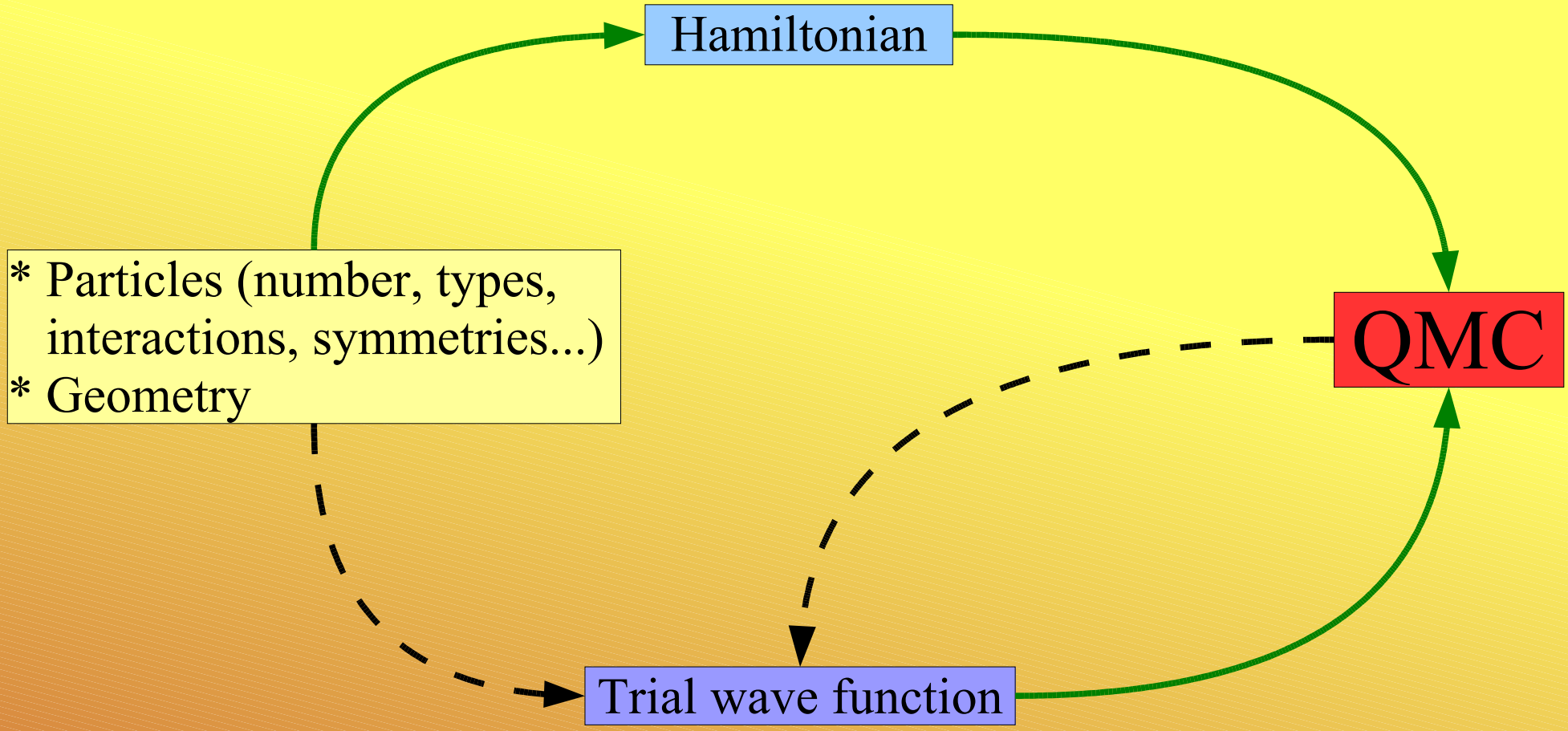
The electron-hole system and QMC

Studying the phases of the electron-hole system

The electron-hole system and QMC

1. How to use QMC to solve a problem.



The electron-hole system and QMC

1. How to use QMC to solve a problem.

Choosing the wave function

For each problem:

* Take known solutions & limits into account

* Combine one-particle orbitals into a compact form which can be optimized easily (Slater-Jastrow, etc.)

* Take all symmetries into account

The electron-hole system and QMC

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The electron-hole system and QMC

2. The electron-hole system

Known limits:

* V=0 : two-component fluid – plane-wave orbitals

* KE=0 : Wigner-Crystal – localized orbitals

* Mean-field : electron-hole pairing – pairing orbitals

The electron-hole system and QMC

2. The electron-hole system

Traditional approach:

* Study the three limits separately using QMC

* The dominant phase is the one with the lowest energy

What's wrong?

The electron-hole system and QMC

2. The electron-hole system

Traditional approach:

* Study the three limits separately using QMC

* The dominant phase is the one with the lowest energy

What's wrong?

We are splitting **one** problem into **three**...

The electron-hole system and QMC

2. The electron-hole system

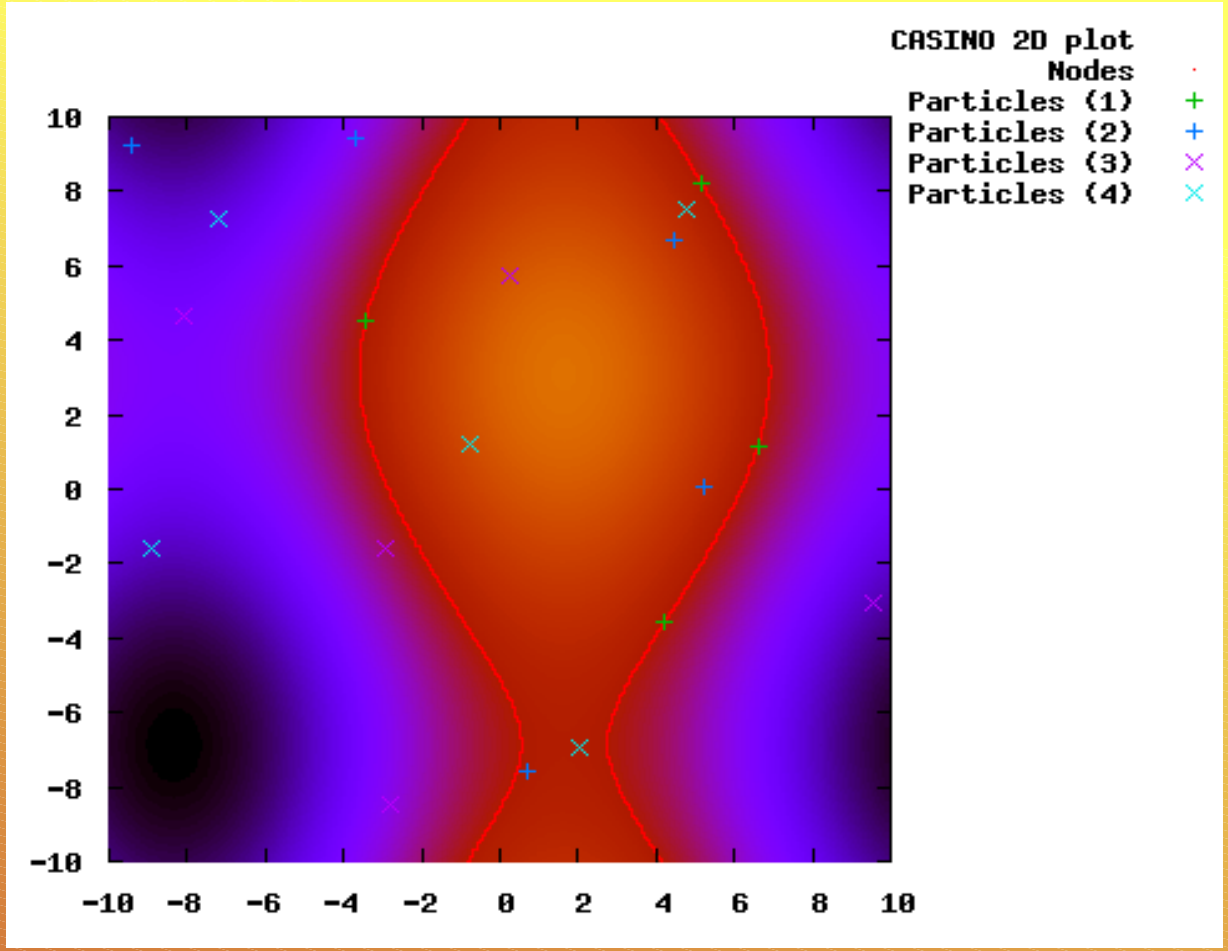
* Is there anything actually wrong with that?

* What is the correct way of proceeding, then?

The electron-hole system and QMC

3. The phase-by-phase approach

* VMC energies are totally determined by the trial wave function, so VMC energies should correspond to the phases



