




Entangled phase of simultaneous fermion and exciton condensations realizedLeeAnn M. Sager  and David A. Mazziotti ^{*}*Department of Chemistry and The James Franck Institute, The University of Chicago, Chicago, Illinois 60637, USA* (Received 8 August 2021; revised 30 December 2021; accepted 22 February 2022; published 8 March 2022)

Fermion-exciton condensates (FECs)—computationally and theoretically predicted states that simultaneously exhibit the character of superconducting states and exciton condensates—are novel quantum states whose properties may involve a hybridization of superconductivity and the dissipationless flow of energy. Here, we exploit prior investigations of superconducting states and exciton condensates on quantum devices to identify a tuneable quantum state preparation entangling the wave functions of the individual condensate states. Utilizing this state preparation, we prepare a variety of FEC states on quantum computers—realizing strongly correlated FEC states on current, noisy intermediate-scale quantum devices—and verify the presence of the dual condensate via postmeasurement analysis. This confirmation of the previously predicted condensate state on quantum devices as well as the form of its wave function motivates further theoretical and experimental exploration of the properties, applications, and stability of FECs.

DOI: [10.1103/PhysRevB.105.L121105](https://doi.org/10.1103/PhysRevB.105.L121105)**I. INTRODUCTION**

It may be possible to create materials that conduct both electric current and exciton excitation energy through the realization a single quantum state that simultaneously demonstrates properties of two different condensates—one composed of Cooper (particle-particle) pairs and the other composed of excitons (particle-hole pairs) [1]. Bose-Einstein condensation allows for multiple bosons aggregating in a single quantum state [2,3] at sufficiently low temperatures, resulting in the superfluidity of the constituent bosons [4,5]. A superconducting quantum phase is created upon the condensation of pairs of fermions into a single quantum state, which results in the frictionless flow of the constituent particle-particle pairs [6,7]. Significant theoretical and experimental investigations [6–28] have centered on superconductors in an effort to determine a commercially viable material supporting superconductivity at sufficiently high temperatures. However, the relatively low energy of the Cooper pairs [6,7] causes them to become unstable, reverting to traditional conductors above a critical temperature too low for commercial applications.

One avenue toward higher-temperature condensate phases has been an examination of condensations composed of particle-hole pairs (excitons) in a single quantum state, which can carry exciton excitation energy without resistance [16,29]. Excitons are more tightly bound than Cooper pairs, meaning that the condensation of excitons can persist at higher temperatures than those at which superconductors form, although the natural recombination of particles and holes is a cause of experimental difficulties in creating stable, high-temperature, ground-state exciton condensates. As such, much recent literature has explored the characteristics of exciton condensation as well as established various methodologies for overcoming the problem of annihilation upon recombination [15–19,30–33]. Specifically, exciton condensates have

been observed in optical traps with polaritons [34–37], the electronic double layers of semiconductors [15,30,38–40] and graphene [19,41,42], and in systems composed of transition-metal chalcogenides [18,43–47].

Here, we present an entangled quantum phase of matter in which a superconductor and an exciton condensate coexist in a single quantum state—a fermion-exciton condensate (FEC). We leverage the ability of quantum computation to explore strongly correlated phenomena [48–53] as well as prior investigation [28,33,54] to prepare a variety of FEC states on quantum devices via a tuneable quantum state preparation—verifying the presence of the condensate state through probing the signatures of particle-particle (λ_D) [55,56] and exciton (λ_G) [17,57] condensations. Our results not only confirm the existence of a unique class of condensates, they verify the theoretical prediction of the form of the wave function of the FEC as well as the phase diagram of the states (see Fig. 1). These results suggest that such condensates can potentially be prepared in physical systems such as twisted graphene bilayers in which forces favoring exciton condensation and superconducting, respectively, are in fierce competition.

Note that while both particle-particle and exciton condensates are known to exist in systems designed to use exciton condensates to mediate the creation of Cooper pairs at higher temperatures [58,59], this coexistence of fermion pair and excitonic condensation occurs in two adjacent systems that interact with one another [59] instead of existing in a joint FEC state.

