Experimental Demonstration of Quantum Tunneling in IBM Quantum Computer

Narendra N. Hegade[1 ¶], Bikash K. Behera[2¶], Prasanta K. Panigrahi[2]
[1] Department of Physics, National Institute of Technology Silchar, Silchar 788010, India
[2] Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, West Bengal, India

According to Feynman, we should make nature to be quantum mechanical to simulate it better. Simulating quantum systems in a computer had been remained a challenging problem to tackle. It's mainly in case of a large quantum system. However, Feynman's 1982 conjecture [1] that 'physics can be simulated using a quantum computer other than using a Turing machine or a classical computer' has been proved to be correct [2]. It is widely known that quantum computers have superior power as compared to classical computers in simulating quantum systems efficiently. Here we report the experimental realization of quantum tunneling through potential barriers by simulating it in the IBM quantum computer, which here acts as a universal quantum simulator. We take a two-qubit system for visualizing the tunneling process, which has a truly quantum nature. We clearly observe the tunneling through a barrier by our experimental results. This experiment inspires us to simulate other quantum mechanical problems which possess such quantum nature.

Quantum simulation is one of the problems that a quantum computer could perform more efficiently than a classical computer as it provides significant improvement in computational resources [2–10]. It has been applied in a wide range of areas of physics like quantum many-body theory [11–14], quantum entanglement [15, 16], quantum phase transitions [17, 18] and molecular physics [19–23] etc. Algorithms have been used in simulating many quantum field theory problems where Hamiltonian of the system [24–39] splits into kinetic and potential energy operators which are then simulated using Trotter's formula [40, 41]. Experimental realizations of quantum simulations have already been made in systems like NMR [11–13, 16, 21, 42–44], ion-trap [45–49], atomic [17, 50] and photonic [51, 52] quantum computers. The current status of this field can be found out from these review papers [53–58].

Quantum tunneling acts as one of the exciting phenomena and the unique fundamental phenomena in quantum mechanics. It has been observed in superconducting Cooper pairs [59]. It has also been utilized in modern technologies [60, 61]. Important science puzzles like lattice quantum chromodynamics can be solved using this tunneling simulation approach. This type of simulation has remained untested in a quantum computer due to the requirement of large number of ancillary qubits and quantum gates. Recently, an algorithm proposed by Sornborger [62] illustrates the simulation by using no ancillary qubits and a small number of quantum gates which motivates the possibility of simulating in today's quantum computer consisting of few qubits. Feng *et al.* [63] have demonstrated the tunneling effect using NMR. Ostrowski [64] has also explicated this process and calculated the transmission and reflection coefficients for the Gaussian wave packet scattered on a rectangular potential. Here, in the present work, we illustrate the simulation using IBM's 5-qubit quantum computer. Using only two qubits and a set of Hadamard and controlled phase gates, we were able to simulate the tunneling process in a double well potential for a single particle.

Quantum Tunneling

The Schrödinger's equation, for a single particle moving in a square well potential in one-dimensional space, is expressed as

$$i\frac{\partial}{\partial t}|\psi(x,t)\rangle = \hat{H}|\psi(x,t)\rangle \tag{1}$$

Here $\hat{H} = \hat{K} + \hat{V}$, where $\hat{K}$ and $\hat{V}$ are kinetic and potential energy operators respectively.

The time evolution for the wave function of the system is given as

$$\begin{aligned} |\psi(x,t+\Delta t)\rangle = &\ e^{-i\hat{H}t}|\psi(x,t)\rangle \\ = &\ e^{-i(\hat{K}+\hat{V})t}|\psi(x,t)\rangle \end{aligned} \tag{2}$$

For digital quantum simulation [65], we discretize the space on a lattice (with spacing Δl) within the boundary region ($0 < x < L$) with a periodic boundary condition $\psi(x+L,t) = \psi(x,t)$. The wave function can be interpreted in terms of n-qubit register as

$$|\psi(x,t)\rangle \rightarrow \sum_{k=0}^{2^n-1} \psi(x_k,t)|k\rangle \tag{3}$$

Here $|k\rangle$ represents the particle location corresponding to binary number k, and $x_k = (k+\frac{1}{2})\Delta l$, $\Delta l = \frac{L}{2^n}$.

¶These authors have contributed equally.