HF wfn, 2CP phase

The electron-hole system and QMC

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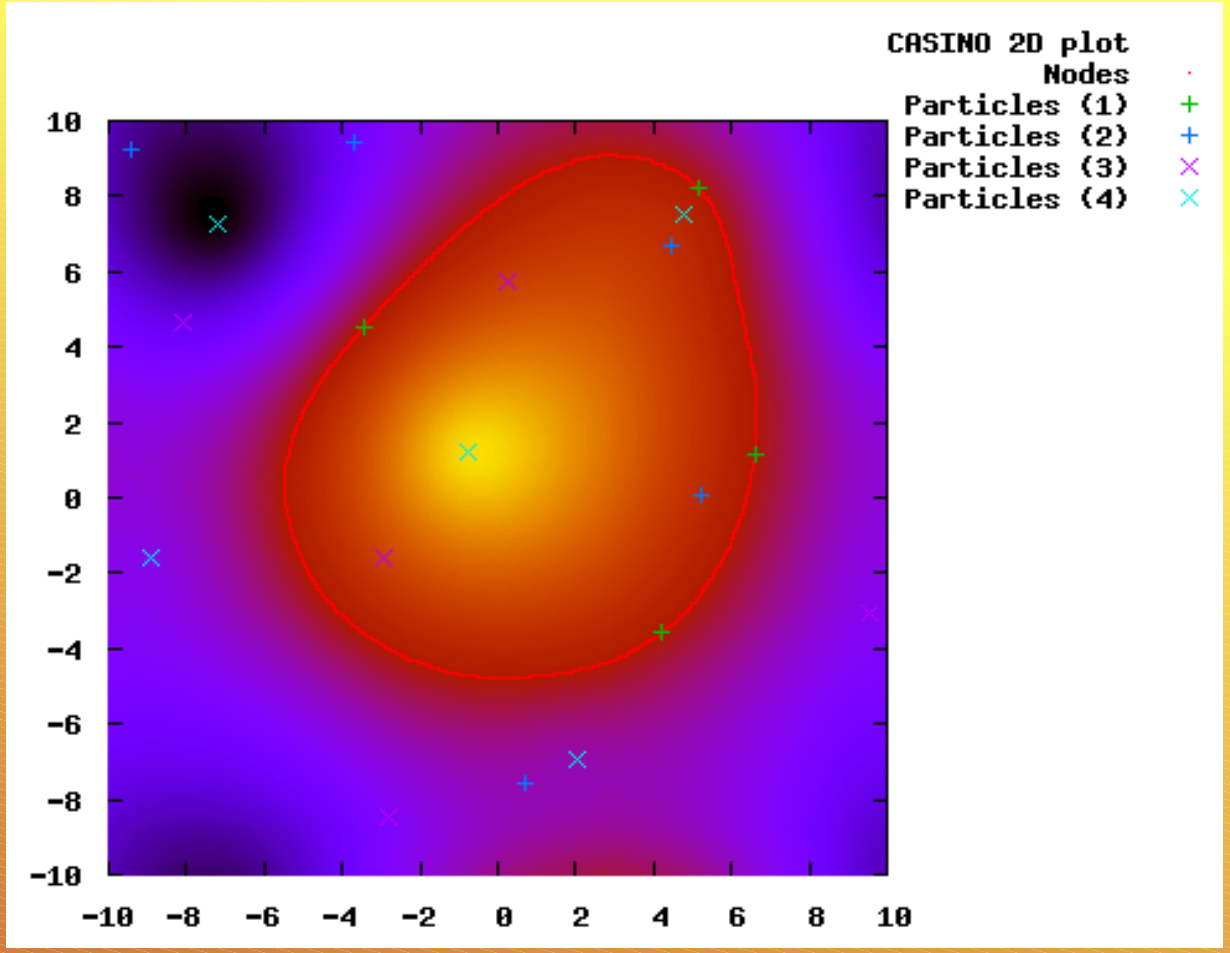
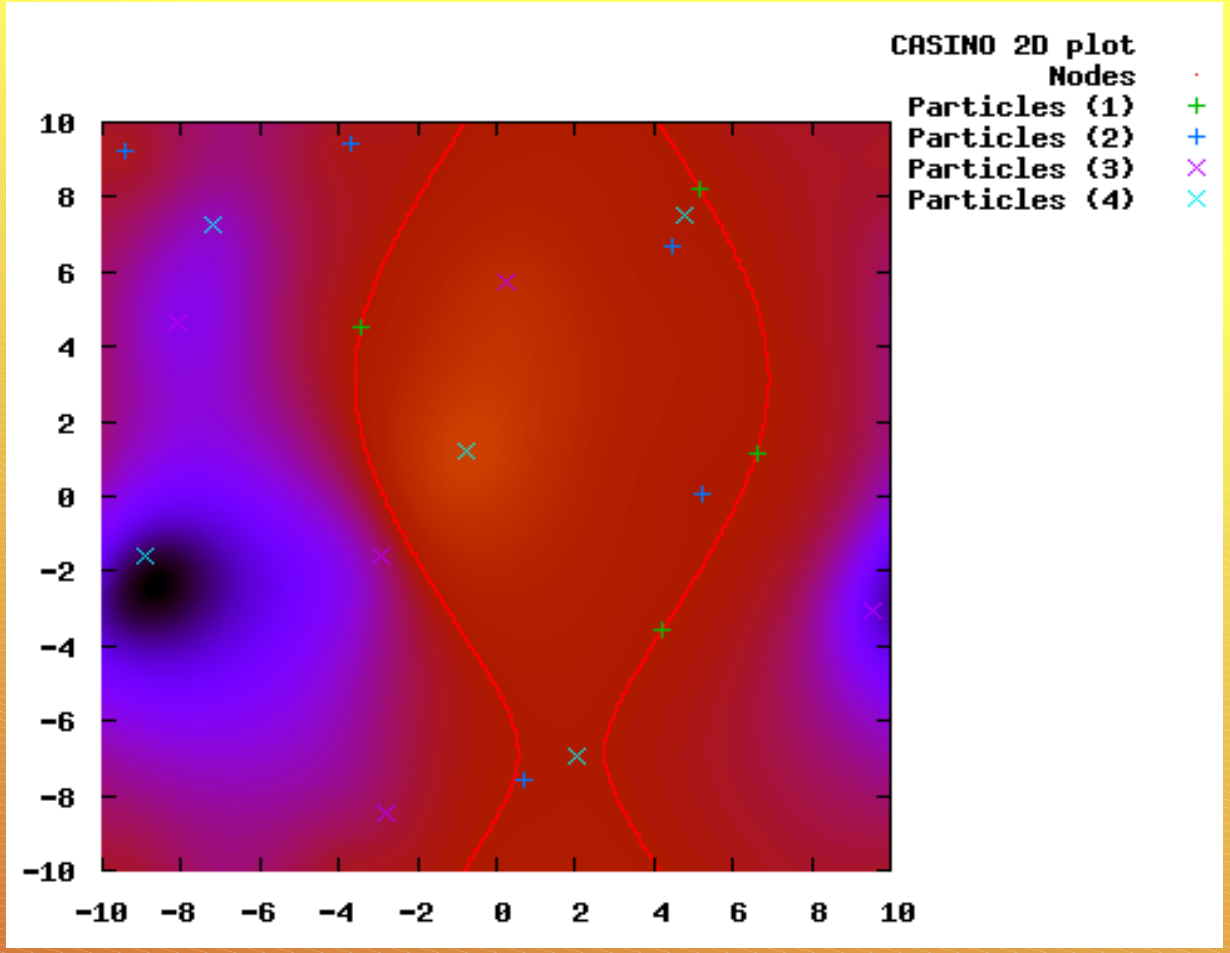


HF wfn, pairing phase

The electron-hole system and QMC

3. The phase-by-phase approach

* But can a Jastrow factor mix up the phases?



SJ wfn, 2CP phase

The electron-hole system and QMC

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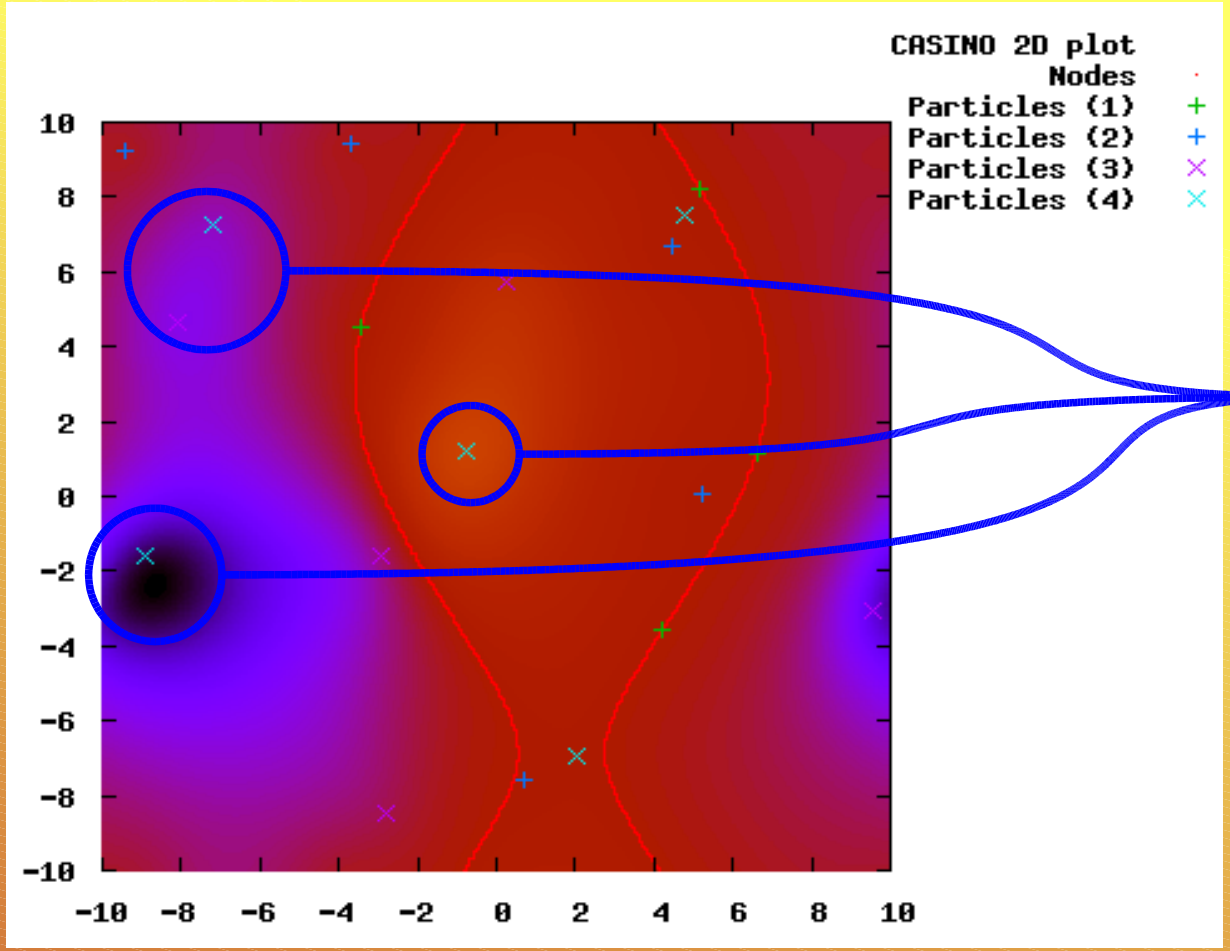

Looks like pairing...

SJ wfn, 2CP phase

The electron-hole system and QMC

3. The phase-by-phase approach

* DMC is equivalent to VMC with the best possible Jastrow. Only the nodes are unaffected (fixed-node approximation).

* Assuming that the nodes are capable of preserving the phase described by the wave function, DMC results can still be correctly assigned to each of the phases.

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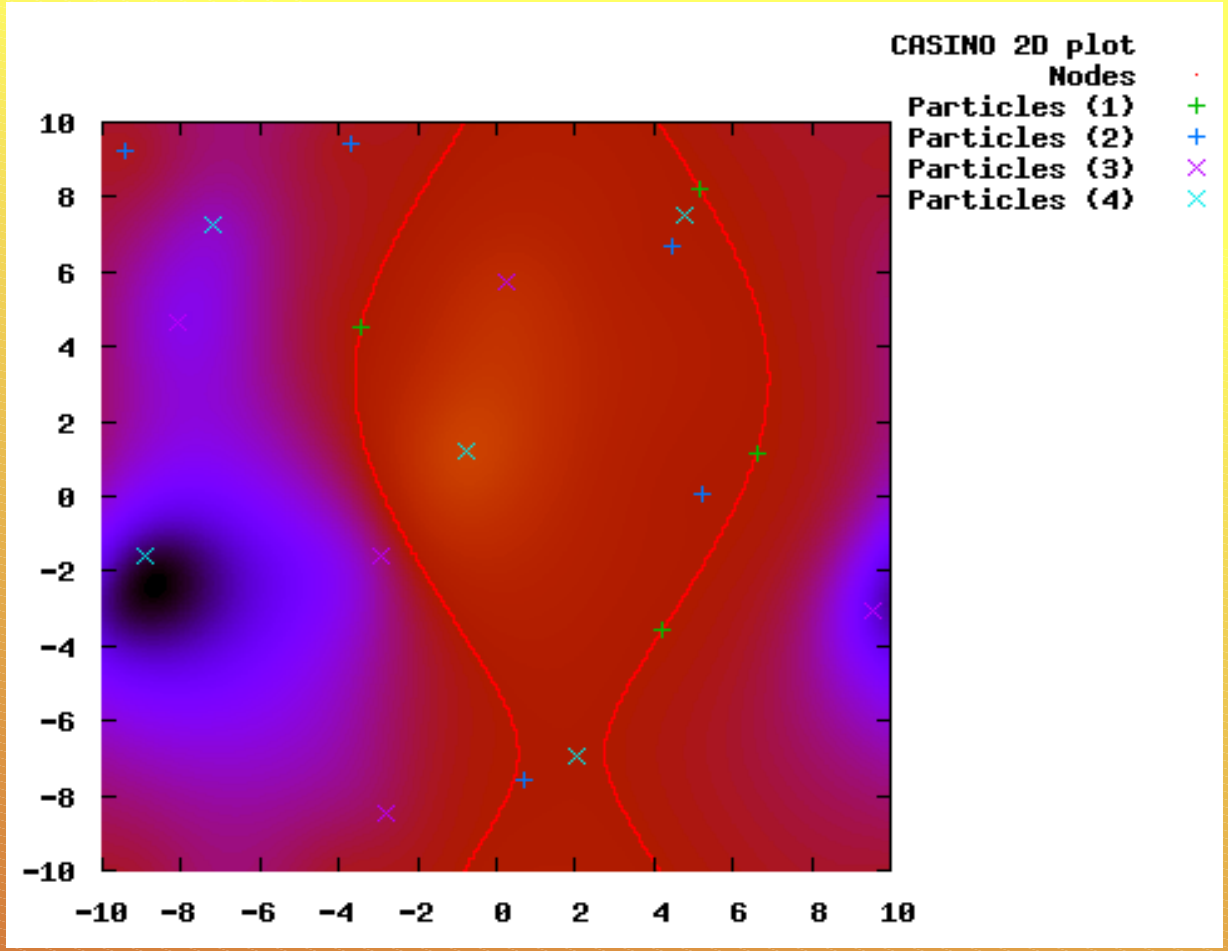
3. The phase-by-phase approach

