Collapse of the electron-hole wave-function in QMC calculations

Pablo López Ríos

Collapse of the electron-hole wave-function in QMC calculations

or,

"understanding why your favourite method gives an unphysical answer"

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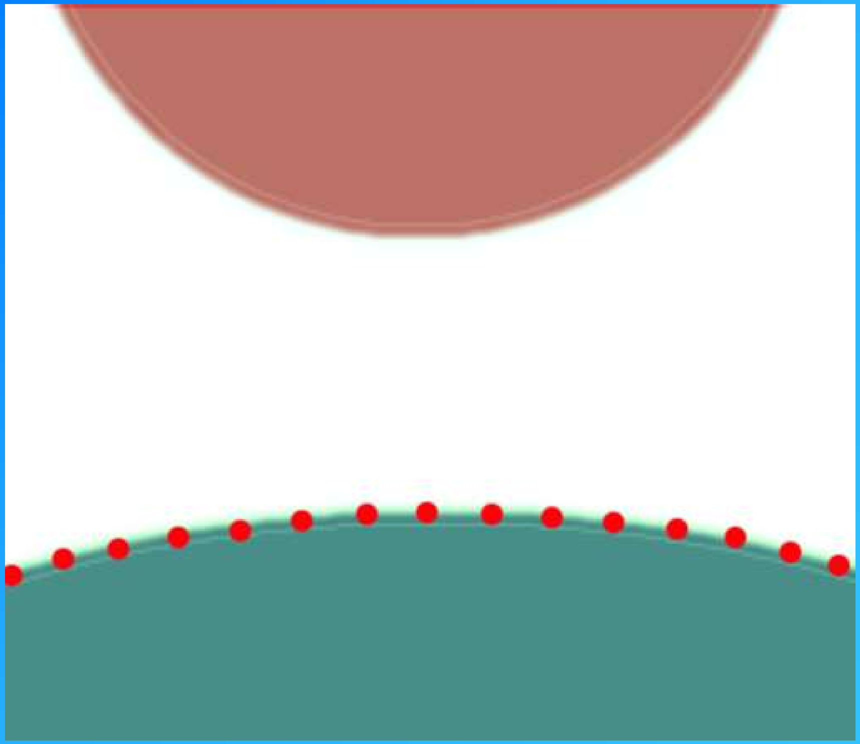
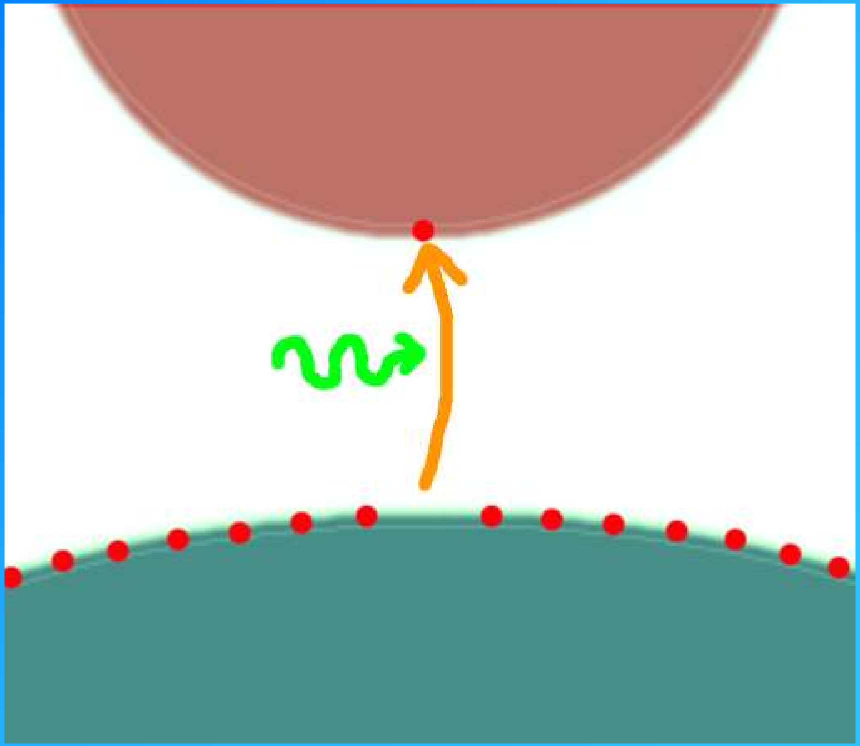
The electron-hole system



The electron-hole system is a model for excited semi-conductors.

When an electron is excited from the valence band into the conduction band, the *hole* left behind can be trated as a particle of charge *-e* and mass given by the effective mass approximation.

The electron-hole system



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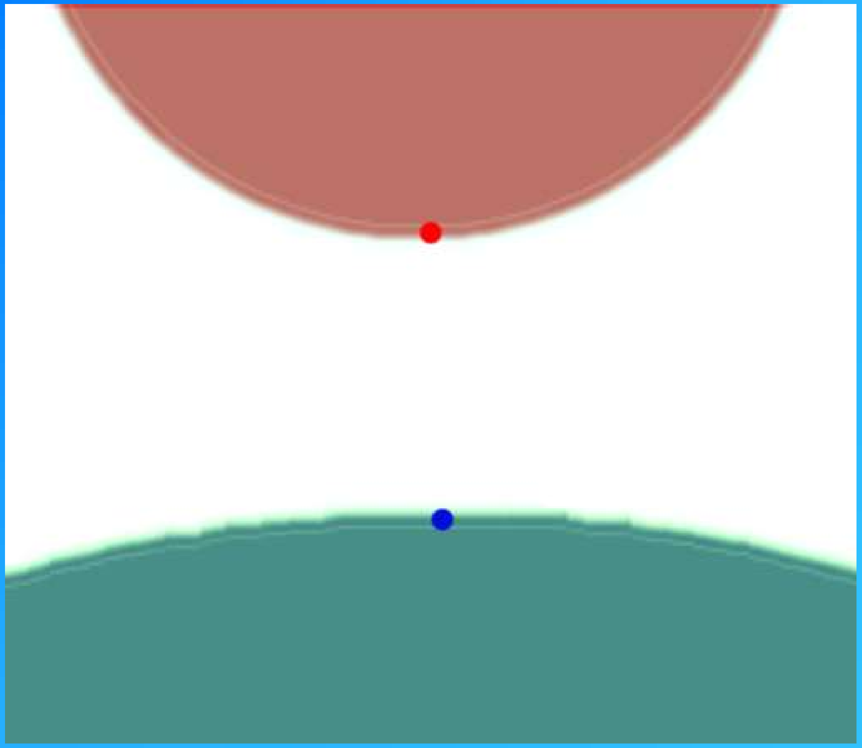

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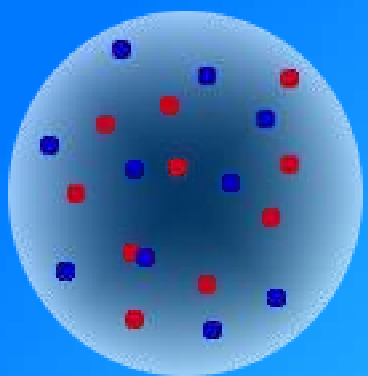
The electron-hole system

The basic phases are:

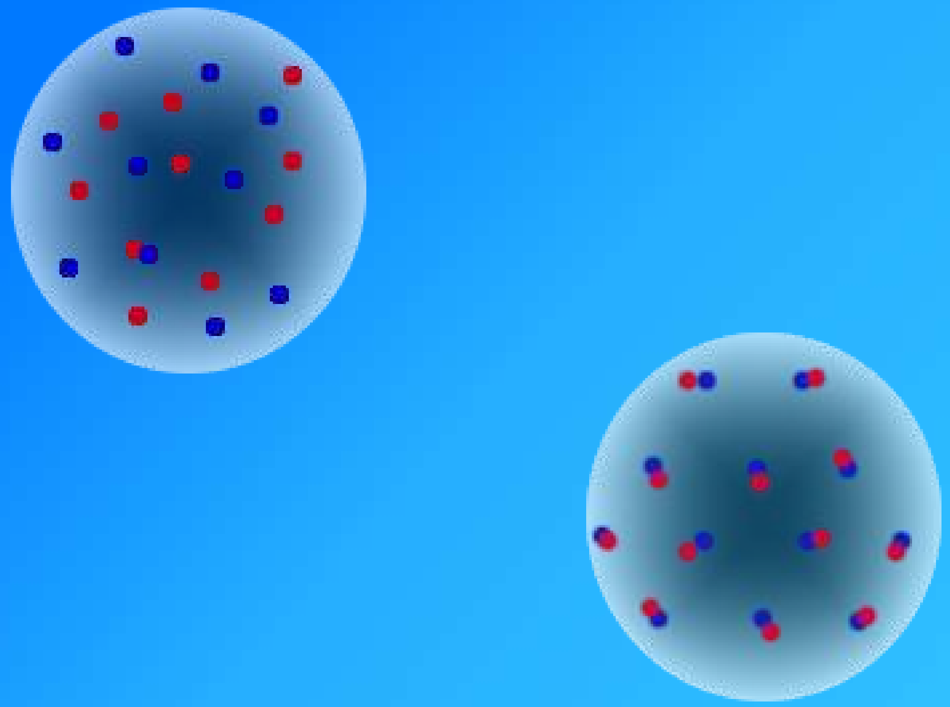
The electron-hole system



The basic phases are:

* Fluid phase
  (high density)

The electron-hole system

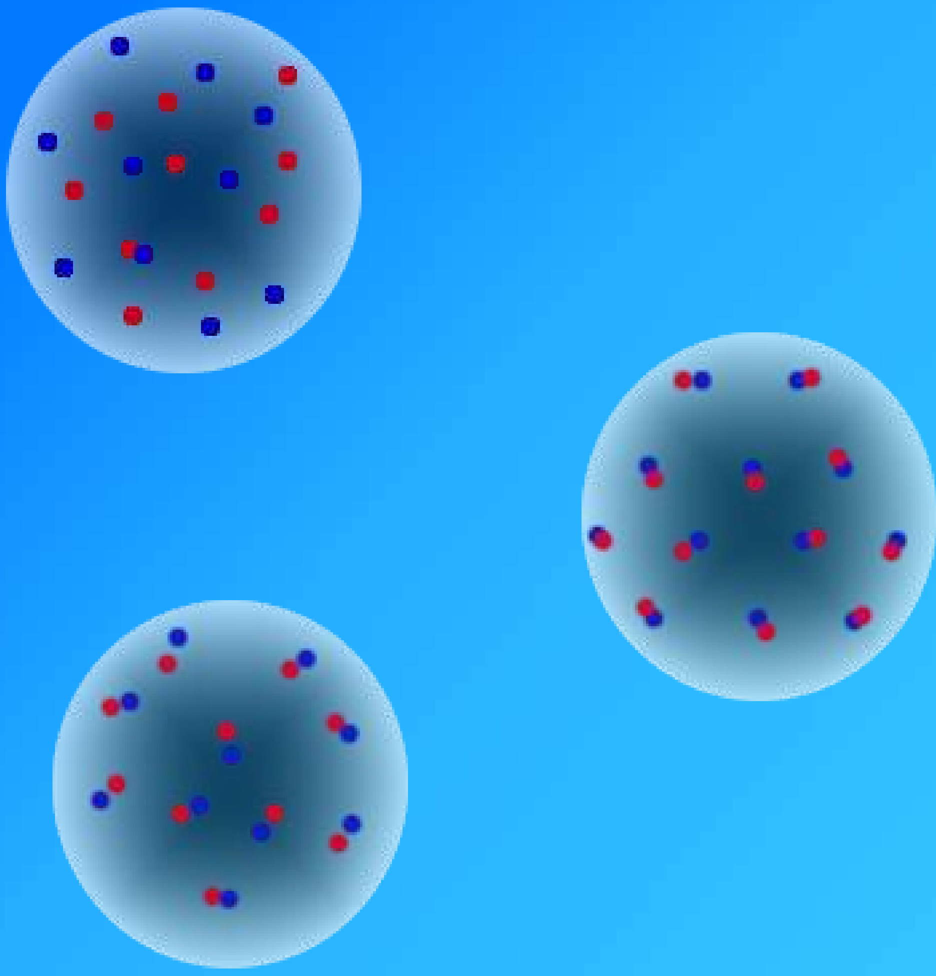


The basic phases are:

* Fluid phase
  (high density)

* Wigner Crystal
  (low density)

The electron-hole system



The basic phases are:

* Fluid phase
  (high density)

* Wigner Crystal
  (low density)

* Excitonic phase

The QMC method

Trial wave-function in Slater-Jastrow form.

$$\Psi = e^{J(\mathbf{R})}\Psi_D$$

QMC is an extremely accurate method.

* VMC:
  Variational principle
  + MC integration.

* DMC:
  Projection of configs
  into imaginary time.
  (exact in principle)

The QMC method

How is the wave-function optimized?

The QMC method

$$\Psi(\{\alpha_i\})$$

How is the wave-function optimized?

1. Set of parameters

The QMC method

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$$\{\mathbf{R}_i\}$$

How is the wave-function optimized?

1. Set of parameters

2. Set of configs distributed according to WF

The QMC method

$$\Psi(\{\alpha_i\})$$

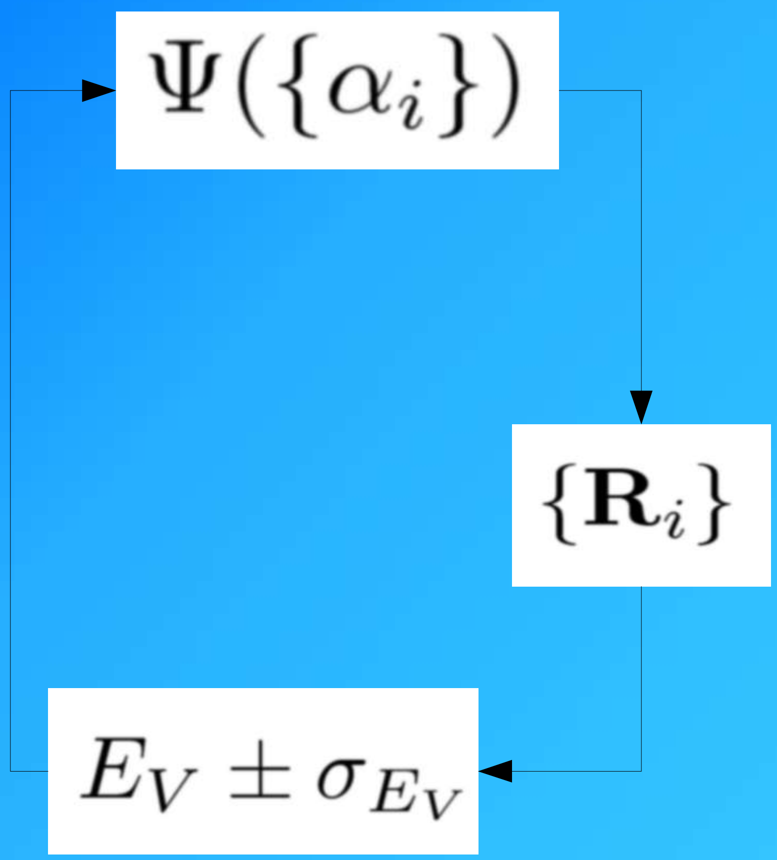
$$\{\mathbf{R}_i\}$$

$$E_V = \frac{\sum_{\mathbf{R}_i} w_i E_L(\mathbf{R}_i)}{\sum_{\mathbf{R}_i} w_i}$$

How is the wave-function optimized?

