Quantum computation of Green's functions

Lin Lin

Department of Mathematics, UC Berkeley
Lawrence Berkeley National Laboratory
Challenge Institute for Quantum Computation

QuCQC,
Useful Quantum Computation For Quantum Chemistry

February 2021

Joint work with

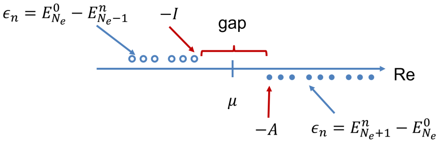
Yu Tong
(Berkeley)

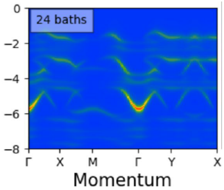
Dong An
(Berkeley → Maryland)

Nathan Wiebe
(Toronto)

Fast inversion, preconditioned quantum linear system solvers, fast Green's function computation, and fast evaluation of matrix functions, (Tong, An, Wiebe, L., 2008.13295)

Spectroscopic information and Green's function





Spectral function, 2D Hubbard model.
$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \operatorname{Im}(G(\mathbf{k}, \omega))$

DMFT calculation: [Mejuto-Zaera, Zepeda-Nunez, Lindsey, Tubman, Whaley, L., 2020]

- Lehmann representation of the single-particle Green's function

$$G(z) = \sum_n \frac{f_n f_n^\dagger}{z - \varepsilon_n + \mathrm{i}\eta \operatorname{sgn}(\varepsilon_n - \mu)}, \quad \eta = 0^+.$$

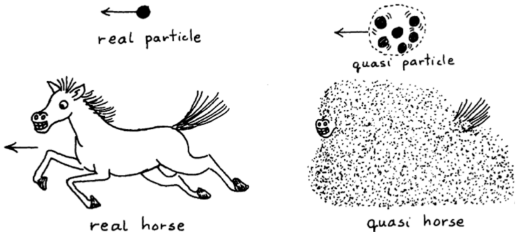
ε_n: quasi-particle energy; f_n: quasi-particle wavefunction

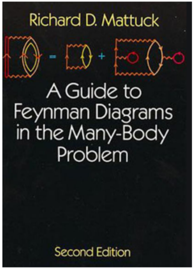
- Poles: ionization potential, electron affinity.

- Many experiments: photoemission spectroscopy; inverse photoemission spectroscopy; ARPES...

Quasi-particle and quasi-horse

"Quasi-horse": bare horse + response of dust (Mattuck, 1976)





Quasi-particle: bare particle + response of material

Quasi-electron: added electron + response

Quasi-hole: removed electron + response ⟸ Photoemission experiment!

Quantum many-body problem

- N sites (spin-orbitals)
- $\hat{a}_i, \hat{a}_i^\dagger, \hat{n}_i$: annihilation, creation, number operator at site i.
- Many-body Hamiltonian (dimension: 2^N)

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{non-interacting}} + \underbrace{\hat{H}_1}_{\text{interacting}}$$

$$\hat{H}_0 = \sum_{ij=1}^{N} T_{ij} \hat{a}_i^\dagger \hat{a}_j, \quad \hat{H}_1 = \sum_{ijkl=1}^{N} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k.$$

- $|\Psi_0\rangle$: ground state with N_e electrons ($N_e \leq 2N$)
  E_0: ground state energy.

Problem we consider: large spectral radius

- Planewave / real space refined spatial discretization: $\left\|\hat{H}\right\| \approx \left\|\hat{H}_0\right\| \gg \left\|\hat{H}_1\right\|$
- Hubbard model, large U limit: $\left\|\hat{H}\right\| \approx \left\|\hat{H}_1\right\| \gg \left\|\hat{H}_0\right\|$
- Schwinger model (Kogut-Susskind, 1975)
- Write $\hat{H} = \hat{A} + \hat{B}$, $\left\|\hat{A}\right\| \gg \left\|\hat{B}\right\|$, but $\hat{A}$ is somewhat easy to manipulate.