* But what would backflow do?



SJ wfn, 2CP phase

The electron-hole system and QMC

3. The phase-by-phase approach

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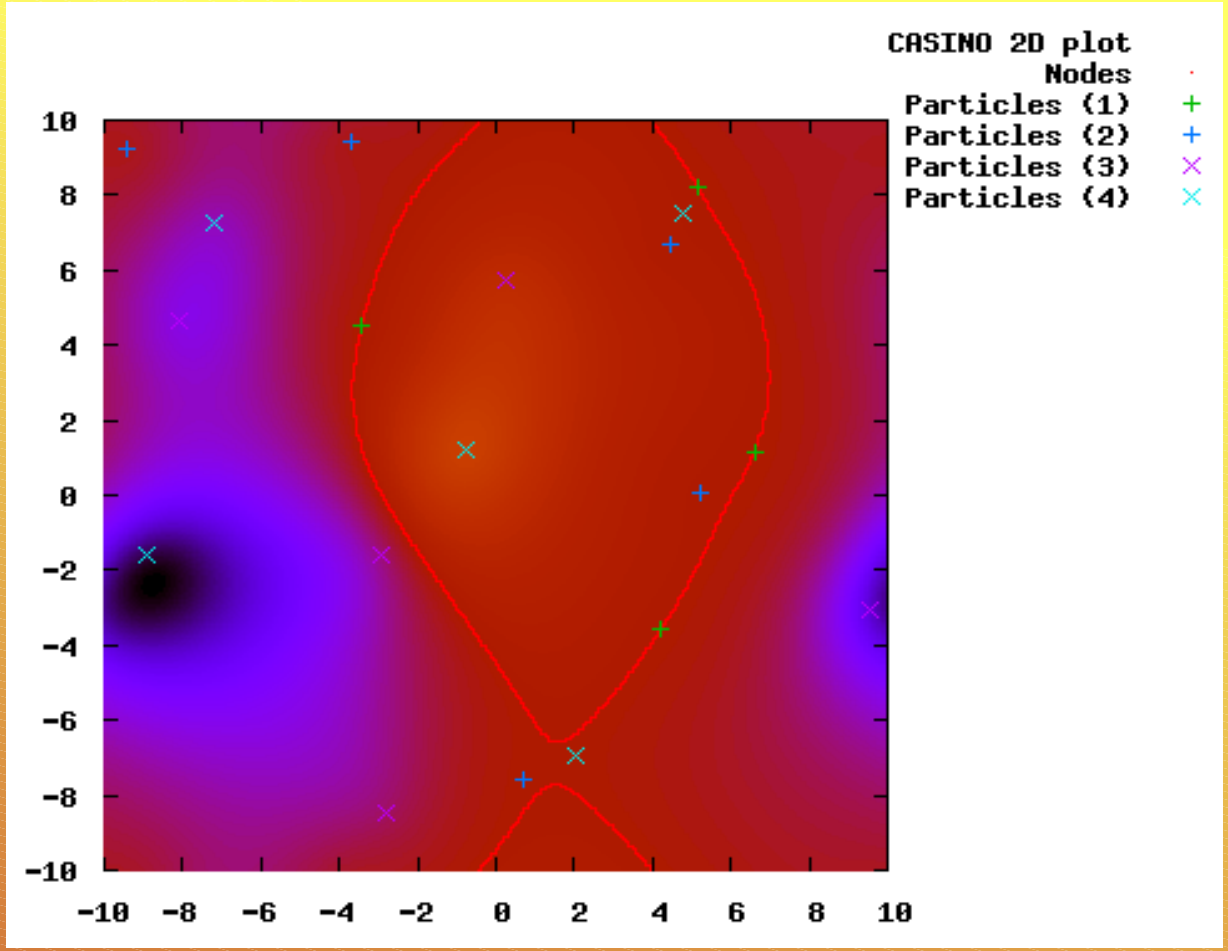

BF wfn, 2CP phase

The electron-hole system and QMC

3. The phase-by-phase approach

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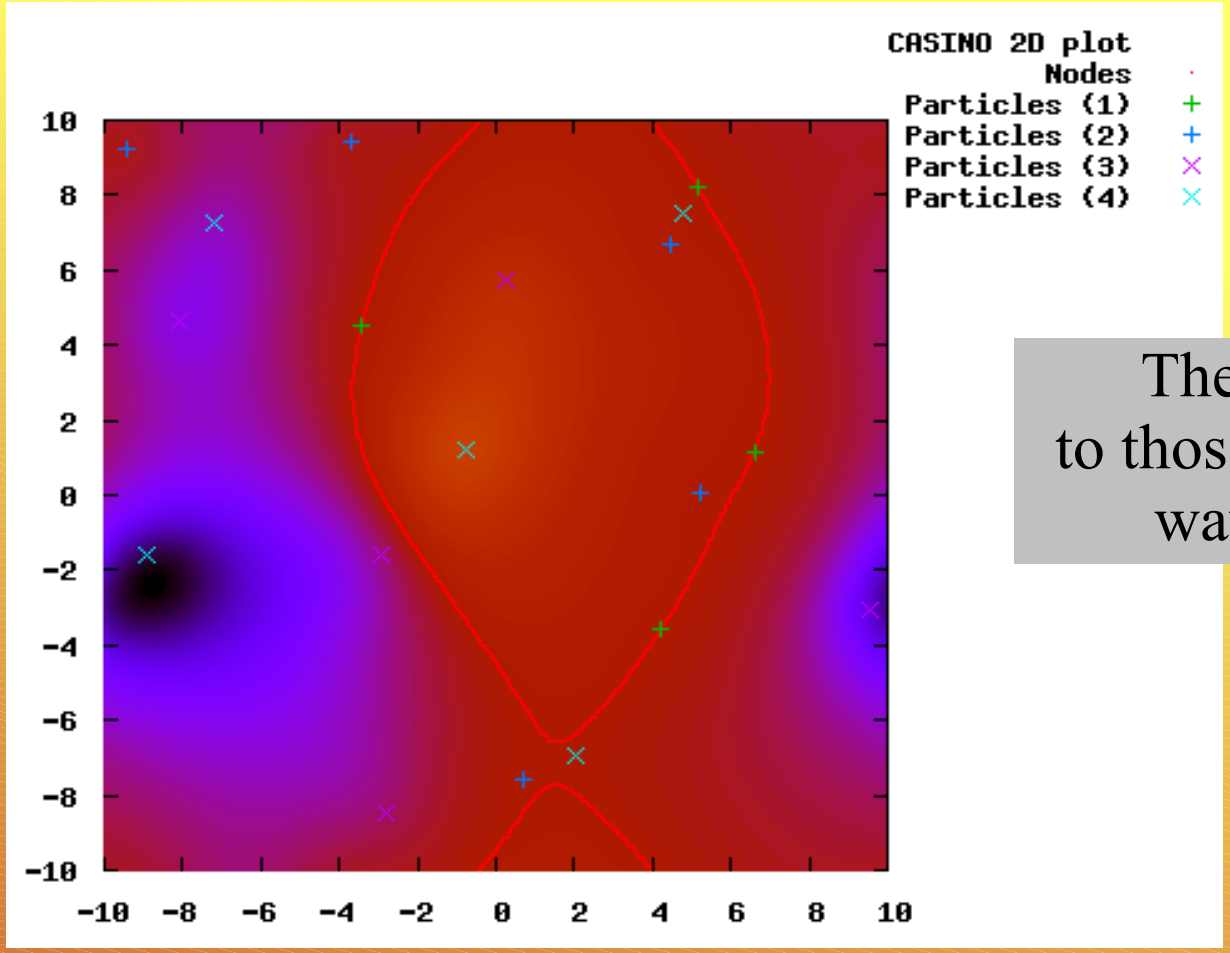


The nodes tend
to those of the pairing
wave function

BF wfn, 2CP phase

The electron-hole system and QMC

3. The phase-by-phase approach

Another problem:

* The mean field solution says all electrons should be paired with all holes, independently of their spin.

* However, one typically uses the following wave function:

$$\Psi_S = D_{e\uparrow h\downarrow} D_{e\downarrow h\uparrow}$$

which is asymmetric with respect to the interchange of, e.g., up and down-spin holes. So this is not the most general wave function.

The electron-hole system and QMC

4. Correct approach #1

Use a wave function with the following determinant part:

$$\Psi_S = c_P \left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow} \right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow} + c_C D^C_{e\uparrow} D^C_{e\downarrow} D^C_{h\uparrow} D^C_{h\downarrow}$$

This form respects the required symmetries, and includes all known limits of the system.

The dominance of one phase over the others must be studied using density matrices.

The electron-hole system and QMC

4. Correct approach #1

Let's ignore the WC limit,

$$\Psi_S = c_P \left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow} \right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

and look at various plots of the above wave function...