1. Set of parameters
2. Set of configs distributed according to WF
3. Variational energy

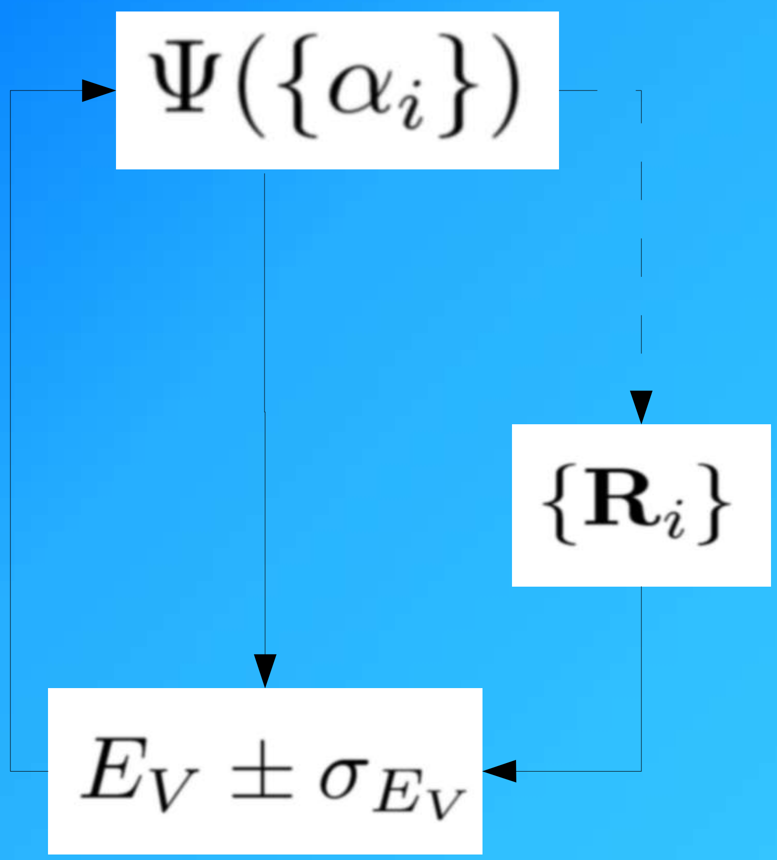
The QMC method



How is the wave-function optimized?

PROBLEM: error in energy is configuration-dependent.

The QMC method

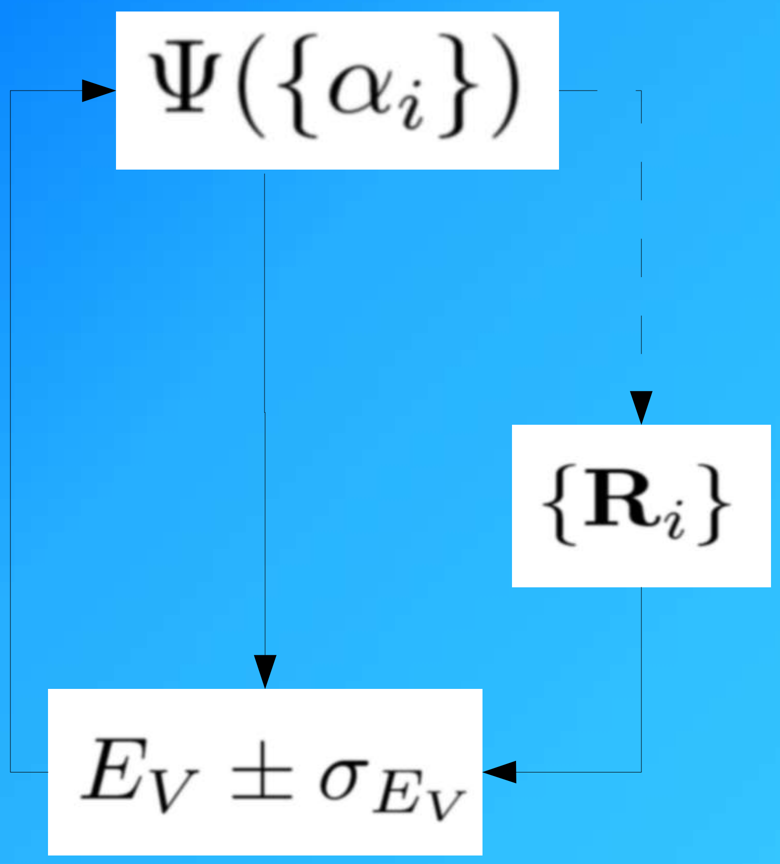


How is the wave-function optimized?

PROBLEM: error in energy is configuration-dependent.

SOLUTION: use correlated sampling.

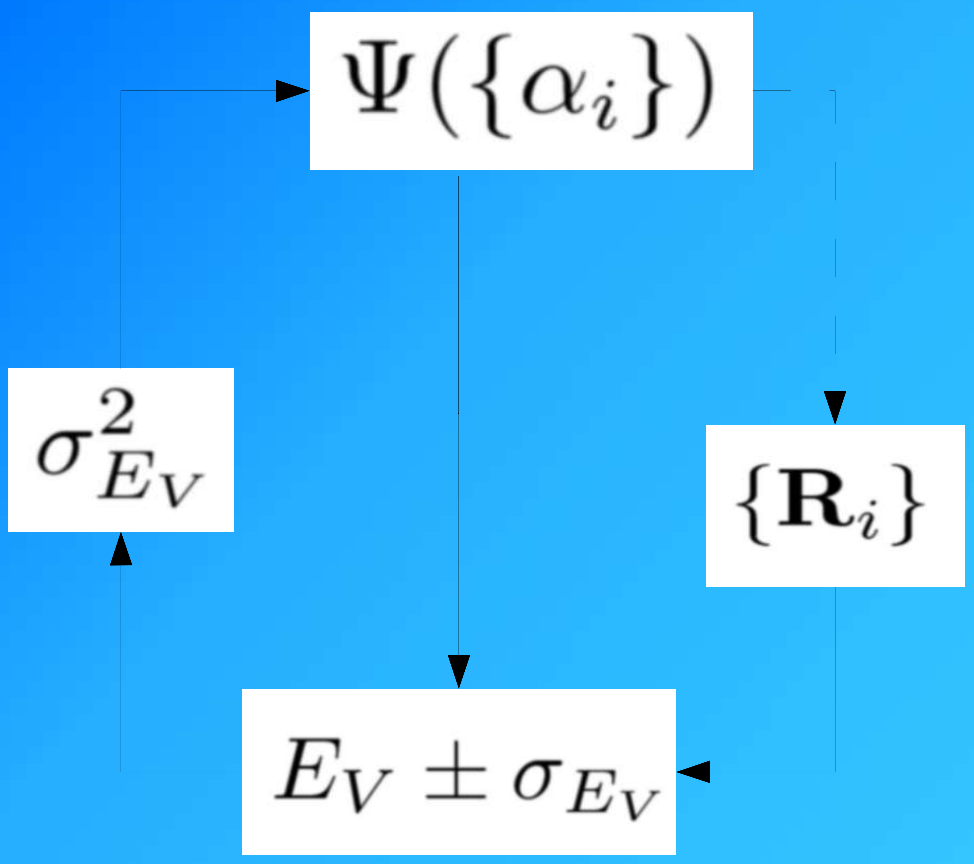
The QMC method



How is the wave-function optimized?

PROBLEM: correlated sampling favours unphysical low-energy configs.

The QMC method



How is the wave-function optimized?

PROBLEM: correlated sampling favours unphysical low-energy configs.

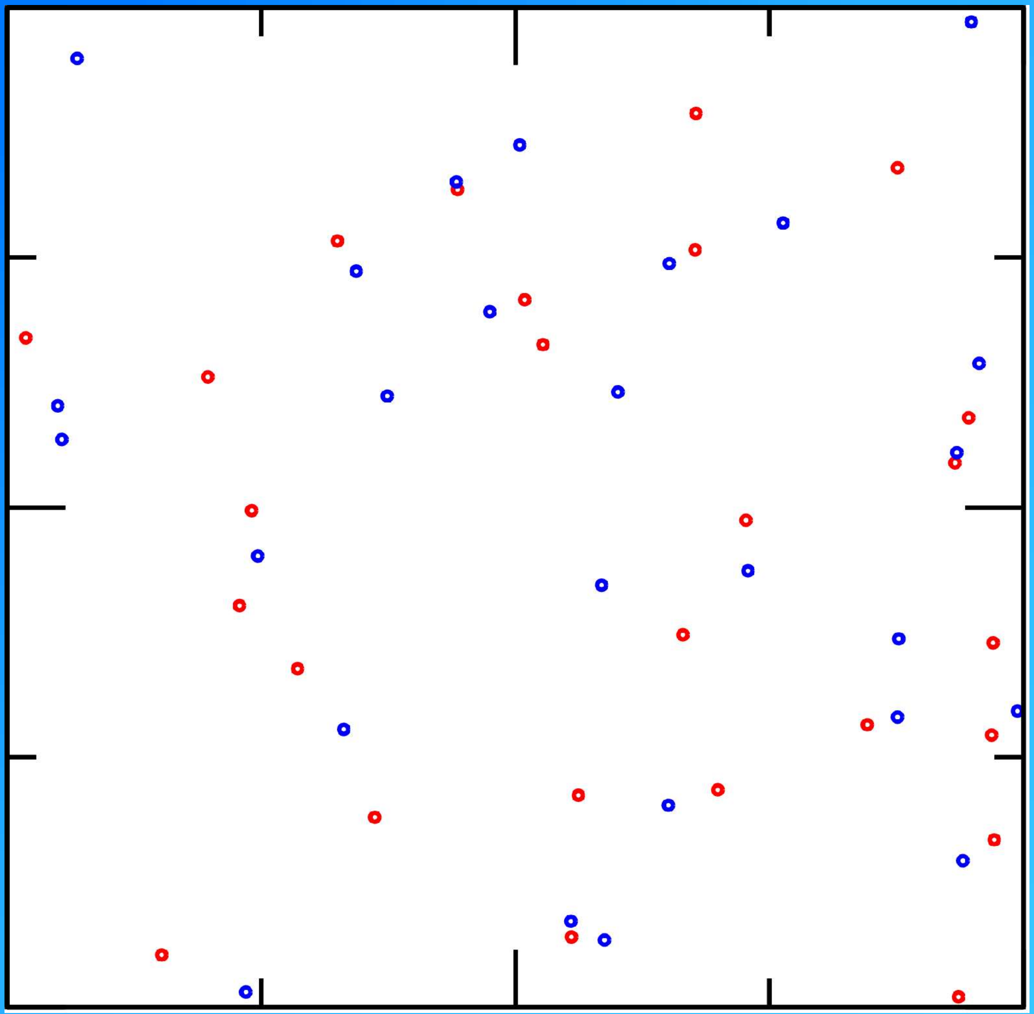
SOLUTION: minimize the variance of the energy.

