

# ALGORITHMIC PERSPECTIVE ON STRONGLY CORRELATED SYSTEMS

(i.e. computational condensed matter)

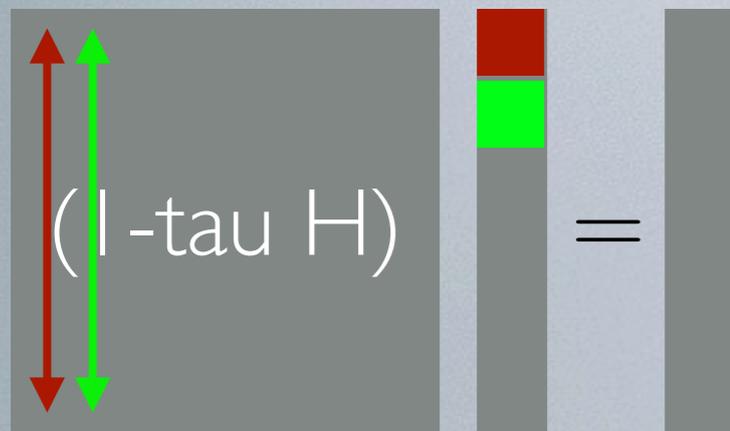
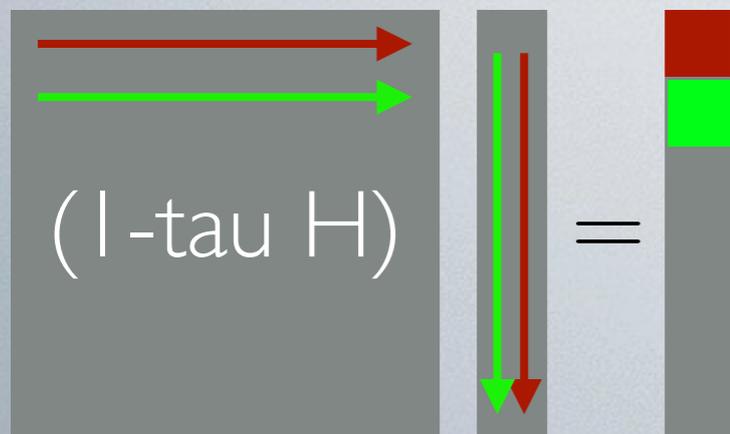
Lecture: Your first QMC Code

Let's go ahead and "write" our first quantum Monte Carlo code.

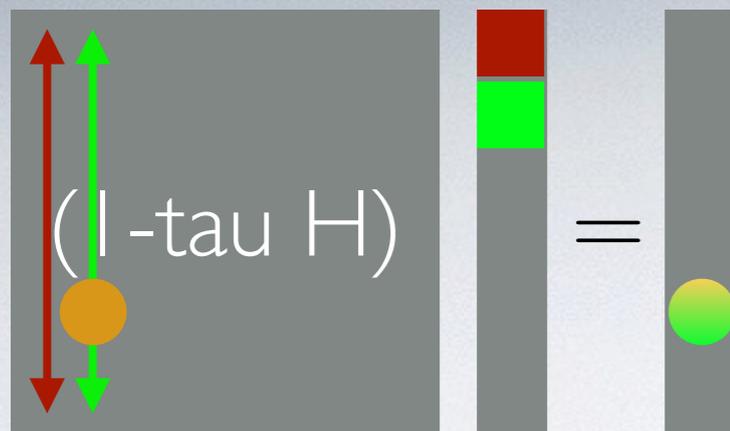
We will do this by slowly morphing the exact diagonalization power method we had seen earlier to a quantum Monte Carlo approach.

The key to the power method is to do matrix-vector multiplication.

Let's figure out how to do this stochastically.