II. THEORY**A. Signatures of condensation**

Condensation occurs when multiple bosons aggregate into a single quantum state [2,3] at temperatures below a certain critical temperature, resulting in the superfluidity of the constituent bosons [4,5]. In a condensation of particle-particle pairs, pairs of fermions condense into a single geminal, a

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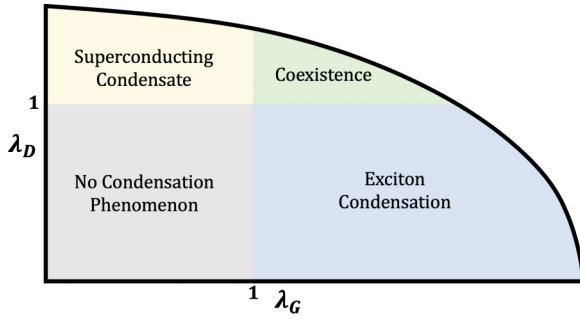


FIG. 1. A figure of the condensate phase diagram in the phase space of the signatures of particle-particle condensation, λ_D , and exciton condensation, λ_G ,—previously presented as Fig. 1 in Ref. [1]—is shown.

two-fermion function directly analogous to a one-fermion orbital [55,56,60–63], resulting in the frictionless flow of the particle-particle pairs [6,7]. As established by Yang [55] and Sasaki [56], a computational signature of such superconducting states—denoted as λ_D —is a large eigenvalue ($\lambda_D > 1$) of the particle-particle reduced density matrix (2-RDM) with elements given by

$${}^2D_{k,l}^{i,j} = \langle \Psi | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k | \Psi \rangle, \quad (1)$$

where $|\Psi\rangle$ is an N -fermion wave function and where \hat{a}_i^\dagger and \hat{a}_i are fermionic creation and annihilation operators for orbital i , respectively. This signature directly probes the presence and extent of nonclassical (off-diagonal) long-range order [61].

Exciton condensation, similarly, results from the condensation of particle-hole pairs (excitons) into a single quantum state [16,29]. A computational signature of exciton condensation—denoted as λ_G —is a large eigenvalue ($\lambda_G > 1$) of a modified version of the particle-hole reduced density matrix [17,57,64], with elements given by

$$\begin{aligned} {}^2\tilde{G}_{k,l}^{i,j} &= {}^2G_{k,l}^{i,j} - {}^1D_j^{i,1} D_k^l \\ &= \langle \Psi | \hat{a}_i^\dagger \hat{a}_j \hat{a}_l^\dagger \hat{a}_k | \Psi \rangle - \langle \Psi | \hat{a}_i^\dagger \hat{a}_j | \Psi \rangle \langle \Psi | \hat{a}_l^\dagger \hat{a}_k | \Psi \rangle, \end{aligned} \quad (2)$$

where 1D is the one-fermion reduced density matrix (1-RDM). Note that this modification removes the extraneous large eigenvalue from a ground-state-to-ground-state transition.

See the Methods section of the Supplemental Material [65] for specifics of how the signatures of superconductivity (λ_D) and exciton condensation (λ_G) are obtained from the result data of a given quantum state preparation.

B. Fermion-exciton condensate

A FEC is a quantum state in which the character of both particle-particle condensation and exciton condensation coexist [1,54]; thus, a FEC exhibits simultaneous large eigenvalues of the particle-particle and modified particle-hole RDMs—i.e., $\lambda_D, \lambda_G > 1$. As we have previously theoretically established in the thermodynamic limit [1], a FEC should result from the entanglement of a wave function exhibiting superconductivity, $|\Psi_D\rangle$, with a wave function exhibiting ex-

citon condensation, $|\Psi_G\rangle$, mathematically represented as

$$|\Psi_{\text{FEC}}\rangle = \frac{1}{\sqrt{2-|\Delta|}} (|\Psi_D\rangle - \text{sgn}(\Delta)|\Psi_G\rangle), \quad (3)$$

where $\Delta = 2\langle \Psi_D | \Psi_G \rangle$ [1].

From our previous work [1,54], we note that a FEC state is accessible in systems as small as four fermions ($N = 4$) in eight orbitals ($r = 8$), and from our investigations of condensate behavior on quantum devices, wave functions demonstrating maximal particle-particle condensation [28] and maximal exciton condensation [33], individually, have been identified, prepared, and probed on quantum devices for $N = 4, r = 8$ systems. Using the forms of these wave functions, we construct a state preparation that allows for the entanglement of the nonzero elements of the separate condensates, which is shown in Fig. 2. The input angles (θ_1, θ_2) are then optimized to generate a FEC with the character of both particle-particle and exciton condensations (i.e., a dual maximization of λ_D and λ_G).