The problem

Variance minimization encounters problems for this case.
[2-D e-h system in fluid phase]

$$
\begin{array}{lll}
\hline
\text{VMC \#1} & E = -0.0540(5)\ a.u. & \sigma^2 = 2.8759\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#2} & E = +0.153(1)\ a.u. & \sigma^2 = 12.85\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#3} & E = -0.1063(2)\ a.u. & \sigma^2 = 0.5071\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#4} & E = +0.316(2)\ a.u. & \sigma^2 = 64.97\ a.u.
\end{array}
$$

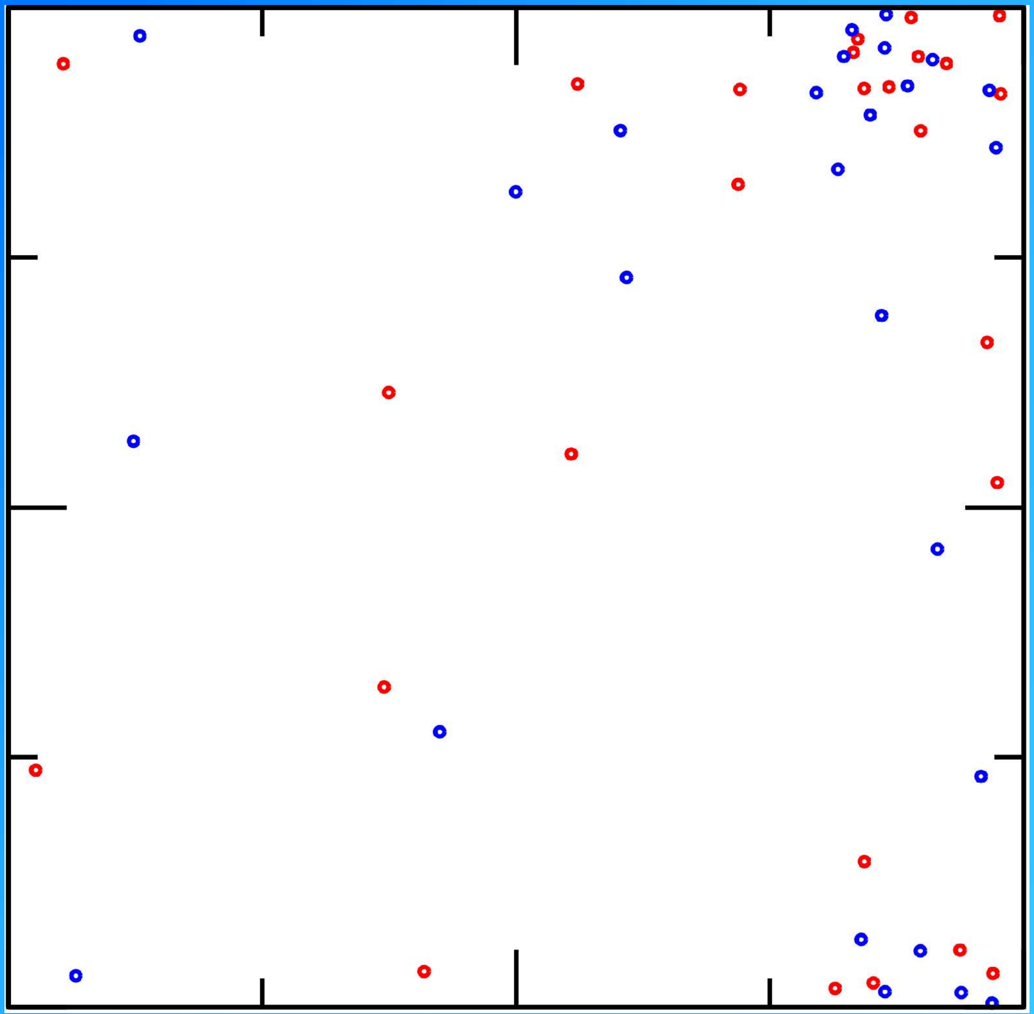
The problem



What happens?

In the first config regeneration we find this behaviour.

The problem



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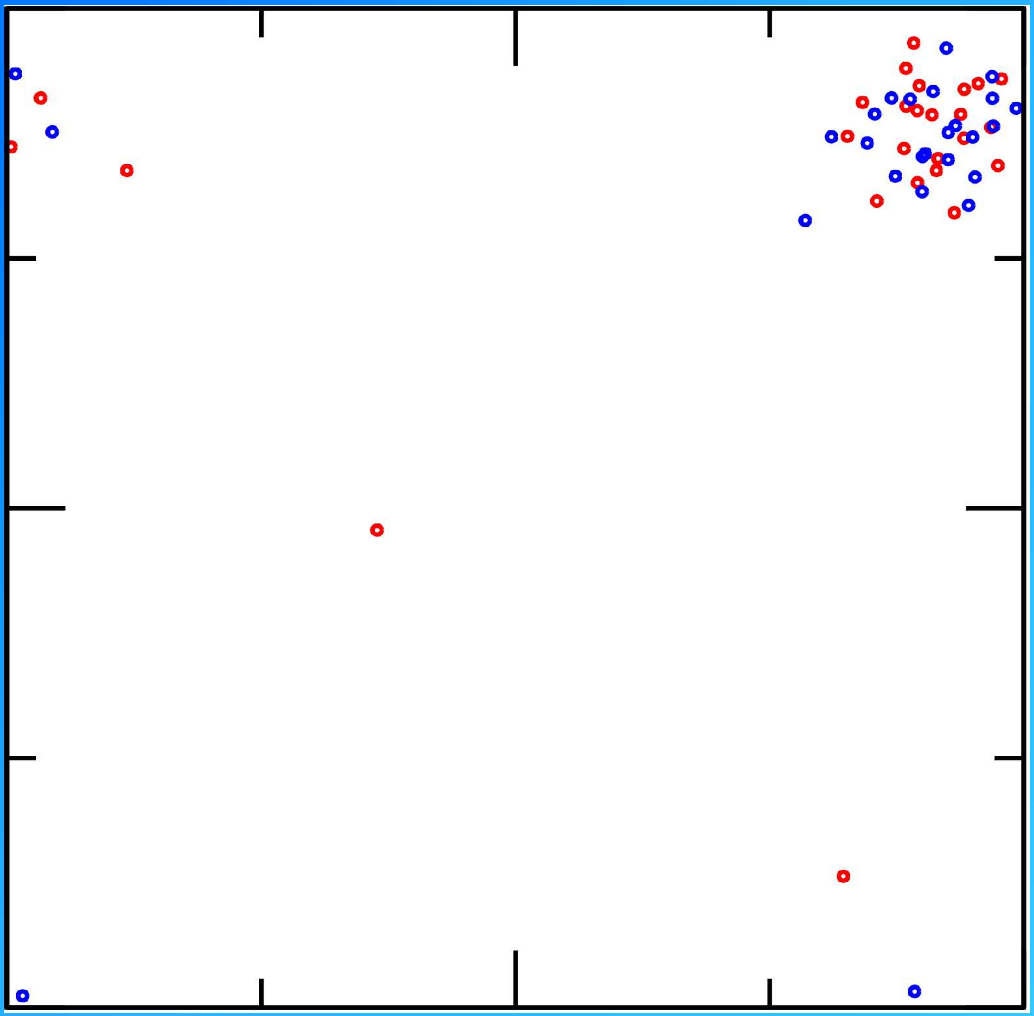