Fast Green's function computation

Main result (informal), 2008.13295

$\hat{H} = \hat{A} + \hat{B}$, with $\widetilde{\sigma}_{\min} = \Omega\left(\eta / \left\|\hat{B}\right\|\right)$, and $\left\|\hat{A}\right\| \gg \left\|\hat{B}\right\|$; $|\operatorname{Im}(z)| \geq \eta > 0$ (broadening parameter)

Algorithm	Queries to block-encodings
HHL	$\widetilde{\mathcal{O}}(\frac{|z|+\left\|\hat{H}\right\|}{\eta^3\epsilon^2})$
LCU/QSVT	$\widetilde{\mathcal{O}}(\frac{|z|+\left\|\hat{H}\right\|}{\eta^2\epsilon})$
Our work	$\widetilde{\mathcal{O}}(\frac{\left\|\hat{B}\right\|}{\widetilde{\sigma}_{\min}^2\epsilon})$

HHL,(Harrow-Hassidim-Lloyd, 2009); Linear combination of unitaries (LCU),(Childs-Kothari-Somma, 2017); Quantum singular value transformation (QSVT) (Gilyén-Su-Low-Wiebe, 2019)

Green's function

- Time-ordered single-particle Green's function (or Green's function for short) in the frequency domain: map $\mathbb{C} \to \mathbb{C}^{N \times N}$

$$G(z) = G^{(+)}(z) + G^{(-)}(z).$$

- Advanced ($G^{(+)}$) and retarded ($G^{(-)}$) Green's functions

$$G_{ij}^{(+)}(z) := \left\langle \Psi_0 \middle| \hat{a}_i \left(z - \left[\hat{H} - E_0 \right] \right)^{-1} \hat{a}_j^\dagger \middle| \Psi_0 \right\rangle$$

$$G_{ij}^{(-)}(z) := \left\langle \Psi_0 \middle| \hat{a}_j^\dagger \left(z + \left[\hat{H} - E_0 \right] \right)^{-1} \hat{a}_i \middle| \Psi_0 \right\rangle .$$

- Assume $|\operatorname{Im}(z)| \geq \eta > 0$ (broadening parameter)

Simplest setting: non-interacting system

- $\hat{H} = \hat{H}_0 = \sum_{ij=1}^{N} T_{ij} \hat{a}_i^\dagger \hat{a}_j$.
- Very simple analytic solution via a (small) matrix inversion

$$G_0(z) = (z - T)^{-1} = \sum_n \frac{f_n f_n^\dagger}{z - \varepsilon_n}, \quad T f_n = \varepsilon_n f_n.$$

- Bare Green's function (bare horse)
- With interaction $\hat{H} = \hat{H}_0 + \hat{H}_1$. $G(z)$: quasi-horse
- Self energy (c.f. Frank Wilhelm-Mauch's talk on Monday)

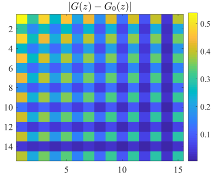
$$\Sigma(z) := G^{-1}(z) - G_0^{-1}(z).$$

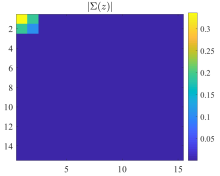
Next simplest setting: quantum impurity

Example: Single-impurity Anderson model (SIAM)

$$\hat{H} = \underbrace{\sum_{\sigma} \epsilon_f \hat{f}_\sigma^\dagger \hat{f}_\sigma + \sum_{\langle j,j'\rangle \sigma} t_{jj'} \hat{c}_{j\sigma}^\dagger \hat{c}_{j'\sigma} + \sum_{j,\sigma} \left(V_j \hat{f}_\sigma^\dagger \hat{c}_{j\sigma} + V_j^* \hat{c}_{j\sigma}^\dagger \hat{f}_\sigma \right)}_{\hat{H}_0} + \underbrace{U \hat{f}_\uparrow^\dagger \hat{f}_\uparrow \hat{f}_\downarrow^\dagger \hat{f}_\downarrow}_{\hat{H}_1}$$

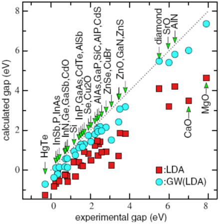
- Perturbation to the Green's function is global.
- Self energy $\Sigma(z)$ is only nonzero on the impurity.
- Foundation of DMFT / CT-QMC etc. "Folk theorem" at least since Feynman (with diagrammatic arguments)
- Non-perturbative proof (for general impurities): [L.-Lindsey, Ann. Henri Poincare 2020]





Computing Green's functions (with general interaction)

- With HF/DFT: essentially a non-interacting picture
- Small $\hat{H}_1$: many-body perturbation theory (MBPT). GF2, GW, SOSEX, GFCC..



van Schilfgaarde et al PRL 96 226402 (2008)

- Large $\hat{H}_1$: exact diagonalization / CI, QMC, DMRG, quantum embedding (DMFT/DMET)..
- Quantum computer

