First quantization scattering on a quantum computer.

DESY. QUANTUM
Center for Quantum Technology and Applications

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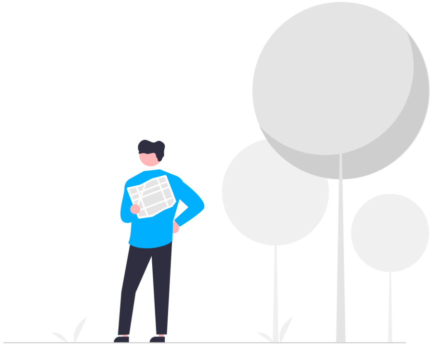

Kitaev-Webb algorithm [1]

- Given a Gaussian wave packet

$$\psi_{\sigma,\mu}(x) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

where μ in the mean of the wave packet and σ is the standard deviation and $\int_{-\infty}^{+\infty} \psi^2(x)dx = 1$

- In order to develop the algorithm on a finite system, we consider the Gaussian to be a function of an integer value *i*,

$$\tilde{\psi}_{\sigma,\mu}(i) = \frac{1}{\sqrt{f(\sigma,\mu)}} e^{-\frac{(i-\mu)^2}{2\sigma^2}}$$

where $f(\mu,\sigma) = \sum_{n=-\infty}^{\infty} e^{-\frac{(n-\mu)^2}{\sigma^2}} \overset{\sigma \gg 1}{\approx} \sigma\sqrt{\pi}$.

[1]A. Kitaev, W.A. Webb, "Wavefunction preparation and resampling using a quantum computer",2009

Kitaev-Webb algorithm

- We define a new periodic function with period 2^N

$$\xi_{\sigma,\mu,N}(i) = \sum_{j=-\infty}^{\infty} \frac{1}{\sqrt{f(\mu,\sigma)}} \exp\left[-\frac{(i+j\cdot 2^N-\mu)^2}{2\sigma^2}\right]$$

  it allows us to define the quantum state

$$|\xi_{\sigma,\mu,N}\rangle = \sum_{i=0}^{2^N-1} \xi_{\sigma,\mu,N}(i)\,|i\rangle$$

- For $\mu, 2^N-\mu \gg \sigma \gg 1$, this state is very close to a Gaussian with mean μ and standard deviation σ.

Kitaev-Webb algorithm

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How can we apply these operations on a quantum circuit?

Quantum Circuits

CLASSICAL

- Fundamental concept: bit
- States: 0 or 1

OFF ON

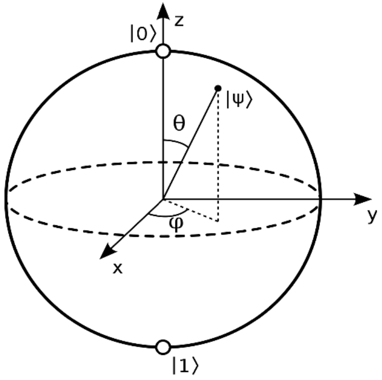
QUANTUM

- Fundamental concept: Qubit
- States: 0, 1 or linear combination

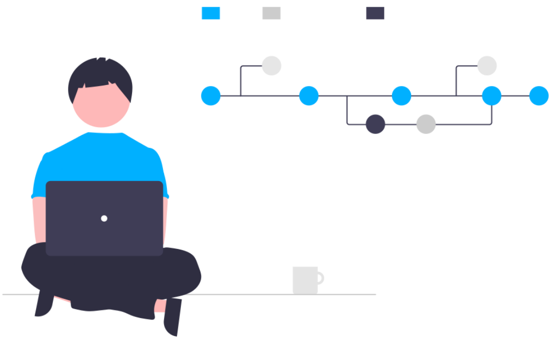
$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

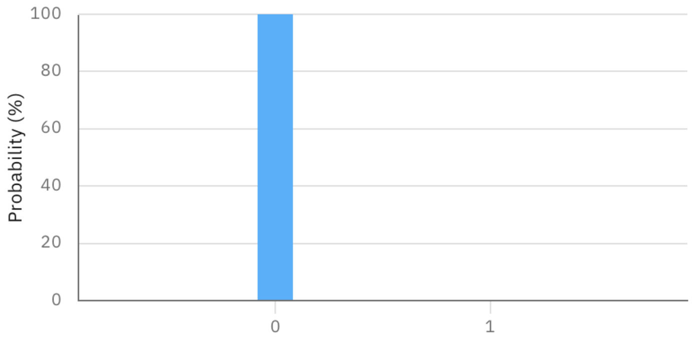
$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}$$

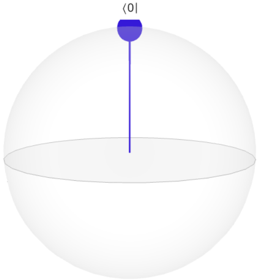
$$|1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$$



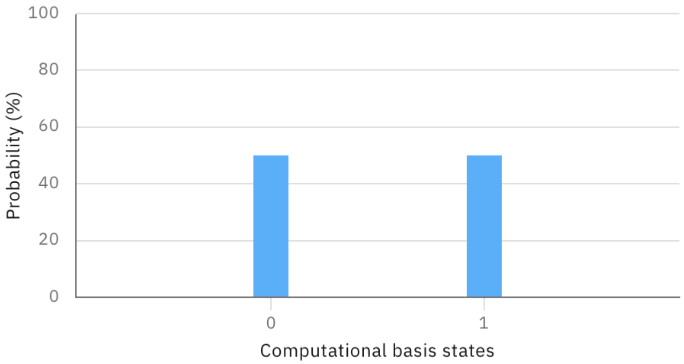
Quantum gates

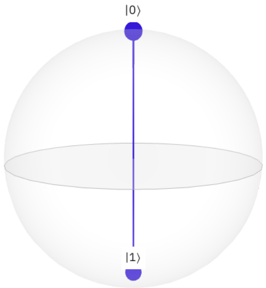






$$RY(\theta) = \exp\left(-i\frac{\theta}{2}Y\right) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$



