Nuclear Structure and Reactions using Quantum Computers

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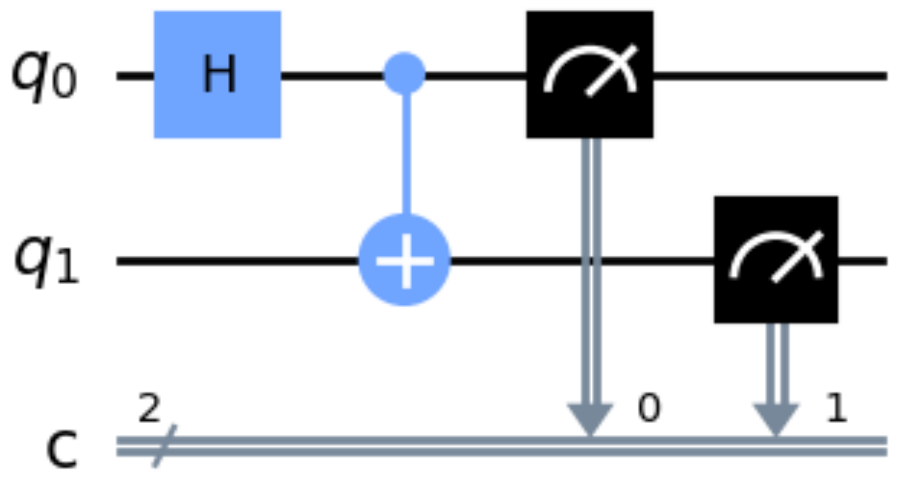
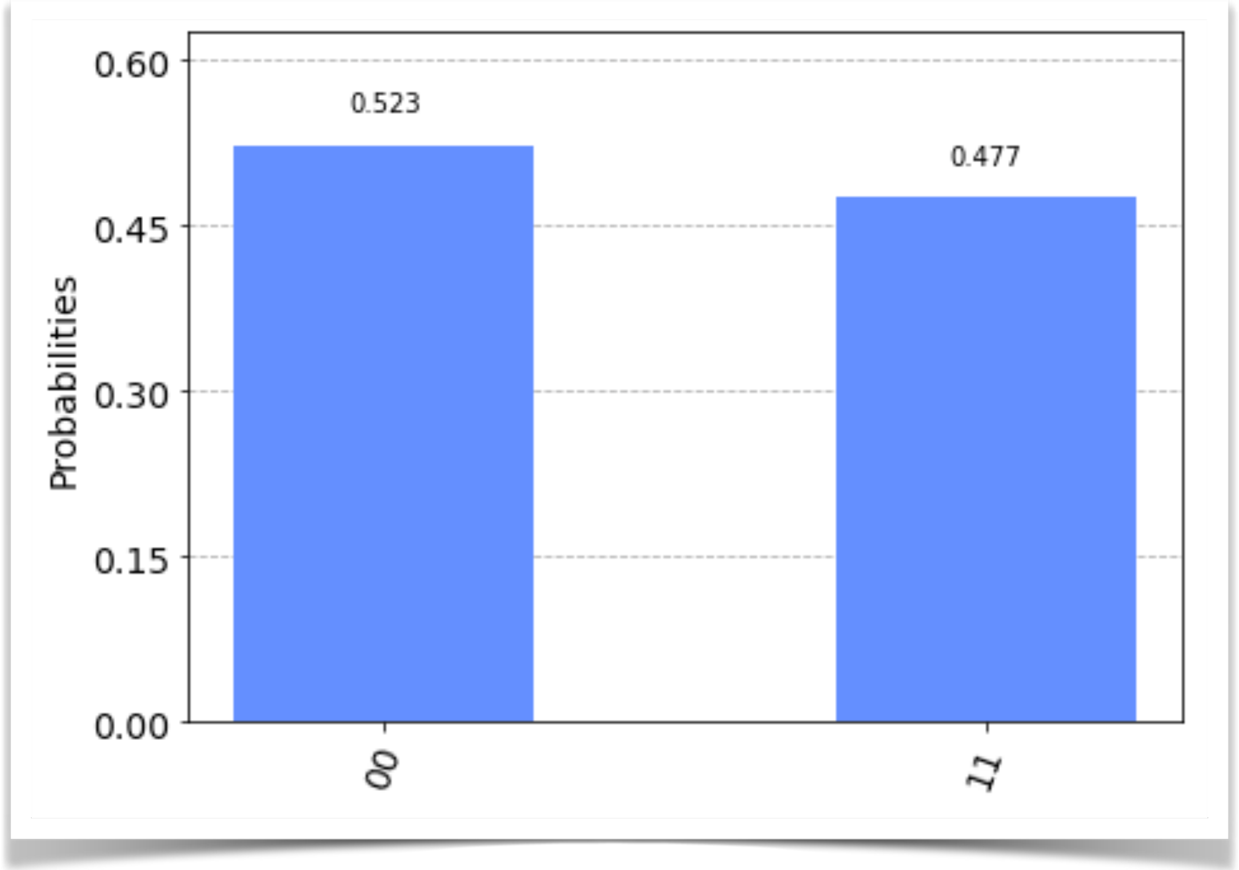
NSF

Quantum Advantage and Challenges

- Realistic many-body classical calculations invariably involve Monte Carlo in imaginary time.
- Fermionic sign problem.
- Loss of real time—-dynamical—-information.



$$\beta_{00} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$



★ Only unitary transformations: Yes, it's Quantum Mechanics. Need paradigm shift in how we do calculations.

★ Qubitization of the theory. Truncating Hilbert spaces, not only space-time, to fit on the qubits.

★ Expensive, noisy hardware: state preparation and unitary evolutions are error prone. Variational methods are inefficient.

Our algorithm is suitable for the NISQ era because it depends on oscillation frequencies in the measurements instead of the amplitude. The former is much less sensitive to noise than the latter.

Fermi's Golden Rule

- Transition matrix element

$$\langle \psi_{\text{final}} | O_T | \psi_{\text{initial}} \rangle$$

determines the rate of many processes of interest in atomic, nuclear and particle physics. They are often accompanied by emission of photons or neutrinos. Ex: $a(b,\gamma)c, a(b,c)d$

- These are the off-diagonal elements of the Hamiltonian

$$H \doteq \begin{pmatrix} \ddots & & & \\ & E_A & \frac{1}{2}\omega_1 & \\ & \frac{1}{2}\omega_1 & E_B & \\ & & & \ddots \end{pmatrix}$$

We have an algorithm to calculate these from the Rabi oscillations that would invariably result from the unitary time evolution on a Quantum Computer.

Algorithm for Inelastic Reactions

The algorithm we propose is as follows:

Counting register

1: Encode the system and add an extra "photon" qubit.

2: Prepare the initial state as $|1\rangle \otimes |E_i\rangle$.

Tensor-product space

3: Evolve initial state with $e^{-iH_T t}$:

$$H_T = \mathbb{1} \otimes H + \frac{\omega}{2}(\mathbb{1} - Z) \otimes \mathbb{1} + c_0\,(\phi^\dagger + \phi) \otimes O_T$$

"Photon" energy

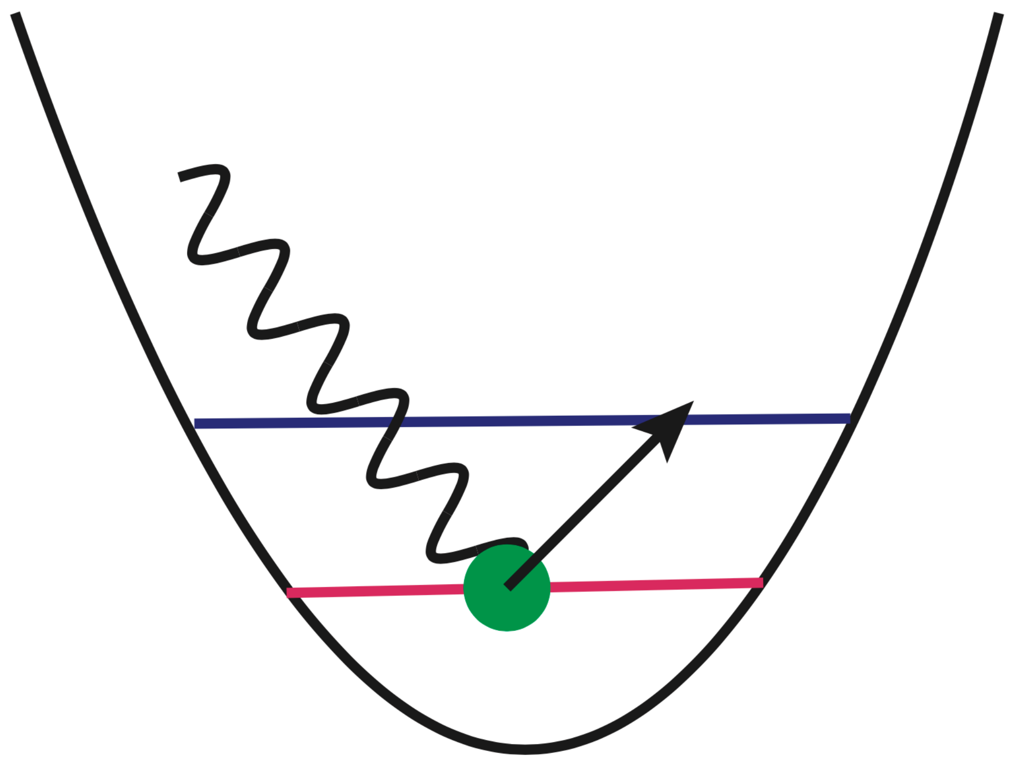
$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

"Photon" creation and annihilation, an X gate

4: Measure the photon qubit.