Using second-order Suzuki-Trotter's formula [66–68], the exponential operator can be decomposed as

$$e^{-i(\hat{K}+\hat{V})\Delta t} = e^{-i\frac{\hat{V}}{2}\Delta t}e^{-i\hat{K}\Delta t}e^{-i\frac{\hat{V}}{2}\Delta t} + O(\Delta t^3) \quad (4)$$

After the quantum Fourier transform, the time evolution takes the following form,

$$e^{-i(\hat{K}+\hat{V})\Delta t} = e^{-i\frac{\hat{V}}{2}\Delta t}Fe^{-i\hat{K}\Delta t}F^{\dagger}e^{-i\frac{\hat{V}}{2}\Delta t} \quad (5)$$

The equivalent quantum circuit for the Fourier transformation operator F can be realized using a series of Hadamard gates and controlled-phase gates [69].

The quantum circuit for one-time step evolution is shown in Fig. 1. The decomposition of the kinetic energy operator, K and potential energy operator, P are illustrated, where $K = FDF^{\dagger}$, $D = e^{-i\hat{K}\Delta t}$ and $P = e^{-i\frac{\hat{V}}{2}\Delta t}$. Here, the double well potential is implemented by operating P on the second qubit q[1].

$$e^{-iV\Delta t} = I \otimes e^{-iv\sigma_z\Delta t} \otimes I..., \quad (6)$$

In our experiment, we take v=0 and 10 for free particle and particle in double well potential respectively, and we set the time interval $\Delta t = 0.1$. Mass of the particle is taken to be 0.5.

The diagonal operation D can be expressed as a product of operators,

$$D = \Phi_{01}Z_1Z_0 \quad (7)$$

where $Z_0 = e^{-i\gamma c_0\sigma_z^0\Delta t}$, $Z_1 = e^{-i\gamma c_1\sigma_z^1\Delta t}$ and $\phi_{01} = e^{-i\gamma c_2 diag(1,1,1,-1)_{01}\Delta t}$. The constant values in the above expression are obtained to be $\gamma = \frac{\pi^2}{8}$, $c_0 = -1$, $c_1 = -4$ and $c_2 = 4$ [62].

EXPERIMENTAL PROCEDURES AND RESULTS

We investigate two qubit quantum simulation for the tunneling process using the IBM 5 qubit quantum processor ibmqx4 whose layout is depicted in Fig. 2.

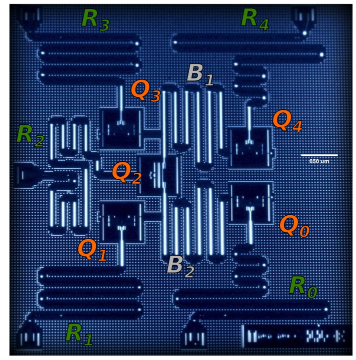

FIG. 2: Two coplanar waveguide (CPW) resonators provide the connectivity between the 5 transmon qubits. For the control and readout of the qubits, a CPW is associated with each qubit.

Qubits	$\omega_i^R/2\pi$ (GHz)	$\omega_i/2\pi$ (GHz)	$\delta_i/2\pi$ (MHz)	$\chi/2\pi$ (kHz)
q[0]	6.52396	5.2461	-330.1	410
q[1]	6.48078	5.3025	-329.7	512
q[2]	6.43875	5.3025	-329.7	408
q[3]	6.58036	5.4317	-327.9	434
q[4]	6.52698	5.1824	-332.5	458

TABLE I: **The table shows some of the parameters of the device ibmqx4.**

The experimental parameters for the device is tabulated in Table I, where ω_i^R, ω_i, δ_i and χ are the resonance frequency, qubit frequency, anharmonicity and qubit-cavity coupling strength for the readout resonator.

The simulation of the quantum tunneling process of the particle is performed on the ibmqx4 chip for 4 time steps, where each step involves the circuit given in Fig. 1. The tunneling process can be clearly observed in Figs. 3 and 4 which explicates the probability distribution of the free particle and the particle in a double well potential in each time step. The particle tunneling through the potential barrier is evident in Fig. 4, where the probability of finding the particle in the barrier is very small. Quantum state tomography (QST) for the initial state and the final state of the particle reveals the comparison between the theoretical and the experimental density matrices. From the graphs shown in Figs. 5 and 6, it is clear that the experimental process is carried out with a high accuracy.