See the Methods section of the Supplemental Material for details of state preparations using both the bosonic representation of a qubit—in which each qubit is interpreted as a two-fermion geminal—and the fermionic representation of a qubit—in which each qubit is interpreted as a one-fermion orbital—as well as the optimization procedure for the input angles. Also note that—as in Ref. [28]—in our fermionic preparation, the pairing of qubits causes the usual difference between fermion and qubit statistics to disappear and hence allows for the direct representation of electron pairs on the quantum computer.

III. RESULTS

Using the bosonic state preparations with input angles that span the region exhibiting dual condensate character, we prepare a FEC on a five-qubit quantum device [66]. As can be seen in Fig. 3(a), with the blue x's representing device data before any error mitigation, various input angles yield quantum states with the signatures of both superconductor (λ_D) and exciton condensate (λ_G) character simultaneously exceeding the Pauli-like bound of one. Moreover, as statistical analysis was conducted with the average and standard deviation determined from a sample size of ten trials per state preparation, these large eigenvalues are not spurious; rather, they are statistically significant within one standard deviation. Further, for several of these unmitigated, experimental FECs, the signature of condensation persists within two standard deviations. (See the Supplemental Material for the standard deviation ranges of the signatures of condensation). Note that divergence from the maximal dual condensate character predicted for these input angles (i.e., the degree to which the reported data deviates from points along the elliptical fit) is likely due to preparation and readout errors on this noisy intermediate-scale quantum (NISQ) computer [67–70]. (See the Supplemental Material for device error specifications).

As shown in Fig. 3(b), using the fermionic state preparation on a noisier, 15-qubit quantum device [71] fails to realize a FEC before error mitigation. Further, as shown in Table I, which presents the λ_D and λ_G values for a range of preparations simulated using four noise models that module errors

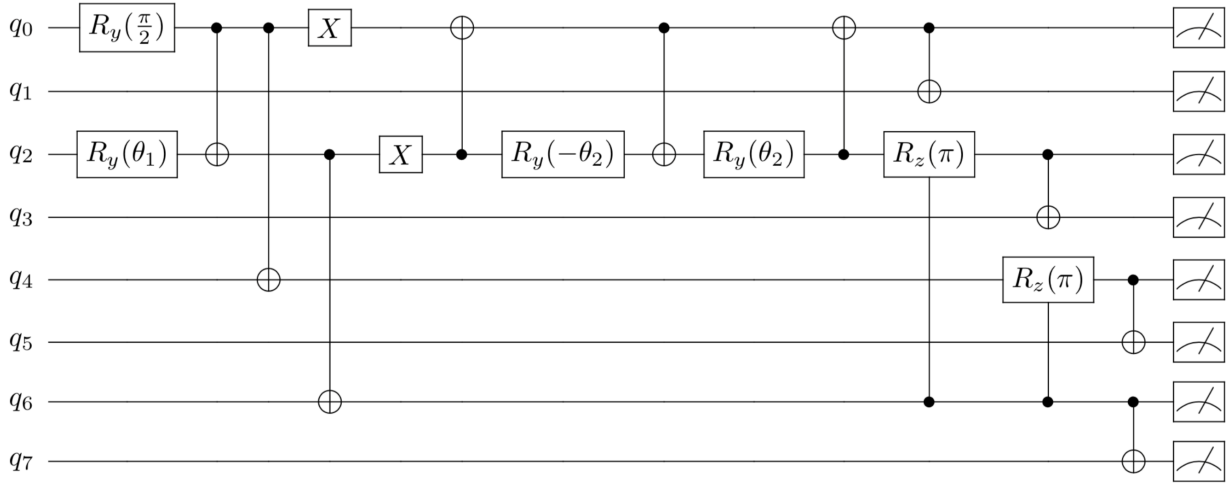


FIG. 2. A schematic demonstrating the fermionic quantum state preparation that yields an entanglement of the nonzero elements of the separate particle-particle and particle-hole condensates [28,33], where R_y and R_z represent rotations about the y and z axes of the Bloch sphere and where two-qubit gates are represented such that the control qubit is specified by a dot connected to the target qubit, which is specified by the appropriate gate. The wave function that results from this state preparation is given in the Supplemental Material. Note that the condensate character—and hence the signatures of condensation λ_G, λ_D —are varied by scanning over input angles (θ_1, θ_2) .

consistent with real-world quantum device back ends, this fermionic preparation would likely not yield FECs on even the newer and less-error-prone Montreal and Mumbai quantum computers. Likely, the four additional two-qubit, CNOT gates introduced into the fermionic state preparation—relative to the bosonic state preparation—introduce a sufficient error to the quantum state such that condensate character is decreased or lost altogether. This is further evidenced by both simulated Montreal and Mumbai being capable of demonstrating dual condensate behavior indicative of a FEC for the bosonic state preparation and by simulated Melbourne demonstrating higher signatures of condensation for the bosonic preparation relative to the fermionic preparation.