The electron-hole system and QMC

4. Correct approach #1

Let's ignore the WC limit,

$$\Psi_S = c_P \left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow} \right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

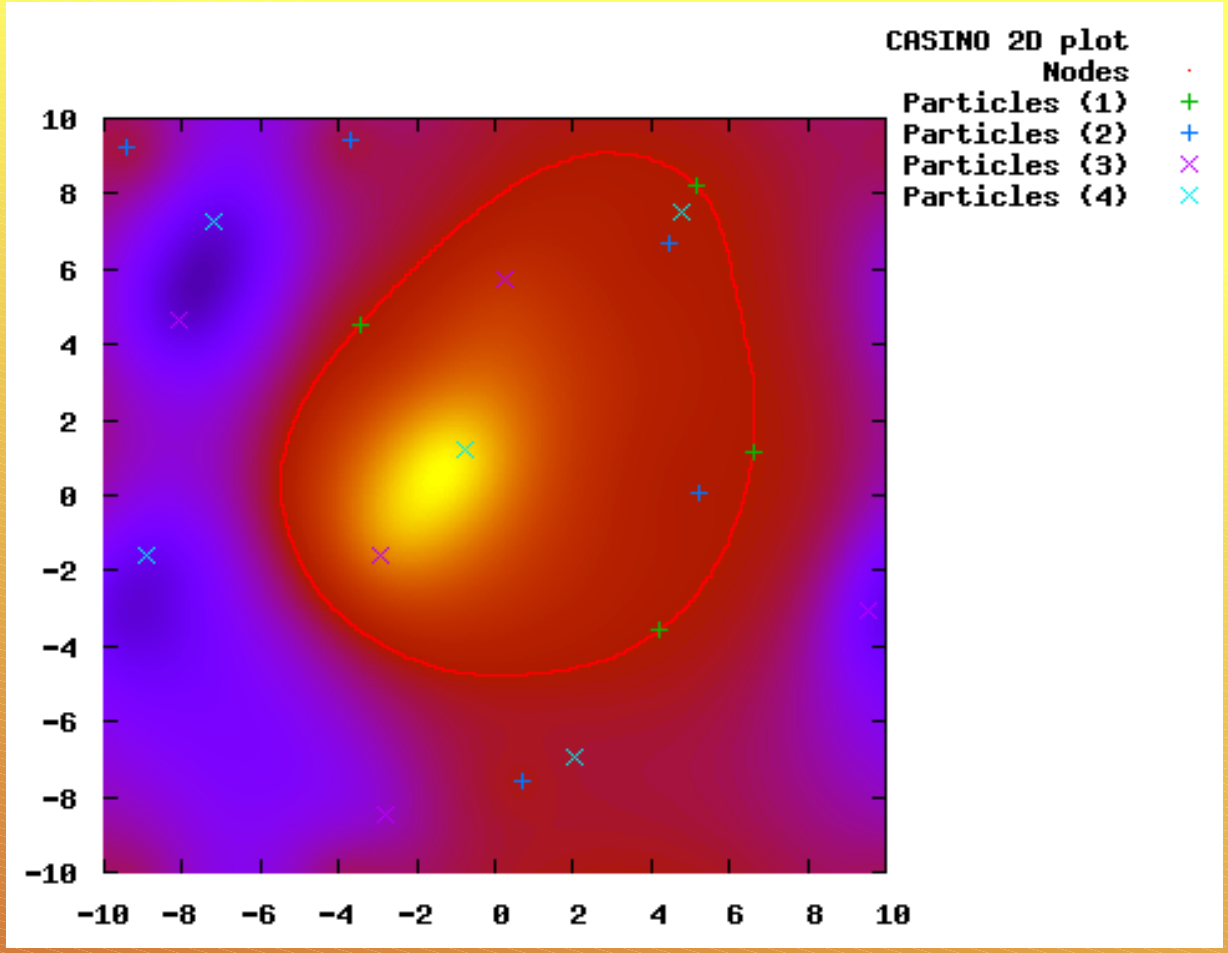
and look at various plots of the above wave function...

...without the symmetrizing pairing determinant.