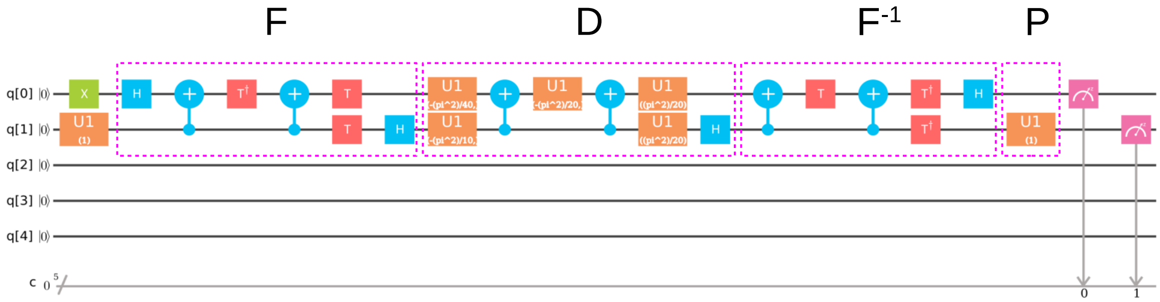

FIG. 1: **The two-qubit quantum circuit for one time step simulation. The quantum circuits for the kinetic ($\mathbf{FDF^{-1}}$) and potential (P) energy operators are depicted.**

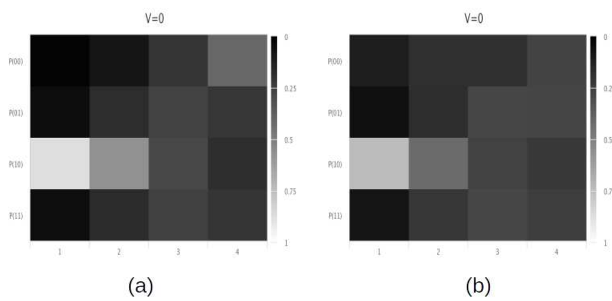

FIG. 3: The figure shows the particle probability distributions for four time steps interval of the free particle (v=0). (a) and (b) are the theoretically calculated and experimentally observed results respectively.

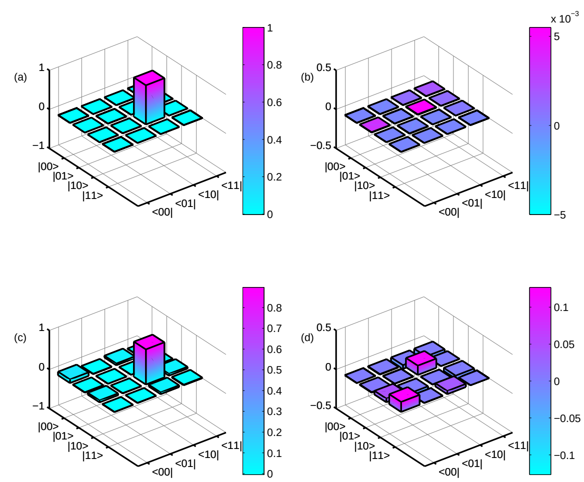

FIG. 5: (a) & (b) are the theoretical real and imaginary parts of the density matrix elements of the $|10\rangle$ state; (c) and (d) are the experimentally reconstructed density matrix elements for the initial $|10\rangle$ state in our two-qubit system.

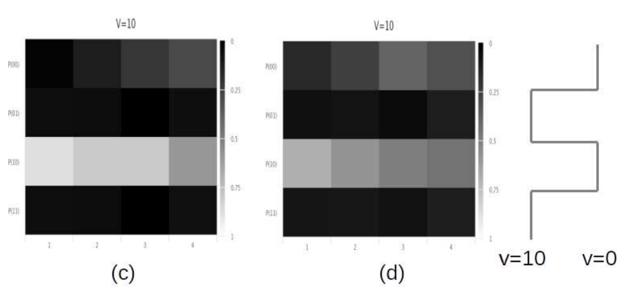

FIG. 4: The figure shows the particle probability distributions for four time steps interval of the particle in double well potential (v = 10). (c) and (d) are the theoretically calculated and experimentally observed results respectively; The two potential wells are at two sites, $|00\rangle$ and $|10\rangle$. After four time steps, the tunneling is clearly shown from $|10\rangle$ to $|00\rangle$.