Quantum strategy: direct computation of G

- Brute-force "matrix-matrix-multiplication"

$$G_{ij}^{(+)}(z) := \left\langle \Psi_0 \middle| \hat{a}_i \left(z - \left[\hat{H} - E_0\right]\right)^{-1} \hat{a}_j^\dagger \middle| \Psi_0 \right\rangle := \langle \Psi_0 | A | \Psi_0 \rangle$$

$$A = \hat{a}_i \left(z - \left[\hat{H} - E_0\right]\right)^{-1} \hat{a}_j^\dagger$$

- $\left(z - \left[\hat{H} - E_0\right]\right)^{-1} \hat{a}_j^\dagger \, |\Psi_0\rangle$: quantum linear system problem (QLSP)

Compare the complexities of QLSP solvers

Significant progress in the past few years: Near-optimal complexity matching lower bounds. All with the promise of $\mathrm{poly}(N)$ complexity for matrix of size 2^N.

Algorithm	Query complexity	Remark
HHL,(Harrow-Hassidim-Lloyd, 2009)	$\widetilde{\mathcal{O}}(\kappa^2/\epsilon)$	w. VTAA, complexity becomes $\widetilde{\mathcal{O}}(\kappa/\epsilon^3)$ (Ambainis 2010)
Linear combination of unitaries (LCU),(Childs-Kothari-Somma, 2017)	$\widetilde{\mathcal{O}}(\kappa^2\mathrm{polylog}(1/\epsilon))$	w. VTAA, complexity becomes $\widetilde{\mathcal{O}}(\kappa \operatorname{poly}\log(1/\epsilon))$
Quantum singular value transformation (QSVT) (Gilyén-Su-Low-Wiebe, 2019)	$\widetilde{\mathcal{O}}(\kappa^2 \log(1/\epsilon))$	Queries the RHS only $\widetilde{\mathcal{O}}(\kappa)$ times
Randomization method (RM) (Subasi-Somma-Orsucci, 2019)	$\widetilde{\mathcal{O}}(\kappa/\epsilon)$	Prepares a mixed state; w. repeated phase estimation, complexity becomes $\widetilde{\mathcal{O}}(\kappa \operatorname{poly}\log(1/\epsilon))$
Time-optimal adiabatic quantum computing (AQC(exp)) (An-L., 2019, 1909.05500)	$\widetilde{\mathcal{O}}(\kappa \operatorname{poly}\log(1/\epsilon))$	No need for any amplitude amplification. Use time-dependent Hamiltonian simulation.
Eigenstate filtering (L.-Tong, 1910.14596, Quantum 2020)	$\widetilde{\mathcal{O}}(\kappa \log(1/\epsilon))$	No need for any amplitude amplification. Does not rely on any complex subroutines.

Near-optimal algorithm for finding the ground energy

		Preparation (bound known)	Ground energy	Preparation (bound unknown)
U_H	Our work	$\mathcal{O}\left(\frac{\alpha}{\gamma\Delta}\log(\frac{1}{\epsilon})\right)$	$\widetilde{\mathcal{O}}\left(\frac{\alpha}{\gamma h}\log(\frac{1}{\vartheta})\right)$	$\widetilde{\mathcal{O}}\left(\frac{\alpha}{\gamma\Delta}\log(\frac{1}{\vartheta\epsilon})\right)$
	GTC19	$\widetilde{\mathcal{O}}\left(\frac{\alpha}{\gamma\Delta}\right)$	$\widetilde{\mathcal{O}}\left(\frac{\alpha^{3/2}}{\gamma h^{3/2}}\right)$	$\widetilde{\mathcal{O}}\left(\frac{\alpha^{3/2}}{\gamma\Delta^{3/2}}\right)$
U_I	Our work	$\mathcal{O}\left(\frac{1}{\gamma}\right)$	$\widetilde{\mathcal{O}}\left(\frac{1}{\gamma}\log(\frac{\alpha}{h})\log(\frac{1}{\vartheta})\right)$	$\widetilde{\mathcal{O}}\left(\frac{1}{\gamma}\log(\frac{\alpha}{\Delta})\log(\frac{1}{\vartheta})\right)$
	GTC19	$\widetilde{\mathcal{O}}\left(\frac{1}{\gamma}\right)$	$\widetilde{\mathcal{O}}\left(\frac{1}{\gamma}\sqrt{\frac{\alpha}{h}}\right)$	$\widetilde{\mathcal{O}}\left(\frac{1}{\gamma}\sqrt{\frac{\alpha}{\Delta}}\right)$
Extra qubits	Our work	$\mathcal{O}(1)$	$\mathcal{O}(\log(\frac{1}{\gamma}))$	$\mathcal{O}(\log(\frac{1}{\gamma}))$
	GTC19	$\mathcal{O}(\log(\frac{1}{\Delta}\log(\frac{1}{\epsilon})))$	$\mathcal{O}(\log(\frac{1}{h}))$	$\mathcal{O}(\log(\frac{1}{\Delta}\log(\frac{1}{\epsilon})))$