Bedaque, Khadka, Rupak, Yusf (2025)

E1 Transition Rates from Qulacs Simulations



Details, details, details :

$$m = 940\,\mathrm{MeV}\,,$$
$$\omega_0 = 8\,\mathrm{MeV}\,,$$
$$\sigma = 11\,\mathrm{MeV}\,,$$
$$L = 21\,,\, a = 0.6\,\mathrm{fm}\,.$$

5000 shots

Charge/coupling q we can choose conveniently

It works

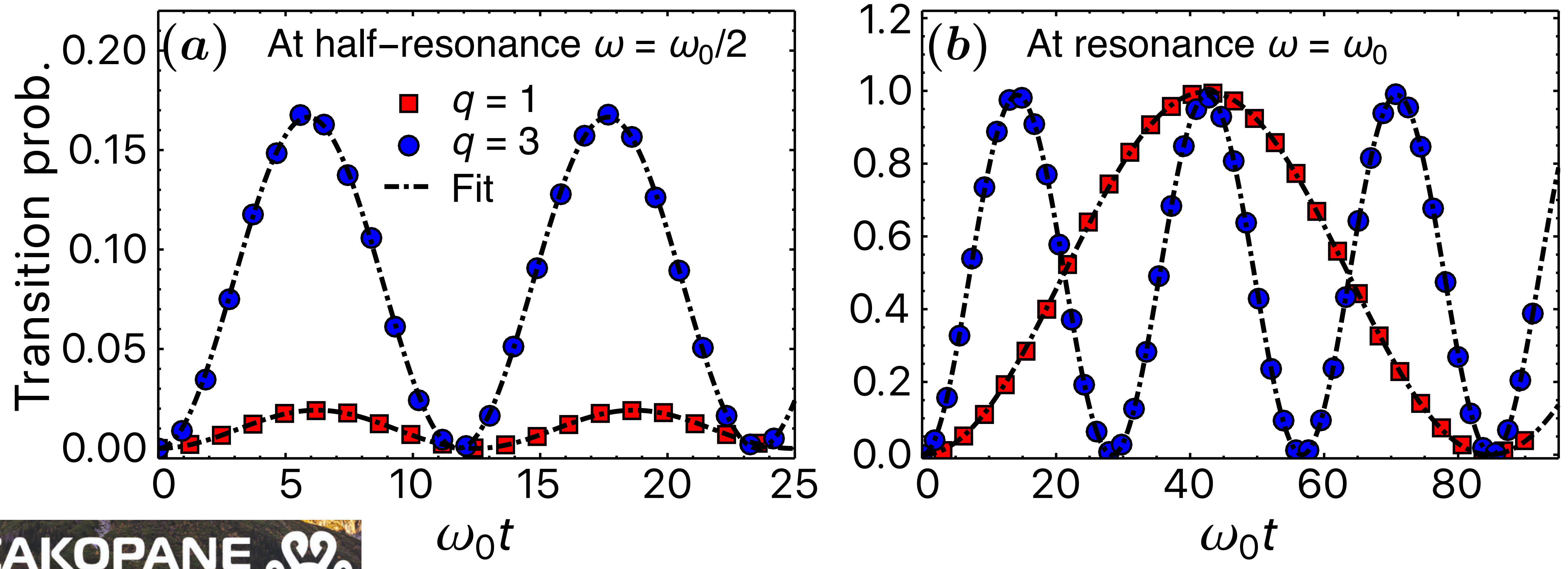
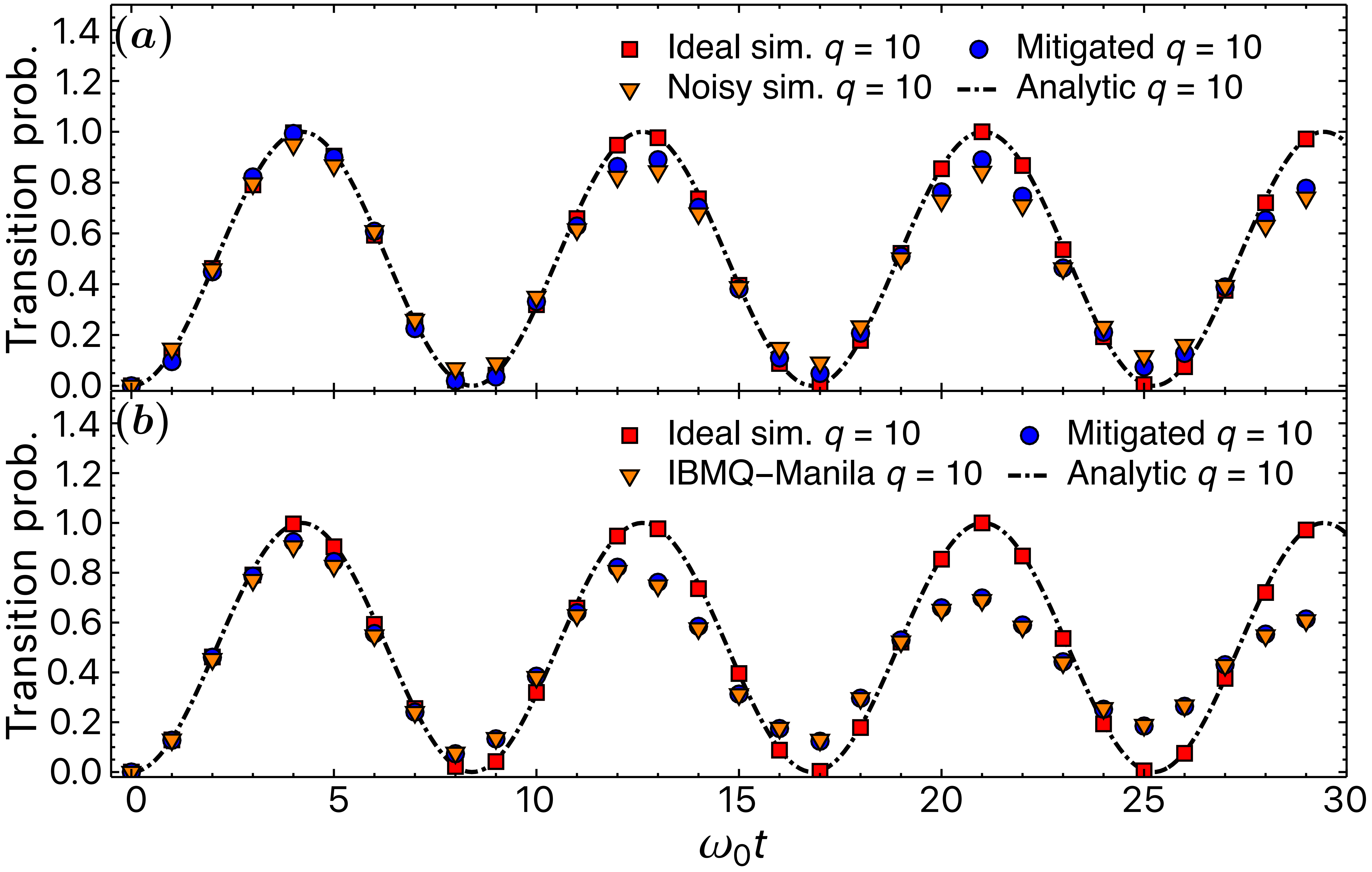


TABLE I. Fit parameter $\Delta\bar{E}$ and $\bar{\omega}_1$ for SHO normalized to expected oscillator frequency $\omega_0 = 8\,\mathrm{MeV}$ and $\omega_1^{(\mathrm{th})}$, respectively. The first set of $(\Delta\bar{E}, \bar{\omega}_1)$ is from fits at $\omega = \omega_0/2$ and the second set with the superscript R is at resonance $\omega = \omega_0$.