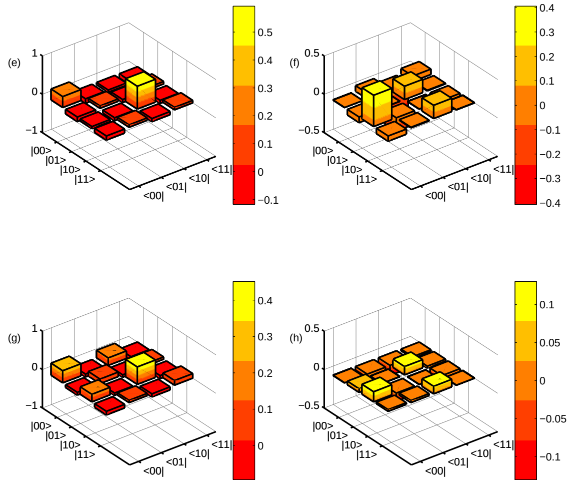

FIG. 6: (e) and (f) are theoretically predicted real and imaginary part of density matrix elements after four time steps of evolution with a double-well potential; (g) and (h) are the experimentally reconstructed density matrix elements after the four time steps in our two qubit-system.

To conclude, we have experimentally demonstrated here the quantum tunneling phenomena of a single particle in a double well potential. We have designed the equivalent quantum circuit for the Hamiltonian of the given system in the real quantum processor ibmqx4. We have shown the architecture of this processor with some device parameters. We have illustrated the tunneling process by running the quantum circuit for four time steps. We have performed quantum state tomography for checking the accuracy of our results. From the experiment, it is observed that the tunneling process is carried out with a high fidelity.

[1] Feynman, R. P. Simulating physics with computers. *Int. J. Theor. Phys.* **21**, 467–488(1982).

[2] Lloyd, S. Universal Quantum Simulators. *Science* **273**, 5278 (1996).

[3] Abrams, D. S., & Lloyd, S. Simulation of many-body Fermi systems on a universal quantum computer. *Phys. Rev. Lett.* **79**, 2586-2589 (1997).

[4] Zalka, C. Simulating quantum systems on a quantum computer. *Proc. R. Soc. Lond. A* **454**, 313-322 (1998).

[5] Berry, D. *et al.* Efficient quantum algorithms for simulating sparse Hamiltonians. *Commun. Math. Phys.* **270**, 359-371 (2007).

[6] Deutsch, D. & Jozsa, R. Rapid solutions of problems by quantum computation. *Proc. R. Soc. Lond. A* **439**, 553 (1992).

[7] Deutsch, D. On the power of quantum computation. *Found. Comput. Sci. 1994 Proc. 35th Annu. Symp.* , 116-123 (1994).

[8] Gerjuoy, E. Shor's factoring algorithm and modern cryptography. An illustration of the capabilities inherent in quantum computers. *Am. J. Phys.* **73**, 523-540 (2005).

[9] Grover, L. K. Quantum Mechanics helps in searching for a needle in a haystack. *Phys. Rev. Lett.* **79**, 325 (1997).

[10] Childs, A. M. *et al.* Exponential algorithmic speedup by quantum walk. *Proc. 35th ACM Symp. Theor. Comput.* , 59-68 (2003).

[11] Tseng, C. H. *et al.* Quantum simulation of a three-body-interaction Hamiltonian on an NMR quantum computer. *Phys. Rev. A* **61**, 012302 (1999).

[12] Negrevergne, C. *et al.* Liquid-state NMR simulations of quantum many-body problems. *Phys. Rev. A* **71**, 032344 (2005).

[13] Peng, X. H., Zhang, J. F., Du, J. F. & Suter, D. Quantum simulation of a system with competing two- and three-body interactions. *Phys. Rev. Lett.* **103**, 140501 (2009).

[14] Peng, G. R., Xu, G. F. & Long, G. L. Experimental realization of nonadiabatic holonomic quantum computation. *Phys. Rev. Lett.* **110**, 190501 (2013).

[15] Zhang, J. F., Wei, T. C. & Laflamme, R. Experimental quantum simulation of entanglement in many-body systems. *Phys. Rev. Lett.* **107**, 010501 (2011).

[16] Peng, X. H., Du, J. F. & Suter, D. Quantum phase transition of ground-state entanglement in a Heisenberg spin chain simulated in an NMR quantum computer. *Phys. Rev. A* **71**, 012307 (2005).

[17] Edwards, E. E. *et al.* Quantum simulation and phase diagram of the transverse-field Ising model with three atomic spins. *Phys. Rev. B* **82**, 060412 (2010).