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

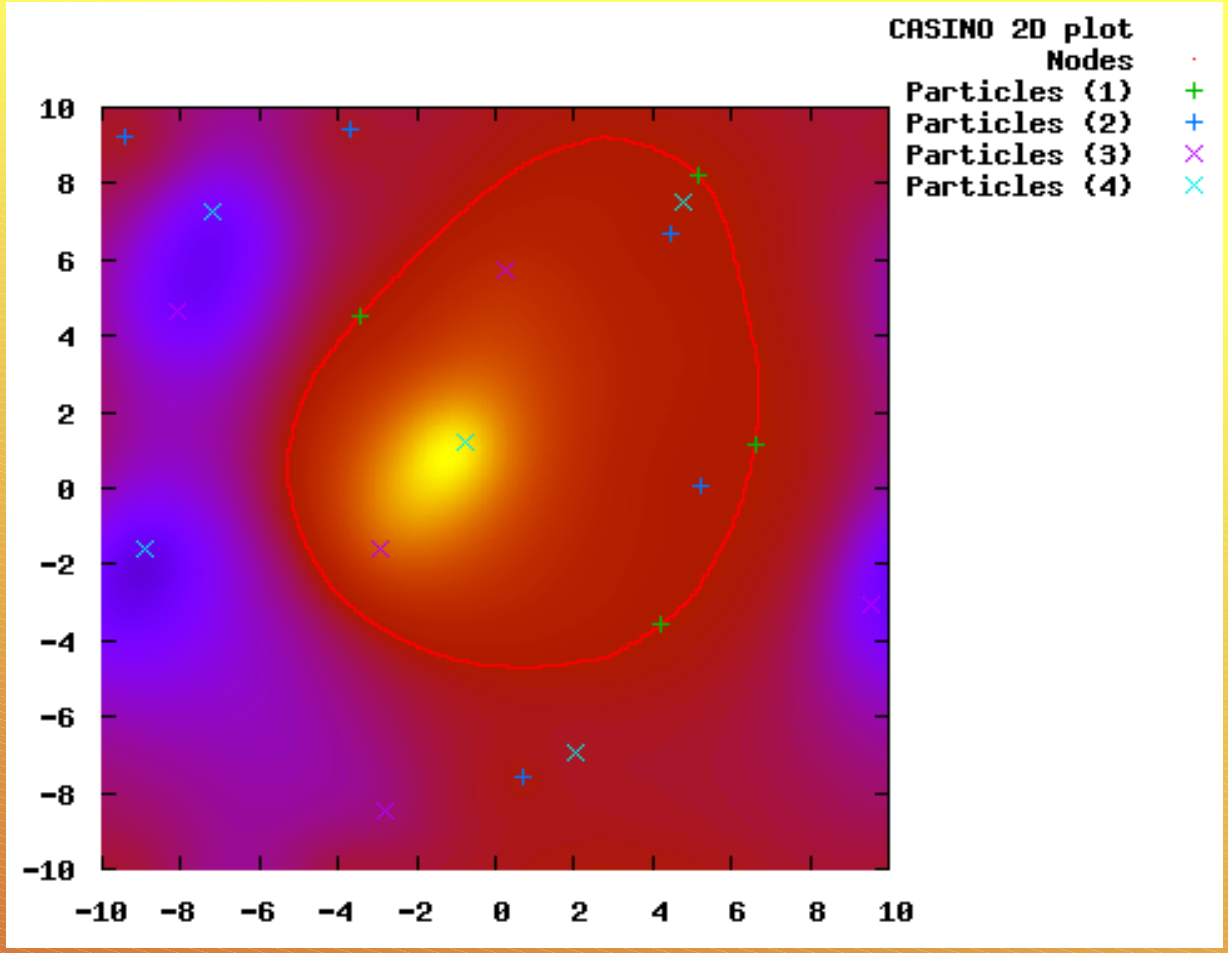


SJ wfn, $c_F/c_P=0$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

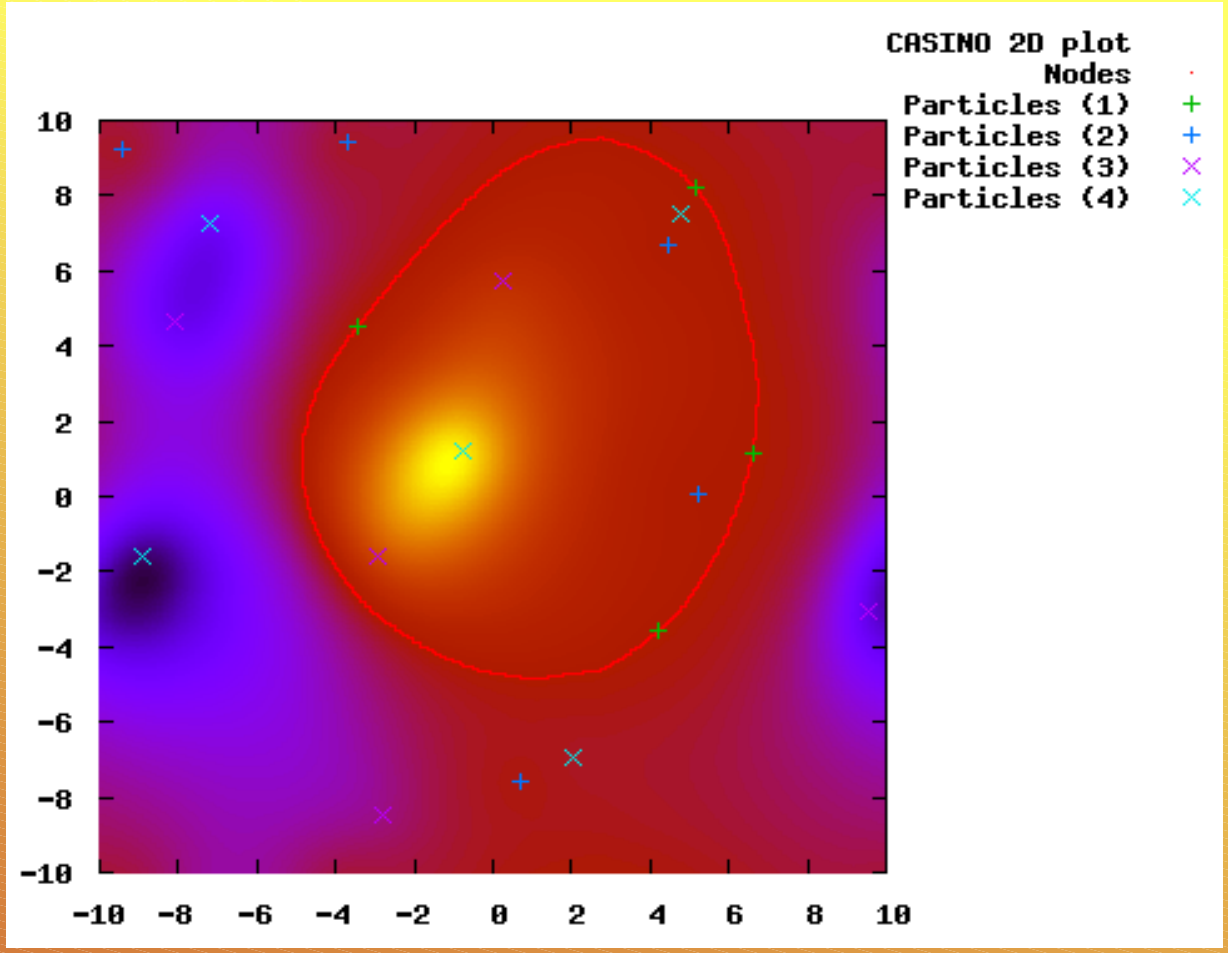


SJ wfn, c_F/c_P=-1

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

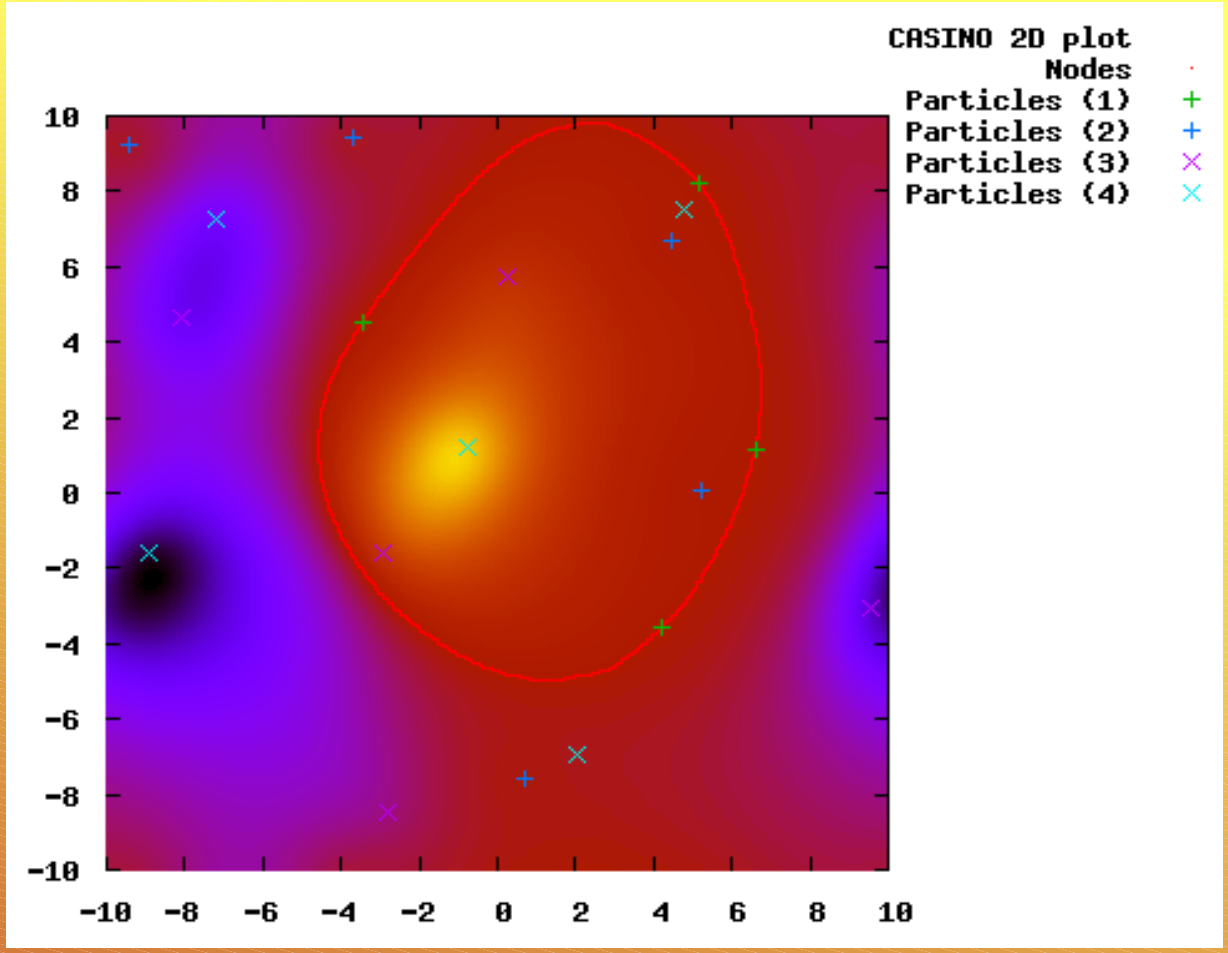


SJ wfn, c_F/c_P=-10

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

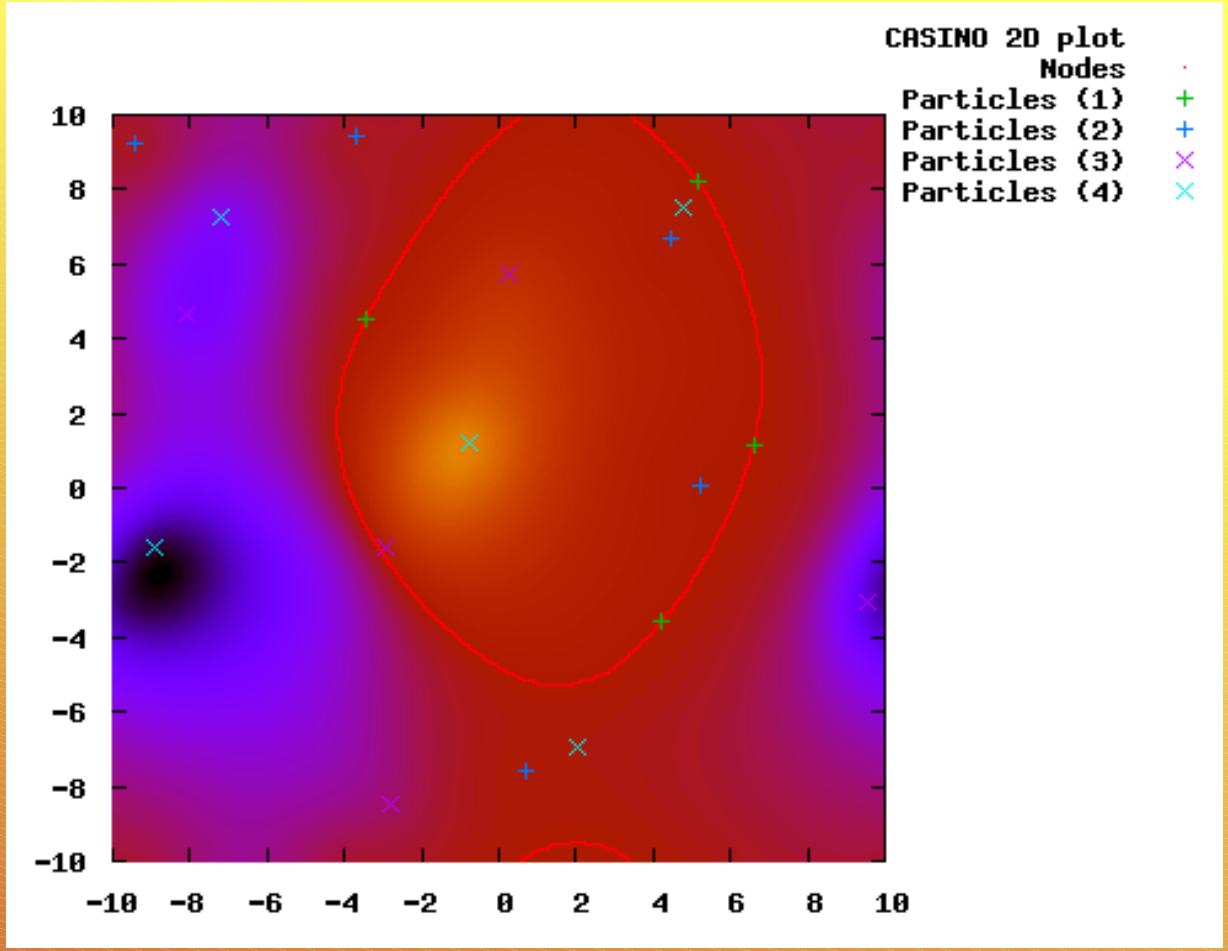