Well-known result: phase estimation; Previous best results: (Ge-Tura-Cirac, 2019)
Our work: (L.-Tong, 2002.12508, Quantum 2020)
h: precision of the ground energy estimate; $1-\vartheta$: success probability
Lower bound for the overlap: $|\langle\phi_0|\psi_0\rangle| \geq \gamma$,
Bounds for the ground energy and spectral gap: $\lambda_0 \leq \mu - \Delta/2 < \mu + \Delta/2 \leq \lambda_1$.

Heisenberg-limited ground state energy estimation for early fault-tolerant quantum computers (L.-Tong, 2102.11340)

Block-encoding

- Quantum gates have to be unitary.
- $A = \hat{a}_i \left(z - \left[\hat{H} - E_0 \right] \right)^{-1} \hat{a}_j^\dagger$ is not unitary.
- Idea: extend n-qubit non-unitary matrix to a $(n+m)$-qubit unitary matrix (Low-Chuang, 2016; called "standard form" initially)

$$U_A \approx \begin{pmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{pmatrix}$$

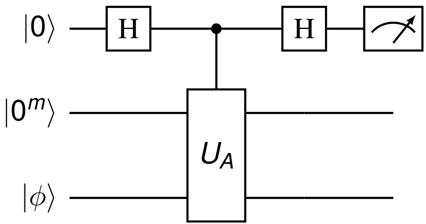
- Many examples of block-encoding: density operators, POVM operators, d-sparse matrices, addition and multiplication of block-encoded matrices (Gilyén-Su-Low-Wiebe, 2019)

Hadamard test for Green's function computation

- If we can block-encode the inverse: $\left(z - \left[\hat{H} - E_0\right]\right)^{-1}$

  $\Rightarrow$ Product of block-encoded matrices
  $A = \hat{a}_i \left(z - \left[\hat{H} - E_0\right]\right)^{-1} \hat{a}_j^\dagger$, call it U_A

- Hadamard test circuit



- Success probability $p(0) = \frac{1}{2}(1 + \mathrm{Re}\,\langle\phi|A|\phi\rangle)$. Similar circuit for the imaginary part.

- Amplitude estimation to improve dependence on ϵ.

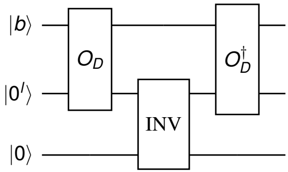
Fast Green's functions computation

Algorithm	Queries to block-encodings
HHL	$\widetilde{\mathcal{O}}(\frac{\lvert z\rvert+\alpha_H}{\eta^3\epsilon^2})$
LCU/QSVT	$\widetilde{\mathcal{O}}(\frac{\lvert z\rvert+\alpha_H}{\eta^2\epsilon})$
Our work	$\widetilde{\mathcal{O}}(\frac{\alpha_B}{\widetilde{\sigma}^2_{\min}\epsilon})$

- $\hat{H} = \hat{A} + \hat{B}$, with $\widetilde{\sigma}_{\min} = \Omega(\eta/\alpha_B)$, and $\left\lVert\hat{A}\right\rVert \gg \left\lVert\hat{B}\right\rVert$.
- Block-encodings in our work involves fast inversion.

Fast inversion of diagonal matrices

- $D = \mathrm{diag}(D_{ii})$: $\left\|D^{-1}\right\| = \min |D_{ii}| = \Omega(1)$, $\|D\| = \max |D_{ii}| \gg 1$
- Assume $O_D \left|i\right\rangle \left|0^l\right\rangle = \left|i\right\rangle \left|D_{ii}\right\rangle, \quad i \in [N]$
- Circuit U_D' for the block-encoding of D^{-1} (classical arithmetic)