q	$\Delta\bar{E}$	$\bar{\omega}_1$	$\Delta\bar{E}^{(R)}$	$\bar{\omega}_1^{(R)}$
1	1.000(6)	0.936(2)	0.996(8)	0.9911(6)
2	0.994(5)	0.967(4)	0.988(11)	0.9866(10)
3	0.987(3)	0.972(3)	0.976(8)	0.9834(9)
4	0.977(2)	0.966(2)	0.961(10)	0.9793(13)
5	0.965(2)	0.958(2)	0.940(10)	0.9735(16)

IBMQ Results



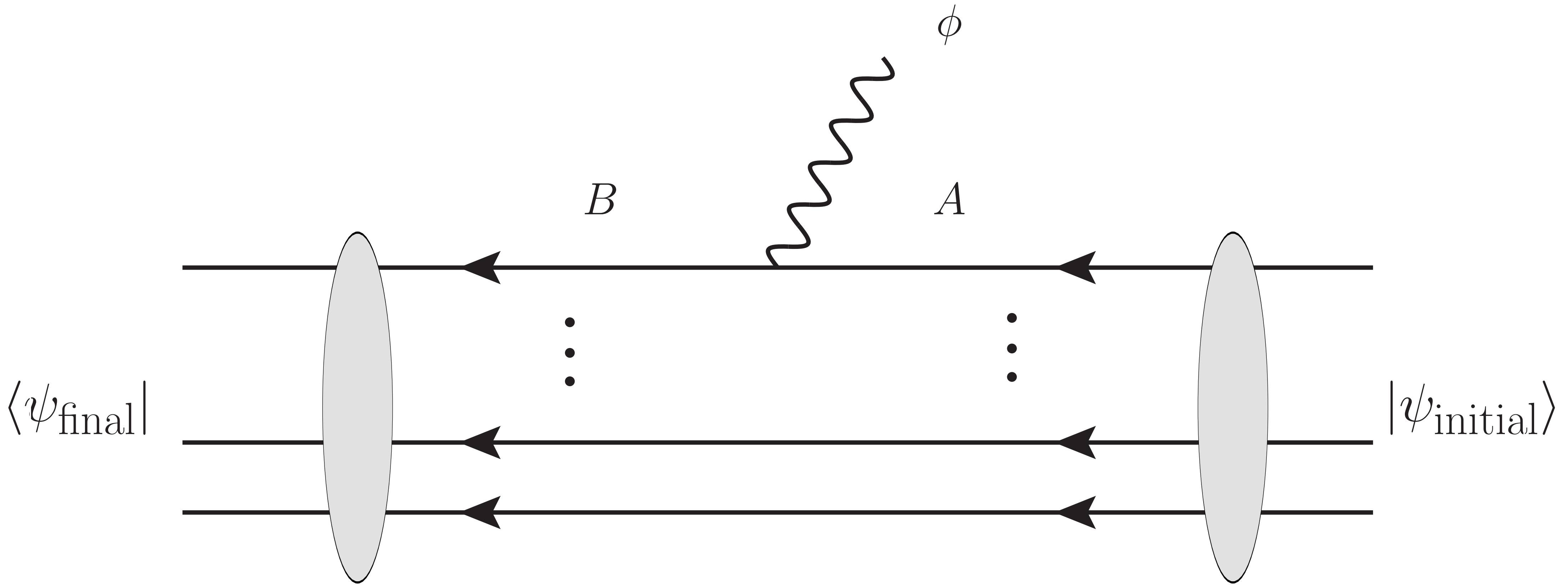
Two-level results from IBMQ-Manila

Qubits 3 and 4 were used for 1024 measurements

Algorithm is robust: Only require the locations of maxima $(2n+1)\pi/t_{\max}$ or minima $2(n+1)\pi/t_{\min}$ for matrix element measurement.

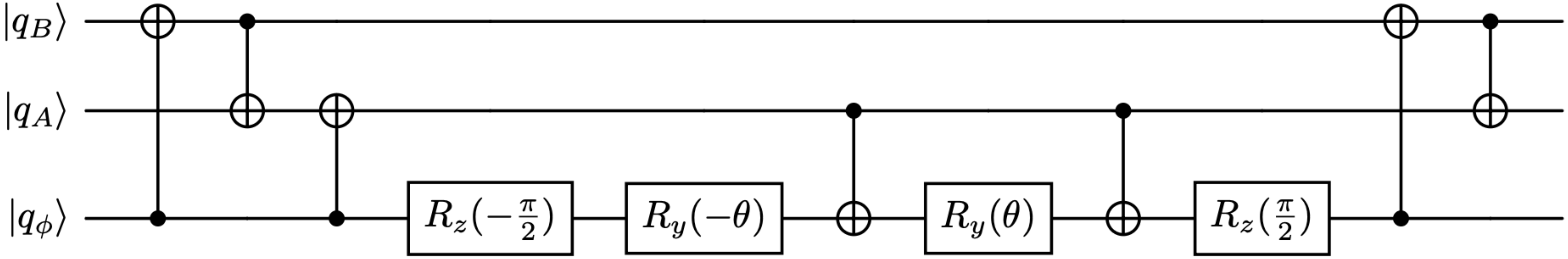
We get $\omega_1^{(\text{meas.})} = 1.03(3)\,\omega_1^{(\text{th})}$

Generic System



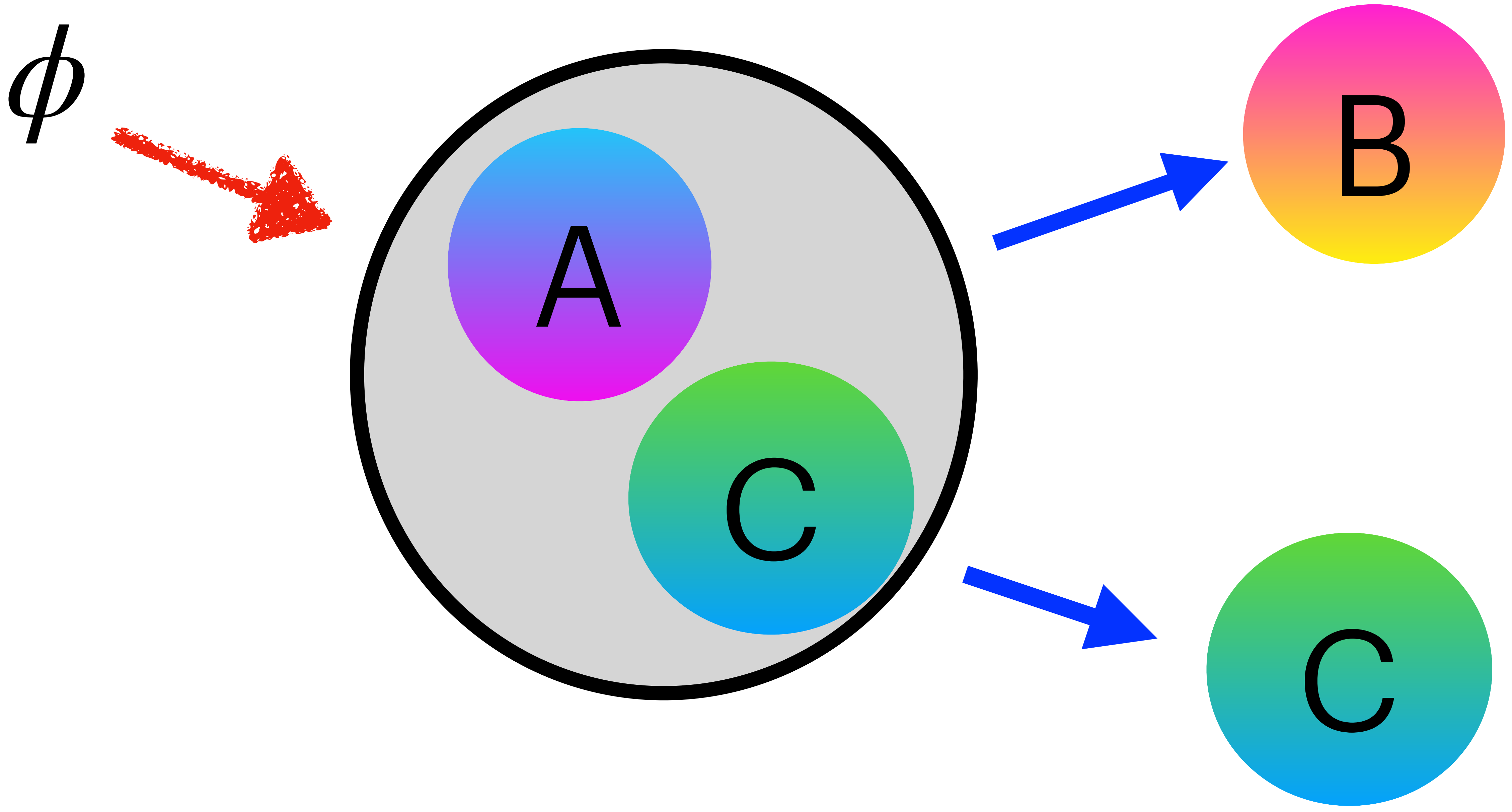
$$X_\phi S_B^\dagger S_A = X_\phi \frac{X_B X_A + Y_B Y_A}{2} \Rightarrow e^{-i\theta X_\phi S_B^\dagger S_A}$$