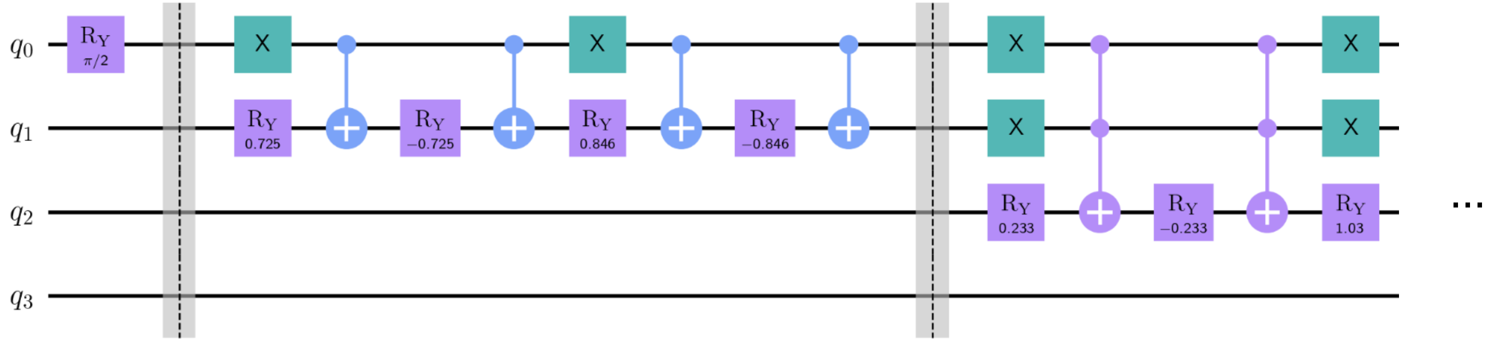


Kitaev-Webb algorithm

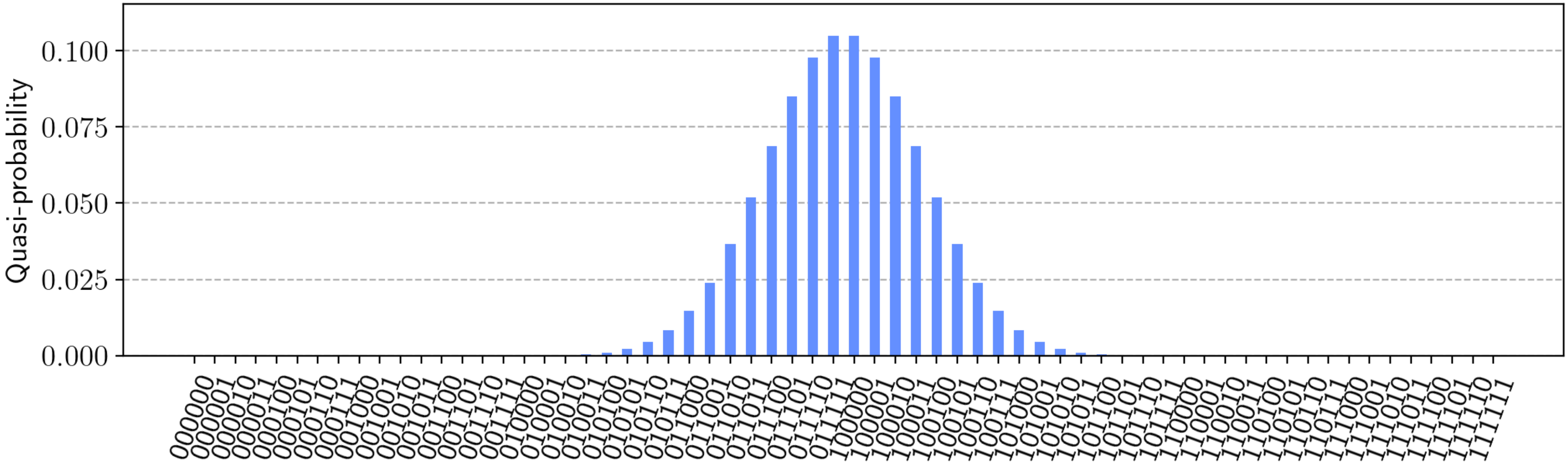
- With a recursive description of the state,

$$|\xi_{\sigma,\mu,N}\rangle = \left|\xi_{\frac{\sigma}{2},\frac{\mu}{2},N-1}\right\rangle \otimes \cos\alpha\,|0\rangle + \left|\xi_{\frac{\sigma}{2},\frac{\mu-1}{2},N-1}\right\rangle \otimes \sin\alpha\,|1\rangle\,,$$

leads to an algorithm for preparing it.



