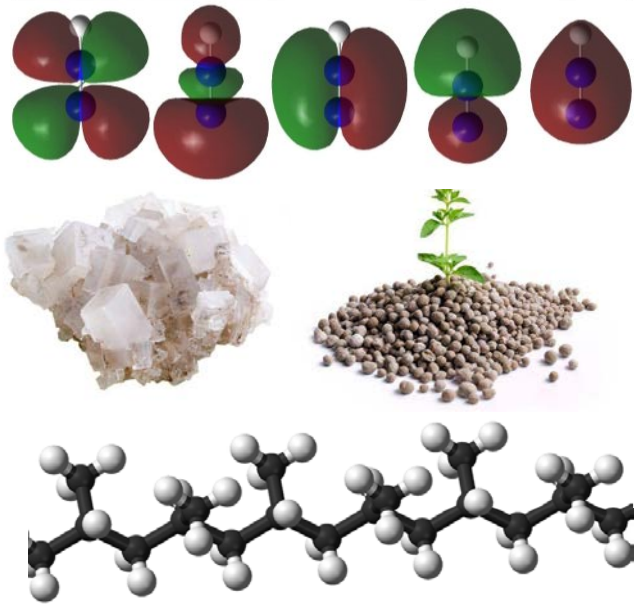
Low Depth Quantum Simulation of Electronic Structure

arXiv:1706.00023



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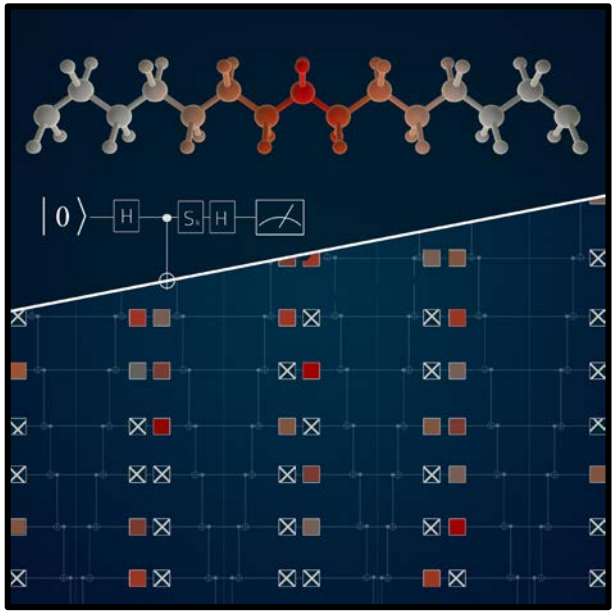
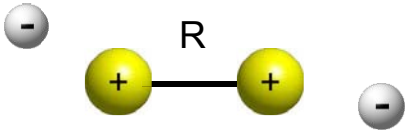


The world is made of atoms. Chemistry arises from interactions of their electrons.

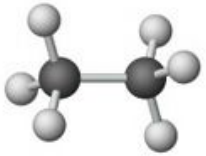
$$H = -\sum_i \frac{\nabla_i^2}{2} + \sum_{i<j} \frac{1}{|r_i - r_j|} + \sum_i U(R, r_i)$$



The electronic structure problem: compute the ground state energy of these systems

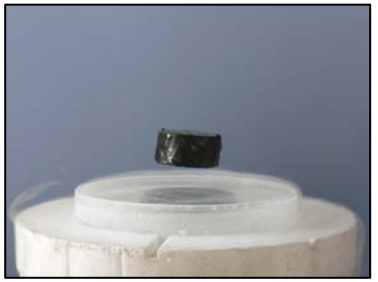
Accurate solutions provide us with rates/mechanisms of chemical reactions

CPU seconds



CPU minutes

CPU days



The prospect of more efficient solutions is both scientifically exciting and valuable

Algorithms for the 2020s and the 2030s face same problems

"Phase estimation to good guess" approach (Aspuru-Guzik 2005) requires error-correction

$$H\left|k\right\rangle = E_k\left|k\right\rangle \qquad e^{-iHt}\left|\psi\right\rangle = \sum_k e^{-iE_k t}\left|k\right\rangle\left\langle k\right|\left.\psi\right\rangle$$

Dominant cost is time-evolution; (Reiher 2017) estimates 10^{15} T gates to solve Fe_2S_2
With error rates at surface code threshold and 1M physical qubits, limit is ~10B T gates
Trotterization bottlenecked by $O(N^4)$ terms in chemistry Hamiltonians

Variational eigensolver for chemistry (Peruzzo 2014) is favored paradigm for near-term