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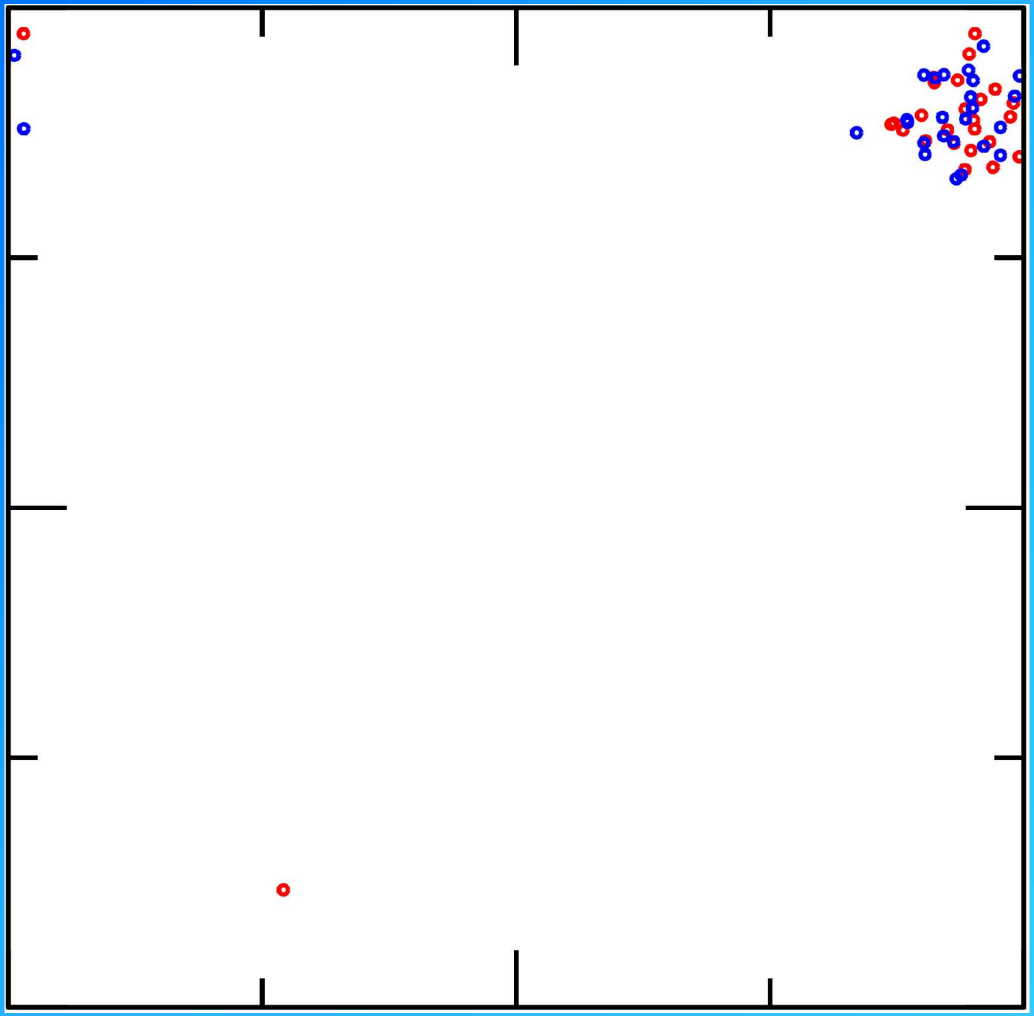
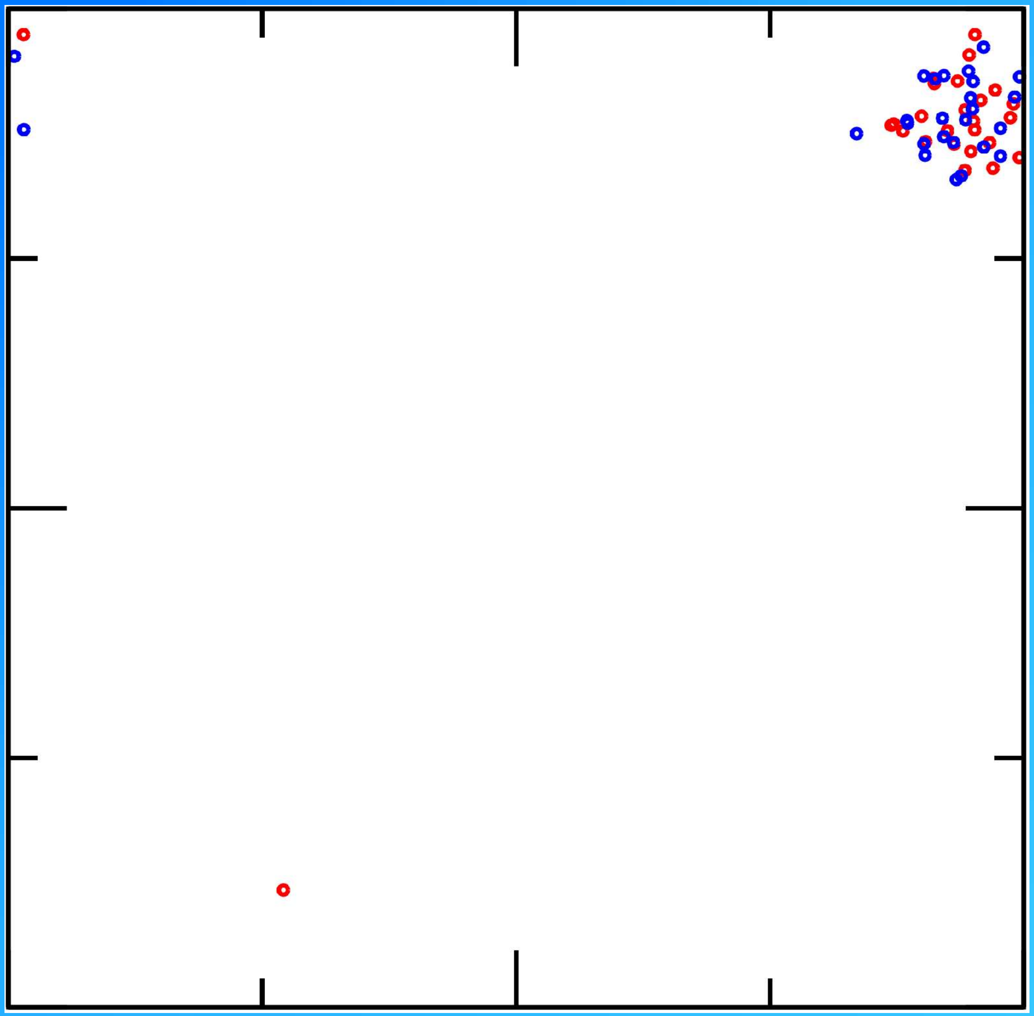


What happens?

In the first config regeneration we find this behaviour.

The optimized WF makes the distribution collapse.

