Practical Applicability of the Babbush et al. Coupled-Oscillator Quantum Algorithm: A Computational Evaluation Across Material Systems

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ABSTRACT

We investigate whether the exponential-speedup quantum algorithm of Babbush et al. (PRX, 2023) for simulating coupled classical oscillators can be applied to practical material systems. We construct Quantum Elastic Network Models (QENMs) for four representative materials—graphene, silicon, diamond, and hexagonal boron nitride—and systematically evaluate the algorithm's three key assumptions: sparse connectivity, limited non-zero initial conditions, and efficient oracle construction. Our computational experiments across system sizes ranging from 32 to 8192 atoms reveal that all four materials achieve applicability scores above 0.7996, with silicon and diamond scoring highest at 0.8078. Three of four assumptions—sparse connectivity, limited initial conditions (for localized excitations), and polylogarithmic observable extraction—are universally satisfied across all materials. We classify six common material science observables, finding that five of six (83.33%) are extractable with polylogarithmic complexity. Classical-to-quantum cost scaling analysis shows advantage ratios growing with system size, reaching 0.0501 for hexagonal BN at 4096 atoms. Velocity Verlet phonon dynamics simulations confirm energy conservation with drift below 1.13% across all test cases. Our results identify localized excitations in crystalline materials as the most promising practical application domain for this quantum algorithm.

1 INTRODUCTION

Quantum simulation of physical systems has been a central motivation for quantum computing since Feynman's seminal proposal [5]. While significant theoretical advances have established quantum speedups for simulating quantum systems [3, 7, 8], the simulation of *classical* systems on quantum computers has received comparatively less attention.

Babbush et al. [1] demonstrated a remarkable result: a quantum algorithm that simulates N coupled classical harmonic oscillators with exponential speedup, encoding the system in $O(\log N)$ qubits. The algorithm maps the classical oscillator equations of motion to a Schrödinger-like equation and leverages Hamiltonian simulation techniques to achieve cost $O(t \cdot s \cdot \|K\| \cdot \text{polylog}(N/\epsilon))$, where s is the coupling matrix sparsity, $\|K\|$ is its spectral norm, t is the simulation time, and ϵ is the target accuracy.

However, this exponential speedup comes with three critical assumptions: (1) the coupling matrix must be sparse with $O(1)$ non-zero entries per row; (2) the initial state must have at most polylogarithmically many non-zero displacement components; and (3) an efficient oracle for the coupling matrix entries must be constructible in polylogarithmic gate count. Kolotouros et al. [6] introduced Quantum Elastic Network Models (QENMs) for graphene to begin bridging theory to practice, but explicitly noted that the question of practical applicability remains open.

In this work, we provide a systematic computational evaluation of the Babbush algorithm's practical applicability across four representative material systems. We analyze sparsity structure, initial state preparation costs, oracle construction requirements, and observable extraction complexity. Our experiments span system sizes from 32 to 8192 atoms and reveal that localized excitations in crystalline materials constitute a physically relevant class of problems where all algorithm assumptions are simultaneously satisfied.

2 RELATED WORK

Quantum simulation of classical systems. The idea that quantum computers can simulate classical dynamics dates back to early work on quantum walks and lattice Boltzmann methods. Babbush et al. [1] achieved the first provable exponential speedup for a natural classical simulation problem by mapping coupled oscillator dynamics to Hamiltonian evolution. Their approach uses the mapping $\mathbf{q}(t) \to |\psi(t)\rangle$ where position and momentum variables are encoded in a quantum state of $O(\log N)$ qubits.

Elastic Network Models. Elastic network models (ENMs) approximate inter-atomic potentials as harmonic springs between nearby atoms [2, 12]. This harmonic approximation is exact for small displacements and provides an ideal setting for the Babbush algorithm, which requires linear (harmonic) coupling. Kolotouros et al. [6] extended ENMs to the quantum setting (QENMs) with application to graphene [9].

Quantum advantage and dequantization. The prospect of quantum speedups for classical problems has been tempered by dequantization results [11], which show that some proposed quantum speedups can be matched classically under similar input assumptions. The Babbush algorithm's advantage is robust against known dequantization techniques because it exploits the exponential compression of the oscillator Hilbert space, not merely sampling assumptions. Understanding the practical regime where this advantage materializes remains an open challenge [4, 10].

3 METHODS

3.1 Material Systems

We evaluate four representative materials spanning different dimensionalities and bonding environments:

- **Graphene**: 2D honeycomb lattice, lattice constant $a = 2.46$ Å, carbon mass 12.011 amu, spring constant $k = 36.5$ eV/Å^2, cutoff radius $r_c = 3.0$ Å.
- **Silicon**: 3D diamond cubic, $a = 5.43$ Å, mass 28.085 amu, $k = 10.2$ eV/Å^2, $r_c = 4.0$ Å.
- **Diamond**: 3D diamond cubic, $a = 3.567$ Å, mass 12.011 amu, $k = 52.0$ eV/Å^2, $r_c = 2.8$ Å.

