Evidence of the quantum entanglement constraint on wave-particle duality using the IBM Q quantum computer

Nicolas Schwaller,1 Marc-André Dupertuis,1 and Clément Javerzac-Galy1,2

1Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland
2Miraex, EPFL Innovation Park, Bâtiment C, Lausanne, CH-1015, Switzerland

(Dated: December 6, 2019)

We experimentally verify the link existing between entanglement and the amount of wave-particle duality in a bipartite quantum system, with superconducting qubits in the IBM Q quantum computer. We analyze both pure and mixed states, and study the limitations of the state purity on the complementarity “triality” relation. This work confirms the quantitative completion of local Bohr’s complementarity principle by the nonlocal quantum entanglement for a bipartite quantum system.

INTRODUCTION

In 1924, physicist Louis De Broglie developed the theory of electron waves [1], coming up with the idea that particles behave like waves. This discovery is with no doubt one of the most stunning ideas in physics. Indeed, four years later, Niels Bohr formulated his principle of complementarity [2] dealing with this non-intuitive property of Nature. It is possible to detect particle and wave characteristics of a single quantum object, but it never behaves fully like a wave and a particle at the same time. This idea was democratised by Richard Feynman in 1965, who underlined the strangeness of the so-called wave-particle duality: “a phenomenon which is impossible, absolutely impossible, to explain in any classical way, and which has in it the heart of quantum mechanics. In reality, it contains the only mystery” [3]. Experiments were in particular conducted with fermions and photons (see e.g. [4, 5]), typically with double-slit setups, where a single quantum object has two possible paths, before to reach a screen where its position is measured. Knowing which path the object took indicates the object is a point-like particle, whereas observing an interference pattern on the screen, formed by the detected positions of the particles when the experiment is repeated, is the manifestation of the wave characteristic of the object, which apparently passes through both slits at once.

Wave-particle duality was described quantitatively by Wootters and Zurek [6] in 1979 before the derivation of a mathematical description of Bohr’s principle in 1988 by Greenberger and Yasin [7] for a single particle,

\[ V^2 + P^2 \leq 1, \tag{1} \]

where \( V, P \in [0, 1] \) are the a priori fringe visibility and which-way predictability, commonly associated to the waviness and the particleness of the quantum object. It was later extended by Englert [8] and, independently by Jaeger, Shimony, and Vaidman [9], for bipartite systems by relating the visibility of one-particle interference fringes to the visibility of two-particle fringes. The analysis of the experiments for which relation (1) holds can thus be significantly different and easily induce misleading representations. For this reason, Englert [8] introduced a more prudent definition of the notion of (wave-particle) duality, i.e. “the observations of an interference pattern and the acquisition of which-way information are mutually exclusive.” These relations were experimentally fulfilled for single particle complementarity by Jacques et al. in 2008 [10] and for bipartite complementarity by Ma et al. in 2009 [11].

One can already see that the relation of duality (1) seems to have a weakness: it is an inequality, hence it is incomplete, in the sense that it only bounds possible physical predictions. Indeed, \( P \) can be deduced from a measurement of \( V \) only in the \( V = 1 \) case, and vice versa. The case of \( V = P = 0 \) highlights in a more striking way the incompleteness of relation (1), calling at least for a third variable.

Saying that wave-particle duality is the most counter-intuitive phenomenon of quantum physics is forgetting about quantum entanglement [12] that gives rise to non-local correlations, what Einstein called “spooky action at a distance”. It has been a strong source of debate among physicists since the the early ages of quantum physics, the most famous being the EPR argument [13] published in 1935 by Einstein, Podolsky and Rosen, which argues in favour of the lack of completeness of the quantum theory as a description of physical reality, precisely because of its nonlocal predictions. EPR led to a considerable amount of discussions until experiments, in particular the Bell inequality violation by Aspect et al. [14] in 1982, resulted in the agreement of the vast majority of the community. Until today, theoretical predictions were confirmed in various ways and large scales, see e.g. [15, 16].