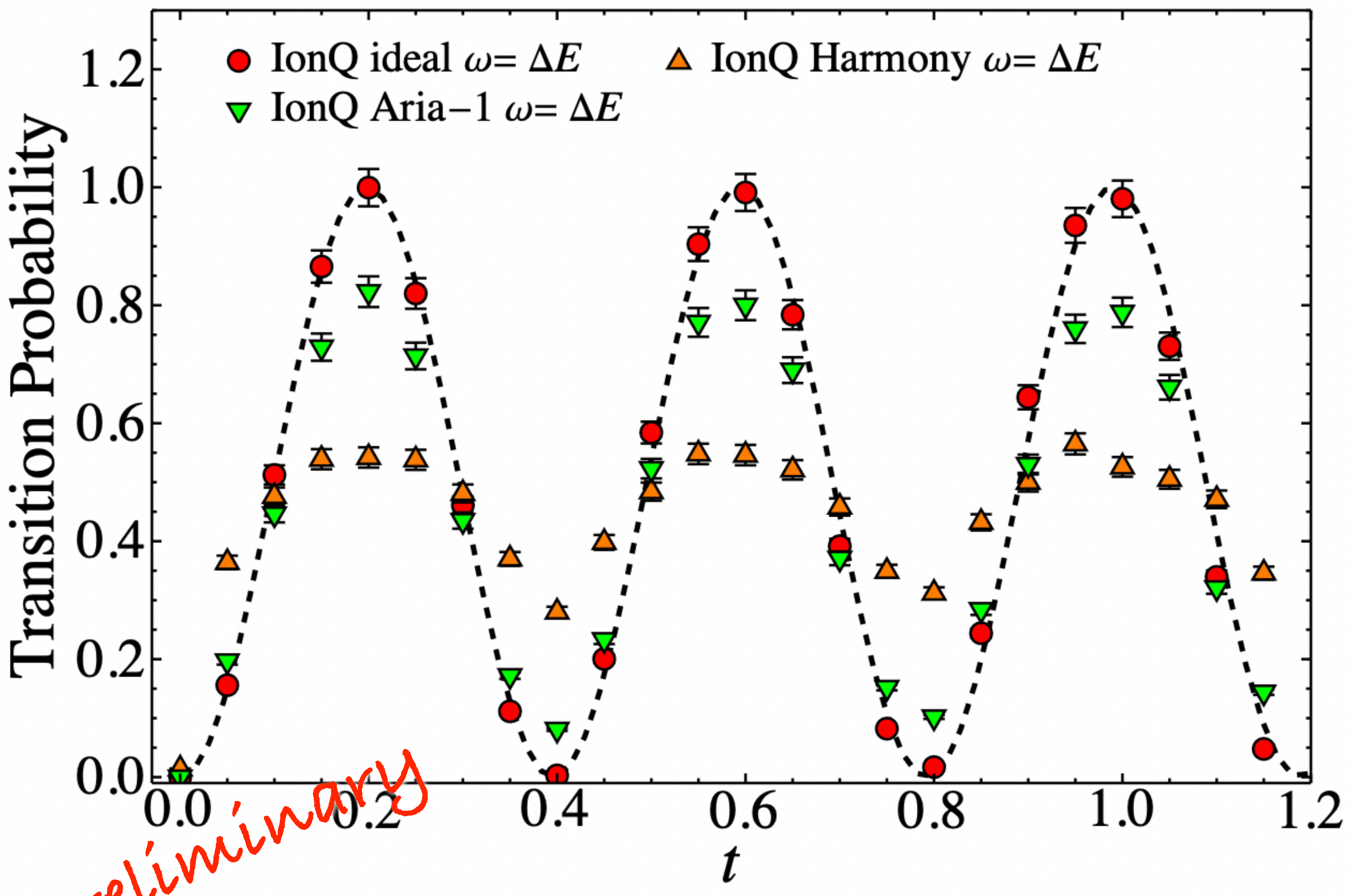
Vatan-Williams (2004)



☑ Advantage of all-to-all connections in trapped ion machines is huge for the “photon”

10-qubit IonQ noisy simulation





Results for bound state to bound state M1 transition with a gap of 1.5 MeV

L	Qubits	CX	1-qubit gate
3	10	70	113
5	16	118	187
9	28	214	335

Bedaque, Rupak (2026)

Mass Gap in Nonlinear $O(3)$ Sigma Model

- Linear sigma model: $\mathscr{L} = \frac{1}{2}\partial_\mu \phi_i \partial^\mu \phi_i - \frac{\lambda}{8}(\phi_i\phi_i - \sigma^2)^2$
- Ground state constant fields, lives on the sphere S^2: $\overrightarrow{\phi} \cdot \overrightarrow{\phi} = \sigma^2$
- Limit $\lambda \to \infty$: All fields, not just in their ground state, satisfy $\overrightarrow{\phi} \cdot \overrightarrow{\phi} = \sigma^2$
- Nonlinear sigma model: $\mathscr{L} = \frac{1}{2g^2}\partial_\mu n_i \partial^\mu n_i$, after rescaling $\overrightarrow{\phi}$

  Known to be asymptotically free Polyakov 1975
- Hamiltonian for qubitization: $\mathscr{H} = \frac{g^2}{2}\Pi_i^2 + \frac{1}{2g^2}(\overrightarrow{\nabla} n_i)^2$

ZAKOPANE CONFERENCE on Nuclear Physics 2026 Extremes of the Nuclear Landscape

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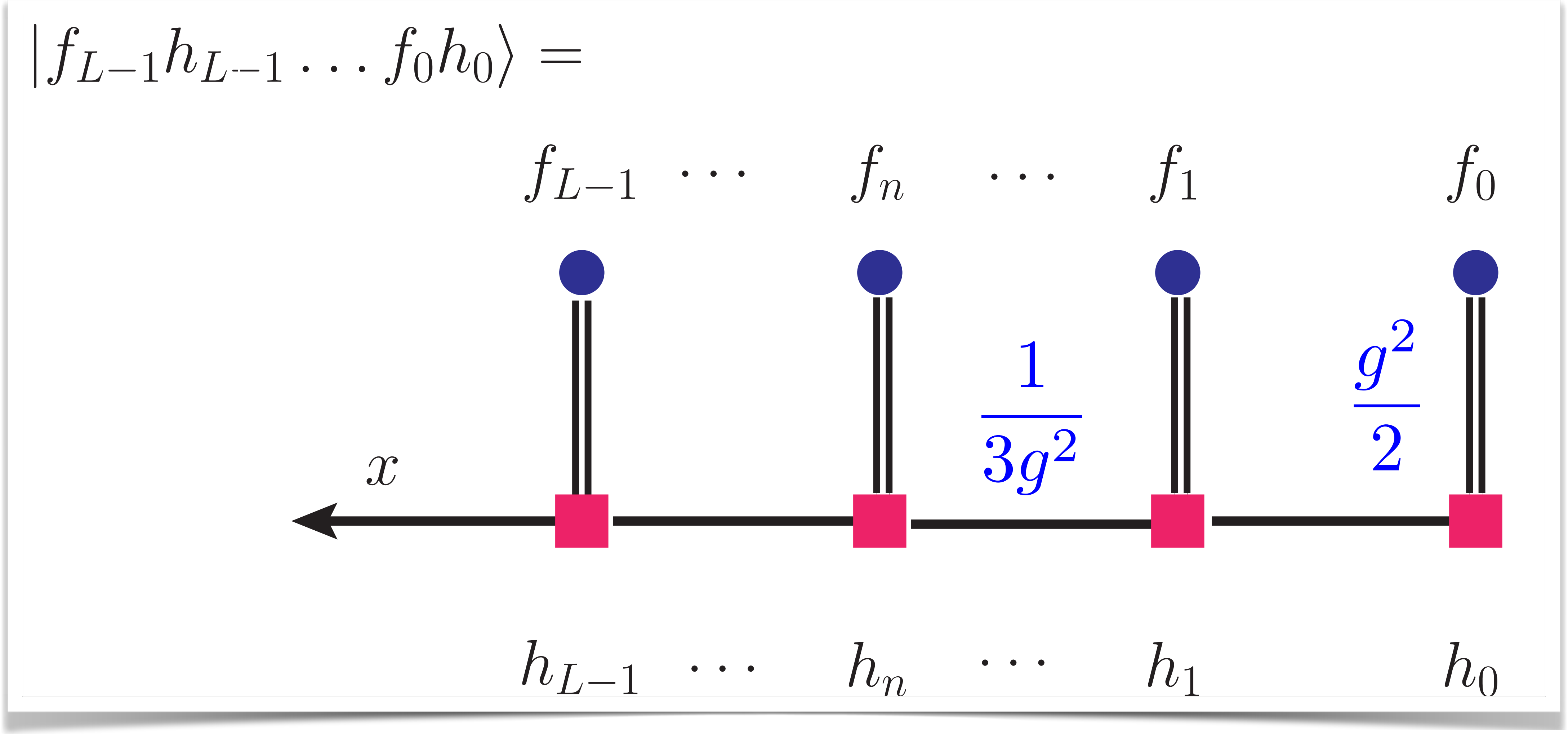
Qubitization of $O(3)$

We need two qubits per lattice site to represent the 4-dimensional Hilbert space.