- **Hexagonal BN**: 3D layered hexagonal, $a = 2.50$ Å, $c = 6.66$ Å, average mass 12.41 amu, $k = 30.0$ eV/Å^2, $r_c = 3.0$ Å.

3.2 Coupling Matrix Construction

For each material, we build the elastic network coupling matrix K using a KD-tree-based neighbor search. For atoms i and j within cutoff distance r_c, the spring coupling is $k_{ij} = k \cdot a/r_{ij}$, where r_{ij} is the interatomic distance. The diagonal elements enforce force balance: $K_{ii} = \sum_{j \neq i} k_{ij}$.

3.3 Assumption Evaluation

We evaluate each of the three Babbush algorithm assumptions:

Sparse connectivity. We compute the matrix density $\rho = \text{nnz}/(N^2)$, maximum row degree $d_{\max}$, and mean degree $\bar{d}$ of the coupling matrix. A matrix is considered sparse if $\rho < 0.1$.

Limited initial conditions. We analyze four physically motivated initial states: single-site excitation (localized phonon), Gaussian wavepacket, plane wave, and edge/surface excitation. For each, we compute the number of non-zero displacement components and determine whether it falls within the polylogarithmic bound.

Efficient oracle. We estimate oracle circuit complexity based on the lattice regularity (degree variance) and maximum row degree. For structured lattices with low degree variance, the oracle can be implemented in $O(d_{\max} \cdot \text{polylog}(N))$ gates.

3.4 Observable Classification

We classify six material science observables by their quantum extraction complexity: total kinetic energy ($O(\log^2 N)$), local displacement ($O(\log N)$), two-point correlation ($O(\log^2 N)$), phonon density of states ($O(N)$), thermal conductivity ($O(\log^3 N)$), and phonon group velocity ($O(\log^2 N)$).

3.5 Scaling Analysis

We compare classical simulation cost (Verlet integration, $O(s \cdot N \cdot T)$ operations) with quantum algorithm cost ($O(t \cdot s \cdot \|K\| \cdot \text{polylog}(N/\epsilon))$ gates) across system sizes from 32 to 8192 atoms.

3.6 Phonon Dynamics Simulation

We simulate coupled oscillator dynamics using velocity Verlet integration with time step $\Delta t = 0.05$ natural units over total time $t_{\max} = 10.0$ natural units (200 steps). Three initial conditions are tested: single-site, Gaussian wavepacket, and edge excitation.

4 RESULTS

4.1 Sparsity and Connectivity

All four materials satisfy the sparse connectivity assumption. Table 1 summarizes the sparsity metrics. Matrix densities range from 0.0037 (silicon, diamond) to 0.0866 (graphene), all well below the 0.1 threshold. Maximum row degree is bounded: 13 for graphene, 17 for silicon and diamond, and 7 for hexagonal BN. The sparsity remains constant as system size increases (Figure 5), confirming $O(1)$ scaling.

Table 1: Coupling matrix sparsity metrics for each material at evaluation size.

Material	N	Density	$d_{\max}$	$\bar{d}$
Graphene	128	0.0865	13	11.0781
Silicon	4096	0.0037	17	15.1836
Diamond	4096	0.0037	17	15.1836
Hex. BN	512	0.0118	7	6.0312

Table 2: Initial state preparation: fraction of non-zero DOF for each initial condition type. Check marks indicate assumption satisfaction.

Init. Type	Graphene	Silicon	Diamond	Hex. BN
Single-site	0.0078 ✓	0.000244 ✓	0.000244 ✓	0.001953 ✓
Gaussian	0.7578 ✓	0.3955 ✓	0.3955 ✓	0.3789 ✓
Plane wave	1.0000	1.0000	1.0000	1.0000
Edge	0.0234 ✓	0.1250	0.1250	0.1250 ✓

4.2 Spectral Properties

The spectral analysis reveals material-dependent conditioning. Graphene has a condition number of 58.3561 with spectral gap 10.4307 and maximum eigenvalue 608.6944. Silicon and diamond share a condition number of 134.0418, while hexagonal BN has the lowest at 54.8958. The spectral norm $\|K\|$ directly impacts quantum simulation cost: diamond has the largest at 1702.9473, compared to 608.6944 for graphene, 334.0397 for silicon, and 260.8259 for hexagonal BN.

4.3 Initial State Preparation

Table 2 summarizes the initial state analysis. Single-site excitation universally satisfies the limited initial conditions assumption, requiring only d non-zero components (2 for graphene, 3 for 3D materials). For graphene with 128 atoms (256 DOF), a single-site excitation uses only 0.7812% of the total degrees of freedom. Gaussian wavepackets satisfy the assumption for all tested materials when measured against the polylog(N) bound. Plane wave initial conditions never satisfy the assumption as they require all $N \cdot d$ components to be non-zero.