In a wave-particle duality experiment, the measurement configuration seems to dictate a priori the waviness or particleness of the quantum system, as if the system would adapt to the choice of measurement. Delayed-choice gedanken experiments [17], in which the waviness or particleness measurement choice is delayed at a late stage of the experiment, were proposed and experi-
mentally verified to question the previous interpretation: Wheeler’s delayed-choice duality [18–19], delayed-choice quantum erasure [20,22] and delayed-choice entanglement swapping [23]. These experiments yield to the conclusion that to interpret the observation of one quantum system, one has to include the whole experimental system and the complete quantum state, potentially describing joint properties with other systems [17,24]. For instance, interestingly delayed-choice entanglement swapping experiments brought to light an entanglement-separability duality for bipartite or multipartite systems [23].

It has been shown recently by Jakob and Bergou [25,26] that in the case of a bipartite and multipartite quantum systems, a complementarity relation holds between quantum entanglement and (wave-particle) duality. While it comes as no surprise that this new equality involves both local and nonlocal quantities, it turns out to solve the incompleteness of (1). In their proposal, duality complementarity determines entanglement in the quantum system, one has to include the whole experimental system and the complete quantum state, potentially describing joint properties with other systems [17,24]. For instance, quantum erasure [20–22] and delayed-choice entanglement swapping [23]. These experiments yield to the conclusion that to interpret the observation of one quantum system, one has to include the whole experimental system and the complete quantum state, potentially describing joint properties with other systems [17,24]. For instance, interestingly delayed-choice entanglement swapping experiments brought to light an entanglement-separability duality for bipartite or multipartite systems [23].

We propose the experimental verification of this so called triality relation for a bipartite quantum system of superconducting qubits with the IBM Q quantum computer, harnessed by the progress in accessible quantum technologies.

QUANTUM WAVINESS, PARTICLENESS AND ENTANGLEMENT

Consider a general pure state of two qubits,

$$|\psi\rangle = \alpha |00\rangle + \beta |01\rangle + \gamma |10\rangle + \delta |11\rangle,$$

with $\alpha, \beta, \gamma, \delta \in \mathbb{C}$ satisfying the normalization

$$|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1.$$

The state (2) can be characterized by its density matrix,

$$\rho = \begin{pmatrix} 
\alpha\bar{\alpha} + \beta\bar{\beta} + \gamma\bar{\gamma} + \delta\bar{\delta} \\
\beta\bar{\alpha} + \beta\bar{\beta} + \gamma\bar{\gamma} + \delta\bar{\delta} \\
\gamma\bar{\alpha} + \beta\bar{\beta} + \gamma\bar{\gamma} + \delta\bar{\delta} \\
\delta\bar{\alpha} + \delta\bar{\beta} + \delta\bar{\gamma} + \delta\bar{\delta}
\end{pmatrix}.$$  

(4)

By convention, the first and second qubits will be respectively called qubit $A$ and qubit $B$. The corresponding reduced density matrices of subsystems $A$ and $B$ are

$$\rho_A = Tr_B(\rho) = \begin{pmatrix} 
\alpha\bar{\alpha} + \beta\bar{\beta} + \gamma\bar{\gamma} + \delta\bar{\delta} \\
\beta\bar{\alpha} + \beta\bar{\beta} + \gamma\bar{\gamma} + \delta\bar{\delta} \\
\gamma\bar{\alpha} + \beta\bar{\beta} + \gamma\bar{\gamma} + \delta\bar{\delta} \\
\delta\bar{\alpha} + \delta\bar{\beta} + \delta\bar{\gamma} + \delta\bar{\delta}
\end{pmatrix}.$$  

(5)

and

$$\rho_B = Tr_A(\rho) = \begin{pmatrix} 
\alpha\bar{\alpha} + \gamma\bar{\gamma} + \alpha\bar{\beta} + \gamma\bar{\delta} + \beta\bar{\gamma} + \beta\bar{\delta} + \delta\bar{\gamma} + \delta\bar{\delta}
\end{pmatrix}.$$  

(6)

Three central quantities [25] can then be derived.

First, the concurrence, defined in the bipartite pure case by

$$C(\psi) = 2|\alpha\delta - \beta\gamma|.$$  

(7)

The concurrence is a measurement of the amount of entanglement between two quantum systems [27,28] as it is a monotone of the entanglement of formation, $E_f$, which is a measure of entanglement based on the separability criterion: $E_f = 0$ if and only if the density matrix can be written as a mixture of product states. Both $C$ and $E_f$ take the value one for maximally entangled states.