SJ wfn, c_F/c_P=-20

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

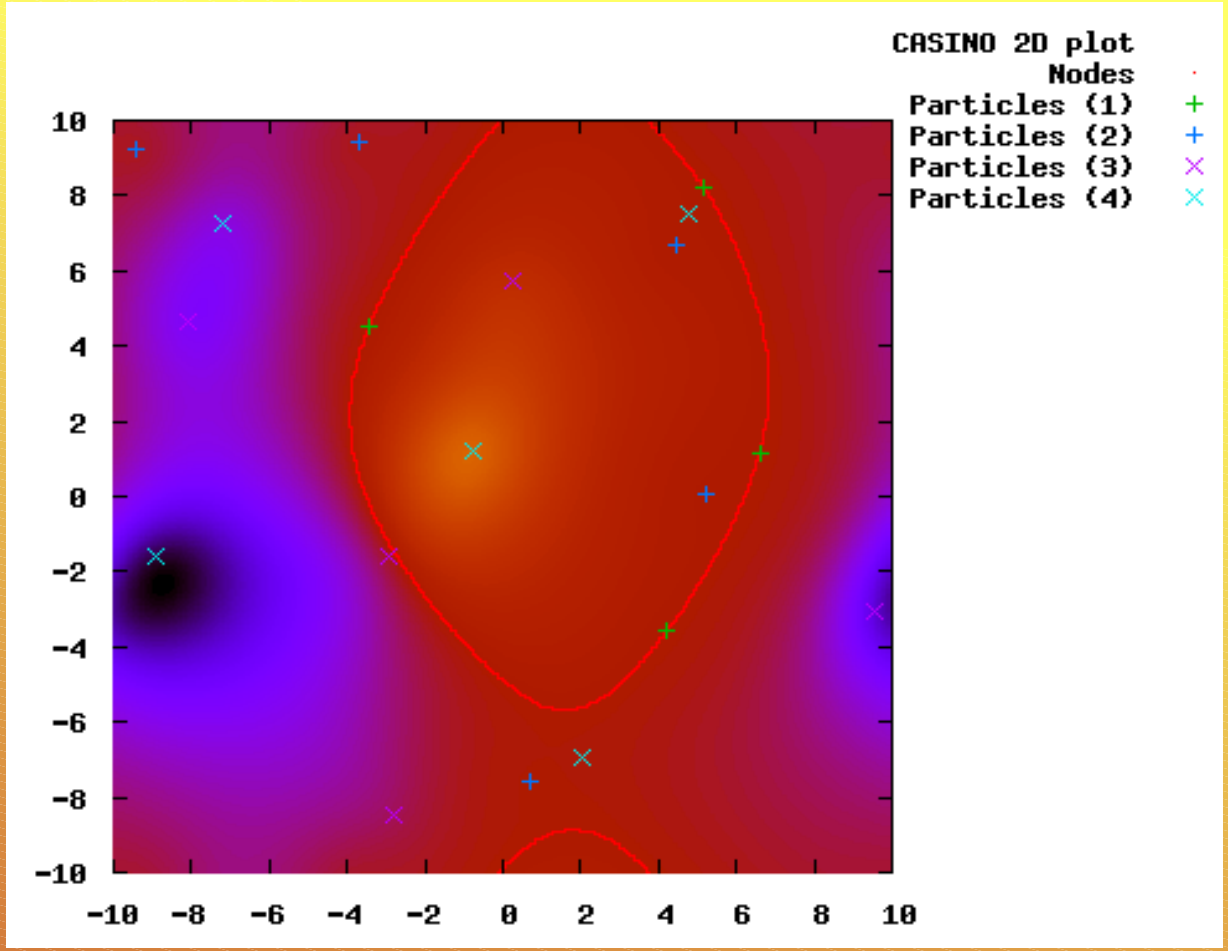


SJ wfn, c_F/c_P=-50

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

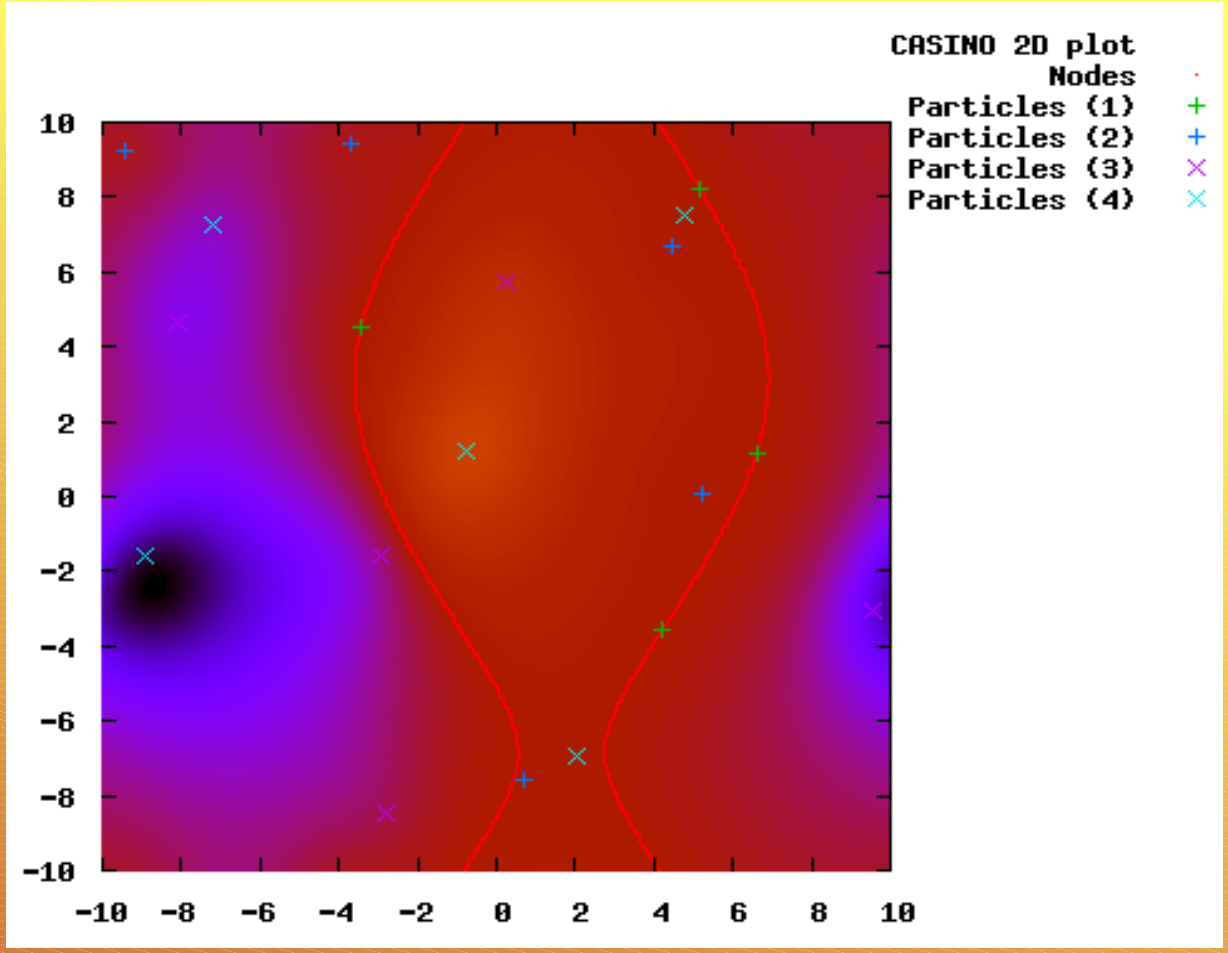


SJ wfn, c_F/c_P=-100

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

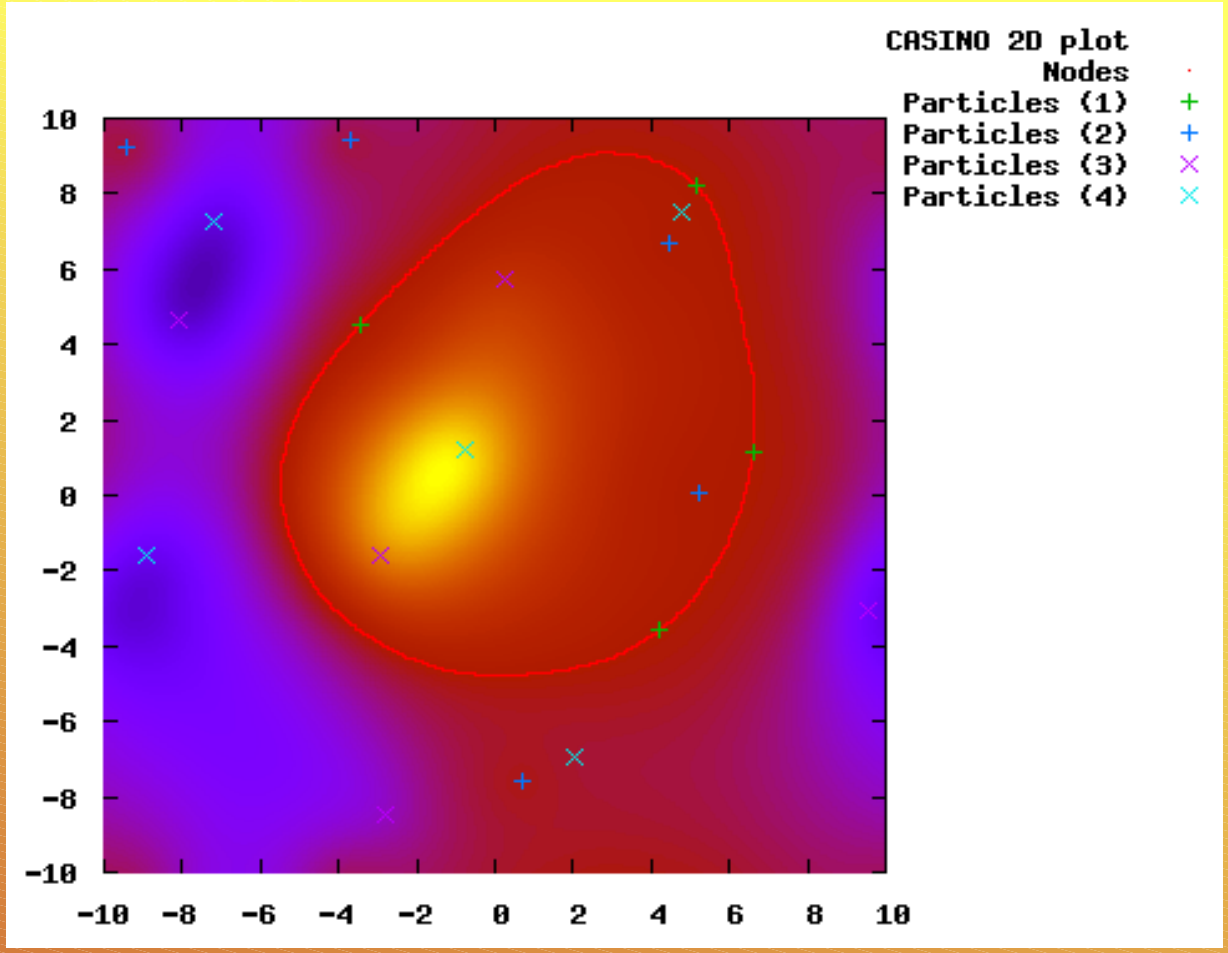


SJ wfn, c_F/c_P = Infinity