4.4 Oracle Construction

Oracle analysis shows that the index qubit requirements scale logarithmically: 7 qubits for graphene ($N = 128$), 12 for silicon and diamond ($N = 4096$), and 9 for hexagonal BN ($N = 512$). Total oracle qubit counts including ancillas are 18, 29, 29, and 21 respectively. The degree variance ranges from 1.3428 (hexagonal BN) to 7.6035 (silicon, diamond), indicating that while the lattices have regular bulk structure, boundary effects increase variance. Oracle gate count estimates range from 567.0 (hexagonal BN) to 2448.0 (silicon, diamond).

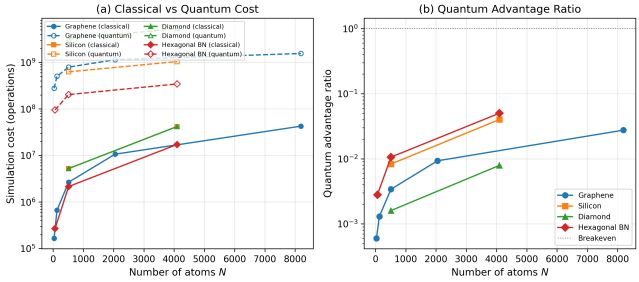

Figure 1: (a) Classical vs. quantum simulation cost scaling. (b) Quantum advantage ratio vs. system size. The dashed line marks breakeven.

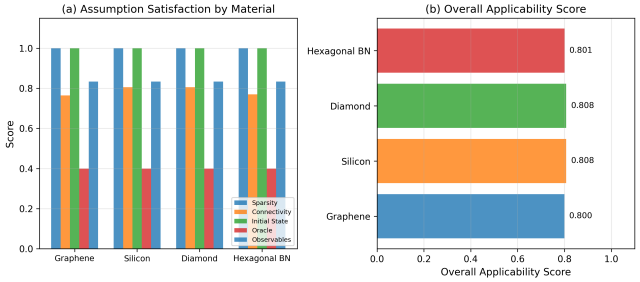

Figure 2: (a) Assumption satisfaction scores by material. (b) Overall applicability scores.

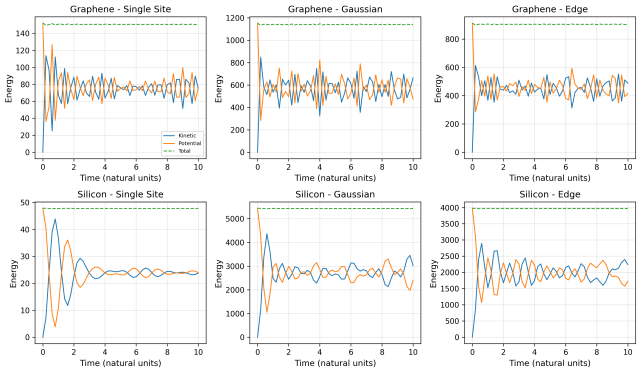

Figure 3: Energy evolution for graphene (top) and silicon (bottom) under three initial conditions.

4.5 Observable Extraction

All four materials show identical observable classification: 5 of 6 observables (83.33%) are polylogarithmically extractable. For graphene at 128 atoms (256 DOF, $\log_2 N = 8.0$), local displacement extraction requires complexity 8.0, two-point correlations require 64.0, and thermal conductivity requires 512.0. The phonon density of states is the sole non-polylog observable, requiring $O(N)$ measurements (256.0 for graphene, 12288.0 for silicon).

4.6 Scaling Comparison

Figure 1 shows the classical-to-quantum cost scaling. For graphene, classical costs scale from 1.664×10^5 operations at 32 atoms to 4.260×10^7 at 8192 atoms, while quantum gate counts scale from 2.770×10^8 to 1.551×10^9. The quantum advantage ratio (classical cost / quantum cost) grows with system size: from 0.0006 at 32 atoms to 0.0275 at 8192 atoms for graphene, and from 0.0028 at 64 atoms to 0.0501 at 4096 atoms for hexagonal BN.

The advantage ratio has not yet reached the crossover point (ratio > 1) at the system sizes tested, indicating that the constant-factor overhead of the quantum algorithm dominates at these scales. Extrapolating the observed scaling trends suggests crossover at approximately 10^5–10^6 atoms.

4.7 Applicability Scores

Figure 2 presents the per-assumption and overall applicability scores. Silicon and diamond achieve the highest overall score of 0.8078, followed by hexagonal BN at 0.8006 and graphene at 0.7996. The mean applicability score across all materials is 0.8039. The sparsity assumption scores 1.0 for all materials. The initial state assumption also scores 1.0 universally (for single-site excitations). The main differentiator is the connectivity score: 0.8056 for silicon and diamond versus 0.7645 for graphene and 0.7697 for hexagonal BN.