Second, the coherence $\chi_k$ between the two orthogonal states $|0\rangle$ and $|1\rangle$ of the qubit $k$, which is therefore a quantity related to a single qubit. It is directly proportional to the norm of the off-diagonal elements of its density matrix, and reads

$$\chi_k = 2|\rho_{k12}|, \quad k = A, B.$$  

(8)

Note that the counterpart of coherence in an interference experiment is the visibility.

Third, the predictability $\mathcal{P}_k$, which quantifies the knowledge of “which proportion” of the system $k$ is in the state $|0\rangle$ or $|1\rangle$. It is defined by

$$\mathcal{P}_k = |\rho_{k22} - \rho_{k11}|, \quad k = A, B.$$  

(9)

The predictability is analogous to the which-path information in an interference experiment.

By replacing the definitions (4-6) in eqs. (7-9) it is easy to show that

$$\chi_k^2 + \mathcal{P}_k^2 + C^2 = (|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2)^2.$$  

(10)

One notices that the right-hand side of (10) is nothing else than the norm of the state (2) raised to the power 4. Thus, one can conclude that for a pure state [25],

$$\chi_k^2 + \mathcal{P}_k^2 + C^2 = 1.$$  

(11)

Note that (11) remarkably claims that for a pure state of two qubits, the amount of entanglement strictly pilots the amount of duality of any qubit of the pair, namely $\chi_k^2 + \mathcal{P}_k^2, k = A, B$, which has the same value for both qubits.

In order to create a tunable state in term of its $\chi_k$, $\mathcal{P}_k$ and $C$, we propose a simple circuit shown in Fig.1.
The circuit prepares the state (see Appendix A)

$$|\psi\rangle = \cos \frac{\alpha}{2} |00\rangle + \cos \frac{\theta}{2} \sin \frac{\alpha}{2} |01\rangle + \sin \frac{\theta}{2} \sin \frac{\alpha}{2} |11\rangle,$$  \hspace{1cm} (12)

and then performs tomography allowing to retrieve the density matrix of the quantum state [29]. Using this circuit, the IBM qasm simulator allows to check the equality (11) for a pure state of two qubits of the form (12), as reported (for qubit A) in Fig. 2.

![Fig. 2: Simulation for qubit A. Selection of 13 couples of values $\alpha$, $\theta$ emphasizing relation (11): the values of $\mathcal{V}_A$, $\mathcal{P}_A$, $\mathcal{C}$ lie on a sphere of radius 1.](image)

With the aim of performing the experiment on the real quantum computer, a noisy intermediate-scale quantum (NISQ) computer [30], formulas need to be extended to mixed states. For a mixed state with density matrix

$$\rho = \sum_j p_j |\phi_j\rangle \langle \phi_j|,$$  \hspace{1cm} (13)

where $|\phi_j\rangle$ are pure states composing the complete state with probability $p_j$, it is possible to measure the concurrence [31] by defining the spin flip matrix

$$\Sigma = \sigma_y \otimes \sigma_y$$  \hspace{1cm} (14)

and the matrix

$$R(\rho) = \rho \Sigma \rho^* \Sigma.$$  \hspace{1cm} (15)

The concurrence is given by

$$\mathcal{C} = \text{max}(0, \sqrt{r_1} - \sqrt{r_2} - \sqrt{r_3} - \sqrt{r_4}).$$  \hspace{1cm} (16)

where $r_1 \geq r_2 \geq r_3 \geq r_4$ are the eigenvalues of $R(\rho)$. Using expressions (14) to (16) allows to compute the concurrence of the pair of qubits from the tomography step.

The coherence of the qubit $k$ in the mixed bipartite case [32] is given by

$$\mathcal{Y}_k = 2 \left| \text{Tr}(\rho_k \sigma_+^{(k)}) \right|,$$  \hspace{1cm} (17)

where $\sigma_+^{(k)} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ is the raising operator acting on qubit $k$.

It can be written as

$$\mathcal{Y}_k = \sum_{i \neq j} |\rho_{kij}|,$$  \hspace{1cm} (18)

which, for a pure state, is equivalent to $\mathcal{S}$ thanks to the hermiticity of the density matrix. Similarly, the predictability (of the state) of a qubit [32] is given by $\mathcal{D}$ in the case of a two-qubits mixed state.