Results for 1 wave packet on 6 qubits

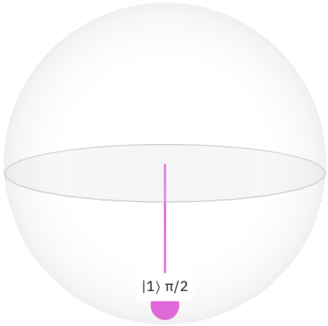


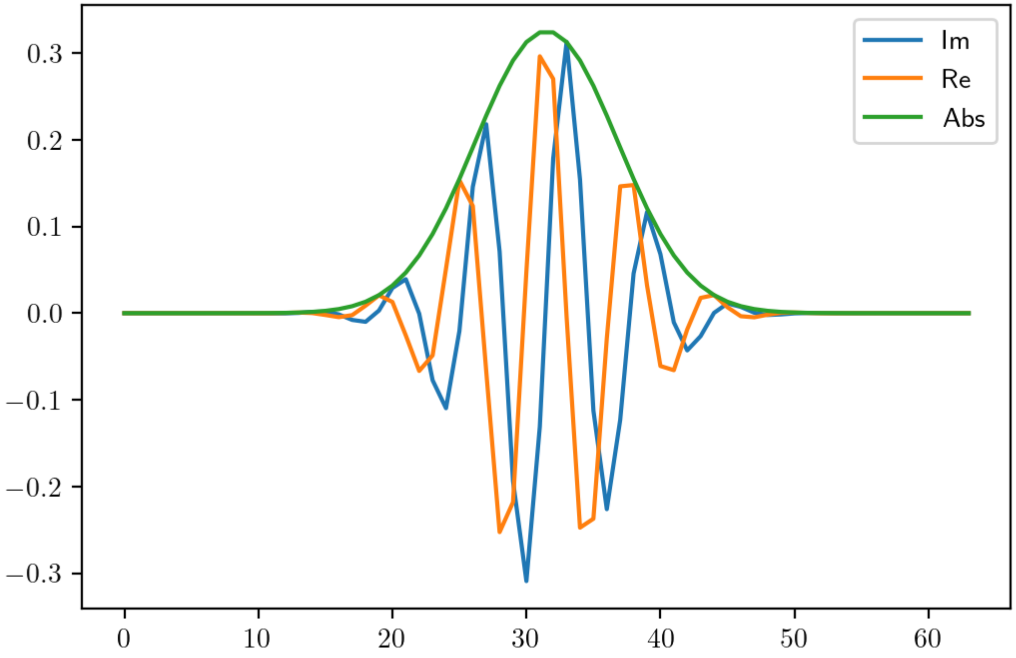
With this method we can exploit the scaling of number of qubits N to represent a large system (2^N)

Results for 1 wave packet: phase [2]

We want to add a phase for the initial state $e^{ip_0 x}$

$$P(\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix}$$



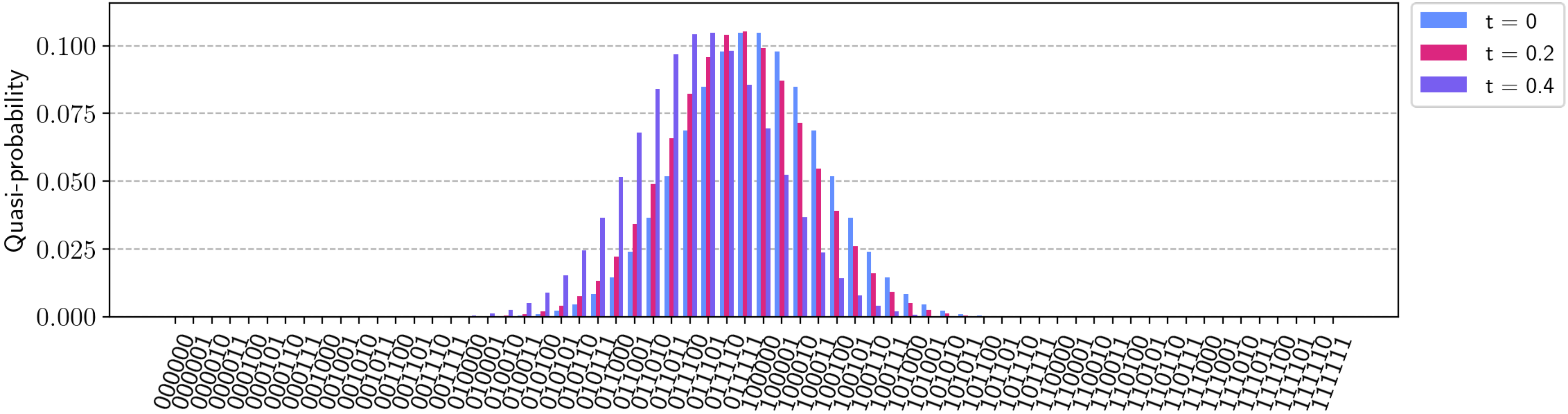


- In this case we get also an Im part.
- This gives an initial momentum to the packet.

[2]A Macridin et al. ,Digital quantum computation of fermion-boson interacting systems, 2018