[18] Zhang, J. F. *et al.* Direct observation of quantum criticality in Ising spin chains. *Phys. Rev. A* **79**, 012305 (2009).

[19] Aspuru-Guzik, A., Dutoi, A. D., Love, P. J. & Head-Gordon, M. Simulated quantum computation of molecular energies. *Science* **309**, 5741 (2005).

[20] Lanyon, B. P., *et al.* Towards quantum chemistry on a quantum computer. *Nat. Chem.* **2**, 106 (2010).

[21] Du, J. F., *et al.* NMR implementation of a molecular hydrogen quantum simulation with adiabatic state preparation. *Phys. Rev. Lett.* **104**, 030502 (2010).

[22] Kassal, I., Whitfield, J. D., Perdomo-Ortiz, A., Yung, M. H. & Aspuru-Guzik, A. Simulating Chemistry using Quantum Computers. *arXiv preprint arXiv:1007.2648* , (2010).

[23] Yung, M. H., Whitfield, J. D., Boixo, S., Tempel, D. G. & Aspuru-Guzik, A. Introduction to quantum algorithms for physics and chemistry. *arXiv preprint arXiv:1203.1331* , (2012).

[24] Büchler, H. P. *et al.* Atomic quantum simulator for lattice gauge theories and ring exchange models. *Phys. Rev. Lett.* **95**, 040402 (2005).

[25] Zohar, E. & Reznik, B. Confinement and lattice quantum-electrodynamic electric flux tubes simulated with ultracold atoms. *Phys. Rev. Lett.* **107**, 275301 (2011).

[26] Szirmai, G. *et al.* Gauge fields emerging from time reversal symmetry breaking for spin-5/2 fermions in a honeycomb lattice. *Phys. Rev. A* **84**, 011611(R) (2011).

[27] Cirac, J. I. *et al.* Cold atom simulation of interacting relativistic quantum field theories. *Phys. Rev. Lett.* **105**, 190403 (2010).

