Use of Quantum Computation to Explore Exciton Condensation Phenomena

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Goal: I aim to develop a methodology to explore the degree of exciton condensation on a quantum computer, determine the preparation(s) that obtain maximum exciton condensation for a given number of qubits, and probe the properties of said exciton condensate states.

Introduction: Condensation phenomena has been an active area of research since 1924 when Einstein and Bose first introduced their ideal "Bose-Einstein" gas.[1] The identical particles comprising this gas (bosons) were proposed to be able to aggregate into a single quantum ground state when sufficiently cooled.[1] Later, London and Tisza attributed Bose-Einstein condensation (BEC) to be the source of superfluidity—the frictionless flow of zero-viscosity fluids—that had been observed in low-temperature liquid helium.[2] In 1940, Pauli established the relationship between spin and statistics, demonstrating that particles with integral spin values obey Bose-Einstein statistics—are bosons—and hence may form a condensate.[2] Extrapolating further, pairs of fermions—particles with half-integer spins—may interact such that the overall two-particle system has integral spin and is hence bosonic. In fact, recent experimental and theoretical investigation has particularly centered around the condensations of one such class of bosons: exciton condensates.[3] *Exciton condensation is defined by the condensation of particle-hole pairs (excitons) into a single quantum state to create a superfluid.* The superfluidity of electron-hole pairs *involves the non-dissipative transfer of energy*, which has applications in energy transport and electronics.[3]

Motivation: While excitons form spontaneously in semiconductors and insulators and while the binding energy of the excitons can greatly exceed their thermal energy at room temperature, they recombine too quickly to allow for formation of a condensate in a simple manner. To combat recombination, the coupling of excitons to polaritons, which requires the continuous input of light,[4] and the physical separation of electrons and holes into bilayers, which involves impractically high magnetic fields and/or low temperatures,[5] are employed. Thus, a *new, more-practical avenue for the creation and study of exciton condensation is desired*; quantum computing offers such an avenue.

A qubit is the basic unit of quantum computing (analogous to the classical bit); the qubit itself is a quantum system whose most-general state is a linear combination of its two basis states ($|0\rangle$ and $|1\rangle$, the classical bit states) with an appropriate phase factor ($e^{i\phi}$) given by[6]

$$|\Psi\rangle = cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}sin\left(\frac{\theta}{2}\right)|1\rangle = \begin{pmatrix} cos\left(\frac{\theta}{2}\right) \\ e^{i\phi}sin\left(\frac{\theta}{2}\right) \end{pmatrix}.$$

If a qubit is considered to be a one-fermion, two-level system in which there is a probability p of the fermion being in the lower-level state ($|0\rangle$) and a probability $1-p$ of the fermion being in the upper-level state ($|1\rangle$) where $p = |cos\left(\frac{\theta}{2}\right)|^2$, then a single qubit can represent two particle-hole paired orbitals. As such, a system of N qubits can be viewed as N fermions in an N-fold degenerate, two-level, particle-hole paired system. As explored in Ref. 7, such a model can demonstrate exciton condensation in systems with as few as 3 fermions in 6 orbitals (i.e., a three qubit system).

Resources: In this work the IBM Quantum Experience devices—which are available online—will be used. Qiskit open-source quantum computing software will be employed for analysis.

Aim-1, Probe the Extent of Exciton Condensation of an Arbitrary Qubit State: *In order to computationally probe the presence and extent of condensation behavior, I aim to measure the largest eigenvalue of the $^2\tilde{G}$ matrix—a calculable, characteristic property of exciton condensation—on the quantum computer.*[8] The elements of the $^2\tilde{G}$ matrix are given by $^2\tilde{G}^{\tilde{i},j}_{\tilde{k},\tilde{l}} =$