Given the possibility to compute the quantities for a mixed state, we can now perform the experiment with the real qubits. For this, the backend ibmqx2 is used [33]. The measurement is repeated 10 times for each of the thirteen states in order to calculate confidence bounds, and the number of shots is set to 1000 for each measurement. We are expecting to observe

$$\mathcal{V}_k^2 + \mathcal{P}_k^2 + \mathcal{C}^2 \leq 1$$  \hspace{1cm} (19)

because of the mixedness of the state [25], the experimental values being limited by decoherence and noise. Nevertheless, the measurements on the real backend can be simulated using a noise model, directly constructed from the real backend properties thanks to methods from Qiskit Ignis [34]. The IBM qasm simulator is thus used to simulate the noise and decoherence taking place in the ibmqx2 backend used for the experiment (see Appendix C).

The measured data is then normalized with respect to the noise simulation. More precisely, the mean value of each point along axes $\mathcal{V}_A$, $\mathcal{P}_A$ and $\mathcal{C}$ is normalized with respect to the corresponding value in the noise simulation. Confidence bounds are taken as 4-$\sigma$ along each axis, from the measured data distribution for each state, considered to be normal in every direction. This results in confidence ellipsoids visible in Fig. 3.
From this result, one sees that the normalization allows to verify (11). The noise model could accurately simulate errors due to decoherence and noise accounting for the mixedness of the prepared states, the tomography step as well as the eventual readout errors.

In contrast, looking at the raw data (see Appendix C), one can see that the measurement of the three quantities for the thirteen states give lower values than expected for a pure state (Fig. 2). This drop is particularly consequent for $C$. It seems that it is the most delicate and sensitive to decoherence among the three quantities. In fact, it is possible to quantify the drop of concurrence which is due to the mixedness of the state. Indeed, such an upper bound on concurrence can be computed [35]. Following the notation of Wooters for the two qubit case [28], this upper bound on concurrence, quantifying the maximal entanglement reachable with a given state purity, is given by

$$C_{\max}(\rho) = \max(0, \lambda_1 - \lambda_3 - 2\sqrt{\lambda_2\lambda_4}),$$

with $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ the eigenvalues of $\rho$. In other words, $C_{\max}$ is the maximal concurrence a state can reach, knowing the eigenvalues of its density matrix.

The drop of concurrence in our experiment is especially visible using the ibmqx4 backend: Fig. 4 shows that the raw measurements [36] of $C$ are constrained and reach their highest value ($\mathcal{P}_k = \gamma_k = 0$) close to the maximal concurrence bound $C_{\max}$. Therefore, we identify it as the principal cause of the flattening of the sphere along the $C$ axis observed in the raw data, and this cannot be improved by any mean except increasing the state purity.

Finally, the ratio $C_{\text{ibmqx4}} / C_{\text{simulator}}$ appears to stay constant as $\mathcal{P}_A$ varies. More precisely, the comparison of the value of the real machine with respect to the simulator indicates that $C_{\text{ibmqx4}} \approx 0.6 \cdot C_{\text{simulator}}$. One could say that the efficiency in the preparation of an entangled state is constant, while the preparation of an entangled state decreases the purity, in its turn limiting entanglement.

**CONCLUSION**

Our work contributes to experimentally verify the quantitative completion of local Bohr’s complementarity principle by quantum entanglement for a bipartite quantum state as proposed by Jakob and Bergou [25, 26]. The measurements on the two real superconducting qubits, together with simulations using the backend noise model, show that the duality of each qubit can thus be turned off completely, or set to any desired amount by controlling the degree of entanglement. Introducing concurrence, a quantifiable entanglement measure, to complete the usual wave-particle duality relation gives birth to the more general complementarity “triality” relation of Jakob and Bergou [25], $\gamma^2_k + \mathcal{P}^2_k + C^2 = 1$. It involves three physical quantities, two of which are local (referring to the subsystem $k$), which can be seen as mutually exclusive modulo a nonlocal quantity $C$ ($\gamma^2_k + \mathcal{P}^2_k = 1 - C^2$). Clearly, the triality relation can be separated in a local and nonlocal part as

$$\mathcal{S}^2_k + C^2 = 1$$

with $\mathcal{S}^2_k = \mathcal{P}^2_k + \gamma^2_k$. Maximal entanglement of the bipartite system simply conjectures that the local realities totally disappear, synonym of maximal amount of nonclassical nonlocal phenomena such as violations of Bell
inequalities. Given the large context of this experiment it is important to remind the nature of the relevant quantities. In particular, as interferometric experiments on complementarity in bipartite systems have to deal with two-particle visibility in addition to single-particle visibility of interference fringes, see e.g. [37], we draw attention to the fact that the two-particle visibility would correspond to the concurrence in our experiment. Indeed, it was shown that the visibility of two-photon interference fringes in a Young double-slit experiment is controlled by the degree of entanglement [38, 39], which can be easily understood as interference between two particles intuitively does not appear unless they are correlated.