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

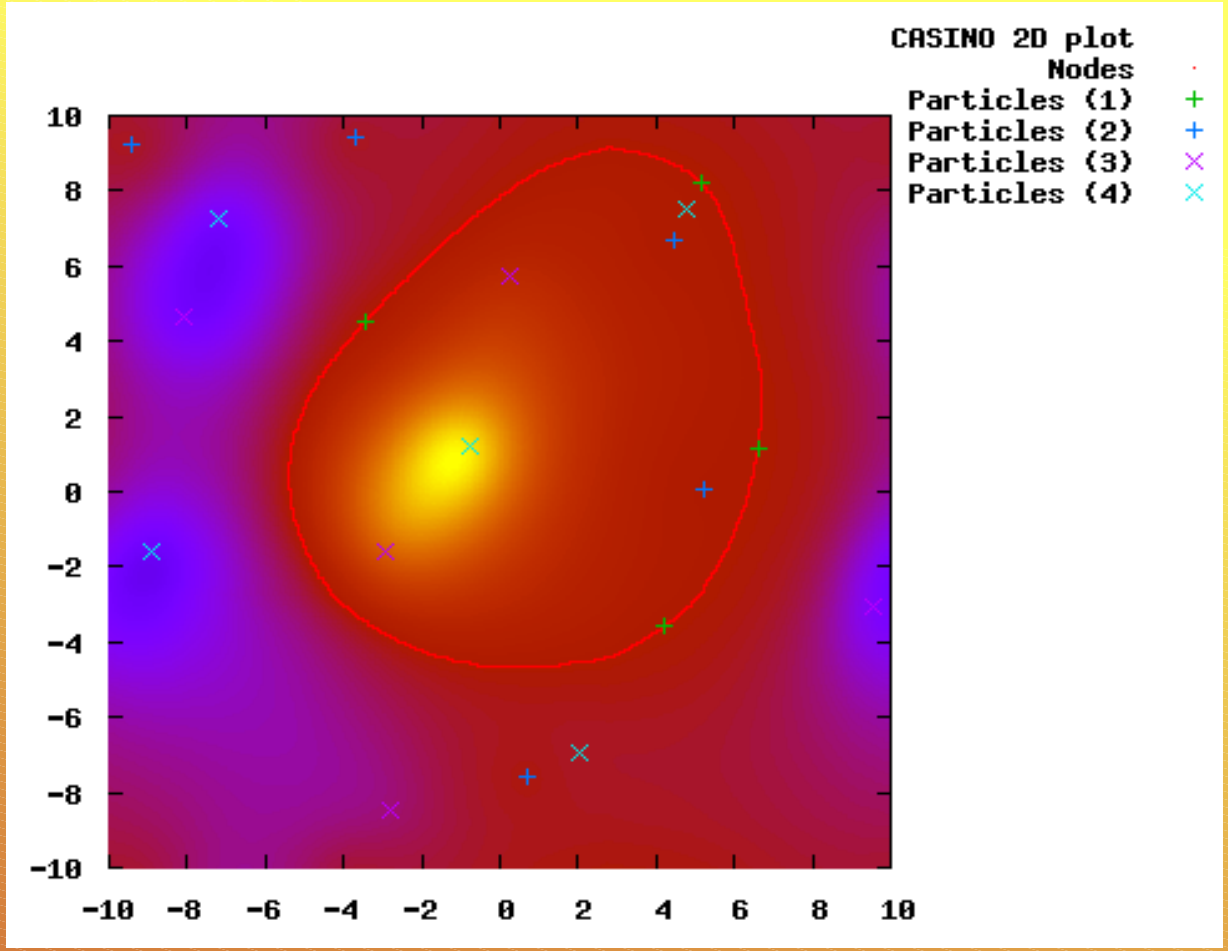


SJ wfn, $c_F/c_P = 0$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

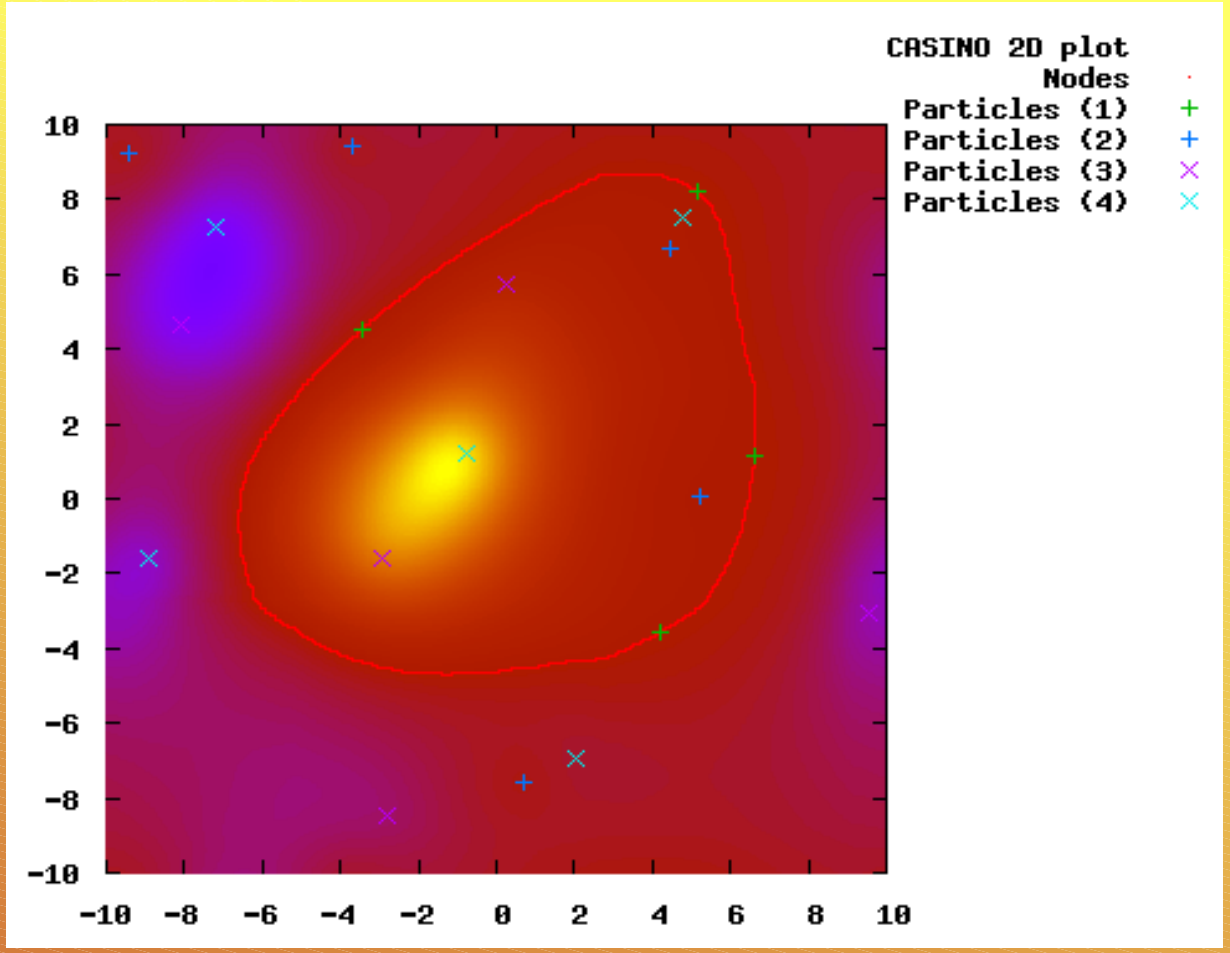


SJ wfn, $c_F/c_P = 1$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

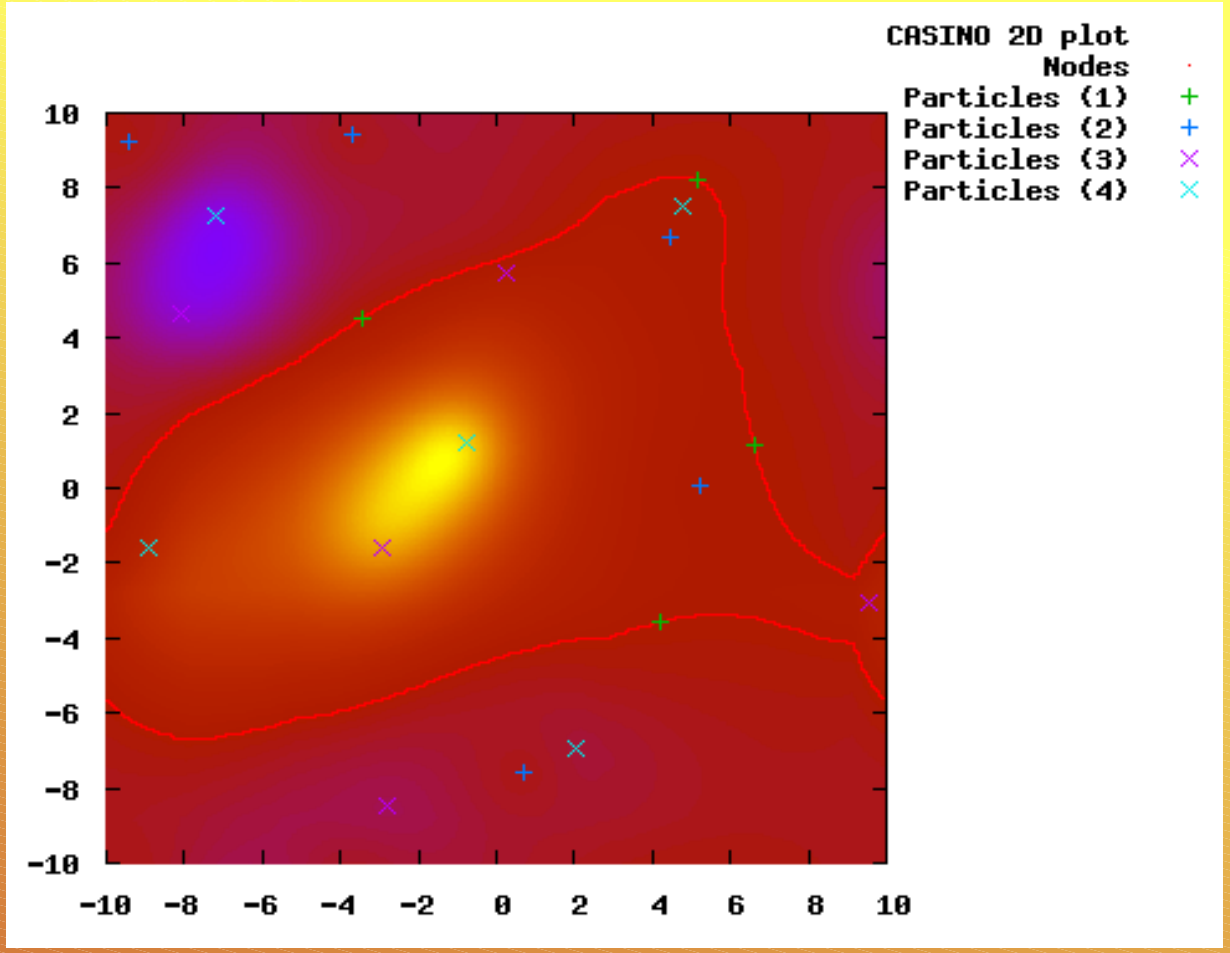


SJ wfn, $c_F/c_P = 10$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

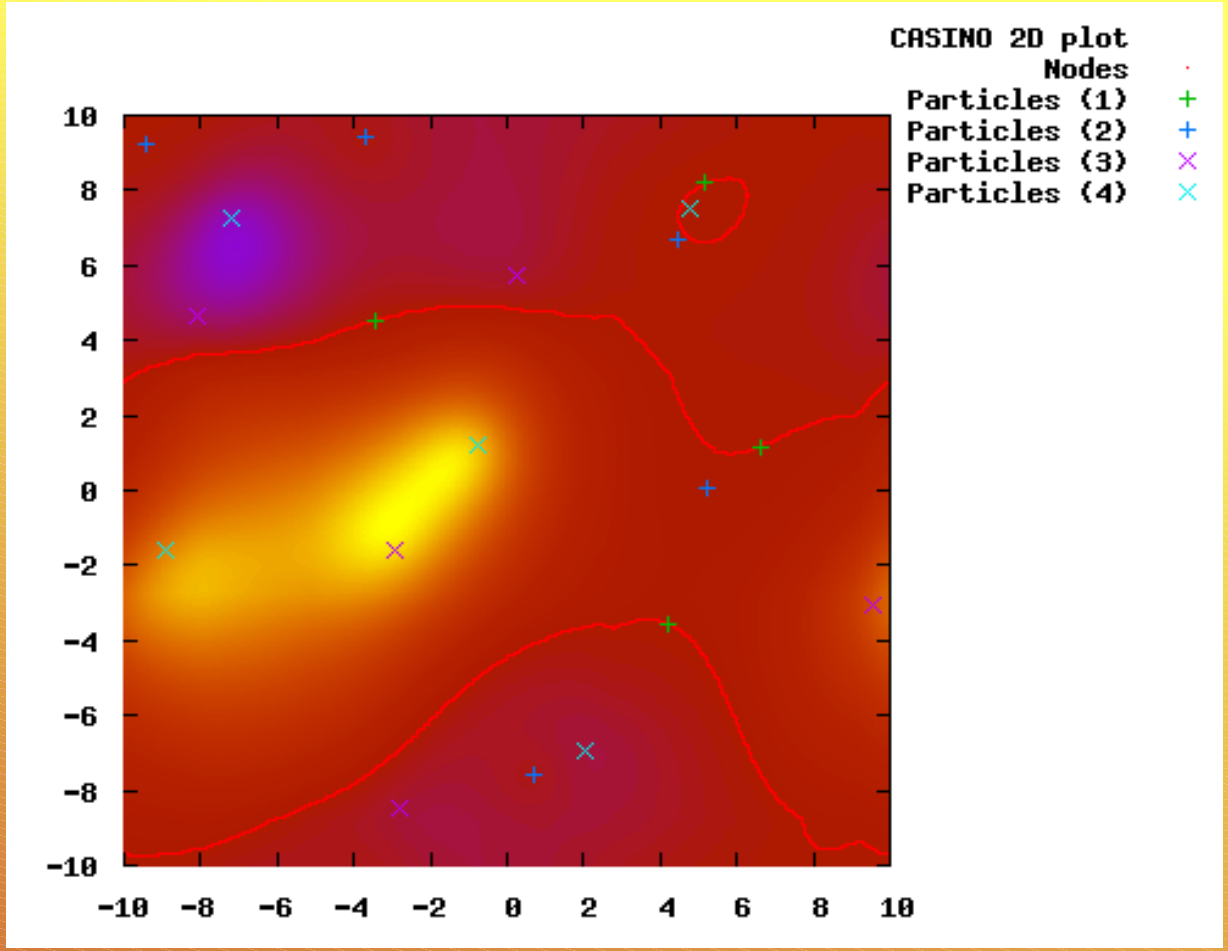