- Circuit depth is independent of $\|D\|$

Fast inversion beyond diagonal matrices

- 1-sparse matrices $A = \Pi D$
- Normal matrices $A = VDV^\dagger$

$$U'_A = (V \otimes I_{l+1}) U'_D (V^\dagger \otimes I_{l+1}).$$

- Example:

$$\sum_{\mathbf{x},\mathbf{y},\sigma} T(\mathbf{x}-\mathbf{y}) \hat{a}^\dagger_{\mathbf{x},\sigma} \hat{a}_{\mathbf{y},\sigma} = \mathrm{FFFT} \left(\sum_{\mathbf{G},\sigma} \hat{T}(\mathbf{G}) \hat{c}^\dagger_{\mathbf{G},\sigma} \hat{c}_{\mathbf{G},\sigma} \right) \mathrm{FFFT}^\dagger$$

Preconditioned quantum linear system solver

- Consider

$$(A+B)\left|x\right\rangle \sim \left|b\right\rangle$$

- Preconditioner: A^{-1}

$$(I+A^{-1}B)\left|x\right\rangle \sim A^{-1}\left|b\right\rangle$$

- Condition number:
$\kappa(I+A^{-1}B) \leq \left(1+\|(A+B)^{-1}\|\|B\|\right)\left(1+\|A^{-1}\|\|B\|\right)$

- Circuit depth: independent of $\|A\|$

Green's function computation for fixed N_e

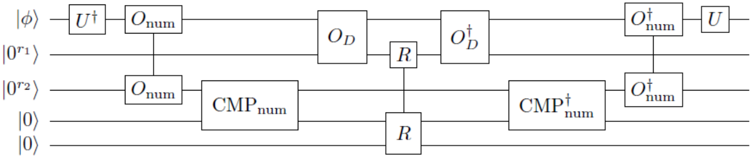
- $[\hat{H}, \hat{P}_{N_e}] = 0$: Preserve the number of electrons N_e ($N_e \ll N$)

- Cost of preconditioned Hubbard solver in second quantization

$$\widetilde{\mathcal{O}}\left(\frac{N^3(\min(|U|,|t|)^3}{\eta^2\epsilon}\log\left(\frac{1}{\delta}\right)\right),$$

- Cost of preconditioned Hubbard solver in second quantization, with N_e scaling

$$\widetilde{\mathcal{O}}\left(\frac{N_e^3(\min(|U|,|t|)^3}{\eta^2\epsilon}\log\left(\frac{1}{\delta}\right)\right),$$



Finite temperature effects (Gibbs state preparation)

- Prepare $\rho_\beta = \frac{1}{Z_\beta} e^{-\beta H}$, $Z_\beta = \mathrm{Tr}(e^{-\beta H})$.
- Purified Gibbs state $|\Psi\rangle = \frac{1}{\sqrt{Z_\beta}} \sum_{x \in [N]} |x\rangle \left(e^{-\beta H/2} |x\rangle\right)$: trace out first register $\quad \Rightarrow \quad$ Obtain ρ_β
- Two new approaches (convert to linear system problems):
  - Cauchy's Contour integral formula:
$$e^{-\beta H} = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma e^{-\beta z} (z - H)^{-1} \,\mathrm{d}z$$
  - Inverse transform:
$$e^{-\beta H} = e^{-\beta (H^{-1})^{-1}}$$

Fast algorithm for preparing $\propto e^{-H}|b\rangle$

	Algorithm	Query complexities
w.o. pre-conditioner	Phase estimation (Poulin-Wocjan, 2009)	$\widetilde{\mathcal{O}}(\frac{\alpha_H}{\xi\epsilon})$
	LCU (van Apeldoorn et al, 2020)	$\widetilde{\mathcal{O}}(\frac{\alpha_H}{\xi}\log(\frac{1}{\epsilon}))$
w. precon-ditioner	This work (contour integral)	$\widetilde{\mathcal{O}}(\frac{\alpha_B}{\xi\widetilde{\sigma}'^2_{\min}}\log(\frac{1}{\epsilon}))$
	This work (inverse transformation)	$\widetilde{\mathcal{O}}\left(\frac{\alpha_B}{\xi\widetilde{\sigma}^2_{\min}}\left[\log\left(\frac{1}{\epsilon}\right)\right]^5\right)$

$\xi = \|e^{-H}|b\rangle\|$, $\widetilde{\sigma}'_{\min} = \Omega(1/\alpha_B)$, $\widetilde{\sigma}_{\min} = \Omega(1/(1+\|(A+B)^{-1}\|\|B\|))$

Acknowledgment

Thank you for your attention!

Lin Lin

https://math.berkeley.edu/~linlin/

U.S. DEPARTMENT OF ENERGY | Office of Science

NSF

CIQC

Google AI Quantum