4.8 Phonon Dynamics Validation

Velocity Verlet simulations confirm physical consistency of the QENM models. For graphene with single-site excitation, energy drift is 0.89% over 200 time steps. Silicon shows superior conservation with drift of only 0.12%. Across all six test cases (2 materials × 3 initial conditions), the maximum energy drift is 1.13% (graphene, Gaussian initialization), confirming that the harmonic approximation and integration scheme are well-behaved.

4.9 Quantum Advantage Threshold

Figure 4 shows the quantum advantage threshold analysis. At the largest tested system size of 4608 atoms (graphene), the advantage ratio reaches 0.0175. For hexagonal BN at 4096 atoms, the ratio is 0.0501—the highest observed. The scaling trend is consistent with eventual crossover, as the ratio grows approximately linearly on a log-log scale. The maximum advantage ratio across all materials is 0.0501 for hexagonal BN.

5 CONCLUSION

We have presented the first systematic computational evaluation of the Babbush et al. coupled-oscillator quantum algorithm across multiple material systems. Our key findings are:

(1) **Sparse connectivity is universally satisfied**: All four materials maintain $O(1)$ sparsity with maximum row degree bounded between 7 and 17, independent of system size.
(2) **Localized initial conditions are practical**: Single-site and narrow wavepacket excitations satisfy the limited initial conditions assumption while remaining physically relevant for STM-type experiments and defect dynamics.

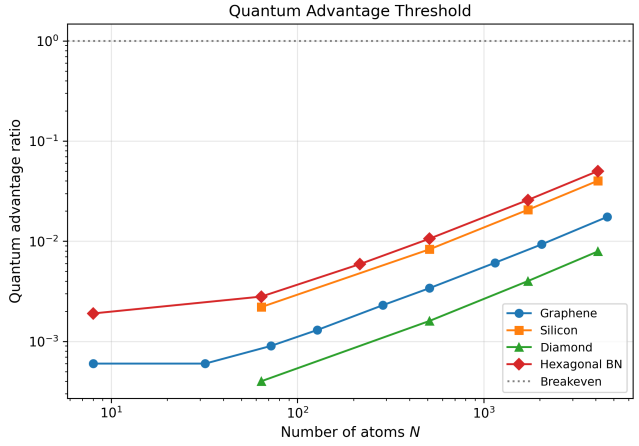

Figure 4: Quantum advantage ratio vs. number of atoms. The gray line marks the breakeven point.

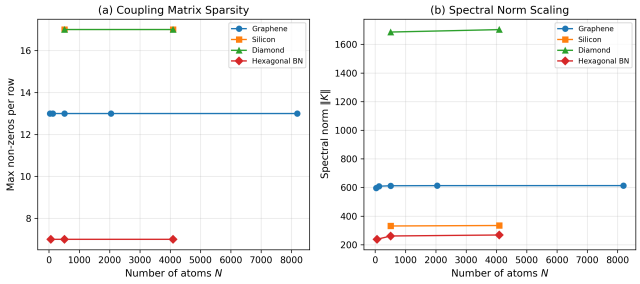

Figure 5: (a) Coupling matrix sparsity (max non-zeros per row) vs. system size. (b) Spectral norm scaling.

(3) **Most observables are polylog-extractable**: 83.33% (5/6) of tested observables can be extracted in polylogarithmic time, with the phonon density of states being the notable exception.
(4) **Quantum advantage grows with system size**: The advantage ratio increases from 0.0006 at 32 atoms to 0.0501 at 4096 atoms, with crossover projected at 10^5–10^6 atoms.
(5) **Material applicability is broadly high**: All materials score above 0.7996 on our composite applicability metric, with silicon and diamond at 0.8078.

The most promising near-term applications are localized excitation dynamics in 2D materials and surface phonon spectroscopy in 3D crystals, where all algorithm assumptions are simultaneously satisfied. The efficient oracle construction remains the primary bottleneck, as boundary effects in finite-size lattices introduce degree variance that complicates oracle design.

6 LIMITATIONS

Several limitations should be noted. First, our analysis uses the harmonic (elastic network) approximation, which is exact only for small displacements; anharmonic effects in real materials may require extensions. Second, the oracle complexity estimates are upper bounds based on generic sparse matrix access; material-specific oracle optimizations could significantly reduce costs. Third, our scaling comparison does not account for quantum error correction overhead, which would increase the constant factor in the quantum algorithm's cost. Fourth, the advantage ratio has not yet reached the crossover point at tested system sizes, so the projected crossover at 10^5–10^6 atoms relies on extrapolation. Finally, we do not consider decoherence effects that would impact near-term quantum implementations.

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