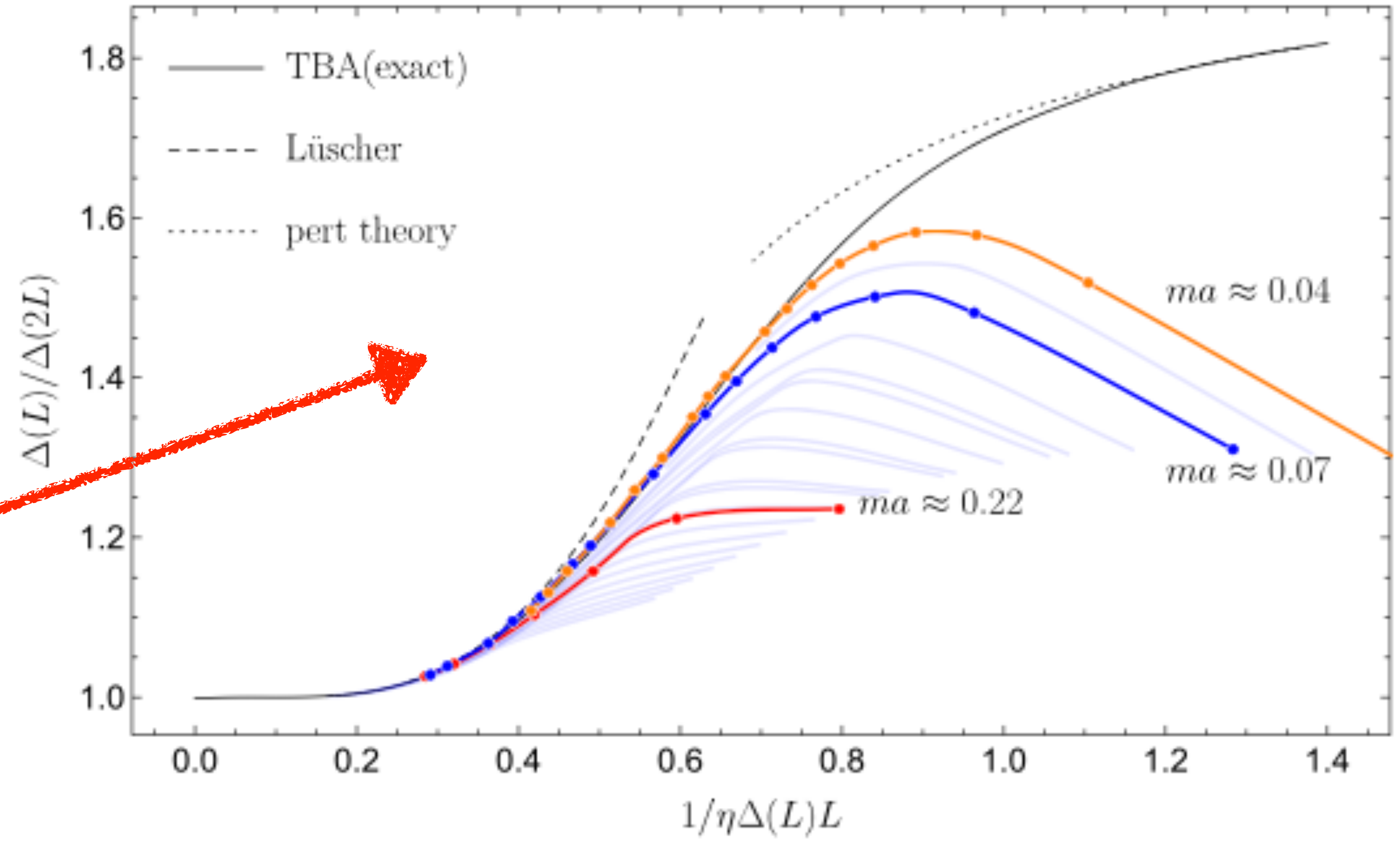
The Hamiltonian in lattice units

$$\hat{H} = \frac{g^2}{2}\sum_{l=0}^{L-1}[X_{2l+1}X_{2l} + Y_{2l+1}Y_{2l} + Z_{2l+1}Z_{2l}]$$
$$+ \frac{1}{3g^2}\sum_{l=0}^{L-1}[X_{2l+2}X_{2l} + Y_{2l+2}Y_{2l} + Z_{2l+2}Z_{2l}]$$

Alexandru, Bedaque, Lamm, Lawrence (2019)
Bhattacharya, Buser, Chandrasekharan (2021)



Do we need to use $j \to \infty$ rep. of $SU(2)$ to recover the continuum limit of nonlinear $O(3)$ sigma model? No!

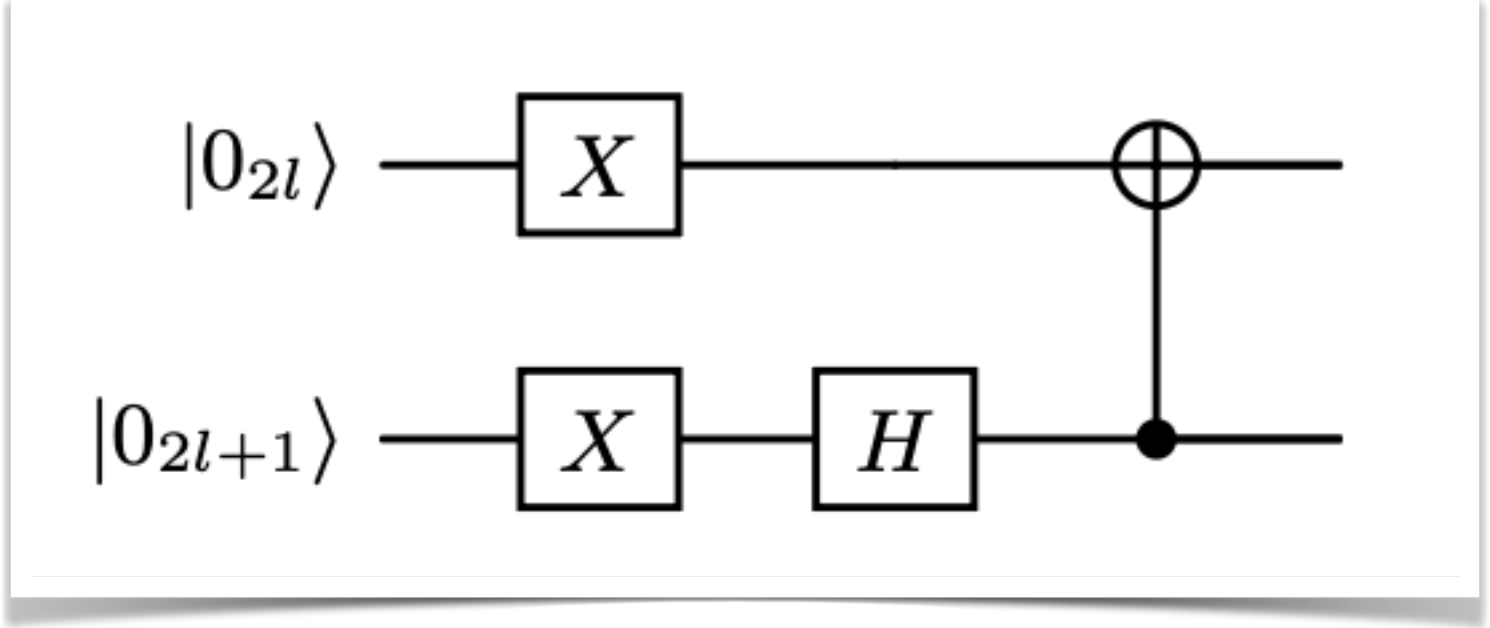


j=1/2 fuzzy theory is in the same universality class as the continuum theory

Alexandru, Bedaque, Carosso, Sheng (2022)

Algorithm for Mass Gap

The algorithm we propose is as follows:



1: Start with approximate ground state. For Example,

$$|\Psi_{\text{strong}}\rangle = \prod_{l=0}^{L-1} \frac{|0_{2l+1}1_{2l}\rangle - |1_{2l+1}0_{2l}\rangle}{\sqrt{2}}, \quad |\Psi_{\text{weak}}\rangle = |\text{antiferro}\rangle \otimes |\text{antiferro}\rangle$$