The problem

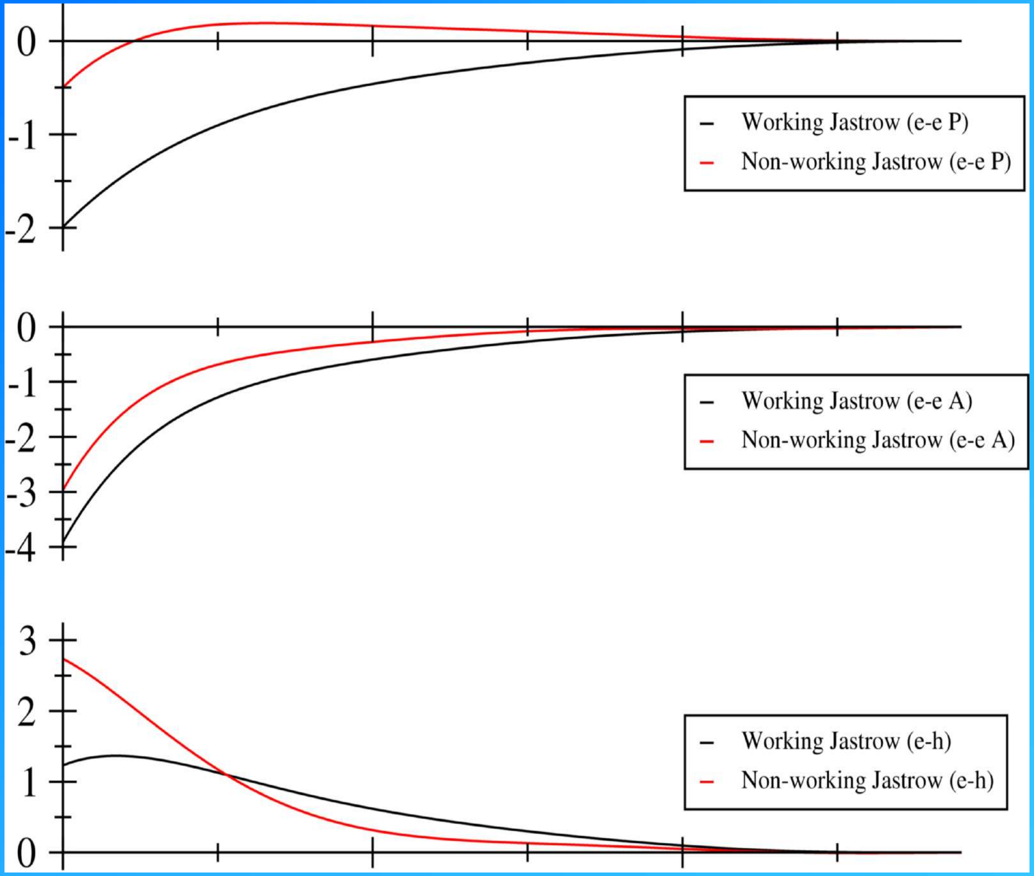


...but WHY?

In this case, the fluid phase is unstable with respect to the EP.

Variance minimization attempts to produce pairing through the Jastrow factor.

The problem



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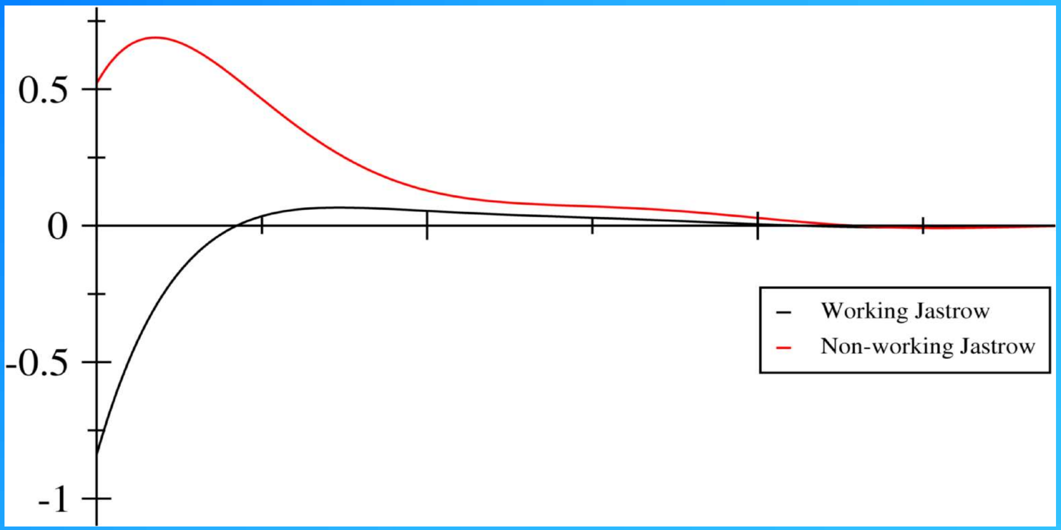
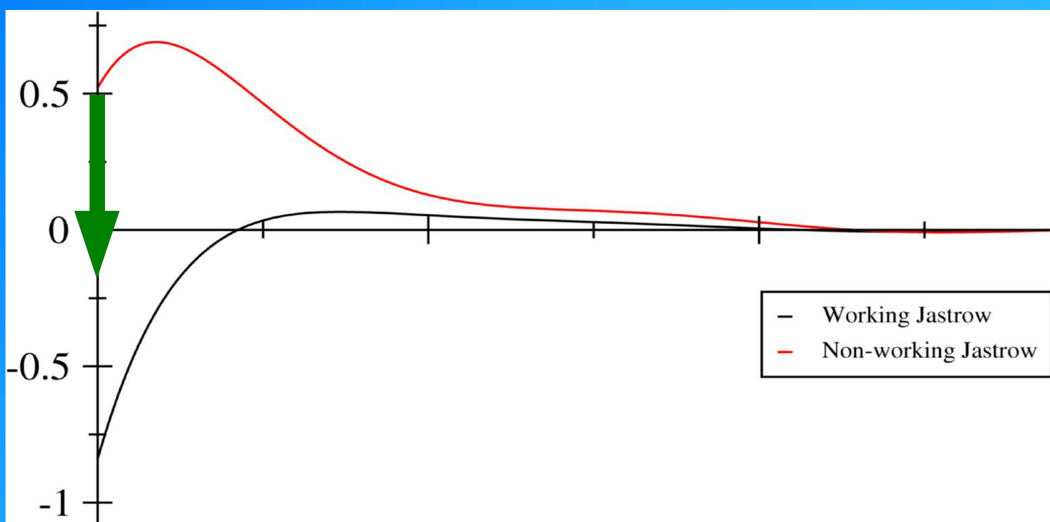


...but WHY?

This is how the total Jastrow factor would look like if all particles were kept at the same distance from each other (this is an approx).

The WF is large at zero distance.

First solution

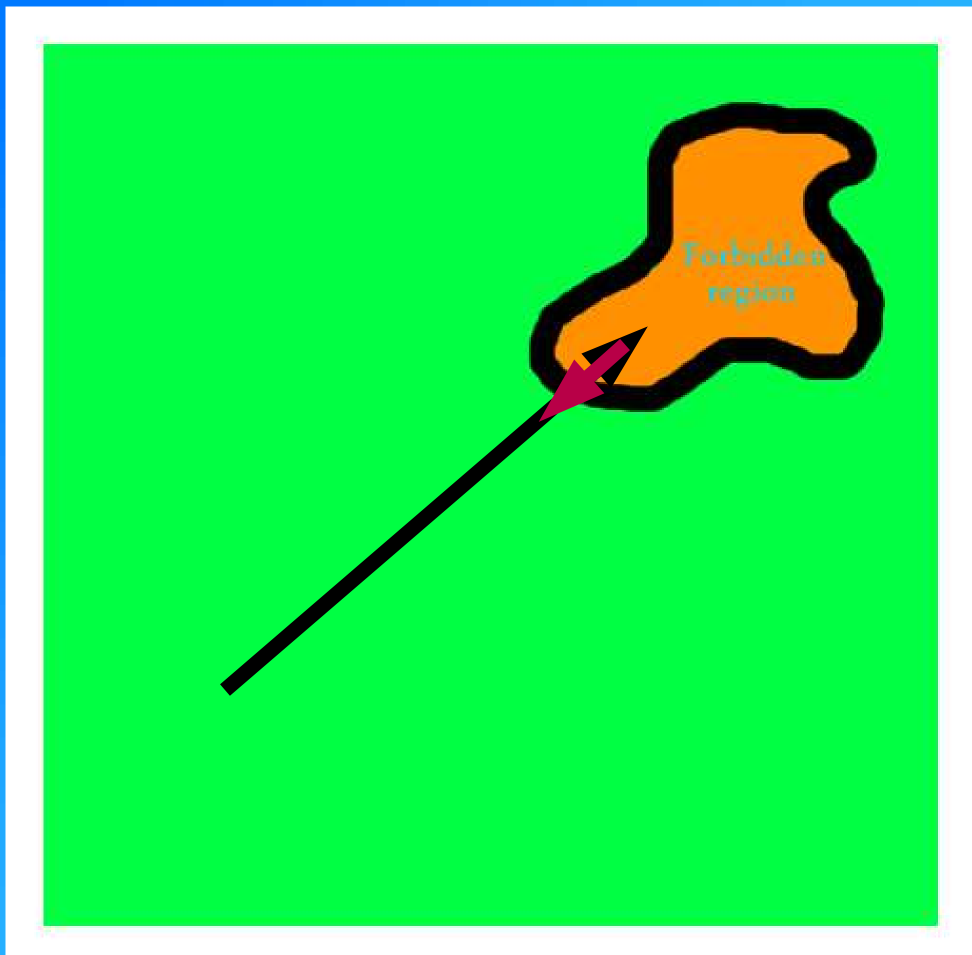


We should try to limit the value of the Jastrow function at r=0.