To use NISQ devices to better model these FEC phases, we introduce an error mitigation scheme. As can be seen in

the Methods section of the Supplemental Material, the state preparations should yield quantum states with only six of the qubit basis states contributing to the overall wave function. Any contribution from states other than these six basis states are unexpected and are directly caused by errors on the quantum devices (or simulators) employed. As such, we perform an error mitigation technique in which we project contributions from the qubit basis states that are not expected to contribute to zero and renormalize the resultant wave function. As can be seen in Fig. 3 and Table I, using this error mitigation technique improves results from both the fermionic and bosonic preparations. Specifically—as can be readily observed from the green x’s representing the mitigated, projected results in Fig. 3—this projection technique leads to values approximating the ideal dual existence of excitonic

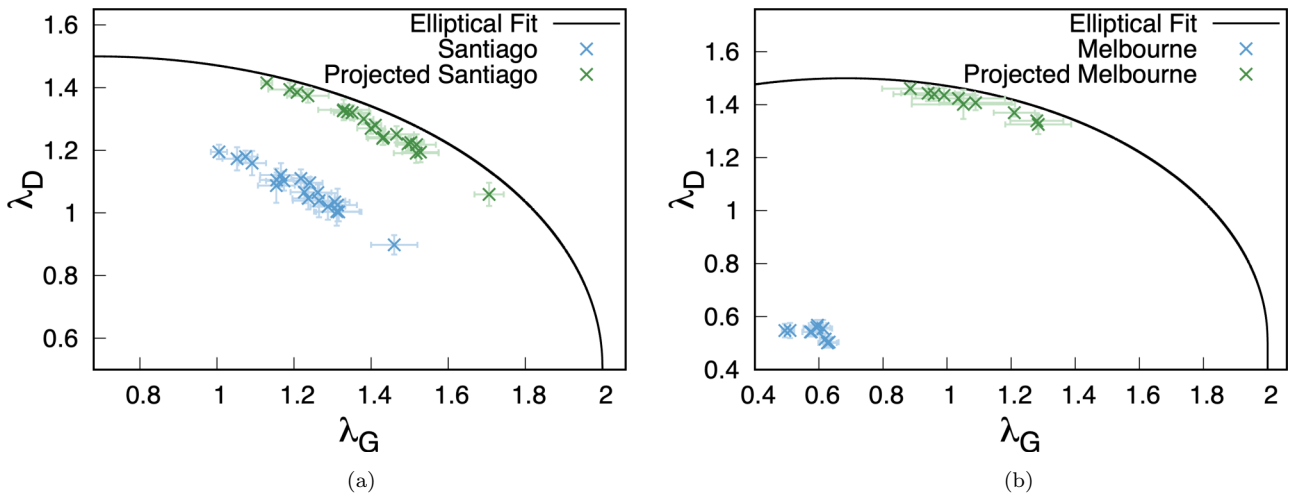


FIG. 3. The eigenvalues of the 2D and ${}^2\tilde{G}$ matrices (λ_D and λ_G , respectively) for various states prepared on IBM Quantum’s (a) Santiago [66] and (b) Melbourne [71] quantum computers before and after error mitigation via projection are plotted against the elliptical fit [1] obtained from the unconstrained scan of λ_D versus λ_G . Note that the average value and standard deviation of ten trials per state preparation are shown.