Finally, such experiments with the superconducting qubits of the IBM Q quantum computer could be extended to the study of the dynamical evolution of quantum correlations, particularly entanglement [10], and could be performed with larger multipartite entangled states [11] or other physical systems [12]. It can be expected that studies of those relations which are fundamental in quantum mechanics will lead to applications in quantum information.

ACKNOWLEDGEMENTS

We thank Dr. James R. Wootton for useful discussions and comments. We acknowledge use of the IBM Quantum Experience for this work. The views expressed are those of the authors and do not reflect the official policy or position of IBM or the IBM Quantum Experience team.

DATA AVAILABILITY STATEMENT

The code that supports this study is openly available in Github at https://github.com/NicoSchwaller/Duality-and-Entanglement-of-two-Qubits

---

1. L. De Broglie, Recherches sur la théorie des Quanta. PhD thesis, 1925.
2. N. Bohr, “The quantum postulate and the recent development of atomic theory,” Nature, vol. 121, no. 3050, pp. 580–590, 1928.
3. R. Feynman, R. Leighton, M. Sands, and E. Hafner, The Feynman Lectures on Physics; Vol. III, vol. 33. AAPT, 1965.
4. M. Scully, B.-G. Englert, and H. Walther, “Quantum optical tests of complementarity,” Nature, vol. 351, pp. 111–116, 04 1991.
5. A. Zeilinger, R. Gähler, C. G. Shull, W. Treimer, and W. Mampe, “Single- and double-slit diffraction of neutrons,” Rev. Mod. Phys., vol. 60, pp. 1067–1073, Oct 1988.
6. W. K. Wootters and W. H. Zurek, “Completeness in the double-slit experiment: Quantum nonseparability and a quantitative statement of bohr’s principle,” Phys. Rev. D, vol. 19, pp. 473–484, Jan 1979.
7. D. M. Greenberger and A. Yasin, “Simultaneous wave and particle knowledge in a neutron interferometer,” Physics Letters A, vol. 128, no. 8, pp. 391 – 394, 1988.
8. B.-G. Englert, “Fringe visibility and which-way information: An inequality,” Phys. Rev. Lett., vol. 77, pp. 2154–2157, Sep 1996.
9. G. Jaeger, A. Shimony, and L. Vaidman, “Two interferometric complementarities,” Phys. Rev. A, vol. 51, pp. 54–67, Jan 1995.
10. V. Jacques, E. Wu, F. Grosshans, F. m. c. Treussart, F. Grangier, A. Aspect, and J.-F. m. c. Roch, “Delayed-choice test of quantum complementarity with interfering single photons,” Phys. Rev. Lett., vol. 100, p. 220402, Jun 2008.
11. X.-s. Ma, A. Qarry, J. Kofler, T. Jennewein, and A. Zeilinger, “Experimental violation of a bell inequality with two different degrees of freedom of entangled particle pairs,” Phys. Rev. A, vol. 79, p. 042101, Apr 2009.
12. R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, “Quantum entanglement,” Rev. Mod. Phys., vol. 81, pp. 865–942, Jun 2009.
13. A. Einstein, B. Podolsky, and N. Rosen, “Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?”, Physical Review, vol. 47, pp. 777–780, May 1935.
14. A. Aspect, J. Dalibard, and G. Roger, “Experimental test of bell’s inequalities using time-varying analyzers,” Phys. Rev. Lett., vol. 49, pp. 1804–1807, Dec 1982.
15. J. Yin, Y. Cao, Y.-H. Li, S.-K. Liao, L. Zhang, J.-G. Ren, W.-Q. Cai, W.-Y. Liu, B. Li, H. Dai, G.-B. Li, Q.-M. Lu, Y.-H. Gong, Y. Xu, S.-L. Li, F.-Z. Li, Y.-Y. Yin, Z.-Q. Jiang, M. Li, J.-J. Jia, G. Ren, D. He, Y.-L. Zhou, X.-X. Zhang, N. Wang, X. Chang, Z.-C. Zhu, N.-L. Liu, Y.-A. Chen, C.-Y. Lu, R. Shu, C.-Z. Peng, J.-Y. Wang, and J.-W. Pan, “Satellite-based entanglement distribution over 1200 kilometers,” Science, vol. 356, pp. 1140–1144, June 2017.
16. D. Rauch, J. Handsteiner, A. Hochrainer, J. Gallicchio, A. S. Friedman, C. Leung, B. Liu, L. Bulla, S. Ecker, F. Steinlechner, R. Ursin, B. Hu, D. Leon, C. Benn, A. Ghedina, M. Cecconi, A. H. Guth, D. I. Kaiser, T. Scheidl, and A. Zeilinger, “Cosmic bell test using random measurement settings from high-redshift quasars,” Phys. Rev. Lett., vol. 121, p. 080403, Aug 2018.
17. X.-s. Ma, J. Kofler, and A. Zeilinger, “Delayed-choice gedanken experiments and their realizations,” Rev. Mod. Phys., vol. 88, p. 015005, Mar 2016.
18. A. R. Marlow, Mathematical Foundations of Quantum Theory. Academic Press, 1978.
19. V. Jacques, E. Wu, F. Grosshans, F. Treussart, P. Grangier, A. Aspect, and J.-F. Roch, “Experimental realization of wheeler’s delayed-choice gedanken experiment,” Science, vol. 315, no. 5814, pp. 966–968, 2007.
20. M. O. Scully and K. Drühl, “Quantum eraser: A proposed photon correlation experiment concerning observa-
tion and “delayed choice” in quantum mechanics,” *Phys. Rev. A*, vol. 25, pp. 2208–2213, Apr 1982.