The e-h contribution has to be limited so that

$J(r=0)<0$.

First solution



We should try to limit the value of the Jastrow function at r=0.

The e-h contribution has to be limited so that

$J(r=0)<0$.

We are creating a "forbidden region" in param space.

First solution

Variance minimization with a limited Jastrow.
Looks quite good...

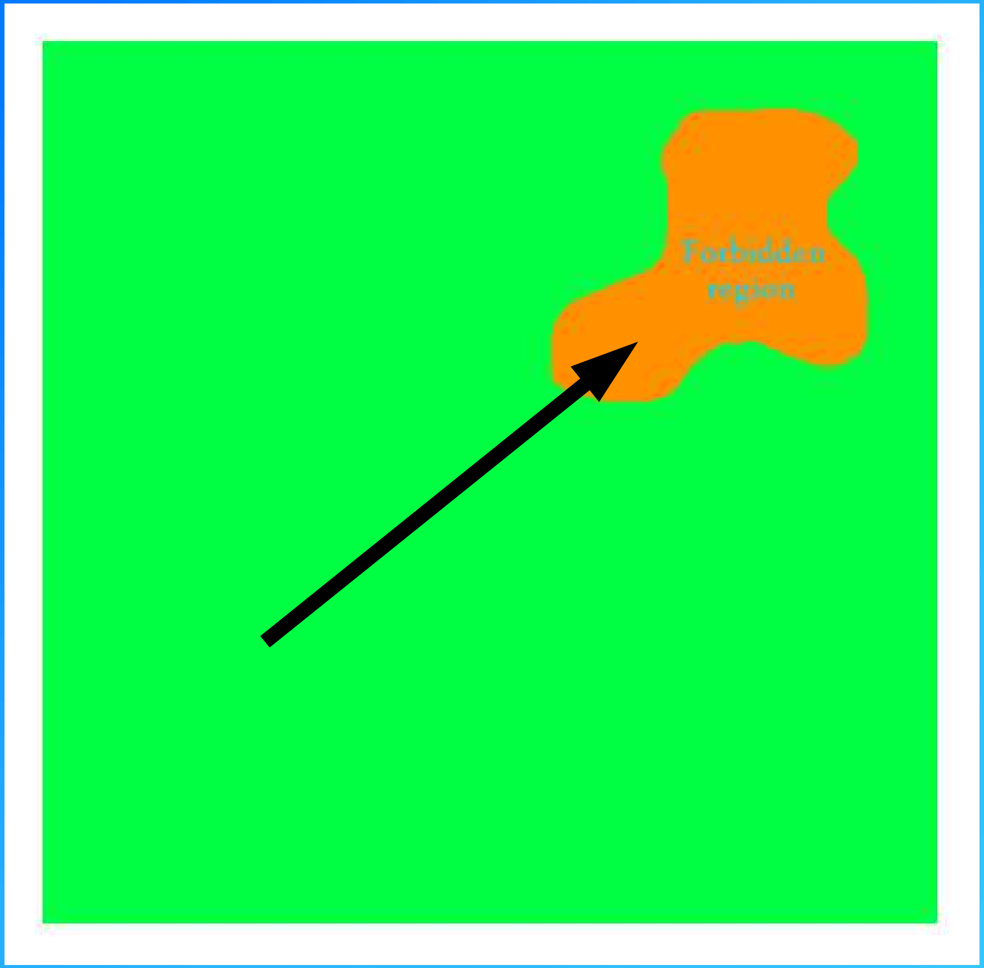
$$\text{VMC \#1} \quad E = -0.0540(5)\ a.u. \quad \sigma^2 = 2.8759\ a.u.$$
$$\Downarrow \text{VM}$$
$$\text{VMC \#2} \quad E = -0.1119(2)\ a.u. \quad \sigma^2 = 0.5526\ a.u.$$
$$\Downarrow \text{VM}$$
$$\text{VMC \#3} \quad E = -0.1020(3)\ a.u. \quad \sigma^2 = 1.0227\ a.u.$$
$$\Downarrow \text{VM}$$
$$\text{VMC \#4} \quad E = -0.1084(2)\ a.u. \quad \sigma^2 = 0.5875\ a.u.$$

First solution

...except when the Jastrow cut-off is large.
In this case, the "forbidden region" is not well characterized.

$$\text{VMC \#1} \quad E = -0.0540(5)\ a.u. \quad \sigma^2 = 1.4756\ a.u.$$
$$\Downarrow \text{VM}$$
$$\text{VMC \#2} \quad E = +1.4825(7)\ a.u. \quad \sigma^2 = 6.5841\ a.u.$$
$$\Downarrow \text{VM}$$
$$\text{VMC \#3} \quad E = +2.089(4)\ a.u. \quad \sigma^2 = 200.71\ a.u.$$
$$\Downarrow \text{VM}$$
$$\text{VMC \#4} \quad E = +1.175(2)\ a.u. \quad \sigma^2 = 46.489\ a.u.$$

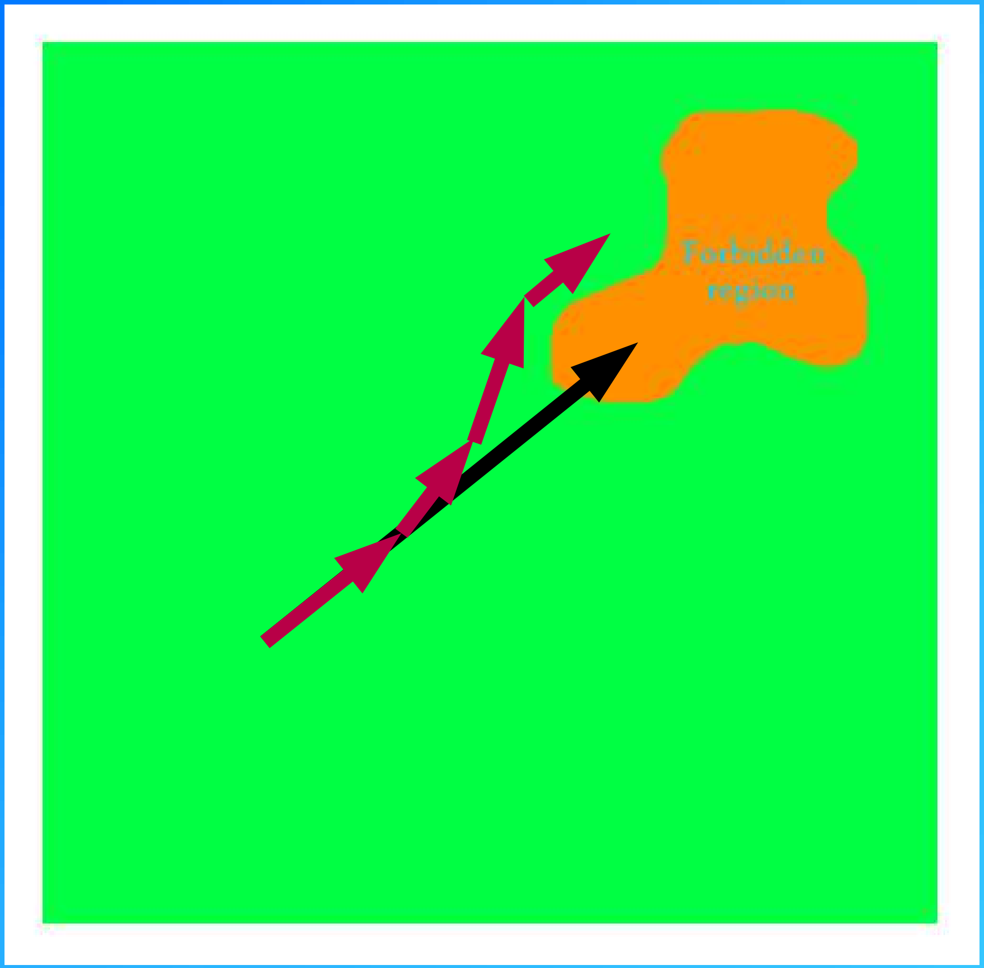
Second solution



Correlated sampling can make regions of parameter space look favourable even if they are not. Old configs inconsistent with new params.