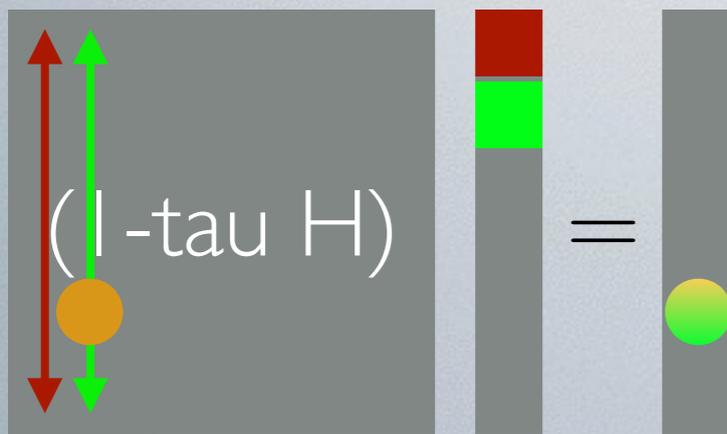
Let's choose where the weight for the green square goes.



Choose an index  $i$  with probability  $P(i) = \frac{|G_{i2}|}{\sum_i |G_{i2}|}$   
 Put the value  $\sum_i |G_{i2}| v_2$  into position  $i$

**Q:** Suppose I loop over all  $i$  many times and sum the resulting vectors. Do I get the right answer?

Q: Suppose I do this over and over again and sum the resulting vectors. Do I get the right answer?

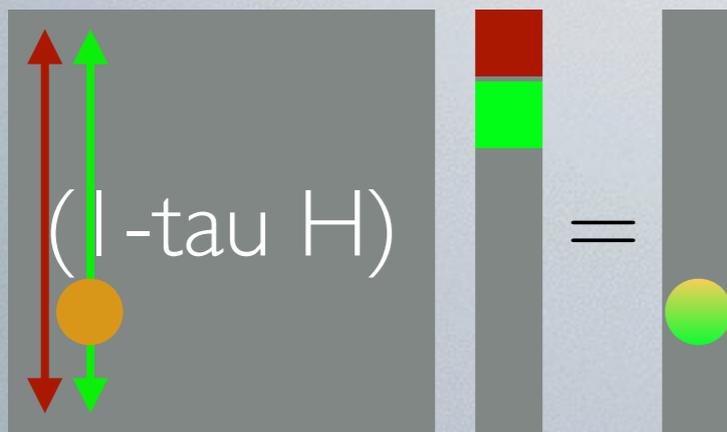


Choose an index  $i$  with probability  $P(i) = \frac{|G_{i2}|}{\sum_i |G_{i2}|}$   
Put the value  $\sum_i |G_{i2}| v_2$  into position  $i$

What is the expectation of the value in  $i$ ?

$$P(i) \left( \sum_i |G_{i2}| v_2 \right) = |G_{i2}| v_2$$

Q: Suppose I don't want to loop over the original vector



Choose a location  $k$  in the original vector with probability  $p(k) = \frac{v_k}{\sum_k v_k}$

Choose an index  $i$  with probability  $P(i) = \frac{|G_{ik}|}{\sum_i G_{ik}}$

Put the value  $\sum_i |G_{ik}| \sum_k v_k$  into position  $i$

What is the expectation of the value in  $i$ ?

$$P(i; k) \sum_i |G_{ik}| \sum_k v_k$$

We now apply this matrix multiplication over and over again...

Q: What do you get out of this algorithm?

You get out a stochastic sample of the vector  $\Psi$

What can you do with a stochastic sample?