2: Prepare the initial state as $|\Psi(0)\rangle = \exp(-id\, t_{\text{prep}})|\Psi_{\text{strong/weak}}\rangle$. We need a dipole operator

that couples to the ground and 1st excited state. Doesn't have to be exact. $d = |E_0\rangle\langle E_1| + |E_1\rangle\langle E_0| + \cdots$

3: Evolve initial state with system Hamiltonian $|\Psi(t)\rangle = c_0 e^{-iE_0 t}|E_0\rangle + c_1 e^{-iE_1 t}|E_1\rangle + \cdots$

4: Measure any operator that doesn't commute with the Hamiltonian. For example the dipole operator:

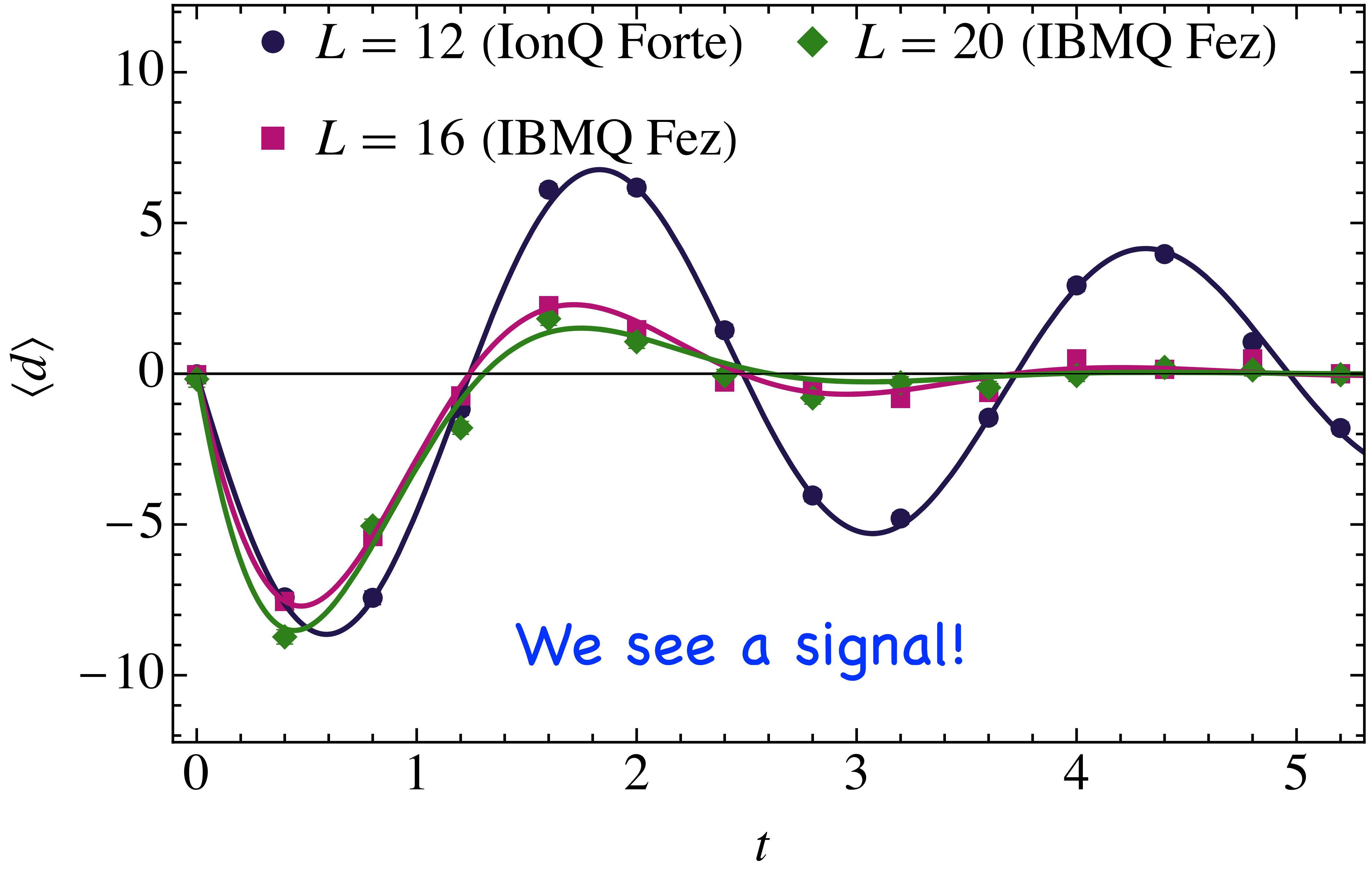
$$\langle\Psi(t)|d|\Psi(t)\rangle = 2\,\text{Re}[c_0 c_1^* e^{i(E_1-E_0)t}]$$

Oscillatory

$$\text{Ehrenfest thm.}: \frac{d}{dt}\langle A\rangle = -\frac{i}{\hbar}\langle [A,H]\rangle$$

Bedaque, Murairi, Rupak, Simonyan (2025)

Strong-coupling $g = 1.2$ result



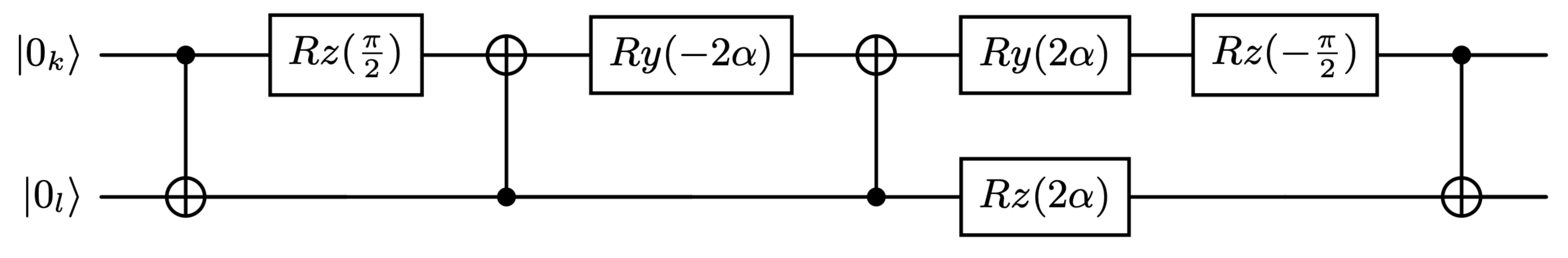


FIG. 3. Circuit for $\exp[-i\alpha(X_l X_k + Y_l Y_k + Z_l Z_k)]$.

$Ae^{-\gamma t} \sin(\omega t)$

TABLE I. Data from IonQ-Forte, IBMQ-Fez Quantum Processor Unit (QPU) and ideal simulator ($L = 12$). The parameters A, γ, ω were obtained from fits to total time $t = 5.2$ at intervals of $\Delta t = 0.4$. We use lattice untis.

L	A	γ	ω	QPU
4	−3.97(17)	0.544(31)	2.64(3)	IonQ
6	−5.45(23)	0.663(36)	2.73(4)	IonQ
8	−7.49(23)	0.534(23)	2.62(2)	IonQ
12	−9.83(21)	0.204(9)	2.54(1)	IonQ
8	−6.80(23)	0.536(25)	2.48(3)	IBMQ
16	−13.12(50)	0.975(45)	2.53(5)	IBMQ
20	−17.47(85)	1.323(72)	2.41(7)	IBMQ
12	−9.87(17)	0.021(6)	2.38(1)	Ideal