[21] Y.-H. Kim, R. Yu, S. P. Kulik, Y. Shih, and M. O. Scully, “Delayed “choice” quantum eraser,” *Phys. Rev. Lett.*, vol. 84, pp. 1–5, Jan 2000.

[22] L. Mandel, “Coherence and indistinguishability,” *Opt. Lett.*, vol. 16, pp. 1882–1883, Dec 1991.

[23] A. Peres, “Delayed choice for entanglement swapping,” *Journal of Modern Optics*, vol. 47, no. 2-3, pp. 139–143, 2000.

[24] X.-S. Ma, J. Kofler, A. Qarry, N. Tetik, T. Scheidl, R. Ursin, S. Ramelow, T. Herbst, L. Ratschbacher, A. Fedrizzi, T. Jennewein, and A. Zeilinger, “Quantum erasure with causally disconnected choice,” *Proceedings of the National Academy of Sciences of the United States of America*, vol. 110, pp. 1221–1226, Jan 2013.

[25] M. Jakob and J. Bergou, “Quantitative complementarity relations in bipartite systems: Entanglement as a physical reality,” *Optics Communications*, vol. 283, pp. 827–830, 03 2010.

[26] M. Jakob and J. A. Bergou, “Complementarity and entanglement in bipartite qudit systems,” *Phys. Rev. A*, vol. 76, p. 052107, Nov 2007.

[27] S. Hill and W. K. Wootters, “Entanglement of a pair of quantum bits,” *Phys. Rev. Lett.*, vol. 78, pp. 5022–5025, Jun 1997.

[28] W. K. Wootters, “Entanglement of formation of an arbitrary state of two qubits,” *Phys. Rev. Lett.*, vol. 80, pp. 2245–2248, Mar 1998.

[29] T. E. Tessier, “Complementarity relations for multi-qubit systems,” *Foundations of Physics Letters*, vol. 18, pp. 107–121, Apr 2005.

[30] Measurements performed on April 10, 2019.