A1: Not very much. The universe doesn't use  $\Psi$   
Instead, the universe uses  $|\Psi|^2$

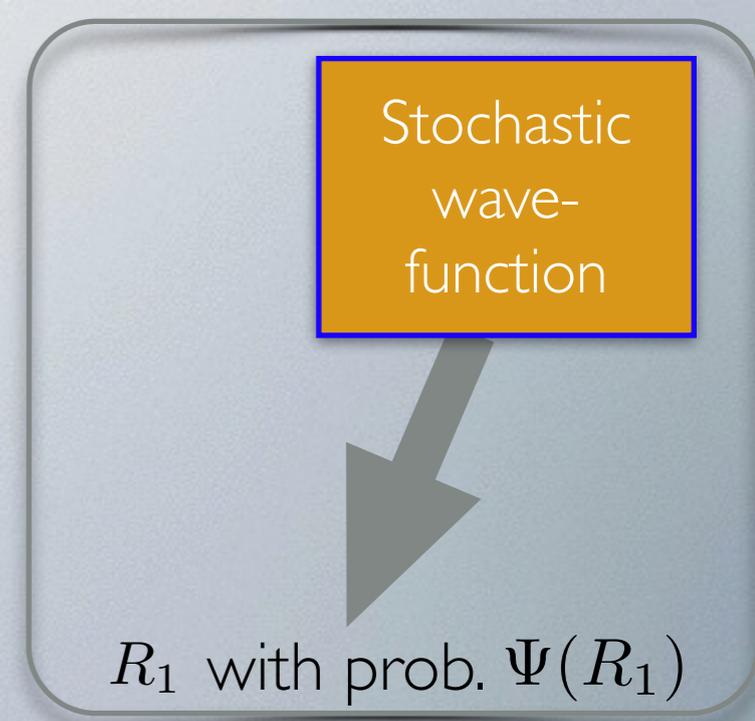
A2: *One exception I know about:* If you are sampling a ground state and if you want the energy, then you only need

How?

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$E = \frac{\sum_R \sum_{R'} \langle \Psi | R \rangle \langle R | H | R' \rangle \langle R' | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

**Note:** This is a more powerful exception than it seems. Why?



Q: Is having access to  $\Psi$  good enough to somehow get  $|\Psi|^2$

Yes. If you could store the whole vector:

Build  $\Psi(R)$

Then square it:  $|\Psi(R)|^2$



Q: Does this work with a stochastic sample?