Instead of not allowing the optimization into this region, let's make it "realize by itself".

Second solution



Correlated sampling can make regions of parameter space look favourable even if they are not. Old configs inconsistent with new params.

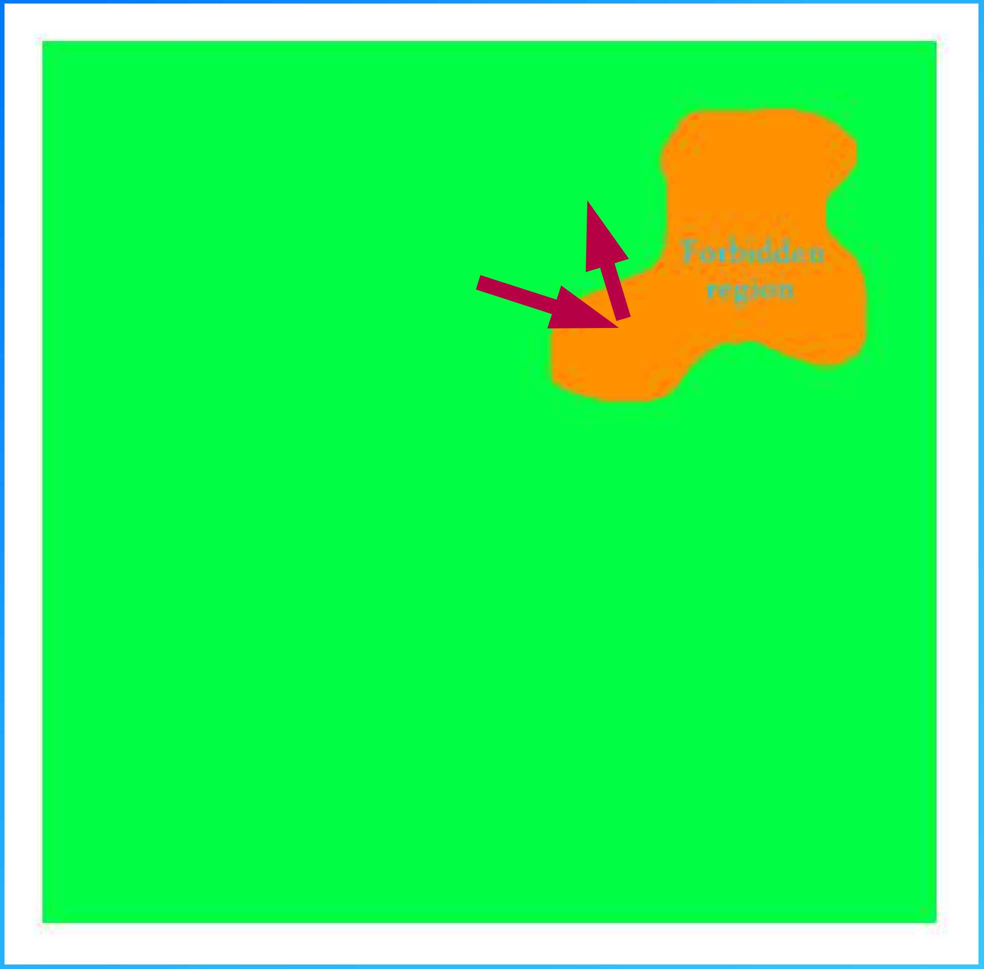
Instead of not allowing the optimization into this region, let's make it “realize by itself”.

Second solution

Results are better than previous solution for variable Jastrow cut-off.
But for a large cut-off...

$$
\begin{array}{lll}
\text{VMC \#1} & E = -0.0540(5)\ a.u. & \sigma^2 = 1.476\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#2} & E = +1.4796(6)\ a.u. & \sigma^2 = 6.503\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#3} & E = +0.7242(9)\ a.u. & \sigma^2 = 10.323\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#4} & E = +0.3965(2)\ a.u. & \sigma^2 = 0.655\ a.u.
\end{array}
$$

Second solution

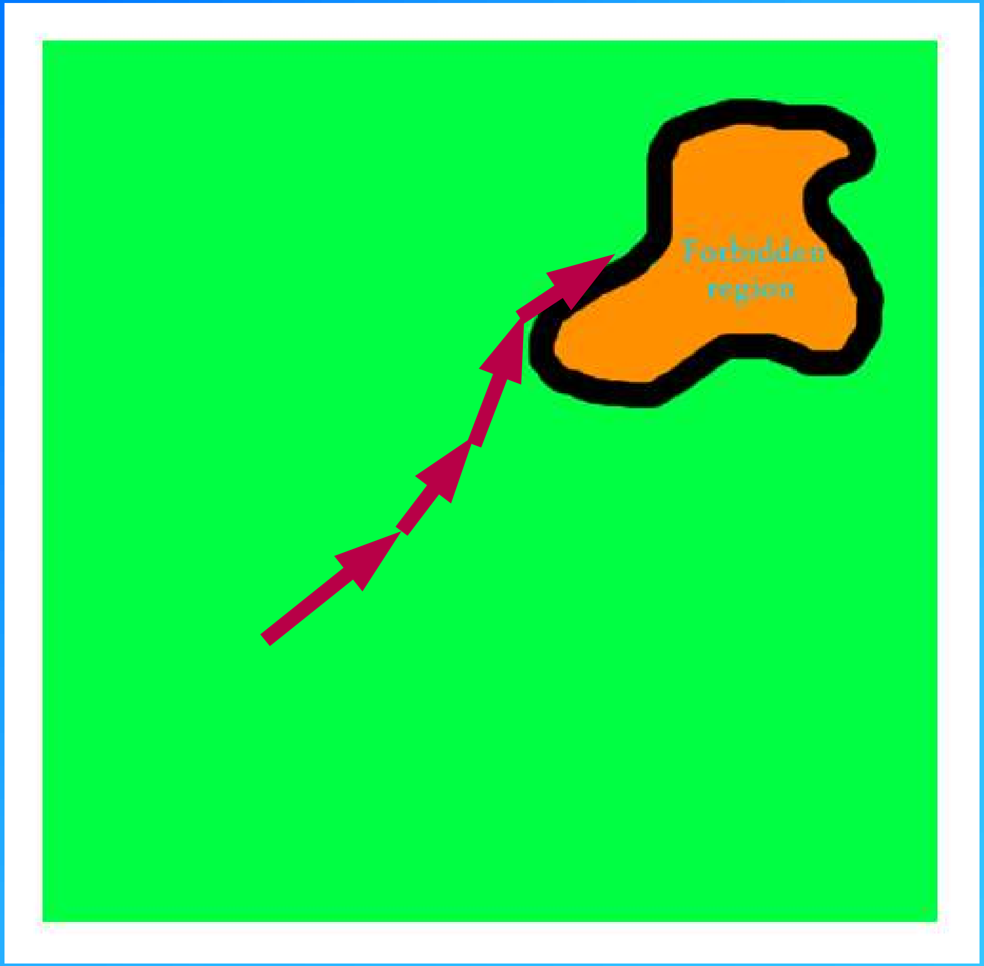


What happens is that the variance changes in shape strongly when close to the "forbidden region".

Iterations go back and forth all the time.

Stepsize cannot be made smaller (still need correlated sampling).

Final solution



First option used too long minimizations and eventually found a way inside the region.

Second option gets inside the region, as it is not forbidden.

So, use both.

Final solution

And the results are good!

$$
\begin{array}{lll}
\text{VMC \#1} & E = -0.0565(5)\ a.u. & \sigma^2 = 1.525\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#2} & E = +1.6651(8)\ a.u. & \sigma^2 = 8.970\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#3} & E = -0.1157(2)\ a.u. & \sigma^2 = 0.3400\ a.u. \\
\Downarrow \text{VM} & & \\
\text{VMC \#4} & E = -0.1330(1)\ a.u. & \sigma^2 = 0.1811\ a.u.
\end{array}
$$