[28] Cirac, L. *et al.* An optical-lattice-based quantum simu-

lator for relativistic field theories and topological insulators. *New J. Phys.* **14**, 015007 (2012).
[29] Kapit, E. & Mueller, E. Optical-lattice Hamiltonians for relativistic quantum electrodynamics. *Phys. Rev. A* **83**, 033625 (2011).
[30] Bermudez, A. *et al.* Wilson fermions and axion electrodynamics in optical lattices. *Phys. Rev. Lett.* **105**, 190404 (2010).
[31] Bermudez, P. & Pachos, J. K. Yang-Mills gauge theories from simple fermionic lattice models. *Phys. Lett. A* **373**, 2542 (2009).
[32] Lepori, L. *et al.* (3+1) massive Dirac fermions with ultracold atoms in frustrated cubic optical lattices. *Euro. Phys. Lett.* **92**, 50003 (2010).
[33] Maeda, K. *et al.* Simulating dense QCD matter with ultracold atomic boson-fermion mixtures. *Phys. Rev. Lett.* **103**, 085301 (2009).
[34] Rapp, À. *et al.* Color superfluidity and baryon formation in ultracold fermions. *Phys. Rev. Lett.* **98**, 160405 (2007).
[35] Weimer, H. *et al.* A Rydberg quantum simulator. *Nat. Phys.* **6**, 382 (2010).
[36] Casanova, J. *et al.* Quantum simulation of quantum field theories in trapped ions. *Phys. Rev. Lett.* **107**, 260501 (2011).
[37] Doucot, B. *et al.* Discrete non-Abelian gauge theories in Josephson junction arrays and quantum computation. *Phys. Rev. B* **69**, 214501 (2004).
[38] Lewenstein, M. *et al.* Ultracold atomic gases in optical lattices: Mimicking condensed matter physics and beyond. *Adv. Phys.* **56**, 243-379 (2007).
[39] Johanning, M. *et al.* Quantum simulations with cold trapped ions. *J. Phys. B* **42**, 154009 (2009).
[40] Jordan, S. P., *et al.* Quantum algorithms for quantum field theories. *Science* **336**, 1130-1133 (2012).
[41] Byrnes, T., & Yamamoto, Y. Simulating lattice gauge theories on a quantum computer. *Phys. Rev. A* **73**, 022328 (2006).
[42] Somaroo, S. *et al.* Quantum simulations on a quantum computer. *Phys. Rev. Lett.* **82**, 5381-5383 (1999).
[43] Khitrin, A. K. & Fung, B. M. NMR simulation of an eight-state quantum system. *Phys. Rev. A* **64**, 032306 (2001).
[44] Brown, K. R. *et al.* Limitations of quantum simulation examined by a pairing Hamiltonian using nuclear magnetic resonance. *Phys. Rev. Lett.* **97**, 050504 (2006).
[45] Friedenauer, A. *et al.* Simulating a quantum magnet with trapped ions. *Nat. Phys.* **4**, 757-761 (2008).
[46] Gerritsma, R. *et al.* Quantum simulation of the Dirac equation. *Nature* **463**, 68-71 (2010).
[47] Gerritsma, R. *et al.* Quantum simulation of the Klein paradox with trapped ions. *Phys. Rev. Lett.* **106**, 060503 (2011).
[48] Lanyon, B. P. *et al.* Universal digital quantum simulation with trapped ions. *Science* **334**, 57-61 (2011).
[49] Lanyon, B. P. *et al.* Towards quantum chemistry on a quantum computer. *Nat. Chem.* **2**, 106-111 (2010).
[50] Kinoshita, T. *et al.* Observation of a one-dimensional Tonks-Girardeau gas. *Phys. Rev. B* **82**, 060412 (2010).
[51] Ma, X. S. *et al.* Quantum simulation of the wavefunction to probe frustrated Heisenberg spin systems. *Nat. Phys.* **7**, 399-405 (2011).
[52] Kassal, I. *et al.* Simulating chemistry using quantum computers. *Annu. Rev. Phys. Chem.* **62**, 185-207 (2011).
[53] Cirac, J. I. & Zoller, P. Goals and opportunities in quantum simulation. *Nat. Phys.* **8**, 264-266 (2012).
[54] Bloch, I. *et al.* Quantum simulations with ultracold quantum gases. *Nat. Phys.* **8**, 267-276 (2012).
[55] Blatt, R. & Roos, C. F. Quantum simulations with trapped ions. *Nat. Phys.* **8**, 277-284 (2012).
[56] Aspuru-Guzik, A. & Walther, P. Photonic quantum simulators. *Nat. Phys.* **8**, 285-291 (2012).
[57] Houck, A. A. *et al.* On-chip quantum simulation with superconducting circuits. *Nat. Phys.* **8**, 292299 (2012).
[58] Brown, K. L. *et al.* Using quantum computers for quantum simulations. *Entropy* **12**, 2268-2307 (2010).
[59] Josephson, B. D. Possible new effects in superconductive tunnelling. *Phys. Lett.* **1**, 251 (1962).
[60] Esaki, L. & Miyahara, Y. A new device using the tunneling process in narrow p-n junctions. *Solid-State Electron.* **1**, 13 (1960).
[61] Binnig, G. & Rohrer, H. Scanning tunneling microscopy. *IBM J. Res. Dev.* **44**, 279-293 (2000).
[62] Sornborger, A. T. Quantum simulation of tunneling in small systems. *Sci. Rep.* **2**, 597 (2012).
[63] Feng, G.-R., Lu, Y., Hao, L., Zhang, F.-H. & Long, G.-L. Experimental simulation of quantum tunneling in small systems. *Sci. Rep.* **3**, 2232 (2013).
[64] Ostrowski, M. Quantum simulation of the tunnel effect *Bull. Pol. Acad. Tech. Sci.* **63**, 0042 (2015).
[65] Benenti, G. & Strini, G. Quantum simulation of the single-particle Schrödinger equation. *Am. J. Phys.* **76**, 657 (2008).
[66] Yoshida, H. Construction of higher-order symplectic integrators. *Phys. Lett. A* **150**, 262-268 (1990).
[67] Sornborger, A. T. & Stewart, E. D. Higher-order methods for simulations on quantum computers. *Phys. Rev. A* **60**, 1956-1965 (1999).
[68] Hatano, N. & Suzuki, M. Quantum Annealing and Other Optimization Methods. *Springer, Heidelberg* , (2005).
[69] Coppersmith, D. An approximate Fourier transform useful in quantum factoring. *IBM Res. Rep.* , (1994).

Acknowledgements BKB acknowledges the support of DST Inspire Fellowship. We are extremely grateful to IBM team and IBM Quantum Experience project.