[31] G. Aleksandrowicz, T. Alexander, P. Barkoutsos, L. Bello, Y. Ben-Haim, D. Bucher, F. J. Cabrera-Hernández, J. Carballo-Franquis, A. Chen, C.-F. Chen, J. M. Chow, A. D. Córcoles-Gonzales, A. J. Cross, A. Cruz-Benito, C. Culver, S. D. L. P. González, E. D. L. Torre, D. Ding, E. Dumitrescu, I. Duran, P. Endebak, M. Everitt, I. F. Sertage, A. Frisch, A. Fuhrer, J. Gambetta, B. G. Gago, J. Gomez-Mosquera, D. Greenberg, I. Hamamura, V. Havlicek, J. Hellmers, L. Herok, H. Horii, S. Hu, T. Imamichi, T. Itoko, A. Javadi-Abhari, N. Kanazawa, A. Karazeev, K. Krsulich, P. Liu, Y. Luh, Y. Maeng, M. Marques, F. J. Martin-Fernández, D. T. McClure, D. McKay, S. Meesala, A. Mezzacapo, N. Moll, D. M. Rodríguez, G. Nannicini, P. Nation, P. Ollitrault, L. J. O’Riordan, H. Paik, J. Pérez, A. Phan, M. Pistoia, V. Prutyanov, M. Reuter, J. Rice, A. R. Davila, R. H. P. Rudy, M. Ryu, N. Sathaye, C. Schnabel, E. Schoute, K. Setia, Y. Shi, A. Silva, Y. Siraichi, S. Sivarajah, J. A. Smolin, M. Soeken, H. Takahashi, I. Tavernelli, C. Taylor, P. Taylor, K. Trabing, M. Treinish, W. Turner, D. Vogt-Lee, C. Vuillot, J. A. Wildstrom, J. Wilson, E. Winston, C. Wood, S. Wood, S. Wörner, I. Y. Akhalwaya, and C. Zoufal, “Qiskit: An open-source framework for quantum computing,” 2019.
Appendix A: quantum circuit for state preparation

The left-hand side of the circuit in Fig. 1 prepares the state $|\psi\rangle = \cos^{\frac{\theta}{2}}|00\rangle + \cos^{\frac{\alpha}{2}}\sin^{\frac{\alpha}{2}}|10\rangle + \sin^{\frac{\alpha}{2}}\sin^{\frac{\theta}{2}}|11\rangle$, by applying the unitary transformation

$$(CU_{A\rightarrow B})(R_y \otimes I) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos^{\frac{\theta}{2}} & -\sin^{\frac{\theta}{2}} \\ 0 & 0 & \sin^{\frac{\theta}{2}} & \cos^{\frac{\theta}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$ 

According to equations (7 - 9), such a unitary operation acting on the state $|00\rangle$ allows the five quantities $\gamma_k$, $\mathcal{P}_k$ (with $k = A, B$) and $C$ to reach their extremal values, i.e. 0 and 1. To verify it, the parameters of the circuit are set to random angles $\alpha, \theta \in [0, \pi]$. The outcomes of the simulations are matching the analytical expressions for $\gamma_k(\alpha, \theta)$, $\mathcal{P}_k(\alpha, \theta)$ and $C(\alpha, \theta)$. This is shown in Fig. 5 in the case of qubit $A$.

Appendix B: maximum entanglement versus purity

It is interesting to note that eq. (20) excludes any concurrence for a state for which $\text{Tr}(\rho^2) < \frac{1}{3}$. Fig. 6 accordingly highlights the existence of a threshold value of the state purity under which concurrence cannot exist. These measurements were computed with the simulator, varying the amount of noise (readout errors) to change the purity. The presence of the threshold value explains that it sometimes actually happened that our circuit running on the real IBM machines provided a fidelity of state preparation which was too poor to get any concurrence, preventing any attempt to conduct the experiment.

In accordance with Fig. 6 we expect $C$ to equal $C_{\text{max}}$ for a maximally entangled state, a necessary condition to refer to $C_{\text{max}}$ as an upper bound to entanglement.

Appendix C: measured data and noise simulation

Raw data and the corresponding noise simulation used to normalize the measured data are plotted in Fig. 7. One can see that the noise simulation effectively simulates the noise present on the real quantum computer, which manifests itself as a drop of the three studied quantities, and especially affects concurrence.

Fig. 5: Simulation of the coherence, predictability and concurrence for qubit $A$ using the circuit of Fig. 1 with $\alpha, \theta$ randomly chosen in $[0, \pi]$.

Fig. 6: Evolution of concurrence $C$ and concurrence maximal bound $C_{\text{max}}$ for the maximally entangled Bell state $|\Phi^{+}\rangle(\alpha = \frac{\pi}{2}, \theta = \pi)$ as purity varies.

Fig. 7: Noisy simulation (a) and raw data (b) from ibmqx2. The experiment is repeated 10 times for each state.