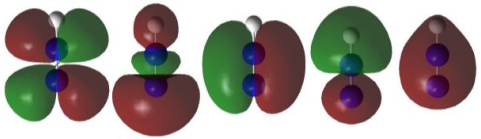
$$\left|\varphi(\vec{\theta})\right\rangle = U_1\left(\theta_1\right)U_2\left(\theta_2\right)\cdots U_n\left(\theta_n\right)\left|\psi\right\rangle \qquad \left\langle\varphi(\vec{\theta})\right|H\left|\varphi(\vec{\theta})\right\rangle \geq \left\langle 0\right|H\left|0\right\rangle$$

Recent experiments (O'Malley 2016, Kandala 2017) represent significant progress
Repetitions required is quadratic in number of Hamiltonian terms (Wecker 2015)
Circuit depth for popular adiabatic state prep ansatz similar to cost of Trotter step

Hamiltonian representation is tied to cost

To represent wavefunctions on computer one must discretize space (confine to grid)
If η electrons confined to N grid points, there are (N choose η) configurations!

Classically it is critical to choose grid where ground state is "compact"
Molecular orbitals (from mean-field solution) are near-optimal for single-molecules

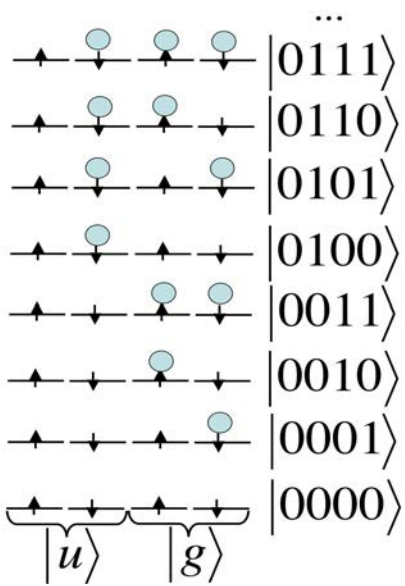


Discretization in MOs leads to O(N^4) Hamiltonian terms at all sizes

$$H = \sum_{p,q} h_{pq}\, a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs}\, a_p^\dagger a_q^\dagger a_r a_s$$

$$h_{pq} = \int dr\, \phi_p^*(r) \left(-\frac{\nabla^2}{2} + U(r) \right) \phi_q(r) \qquad h_{pqrs} = \int dr_1\, dr_2\, \phi_p^*(r_1)\, \phi_q^*(r_2)\, \frac{1}{|r_1 - r_2|} \phi_r(r_2)\, \phi_s(r_1)$$

A spatially disjoint basis leads to O(N^2) terms
But such basis sets are not compatible with Galerkin discretization



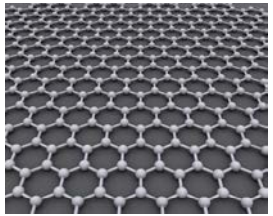
The plane wave basis with N^3 terms

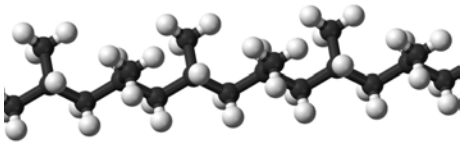
$$\varphi_\nu(r) = \sqrt{\frac{1}{\Omega}} e^{i k_\nu \cdot r}$$

$$k_\nu = \frac{2\pi\,\nu}{\Omega^{1/3}} \qquad V = \frac{2\pi}{\Omega} \sum_{\substack{p \neq q \\ \nu \neq 0}} \frac{c_p^\dagger c_q^\dagger c_{q+\nu} c_{p-\nu}}{k_\nu^2} \qquad V(r_p, r_q) = \frac{4\pi}{\Omega} \sum_{\nu \neq 0} \frac{\cos\left[k_\nu \cdot (r_p - r_q)\right]}{k_\nu^2}$$

Ideal for periodic systems

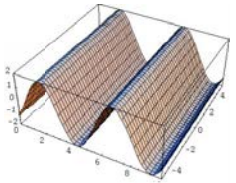
Twice as many PWs required for each non-periodic dimension





What about basis set discretization error?