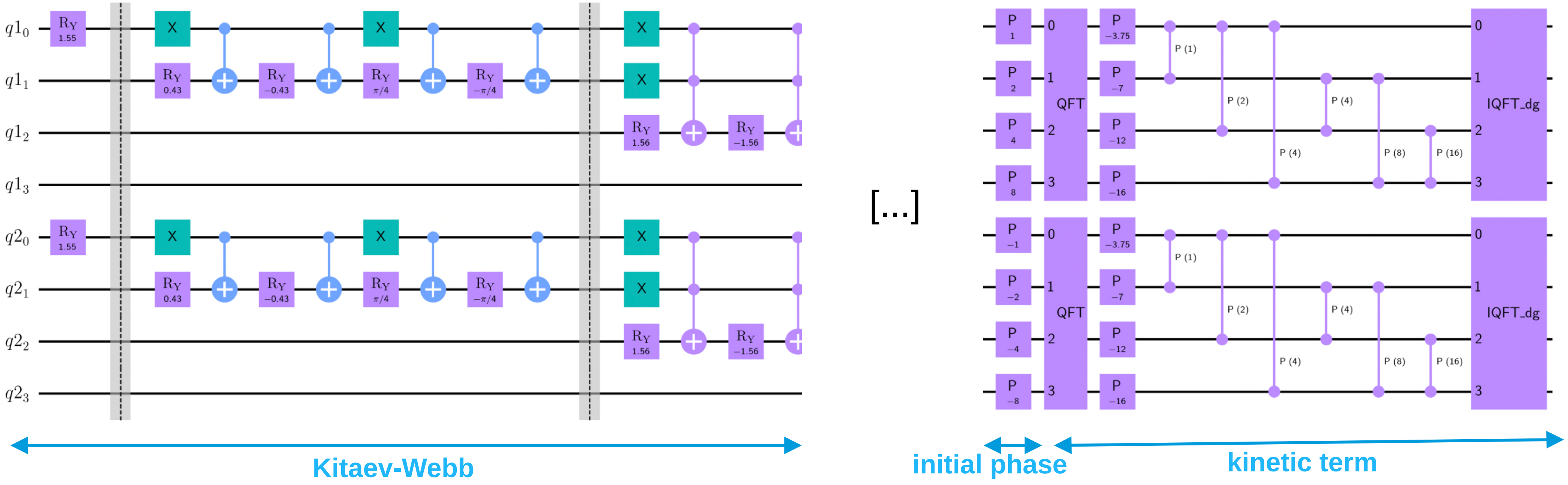
Results for 1 wave packet: time evolution

By applying the QFT and a set of phase gates we get



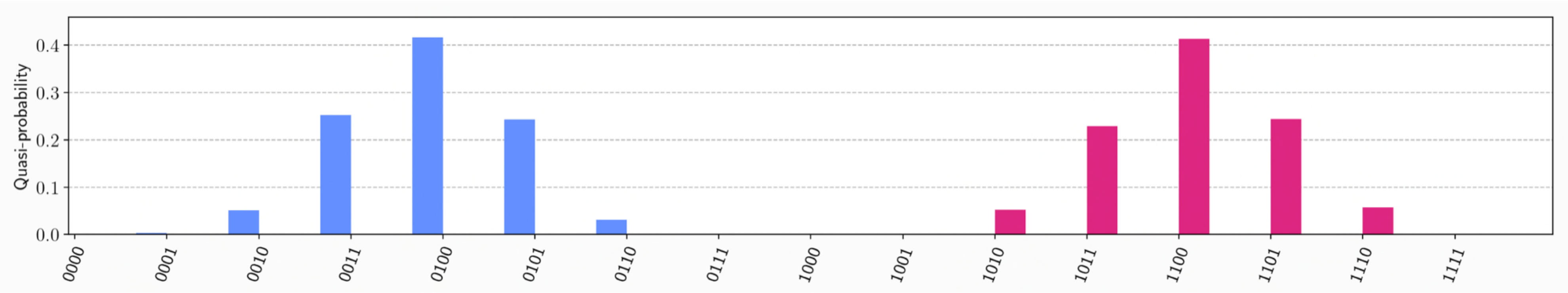
Results for 2 wave packets

We want the dynamics of 2 systems, so we generalise the previous algorithm:

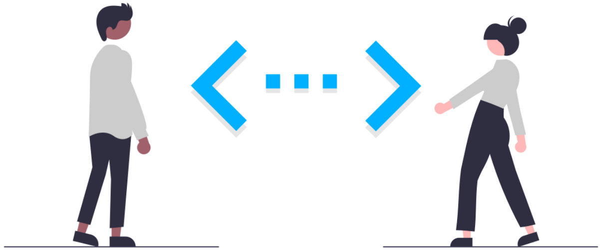


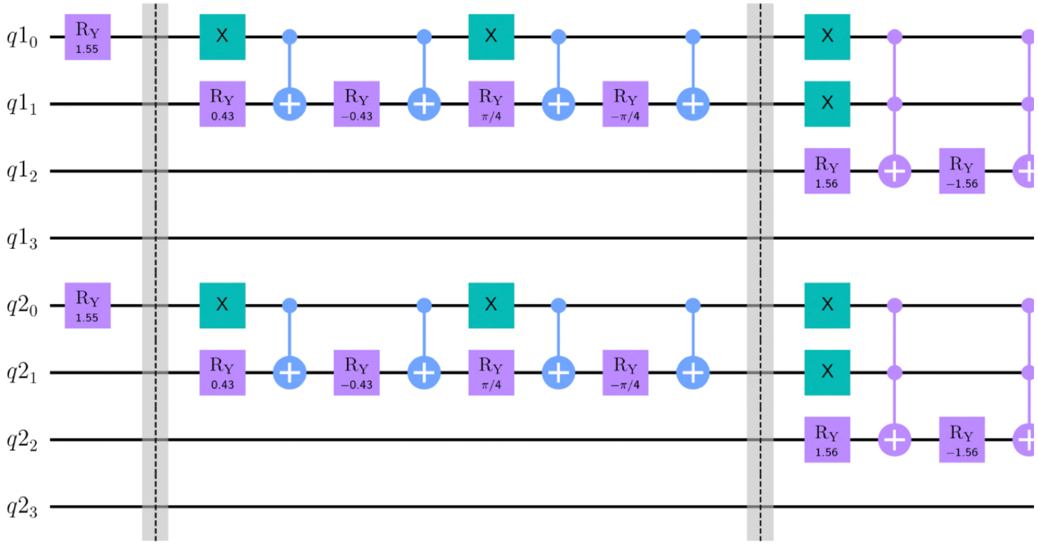
Results for 2 wave packets

With the previous circuit we obtain two Gaussians:

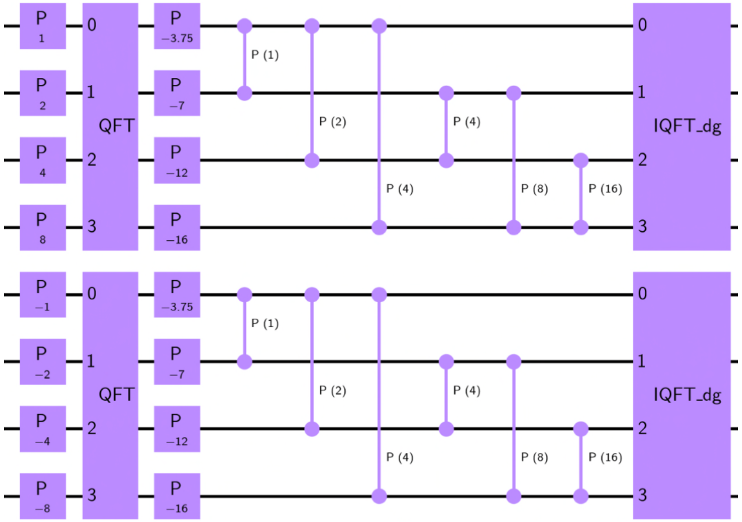


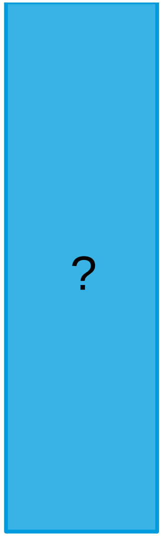
Next step: interaction





[...]





Next step: interaction

General solution of the time evolution of two interacting harmonic oscillators

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[4] *School of Mathematical Sciences, University of Nottingham, NG7 2RD, Nottingham, UK*[‡]
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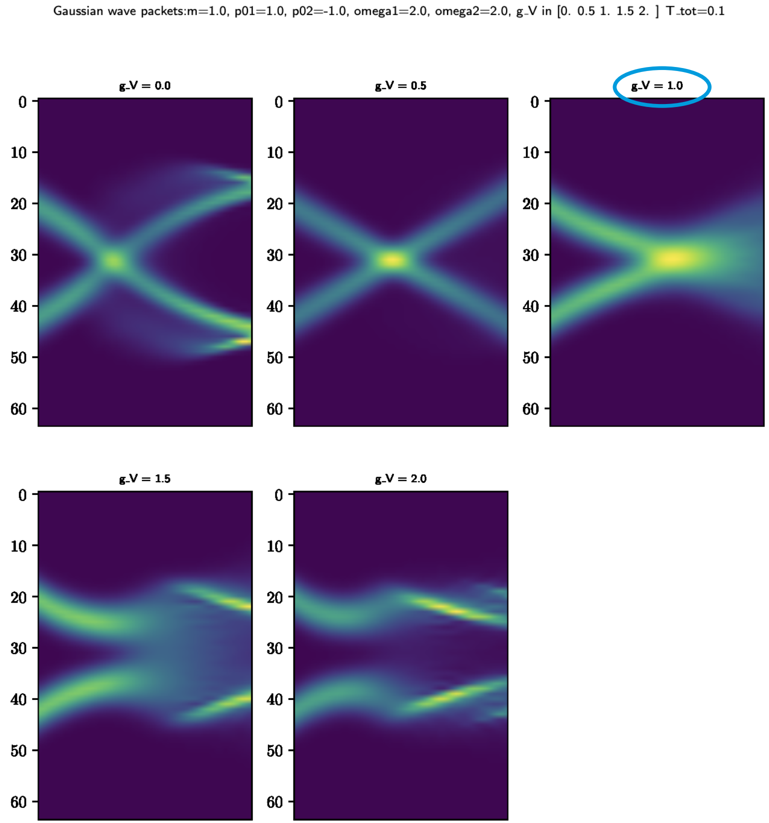
(Dated: February 15, 2021)

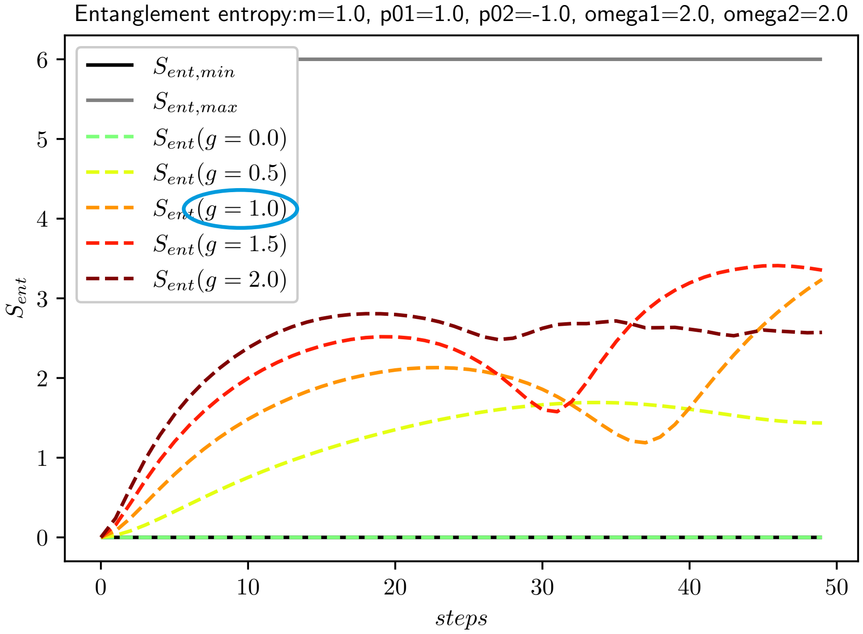
$$\hat{H} = \hat{H}_0 + V(\hat{a}, \hat{b}, \hat{a}^\dagger, \hat{b}^\dagger), \tag{3}$$

where $\hat{H}_0 = \hbar\,\omega_{\mathrm{a}}\,\hat{a}^\dagger\,\hat{a} + \hbar\,\omega_d\,\hat{b}^\dagger\,\hat{b}$ denotes the free Hamiltonian (we have discarded the zero point energy constant), and now the potential V is obtained as a combination of terms that are quadratic in the new operators.