**Q:** Is having access to  $\Psi$  good enough to somehow get  $|\Psi|^2$

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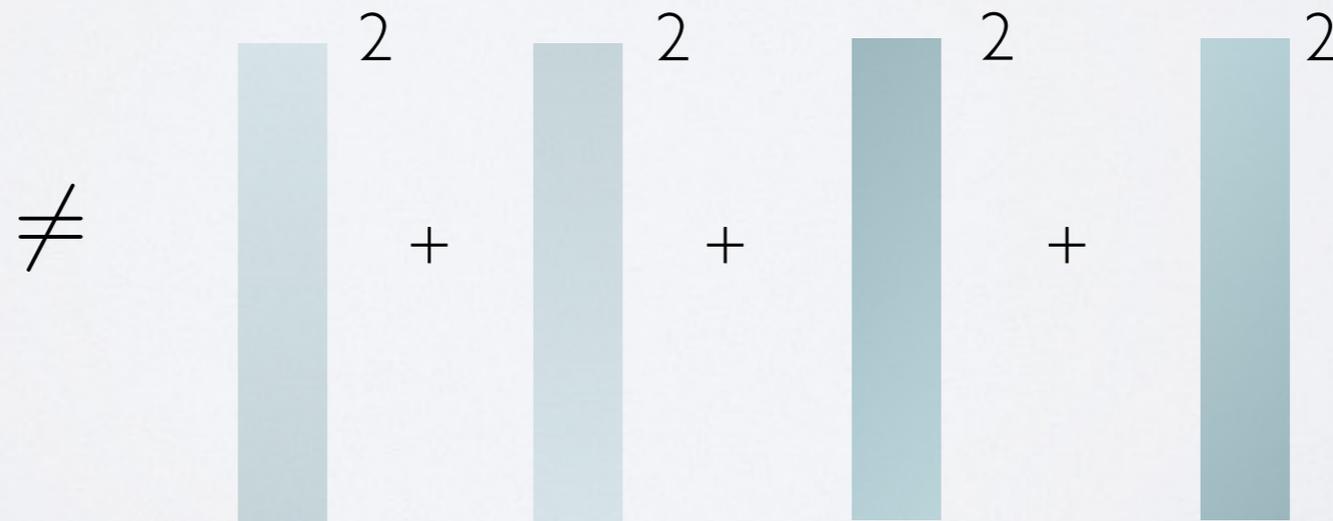
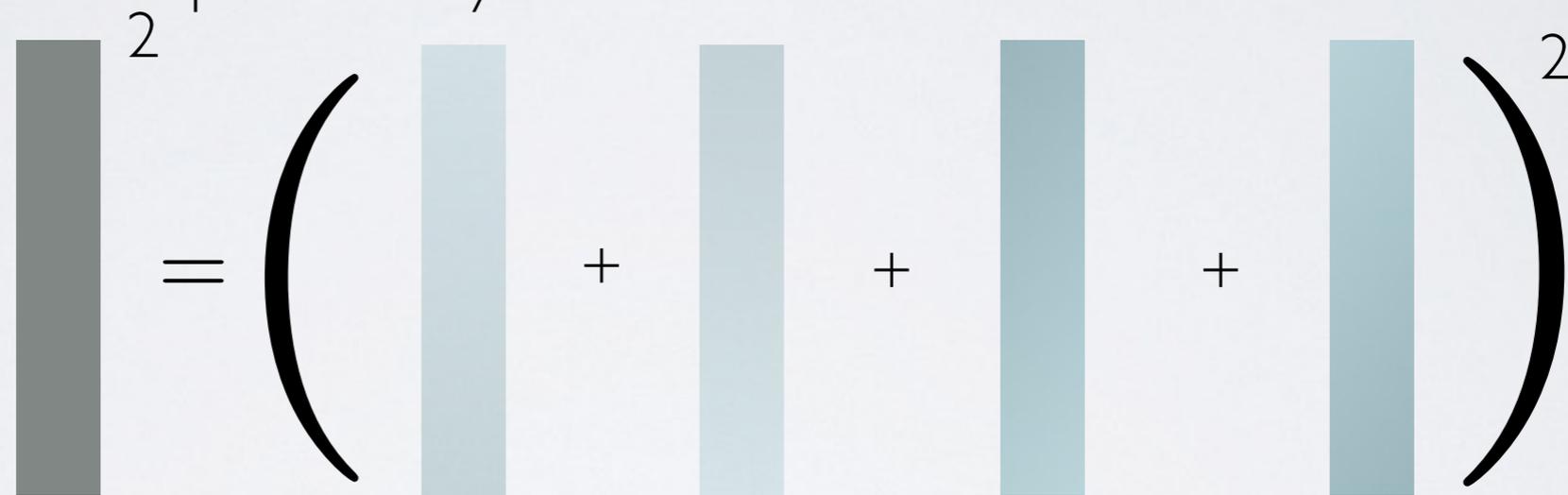
Build  $\Psi(R)$

Then square it:  $|\Psi(R)|^2$



**Q:** Does this work with a stochastic sample?

No. A stochastic sample means you have a bunch of vectors which sum to the right one.



# Aside: Sampling discrete $p(x)$

## (1) Discrete Distributions

pdf:

<b>0.1</b>	<b>0.3</b>	<b>0.1</b>	<b>0.05</b>	<b>0.05</b>	<b>0.1</b>	<b>0.3</b>
$r_1$	$r_2$	$r_3$	$r_4$	$r_5$	$r_6$	$r_7$

cdf:

<b>0.1</b>	<b>0.4</b>	<b>0.5</b>	<b>0.55</b>	<b>0.6</b>	<b>0.7</b>	<b>1.0</b>
$r_1$	$r_2$	$r_3$	$r_4$	$r_5$	$r_6$	$r_7$

Choose a uniform random number:

**0.34**  $\longrightarrow$   $r_2$

**0.8**  $\longrightarrow$   $r_7$

**Bisection:  $\log(N)$**