Asymptotically determined by wavefunction cusps (Kato 1957)



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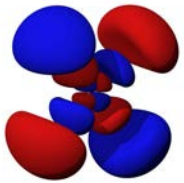


Gaussians centered on nuclei: suppress errors at nuclear cusp as $O(\exp[-\alpha N^{1/2}])$

Pseudopotentials restore analyticity at nuclei: Fourier transform error scales as $O(e^{-\kappa N})$

The real problem is the electron-electron cusp; single-particle bases converge as O(1/N)

The dual basis with N^2 terms

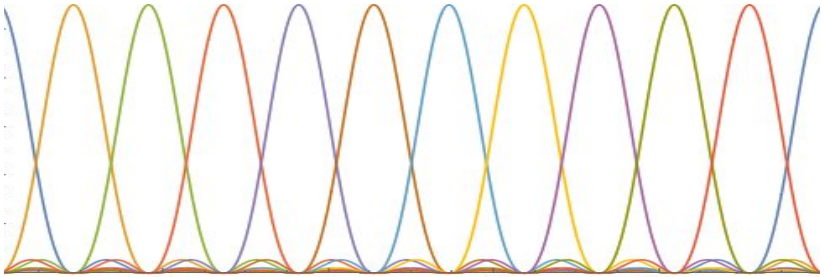
What happens when we Fourier transform the plane wave basis?

We get "dual basis" with diagonal potential and N^2 terms!

$$c_\nu^\dagger = \sqrt{\frac{1}{N}} \sum_p a_p^\dagger e^{-i\, k_\nu \cdot r_p}$$

$$H = \sum_{pq} T_{pq} a_p^\dagger a_q + \sum_p U_p n_p + \sum_{p \neq q} V_{pq} n_p n_q$$

$$V_{pq} = \frac{2\pi}{\Omega} \sum_{\nu \neq 0} \frac{\cos\left[k_\nu \cdot (r_p - r_q)\right]}{k_\nu}$$



Jordan-Wigner Hamiltonian still looks challenging to simulate

$$H = \sum_{p \neq q} \tilde{T}_{pq} \left(X_p Z_{p+1} \cdots Z_{q-1} X_q + Y_p Z_{p+1} \cdots Z_{q-1} Y_q\right) + \sum_{p \neq q} \tilde{V}_{pq} Z_p Z_q + \sum_p \tilde{U}_p Z_p$$

O(N) depth Trotter step possible for H = T + V; T diagonal in plane waves, V diagonal in dual

Fourier transform on mode operators in O(N) depth on planar lattice

We bound number of Trotter steps at $O(N^{5/2})$

Linear Trotter steps by fermionic swap network (arXiv:1711.04789)

$$H = \sum_{p \neq q} \tilde{T}_{pq} \left(X_p Z_{p+1} \cdots Z_{q-1} X_q + Y_p Z_{p+1} \cdots Z_{q-1} Y_q \right) + \sum_{p \neq q} \tilde{V}_{pq} Z_p Z_q + \sum_p \tilde{U}_p Z_p$$

Our strategy makes use of the fermionic swap:

$$f_{\text{swap}}^{p,q} a_p^\dagger \left(f_{\text{swap}}^{p,q} \right)^\dagger = a_q^\dagger \qquad f_{\text{swap}}^{p,q} a_p \left(f_{\text{swap}}^{p,q} \right)^\dagger = a_q$$

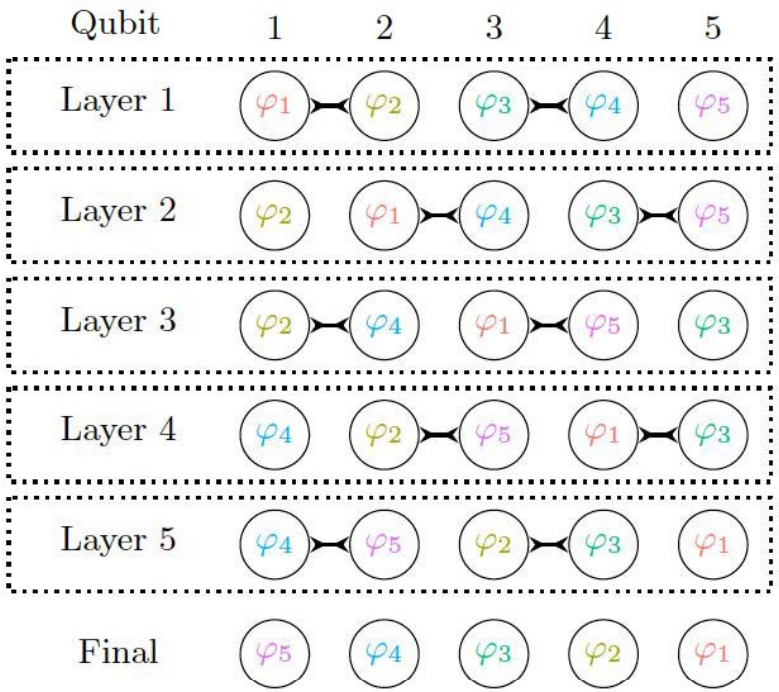
Both fswap and T_{pq} term are 2-local qubit operators if applied to neighbor orbitals under Jordan-Wigner