The potential can take, for example, the form $V(\hat{a}, \hat{b}, \hat{a}^\dagger, \hat{b}^\dagger) = g\,(\hat{a}\,\hat{b}^\dagger + \hat{a}^\dagger\,\hat{b} + \hat{a}\,\hat{b} + \hat{a}^\dagger\,\hat{b}^\dagger)$, and in this

Next step: interaction

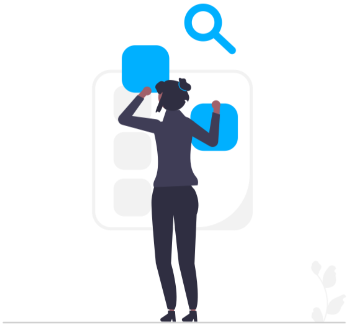




to be continued..

Thank you.

Questions?



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Superpositions of integrable probability distributions [1]

- Given a probability $\{p_i\}$ how can we create a quantum superposition of the form $|\psi(\{p_i\})\rangle = \sum_i \sqrt{p_i}\,|i\rangle$ (where *i* in range of *N* values and $\{p_i\}$ discretized version of $p(x)$) ?

[1] Lov Grover and Terry Rudolph, 2002

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1) Assume the distribution is divided into 2^m regions and that we have a *m* qubit state,

$$|\psi_m\rangle = \sum_{i=0}^{2^m-1} \sqrt{p_i^{(m)}}\,|i\rangle$$

probability for random variable *x* to lie in region *i* ($p_0^{(m)} \equiv$ probab. x to lie in leftmost region
$p_1^{(m)} \equiv$ probab. to lie in region adjacent to this)

Superpositions of integrable probability distributions [1]

2) Goal: show that we can subdivide these 2^m regions to a 2^{m+1}region discretisation of $p(x)$, i.e. we want to add 1 qubit to the previous expression to achieve

$$\sqrt{p_i^{(m)}}\,|i\rangle = \sqrt{\alpha_i}\,|i\rangle\,|0\rangle + \sqrt{\beta_i}\,|i\rangle\,|1\rangle$$

with $\alpha_i(\beta_i)$ probability for *x* to lie in left (right) half of region.

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3) if we can achieve this, then we have the state of *m+1* qubits:

$$|\psi_{m+1}\rangle = \sum_{i=0}^{2^{m+1}-1} \sqrt{p_i^{(m+1)}}\,|i\rangle$$

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4) repeat until $2^m = N$.

Superpositions of integrable probability distributions

- **Example** of distribution $f(i) = \frac{\int_{x_L^i}^{\frac{x_R^i - x_L^i}{2}} p(x)dx}{\int_{x_L^i}^{x_R^i} p(x)dx}$, (x_L^i / x_R^i left/right boundaries of region i)

  gives probability that, given x in region i, it also lies in <u>left half</u>.

- With a controlled rotation angle on qubit m+1, we obtain

$$\sqrt{p_i^{(m)}} \left| i \right\rangle \left| 0 \right\rangle \rightarrow \sqrt{p_i^{(m)}} \left| i \right\rangle (\cos\theta_i \left| 0 \right\rangle + \sin\theta_i \left| 1 \right\rangle)$$

  with $\theta_i \equiv \arccos\sqrt{f(i)}$

Kitaev-Webb algorithm

- $(N = 1)$:

$$|\xi_{\sigma,\mu,1}\rangle = \xi_{\sigma,\mu,1}(0)\,|0\rangle + \xi_{\sigma,\mu,1}(1)|1\rangle$$

$$\xi_{\sigma,\mu,1}(0) = \sum_{j=-\infty}^{\infty} \frac{1}{\sqrt{f(\mu,\sigma)}} \exp\left[-\frac{(j\cdot 2-\mu)^2}{2\sigma^2}\right] = \frac{1}{\sqrt{f(\mu,\sigma)}} \sum_{j=-\infty}^{\infty} \exp\left[-\frac{(j-\frac{\mu}{2})^2}{2\frac{\sigma^2}{2}}\right] = \frac{\sqrt{f(\frac{\mu}{2},\frac{\sigma}{2})}}{\sqrt{f(\mu,\sigma)}}$$

$$\xi_{\sigma,\mu,1}(1) = \sum_{j=-\infty}^{\infty} \frac{1}{\sqrt{f(\mu,\sigma)}} \exp\left[-\frac{(1+j\cdot 2-\mu)^2}{2\sigma^2}\right] = \frac{\sqrt{f(\frac{\mu-1}{2},\frac{\sigma}{2})}}{\sqrt{f(\mu,\sigma)}}$$

- the wavefunction has 2 components with the sum over probabilities $f(\mu,\sigma) = f(\frac{\mu}{2},\frac{\sigma}{2}) + f(\frac{\mu-1}{2},\frac{\sigma}{2})$.