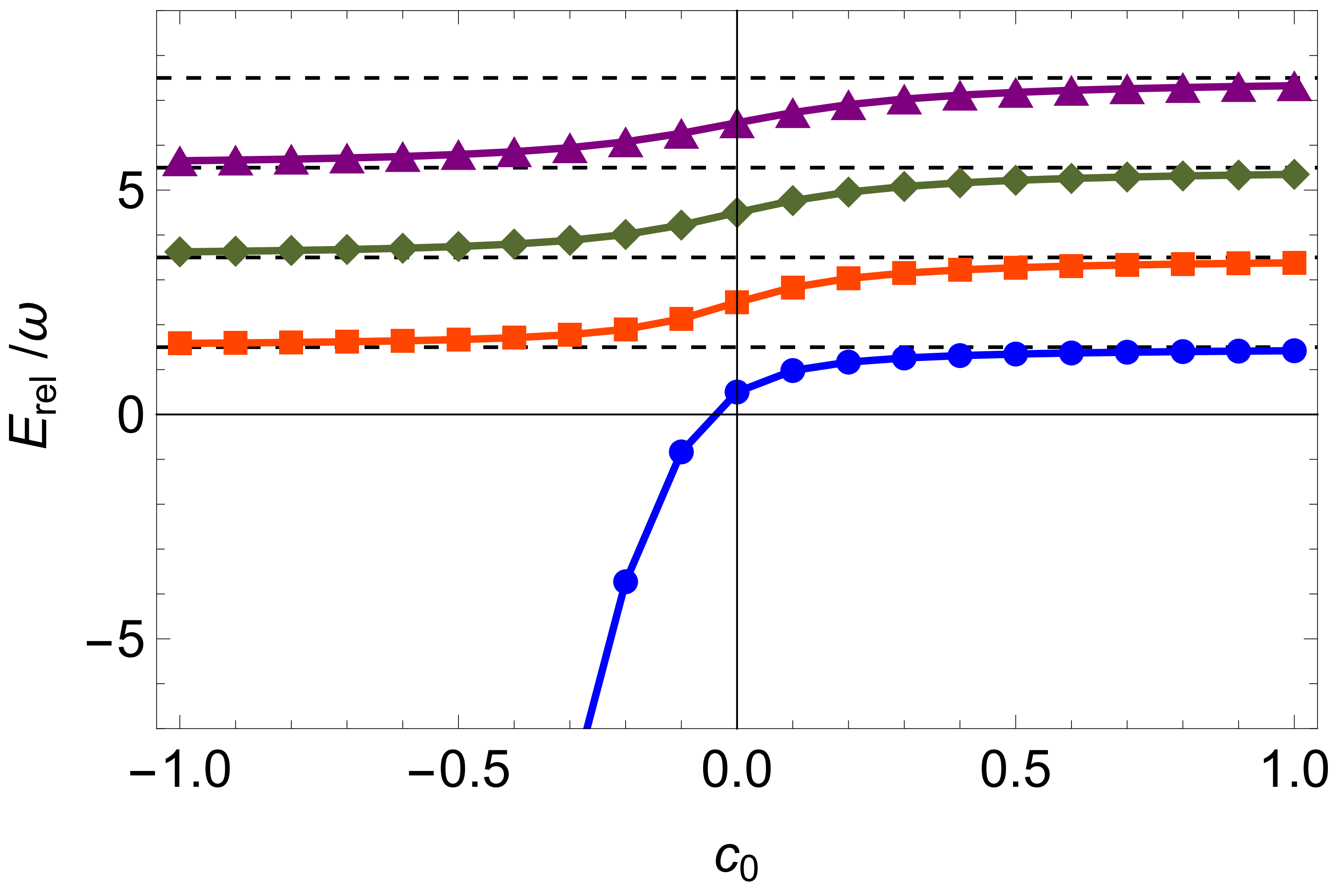
Hilbert space of 2^{40}

How well did we do? Ave $\omega = 2.56(2)$, compared to exact $\omega_{\text{exact}} = 2.34$ from $L \leq 12$ diagonalization

Neutron-Proton Elastic Scattering (1D)

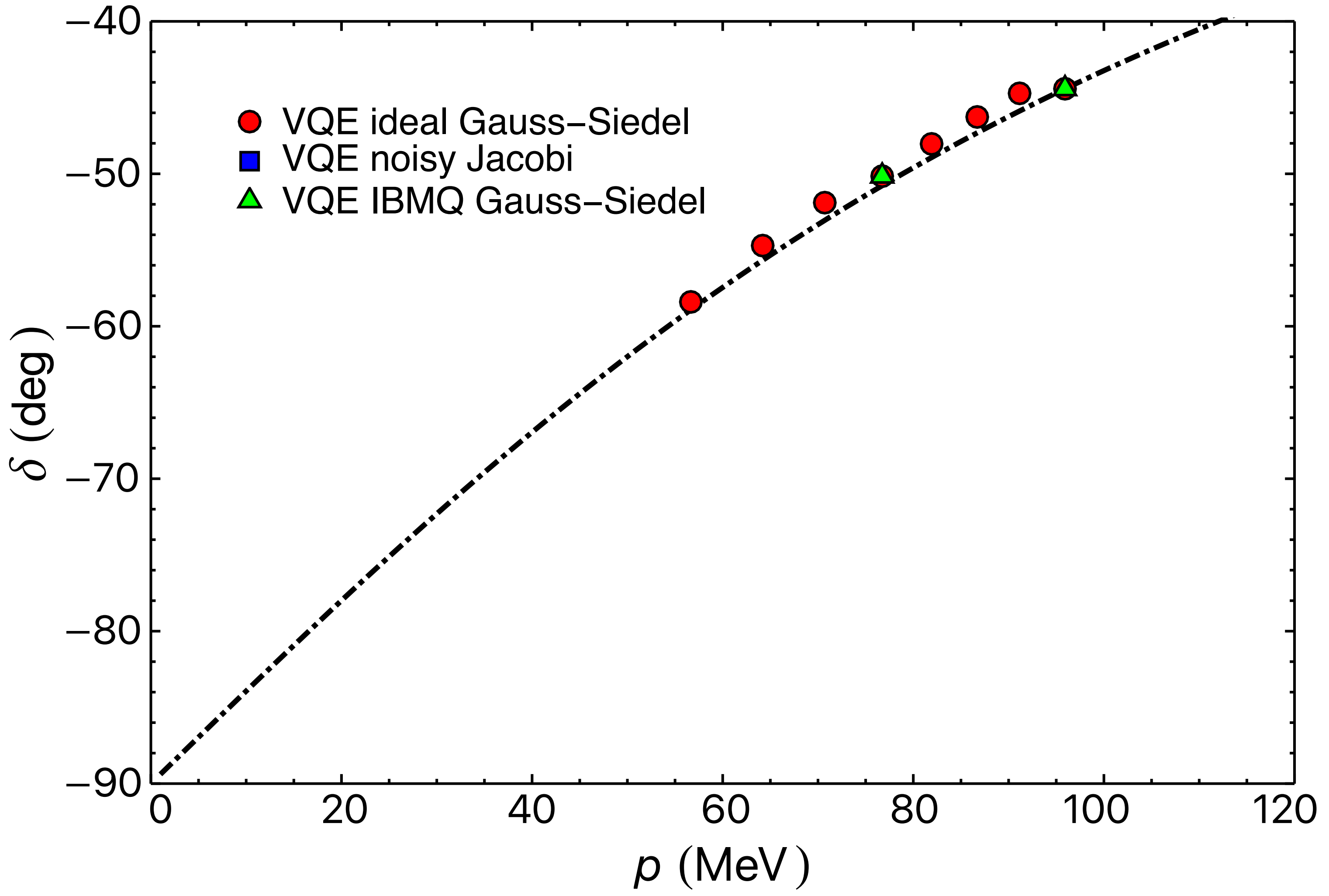
Energy shifts in a harmonic trap (Busch-Englert-Rzażewski-Wilkens)

$$p\cot\delta = -\frac{p^2}{\mu c_0} = \frac{1}{2}\frac{p^2}{\sqrt{\mu\omega}}\frac{\Gamma(\frac{1}{4}-\frac{p^2}{4\mu\omega})}{\Gamma(\frac{3}{4}-\frac{p^2}{4\mu\omega})}$$



Yusf, Gan, Moffat, Rupak (2025)

Hybrid quantum-classical



$$\hat{\Psi}^{(\text{new})}_{i_1,i_2} = \frac{4\hat{h}\langle\hat{\Psi}_{i_1,i_2}\rangle}{4\hat{h}+\hat{V}_{i_1,i_2}-\hat{E}_{\text{total}}}$$

Schroeder (2017)
Jackson, 3rd Ed (1998)

