at different values of ℓ , effectively splitting J_{ij} and h_i into $N \times N$ sub-blocks. To do this we will utilize the Ising-chain domain wall representation introduced in [30]. That is for every position ℓ we add to the Hamiltonian

$$H_\ell^{(\text{chain})} = -\Lambda \left(\sum_{j=1}^{N-1} \sigma_{\ell N+j}^Z \sigma_{\ell N+j+1}^Z - \sigma_{\ell N+1}^Z + \sigma_{\ell N+N}^Z \right). \quad (11)$$

As shown in [30], taking Λ to be much larger than every other energy scale in the overall Hamiltonian, these terms will constrain the system to remain in the ground subspace of the Hamiltonian, where exactly one spin position, α_ℓ say, is frustrated for each ℓ . These states are of the form

$$|11\dots 100\dots 0\rangle_\ell \Rightarrow \phi(\rho_\ell) = \phi_0 + \alpha_\ell \xi, \quad (12)$$

where in the above the discretized field value is represented by the position α_ℓ of the frustrated domain wall. Conversely the field value at the ℓ 'th position can be found by making the measurement

$$\phi(\rho_\ell) = \frac{1}{2} \sum_{j=1}^{N-1} (\phi_0 + j\xi) \langle \sigma_{\ell N+j+1}^Z - \sigma_{\ell N+j}^Z \rangle, \quad (13)$$

which only receives a contribution from frustrated spin position with $j = \alpha_\ell$. For later, it is useful to note that this is equivalent to

$$\phi(\rho_\ell) = \phi_0 + \frac{N\xi}{2} - \frac{\xi}{2} \sum_{j=1}^N \langle \sigma_{\ell N+j}^Z \rangle. \quad (14)$$

In terms of J_{ij} and h_i , adding the full set of Ising-chain Hamiltonians given by Eq. (11) corresponds to

V. IMPLEMENTATION ON A QUANTUM SPIN DEVICE AS A GENERAL ISING MODEL

In Sec. III we have devised a method which encodes the problem of finding a solution to a quantum field theoretical problem, i.e., of finding a solution to Eq. (6), into finding the ground state of the Hamiltonian of an Ising model. The latter can then be given an interpretation as the solution to Eq. (6) through Eq. (12), for each ρ_l with $l \in [1, \dots, M]$. To show that our approach is valid and converges to the correct solution $\phi(\rho)$, we now implement the method onto various annealing samplers, as provided by D-Wave [33].

As discussed quantum annealers [28,34] perform continuous time quantum computations in Ising systems, so they are extremely well-suited to the problem at hand (although our discussion could ultimately be adapted to gate-model quantum computers as well) [35–47]. In contrast with the quantum-gate devices, they are already quite large, 2048 qubits in the current generation, with work ongoing to develop much more connected 5,000 qubit machines. D-Wave devices have been able successfully to simulate condensed matter systems, sometimes showing advantages over classical counterparts [48–50].

The quantum states are characterized by NM -tuples of the form $|11\dots100\dots0\rangle$ and the Hilbert space of the Ising model is therefore 2^{NM} dimensional. Sampling such a large vector space classically, with an exact sampler, while calculating the expectation value $\langle \mathcal{H} \rangle$ for each state quickly becomes a computationally prohibitive task for $NM \gg 20$. Conversely, a discretization with $NM \lesssim 20$ cannot give a reasonable approximation for the derivatives of Eq. (19).

Yet, not unlike protein-folding, in which a unique ground state is selected from an estimated number of 3^{300} so-called conformations within microseconds (known as Levinthal's paradox [51]), a quantum annealer can in principle find a ground state of a Hamiltonian acting on a highly complex Hilbert space on a similar time scale, assuming there is a gap between the ground state and the other states of the system.

While the next generation of annealing processors will have approximately 5,000 qubits, they will have limited connectivity [52]. Therefore in order to accommodate the more general Ising model required for our encoding, we resorted to a hybrid asynchronous decomposition sampler

(the Kerberos solver [53–55]), which can solve problems of complex structure and size. To find the ground state efficiently, it applies in parallel classical tabu search algorithms, simulated annealing and D-Wave subproblem sampling on variables that have high-energy impact. Using this method we calculate the solution $\phi(\rho)$ to Eq. (6) for $N = M = 50$ in Fig. 2(b). We observe that the discretized field theory has minimized at the expected tunneling solution, and the field theory and its Hamiltonian are successfully encoded in the Ising model.

VI. CONCLUSION

We conclude that near-term applications of quantum devices already allow the implementation of a wide class of scalar field theories. By encoding them as an Ising model, as described in Sec. III, we have been able to find tunneling solutions on a D-Wave quantum annealer, which match very precisely with the classical instanton solution. It is important to appreciate that our end result is essentially an experimental one: it is a genuine field theory relaxing to the predicted solution. Thus the method is a novel, highly flexible and possibly transformative way to probe non-perturbative aspects of a wide class of field theories.

Our method has the potential to consider theories and processes that are not easy to simulate and cannot be treated analytically either. The variety of theory that can be studied in this laboratory appears to be limited mainly by the number and connectivity of the qubits in the generalized Ising model. For example the Ising encoding of fermions and of gauge theories is a longstanding topic (see for example [56,57]). It is important to realize that these encodings represent genuine condensed matter field theories constructed from a set of aligned quantum spins. In this sense although the toy problem discussed here is an optimization that can be done classically, depending on the set-up these configurations can be morally different from a simulation. For example the system can support actual dynamical quantum tunneling rather than a simulation of it [58].

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