We can fswap and simulate at the same time:

$$-e^{-iV_{pq}/4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i \sin T_{pq} & \cos T_{pq} & 0 \\ 0 & \cos T_{pq} & i \sin T_{pq} & 0 \\ 0 & 0 & 0 & -e^{iV_{pq}} \end{pmatrix}$$

$N^2/2$ gates, fully parallel on linear array = N depth

Appears optimal even for arbitrary connectivity!



TL;DR: We can also implement arbitrary orbital basis change on linear array in depth N/2!

$O(N^{1/2})$ depth Trotter step / state prep for Hubbard model on linear array

Cost of post-Trotter methods depends on term structure

Post-Trotter methods like Tayor series (Berry 2015) and signal processing (Low 2017) have no explicit polynomial dependence on number of Hamiltonian terms

$$H = \sum_\gamma a_\gamma U_\gamma \qquad \text{SELECT} \left|\gamma\right\rangle \left|\psi\right\rangle = \left|\gamma\right\rangle U_\gamma \left|\psi\right\rangle \qquad \text{PREPARE} \left|0\right\rangle = \sum_\gamma \sqrt{a_\gamma / \lambda} \left|\gamma\right\rangle \qquad \lambda = \sum_\gamma |a_\gamma|$$

With λ t queries to SELECT and 2 λ t queries to PREPARE one can *exactly* implement evolution under arcsin(H) for time t; this is sufficient for PEA (arXiv:1711.10460)

(Babbush 2015) showed SELECT with $\tilde{O}(N)$ gates for molecular orbital chemistry
Costly part is PREPARE because coefficients were determined by integrals

$$\frac{1}{2N} \sum_{\nu,p,q,\sigma} k_\nu^2 \cos\left[k_\nu \cdot r_{q-p}\right] a_{p,\sigma}^\dagger a_{q,\sigma} - \frac{4\pi}{\Omega} \sum_{\substack{p,\sigma \\ j,\nu \neq 0}} \frac{\zeta_j \cos\left[k_\nu \cdot (R_j - r_p)\right]}{k_\nu^2} n_{p,\sigma} + \frac{2\pi}{\Omega} \sum_{\substack{(p,\sigma) \neq (q,\sigma') \\ \nu \neq 0}} \frac{\cos\left[k_\nu \cdot r_{p-q}\right]}{k_\nu^2} n_{p,\sigma} n_{q,\sigma'}$$

Only O(N) unique coefficients; index with O(log N) ancilla; PREPARE costs O(N)
We prove $\lambda = O(N^{8/3})$ but [unpublished] numerics indicate this is very loose!

Summary

By changing the basis we quadratically reduced number of Hamiltonian terms
Non-periodic system (e.g. single molecules) requires constant factor more qubits
We extended quantum simulation methods for this problem to periodic systems

Practical and asymptotic improvements for all known approaches
Best rigorous Trotter PEA circuit size improved from $O(N^8)$ to $O(N^{9/2})$
Best empirical Trotter PEA circuit size improved from $O(\sim N^{5.5})$ to $O(\sim N^{3.5})$ [unpublished]
Best post-trotter PEA circuit size improved from $\tilde{O}(N^5)$ to $\tilde{O}(N^{11/3})$ [empirically loose]
Circuit repetitions for measurements required reduced from $O(N^8)$ to $O(N^4)$
Trotter based variational ansatz reduced from $O(N^5)$ to $O(N)$ depth on linear array

We suggest jellium as target for first useful supremacy in electronic structure
System has deep connections to study of FQHE and DFT, plane waves are optimal
Canonical benchmark for classical methods, unbiased solution intractable at 100 qubits
Trotter/PEA algorithm require fewer than 1 billion T gates [unpublished]