Schmidt decomposition

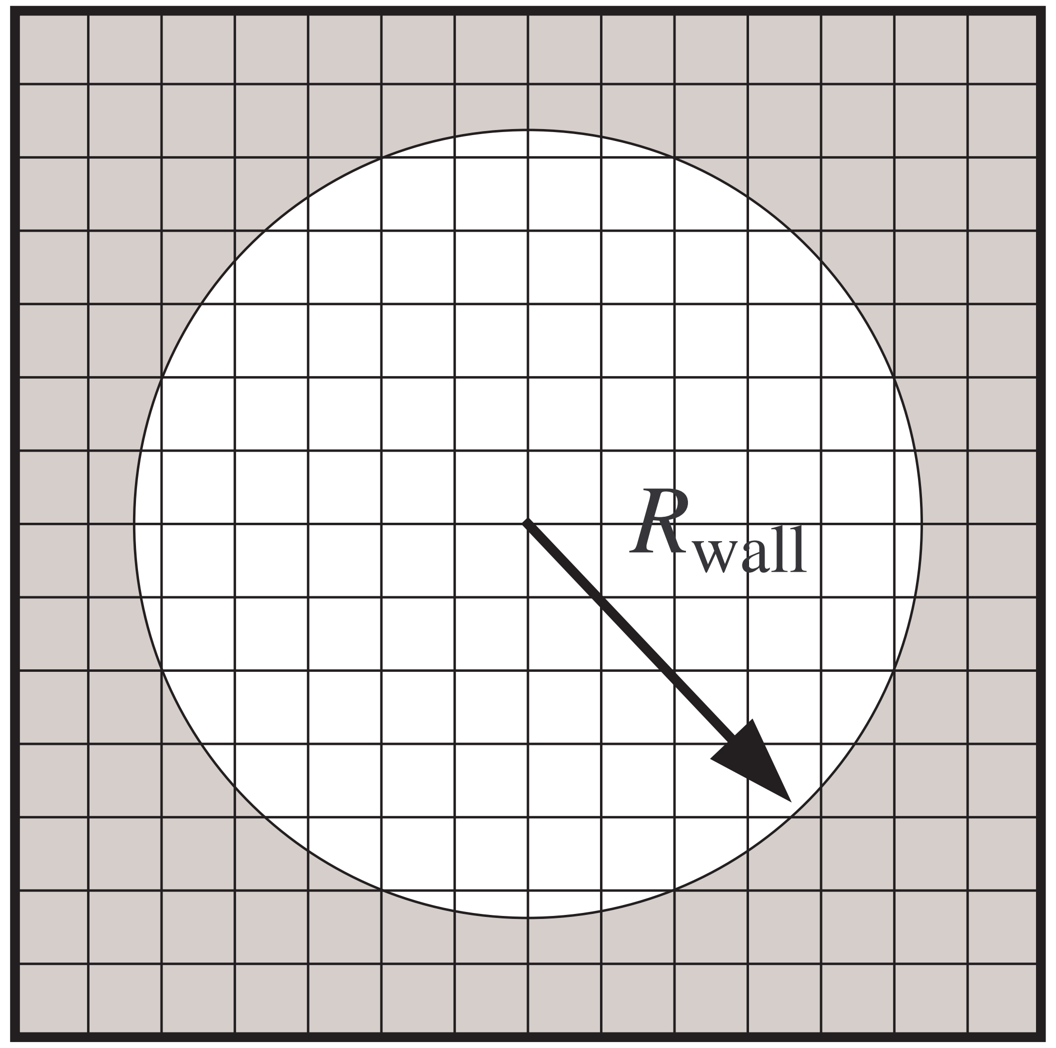
$$|\psi\rangle = \sum_{i=1}^{r\leq A}\lambda_i|i\rangle_A\otimes|i\rangle_B$$

Run	L	b (fm)	ω (MeV)	c_0	Exact (MeV)	Full ideal	Full QPU	SVD ideal	SVD QPU
1	5	1.5	5	0.2	21.33	1.003	1.873	0.9599	1.009
2	13	0.8	10	0.2	22.33	—	—	0.9905	1.459

Proton-Proton s-wave Scattering

Spherical wall

$$\delta_0(p) = \tan^{-1}\left[-\frac{F_0(\eta_p, R_{\rm wall}\, p)}{G_0(\eta_p, R_{\rm wall}\, p)}\right]$$



Brassy, Epelbaum, Krebs, Lee Meißner (2007)

Carlson, Pandharipande, Wiringa (1984)

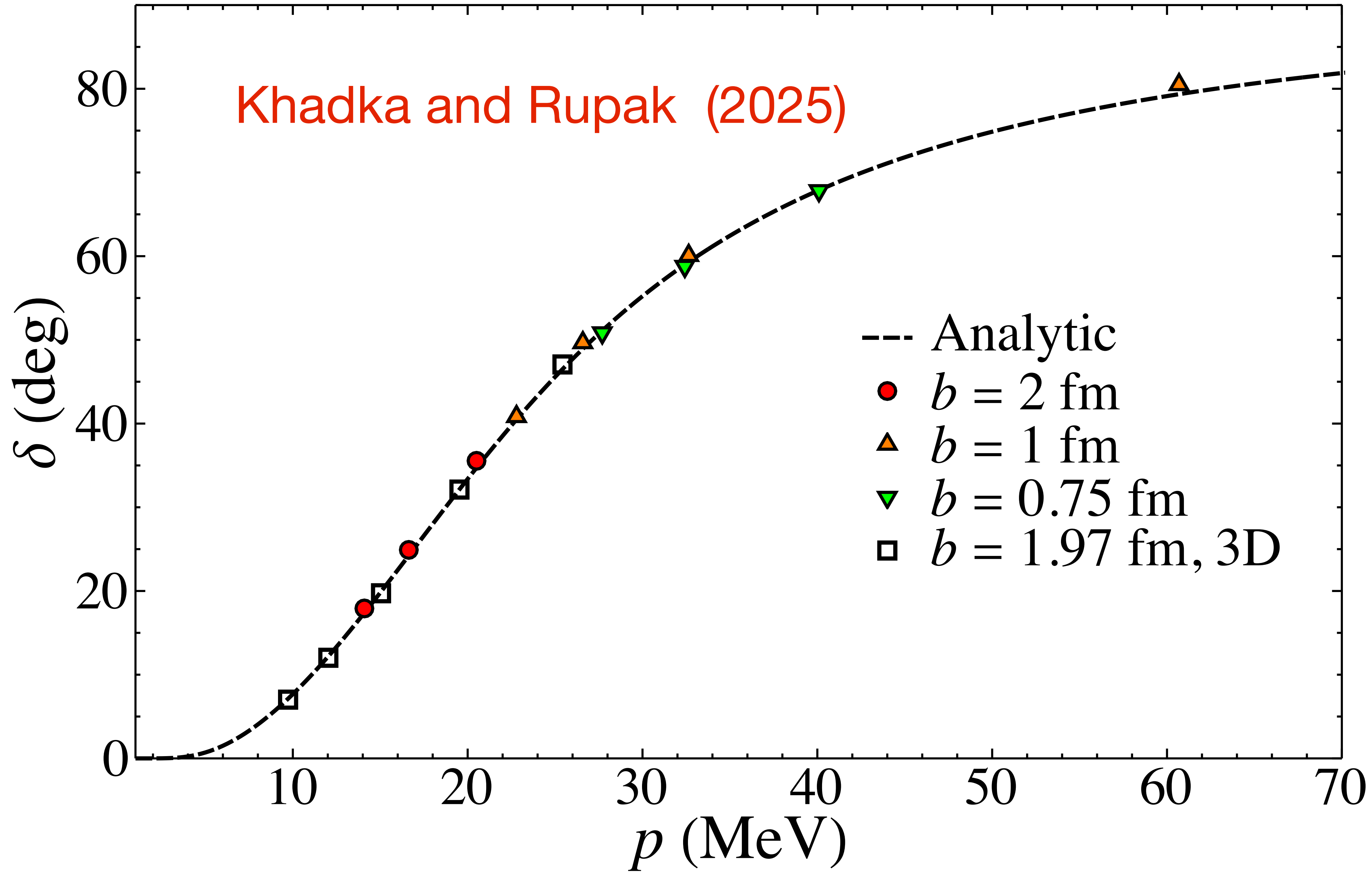


TABLE I. IBMQ-Brisbane measurements were done with 5000 shots (quantum measurements) with `optimization_level=3`. The last five columns are energy measurements relative to the exact energy in the 4th column. The ideal simulations were performed with 5000 shots as well, except for the simulations in column 8 that were done with 20000 shots, as indicated.

L	b (fm)	c_0	Exact (MeV)	Full ideal	Full QPU	SVD ideal	SVD ideal (20000)	SVD QPU
15	2.0	-0.0449	5.809	—	—	1.090	1.038	1.323
20	2.0	-0.0449	5.809	—	—	1.122	1.022	1.464
25	2.0	-0.0449	5.809	—	—	1.120	1.032	1.407
7	1.0	-0.1112	22.13	0.9798	20.64	1.046	1.048	1.287
15	1.0	-0.1112	22.13	—	—	1.095	1.040	1.268
20	1.0	-0.1112	22.13	—	—	1.127	1.023	1.207
25	1.0	-0.1112	22.14	—	—	1.126	1.034	1.160
15	0.75	-0.1540	38.91	—	—	1.096	1.040	1.190
20	0.75	-0.1540	38.91	—	—	1.128	1.023	1.114
25	0.75	-0.1540	38.91	—	—	1.127	1.035	1.133

Conclusions

1. Quantum computing provides an advantage in real-time calculation of electro-weak processes. Efforts in this direction is important.

2. A generic algorithm for inelastic processes, final/excited state preparation was presented.
    a. Work is in progress to calculate $p(n, \gamma)d$, building from lower to higher dimensions.
    b. The current algorithm can be used to prepare excited state efficiently near the resonance.

3. An algorithm for mass gap calculation.
    a. Demonstrated for the non-linear $O(3)$ sigma model at strong coupling on NISQ devices.
    b. Proof of concept at weak coupling on ideal simulator in non-linear $O(3)$ sigma model.
    c. Flexibility in observable measurements.

4. Hybrid quantum-classical algorithms for two-particle scattering using physics aware optimizer.