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$\langle\Psi|\hat{\psi}_i^\dagger\hat{\psi}_j\hat{\psi}_{\tilde{l}}^\dagger\hat{\psi}_{\tilde{k}}|\Psi\rangle - \langle\Psi|\hat{\psi}_i^\dagger\hat{\psi}_j|\Psi\rangle\langle\Psi|\hat{\psi}_{\tilde{k}}^\dagger\hat{\psi}_{\tilde{l}}|\Psi\rangle$ where $|\Psi\rangle$ is the N-fermion wavefunction; $i, j, \tilde{l}, \tilde{k}$ represent spin orbitals; and $\hat{\psi}^\dagger$ and $\hat{\psi}$ are the creation and annihilation operators. Due to the particle-hole pairing of each qubit, the spin orbitals denoted by i and j and the spin orbitals denoted by $\tilde{k}$ and $\tilde{l}$ must correspond to the same qubit to be non-zero, simplifying the matrix. In order to obtain the ${}^2\tilde{G}$ matrix on a quantum computer, these elements must be translated into the basis of Pauli matrices. The expectation values of the Pauli matrices can be obtained through direct measurement from a quantum computer, and the matrix elements can then be calculated through use of the appropriate conversion. The largest eigenvalue can be computed from the matrix obtained.

Aim-2, Determine Preparation(s) for State(s) with Maximum Exciton Condensation: A quantum state of qubits can be prepared on a quantum computer by the application of a unitary transformation, $\hat{U}_i$, such that $|\Psi_i(1,2,\ldots,N)\rangle = \hat{U}_i|\Psi_0(1,2,\ldots,N)\rangle$ describes the preparation of an N-qubit state from the initial state $|\Psi_0\rangle = |00\cdots0\rangle$. *I aim to determine the appropriate unitary transformation for a given number of qubits that corresponds with the maximum condensation of excitons*—the largest eigenvalue. One particular N-qubit state that may be of interest on this search is the GHZ state—the state in which all qubits are in the $|0\rangle$ state or the $|1\rangle$ state with equal probability (i.e., $|\Psi_{GHZ}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle^{\otimes N} + |1\rangle^{\otimes N}\right)$);[6] this state is highly entangled and is hence an ideal candidate for exciton condensation.

Aim-3, Probe Properties of Exciton Condensates: Any physical, measurable property of a system corresponds to a Hermitian matrix ($\hat{A}$) such that the eigenvalues of $\hat{A}$ are the possible outcomes of measurement of said property. The elements of these Hermitian matrices can be written in terms of the expectation values of Pauli matrices and can therefore be obtained for a given qubit preparation. From this matrix, the probability of a given measurement ($\langle\Psi_i|a_n\rangle$) and the expectation value of that property ($\langle\Psi_i|\hat{A}|\Psi_i\rangle$) can be obtained where $|a_n\rangle$ is the eigenstate corresponding to a given measurement a_n and $|\Psi_i\rangle$ is an N-qubit state prepared by the unitary matrix $\hat{U}_i$. For example, the energetics of a prepared qubit state can be probed by obtaining the eigenvalues/eigenstates of the two-fermion reduced Hamiltonian matrix given by ${}^2K = \frac{1}{N-1}\left(-\frac{1}{2}\nabla_1^2 - \sum_j \frac{Z_j}{r_{1j}}\right) + \frac{1}{2}\frac{1}{r_{12}}$.

Intellectual Merit: *This project aims to expand our understanding of exciton condensation phenomena.* Should these approaches prove successful, a reliable and facile preparation for exciton condensate states will be achieved, and properties of such condensates will be able to be probed in a straightforward manner.

Broader Impacts: The superfluidity of excitons in a condensate allows for the frictionless transport of the excitation energy, released upon recombination of the particle and hole. Additionally, such superfluidity in a bilayer—with electrons in one layer and holes in another—allows for the frictionless transfer of charge as long as current is directed in opposite directions in the two layers—a phenomenon known as counterflow superconductivity.[3] Understanding and exploiting the superfluid properties of exciton condensates may hence be instrumental in the effort to design wires and electronic devices with minimal loss of energy, decreasing overall energy consumption.

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