TABLE I. Table of eigenvalues for the ${}^2\tilde{G}$ (λ_G) and 2D (λ_D) matrices obtained from noise models simulating errors from real-world quantum computers both before (full) and after (projected) error mitigation via projection of appropriate components to zero.

| Computer | quantum volume | Full | | Projected | |
|------------------|--------------------|-------------|-------------|-------------|-------------|
| | | λ_G | λ_D | λ_G | λ_D |
| Fermionic | preparation | | | | |
| Melbourne | 8 | 0.804 | 0.994 | 1.191 | 1.352 |
| | | 0.921 | 0.597 | 1.387 | 1.303 |
| | | 0.934 | 0.581 | 1.440 | 1.271 |
| | | 0.910 | 0.567 | 1.461 | 1.261 |
| Montreal | 128 | 0.918 | 1.134 | 1.169 | 1.329 |
| | | 1.193 | 0.868 | 1.472 | 1.255 |
| | | 1.241 | 0.849 | 1.527 | 1.215 |
| | | 1.267 | 0.824 | 1.580 | 1.176 |
| Mumbai | 128 | 0.866 | 1.051 | 1.217 | 1.334 |
| | | 0.928 | 0.697 | 1.360 | 1.319 |
| | | 0.925 | 0.636 | 1.435 | 1.278 |
| | | 1.113 | 0.721 | 1.537 | 1.212 |
| Bosonized | preparation | | | | |
| Melbourne | 8 | 0.875 | 1.256 | 1.130 | 1.377 |
| | | 1.013 | 0.919 | 1.328 | 1.334 |
| | | 1.077 | 0.906 | 1.409 | 1.289 |
| | | 1.094 | 0.914 | 1.422 | 1.281 |
| Montreal | 128 | 1.126 | 1.281 | 1.244 | 1.310 |
| | | 1.306 | 1.107 | 1.454 | 1.265 |
| | | 1.400 | 1.066 | 1.547 | 1.205 |
| | | 1.406 | 1.041 | 1.567 | 1.188 |
| Mumbai | 128 | 0.934 | 1.295 | 1.138 | 1.364 |
| | | 1.160 | 1.022 | 1.408 | 1.293 |
| | | 1.080 | 0.965 | 1.376 | 1.311 |
| | | 1.233 | 0.990 | 1.497 | 1.238 |
| Santiago | 32 | 1.169 | 1.278 | 1.264 | 1.304 |
| | | 1.344 | 1.130 | 1.465 | 1.260 |
| | | 1.390 | 1.100 | 1.517 | 1.225 |
| | | 1.460 | 1.060 | 1.589 | 1.174 |

and fermionic behavior along the elliptical fit, allowing us to prepare and probe ideal FECs despite significant amounts of error on the NISQ quantum devices.

One interesting aside is that—for both the raw and projected data—the trade-off between the character of a superconductor and that of an exciton condensate first noted in Ref. [1] is also observed here. This trade-off appears to be elliptical in nature—consistent with the convex nature of the 2-RDMs when projected onto two dimensions [72–74]—even for the noisy, nonmitigated Santiago results, and nearly the exact elliptical fit established in Ref. [1] is observed when the contributions from the components that should not contribute are projected to zero. (See Ref. [1] for additional details). This

trade-off is significant as it precludes a FEC with maximal condensate character of both particle-particle and exciton condensations. However, as the trade-off is elliptical in nature and as the maximal λ_D and λ_G values increase with system size (N), the lengths of the major and minor axes of the elliptical fit will increase as the size of the system is increased, causing the trade-off to become less and less stark.

IV. CONCLUSIONS

In this paper, we prepare a FEC—a single quantum state demonstrating both superconductivity and exciton condensation—on a quantum device. This both realizes a highly correlated state of matter on a noisy intermediate-scale quantum device and verifies the theoretical hypothesis from Ref. [1] that such a state can be generated by entangling wave functions that separately exhibit particle-particle and exciton condensation. Further, the error mitigation technique introduced leads to signatures of fermion-pair (λ_D) and exciton condensation (λ_G) approaching the ideal dual existence of excitonic and fermionic behavior along the elliptical fit on NISQ devices, allowing for better modeling of these highly correlated dual condensate phases on even extremely noisy devices.

An experimental system that may result in such an entanglement may be a bilayer system—as bilayers are often known to exhibit exciton condensation—in which the geometric orientation of the layers such as the twist angles are optimized to generate competition between forces favoring an exciton condensate and a superconductor. It may also be possible to consider bilayers in which each layer is composed of a traditional superconductor, which can demonstrate particle-particle condensation. These systems should be studied both computationally and experimentally, as there are many open questions regarding the formation, properties, application, and stability of FECs. The possibility of a hybridization of the properties of superconductors with those of an exciton condensate definitely motivate further examination of this state of matter.

Data will be made available upon reasonable request. Code will be made available on a public Github repository upon publication [75].

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