Kitaev-Webb algorithm

- $(N=1)$:
  the quantities, $\xi_{\sigma,\mu,1}(0) = \frac{\sqrt{f(\frac{\mu}{2},\frac{\sigma}{2})}}{\sqrt{f(\mu,\sigma)}}$ and $\xi_{\sigma,\mu,1}(1) = \frac{\sqrt{f(\frac{\mu-1}{2},\frac{\sigma}{2})}}{\sqrt{f(\mu,\sigma)}}$

  can be written in term of one angle

$$\alpha = \arccos\sqrt{f\left(\frac{\mu}{2},\frac{\sigma}{2}\right)/f(\mu,\sigma)} = \arcsin\sqrt{f\left(\frac{\mu-1}{2},\frac{\sigma}{2}\right)/f(\mu,\sigma)}$$

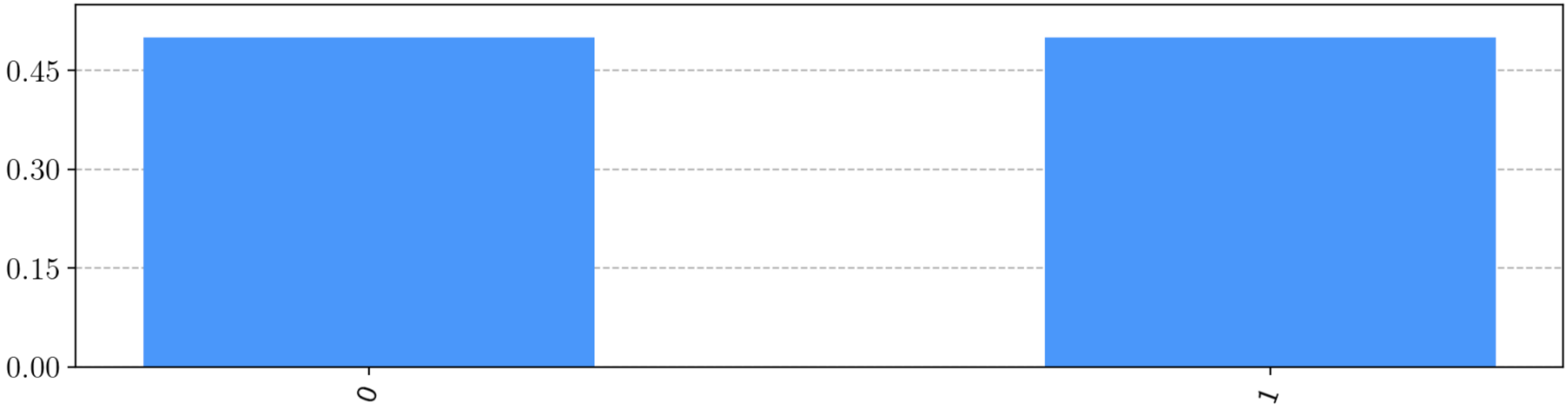
- Let's define: $C(\mu,\sigma) \equiv \frac{\sqrt{f(\frac{\mu}{2},\frac{\sigma}{2})}}{\sqrt{f(\mu,\sigma)}}$ and $S(\mu,\sigma) \equiv \frac{\sqrt{f(\frac{\mu-1}{2},\frac{\sigma}{2})}}{\sqrt{f(\mu,\sigma)}}$

Superpositions of integrable probability distributions

- **Example** of Gaussian distribution (μ=0.5, σ=1.0)

$(N = 1)$

$$|\xi_{\sigma,\mu,1}\rangle = \xi_{\sigma,\mu,1}(0)\,|0\rangle + \xi_{\sigma,\mu,1}(1)\,|1\rangle$$



Kitaev-Webb algorithm

- $(N=2)$:

$$|\xi_{\sigma,\mu,1}\rangle = \frac{\sqrt{f(\frac{\mu}{4},\frac{\sigma}{4})}}{\sqrt{f(\mu,\sigma)}}|00\rangle + \frac{\sqrt{f(\frac{\mu-1}{4},\frac{\sigma}{4})}}{\sqrt{f(\mu,\sigma)}}|01\rangle + \frac{\sqrt{f(\frac{\mu-2}{4},\frac{\sigma}{4})}}{\sqrt{f(\mu,\sigma)}}|10\rangle + \frac{\sqrt{f(\frac{\mu-3}{4},\frac{\sigma}{4})}}{\sqrt{f(\mu,\sigma)}}|11\rangle$$

$$= \left[C(\frac{\mu}{2},\frac{\sigma}{2})|0\rangle + S(\frac{\mu}{2},\frac{\sigma}{2})|1\rangle\right] \otimes C(\mu,\sigma)|0\rangle + \left[C(\frac{\mu-1}{2},\frac{\sigma}{2})|0\rangle + S(\frac{\mu-1}{2},\frac{\sigma}{2})|1\rangle\right] \otimes S(\mu,\sigma)|1\rangle$$

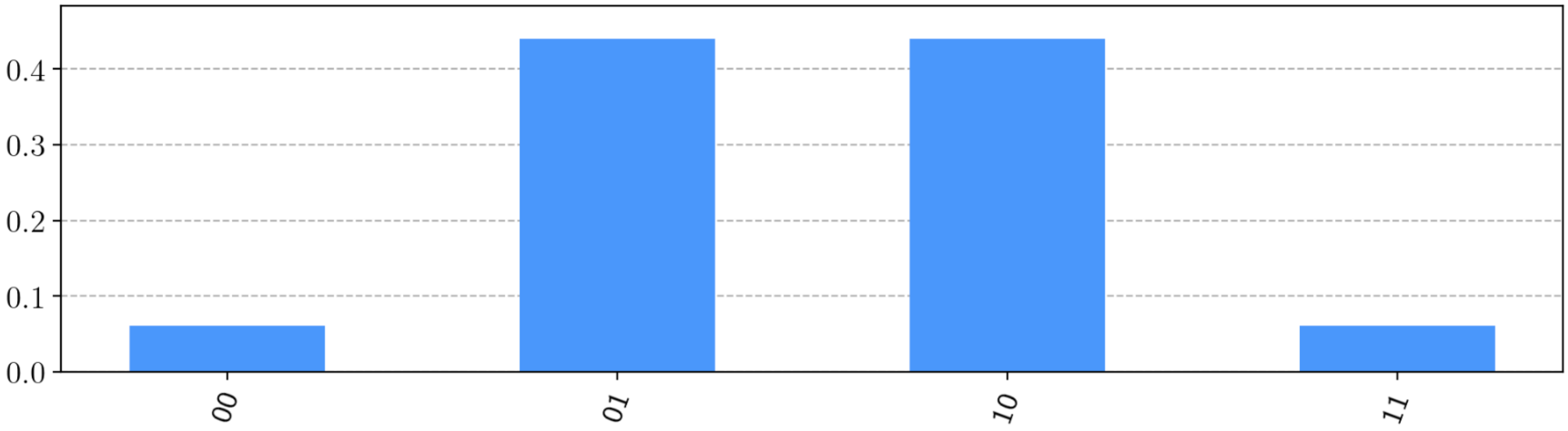
etc.