Year	arXiv Number	Representation	Algorithm	Layout	Primitive Depth	Repetitions	Total Depth
2005	quant-ph/0604193	JW Gaussians	Trotter	Arbitrary	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$
2010	1001.3855	JW Gaussians	Trotter	Arbitrary	$\Theta(N^5)$	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$
2012	1208.5986	BK Gaussians	Trotter	Arbitrary	$\widetilde{\Theta}(N^4)$	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$
2013	1304.3061	JW Gaussians	UCC	Arbitrary	$\Theta(N^5)$	Variational	$\Omega(N^5)$
2013	1312.2579	CI Gaussians	Trotter	Arbitrary	$\Theta(\eta^2 N^3)$	$\mathcal{O}(\text{poly}(N))$	$\mathcal{O}(\text{poly}(N))$
2013	1312.1695	JW Gaussians	Trotter	Arbitrary	$\Theta(N^5)$	$\mathcal{O}(N^5)$	$\mathcal{O}(N^{10})$
2014	1403.1539	JW Gaussians	Trotter	Arbitrary	$\Theta(N^4)$	$\mathcal{O}(N^4)$	$\mathcal{O}(N^8)$
2014	1406.4920	JW Gaussians	Trotter	Arbitrary	$\Theta(N^4)$	$\mathcal{O}(\sim N^2)$	$\mathcal{O}(\sim N^6)$
2014	1407.7863	JW Gaussians	Trotter	Arbitrary	$\mathcal{O}(\sim N^3)$	$\mathcal{O}(N^3)$	$\mathcal{O}(\sim N^6)$
2014	1410.8159	JW Gaussians	Trotter	Arbitrary	$\Theta(N^4)$	$\mathcal{O}(\sim N)$	$\mathcal{O}(\sim N^5)$
2015	1506.01020	JW Gaussians	Taylor	Arbitrary	$\widetilde{\Theta}(N)$	$\widetilde{\mathcal{O}}(N^4)$	$\widetilde{\mathcal{O}}(N^5)$
2015	1506.01029	CI Gaussians	Taylor	Arbitrary	$\widetilde{\Theta}(N)$	$\widetilde{\mathcal{O}}(\eta^2 N^2)$	$\widetilde{\mathcal{O}}(\eta^2 N^3)$
2015	1507.08969	JW Gaussians	UCC	Arbitrary	$\Theta(N^4)$	Variational	$\Omega(N^4)$
2016	1509.04279	BK Gaussians	UCC	Arbitrary	$\widetilde{\Theta}(\eta^2 N^2)$	Variational	$\widetilde{\Omega}(\eta^2 N^2)$
2017	1706.00023	JW Plane Waves	Taylor	Arbitrary	$\widetilde{\Theta}(N)$	$\mathcal{O}(N^{2.67})$	$\widetilde{\mathcal{O}}(N^{3.67})$
2017	1706.00023	JW Plane Waves	Trotter	Planar	$\Theta(N)$	$\mathcal{O}(\eta^{1.83} N^{0.67})$	$\mathcal{O}(\eta^{1.83} N^{1.67})$
2017	1706.00023	JW Plane Waves	TASP	Planar	$\Theta(N)$	Variational	$\Omega(N)$
2017	1711.04789	JW Plane Waves	TASP	Linear	$\Theta(N)$	Variational	$\Omega(N)$
2018	Unpublished	JW Plane Waves	Trotter	Linear	$\Theta(N)$	$\mathcal{O}(\sim N^{1.5})$	$\mathcal{O}(\sim N^{2.5})$

TABLE I. N is number of orbitals and $\eta < N$ is number of particles. $\mathcal{O}$ indicates an upper-bound, Ω indicates a lower-bound and Θ indicates both. $\sim$ on top of the bound indicates suppression of polylogarithmic factors and $\sim$ inside of the bound indicates an empirical bound from numerics. Fermionic encodings are abbrivieated as JW (second-quantized Jordan-Wigner), BK (second-quantized Bravyi-Kitaev), and CI (first-quantized Configuration Interaction). Variational ansatze are abbreviated as UCC (Unitary Coupled Cluster) and TASP (Trotterized Adiabatic State Preparation).

Jellium as target for supremacy in electronic structure

The uniform electron gas (jellium) is a canonical benchmark for new classical methods
System has deep connections to study of FQHE and DFT, plane waves are optimal

$$H = \frac{1}{2}\sum_{p,\sigma} k_p^2\, c_{p,\sigma}^\dagger c_{p,\sigma} + \frac{2\pi}{\Omega} \sum_{\substack{(p,\sigma)\neq(q,\sigma') \\ \nu\neq 0}} \frac{c_{p,\sigma}^\dagger c_{q,\sigma'}^\dagger c_{q+\nu,\sigma'} c_{p-\nu,\sigma}}{k_\nu^2}$$

Classically intractable jellium requires about 100 qubits

Trotter/PEA algorithm require fewer than 1 billion T gates

Compelling variational algorithm requires about 150 layers of gates