Superpositions of integrable probability distributions

- **Example** of Gaussian distribution (μ=1.5, σ=1.0)

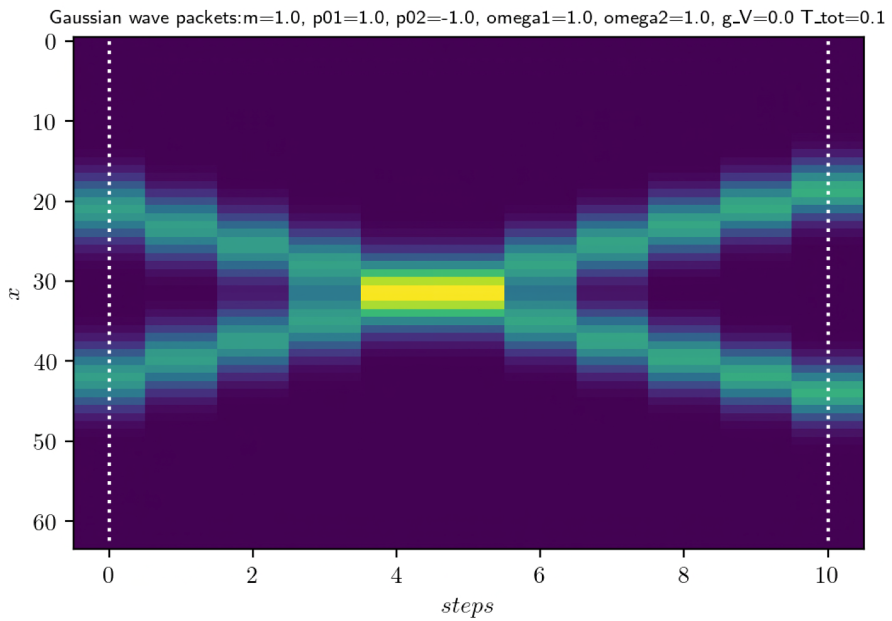
$(N = 2)$

$$|\xi_{\sigma,\mu,1}\rangle = \frac{\sqrt{f(\frac{\mu}{4},\frac{\sigma}{4})}}{\sqrt{f(\mu,\sigma)}}|00\rangle + \frac{\sqrt{f(\frac{\mu-1}{4},\frac{\sigma}{4})}}{\sqrt{f(\mu,\sigma)}}|01\rangle + \frac{\sqrt{f(\frac{\mu-2}{4},\frac{\sigma}{4})}}{\sqrt{f(\mu,\sigma)}}|10\rangle + \frac{\sqrt{f(\frac{\mu-3}{4},\frac{\sigma}{4})}}{\sqrt{f(\mu,\sigma)}}|11\rangle$$

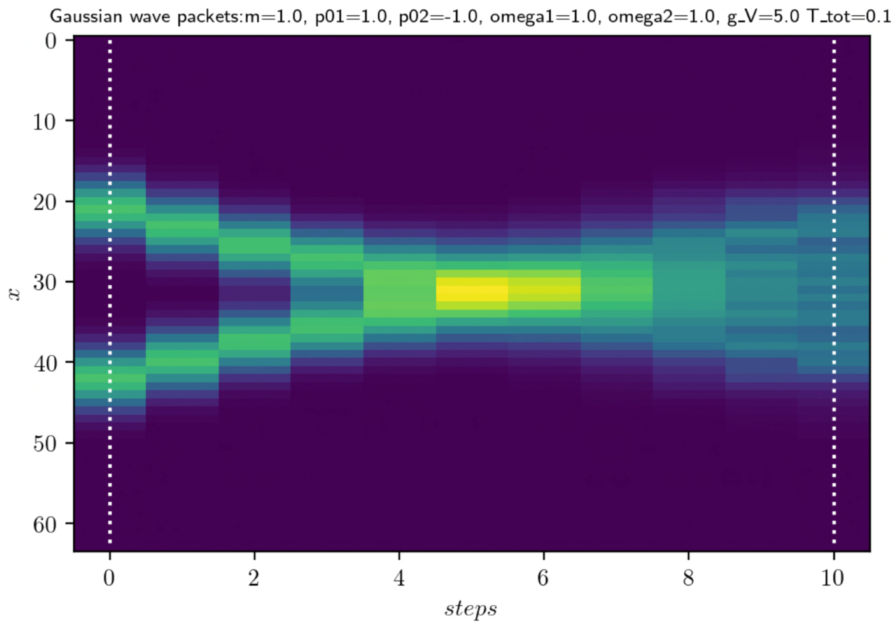


Next step: interaction

Interaction off



Interaction on



to be continued..