SJ wfn, $c_F/c_P = 20$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

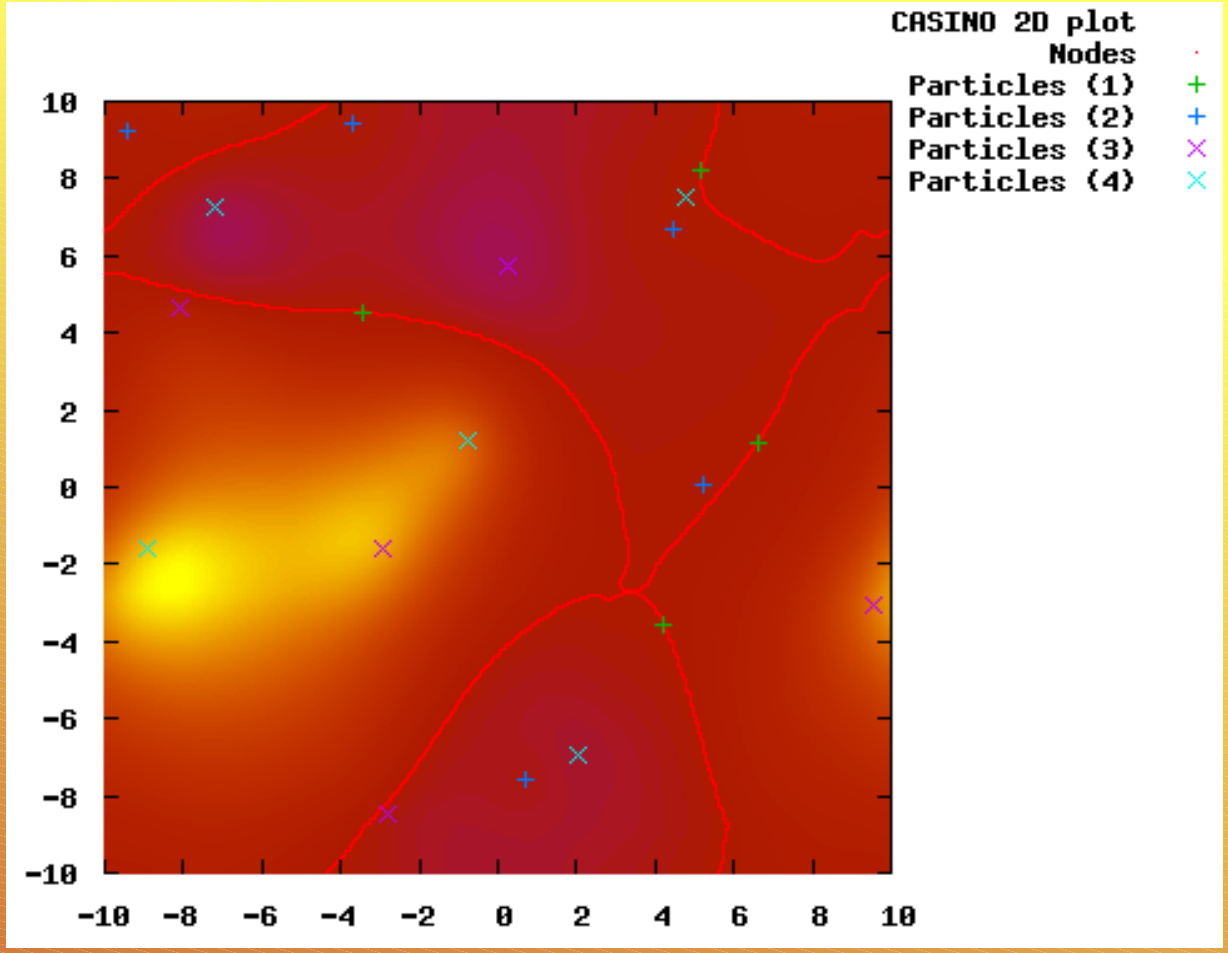


SJ wfn, $c_F/c_P = 30$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

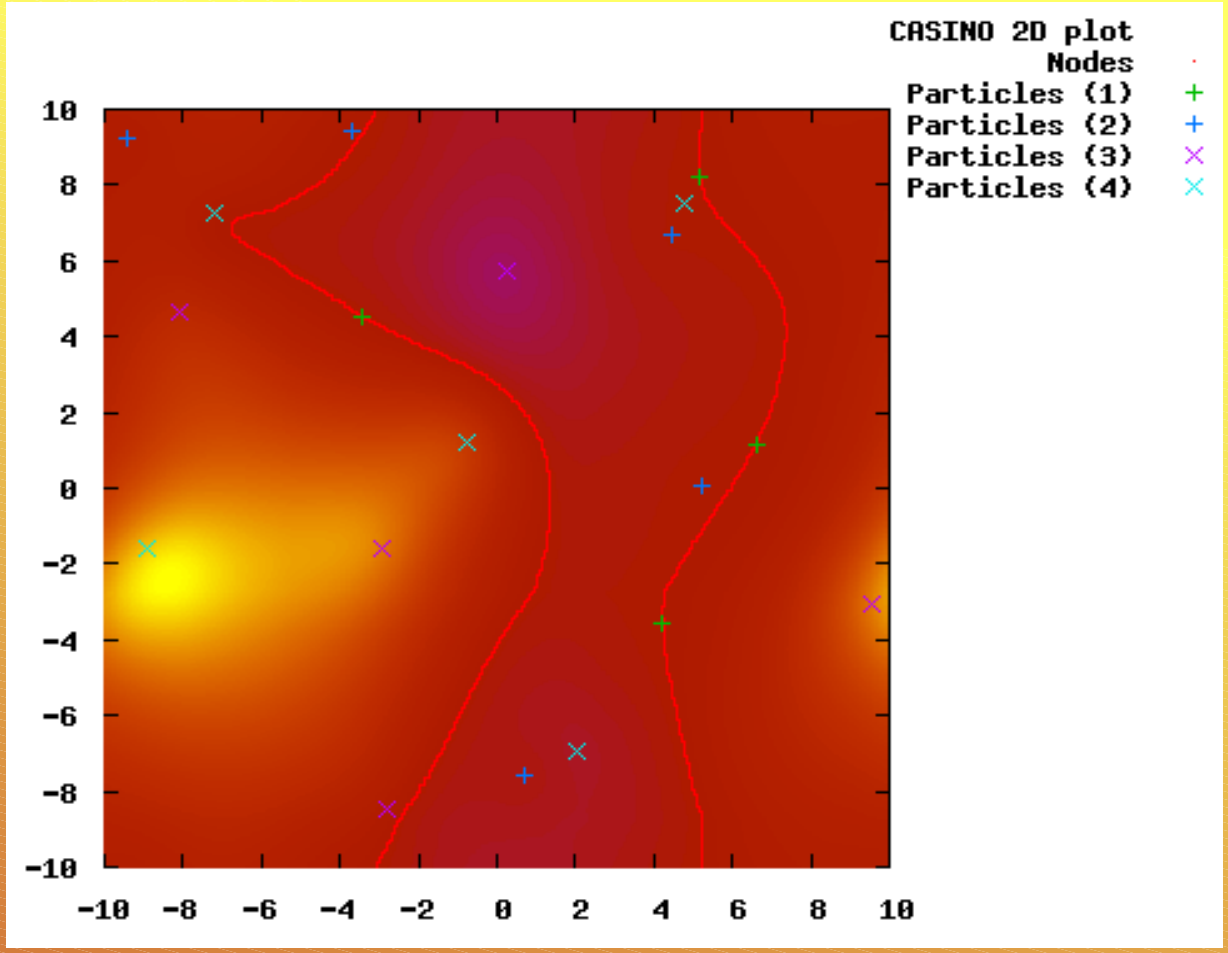


SJ wfn, $c_F/c_P = 40$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

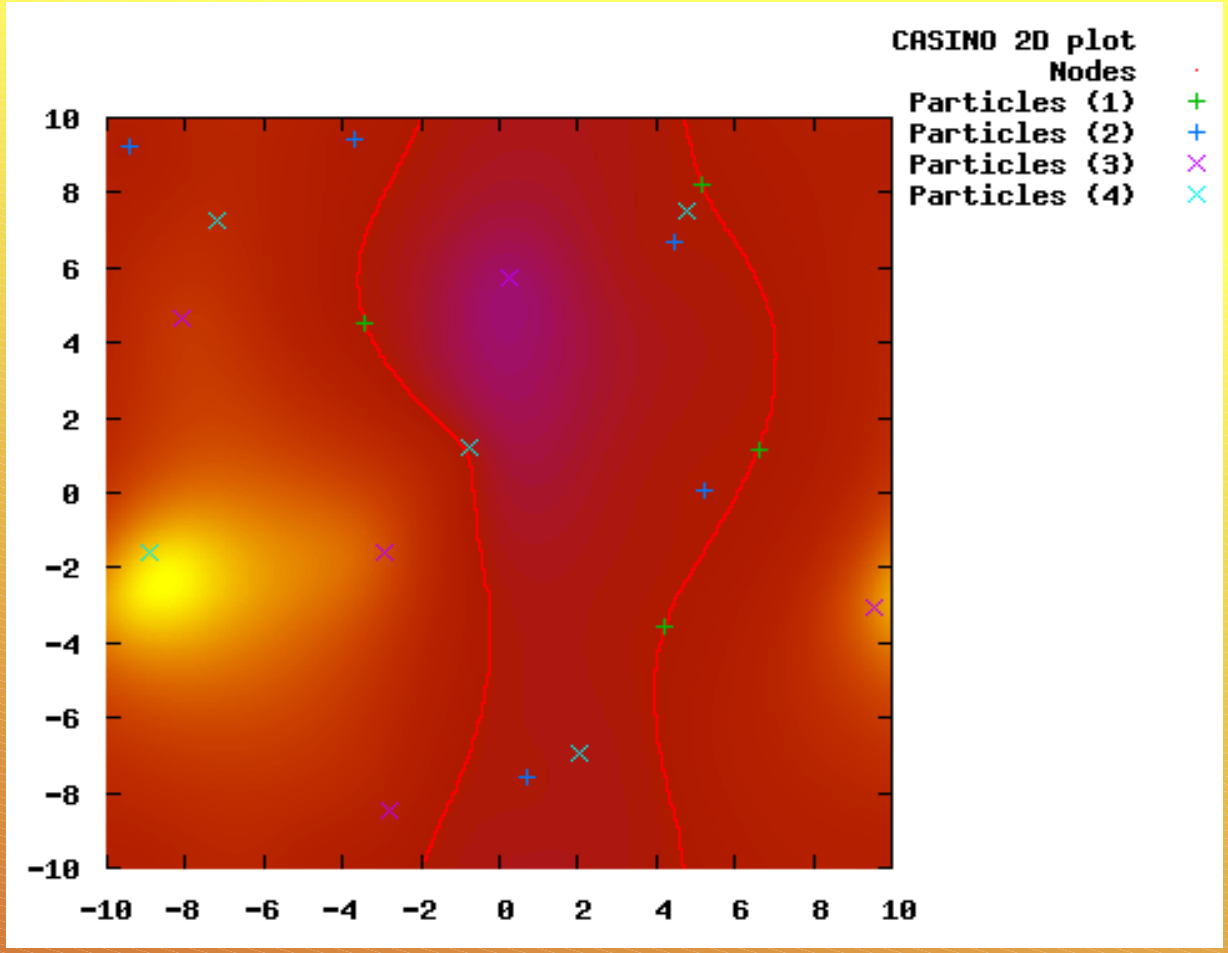


SJ wfn, $c_F/c_P = 50$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

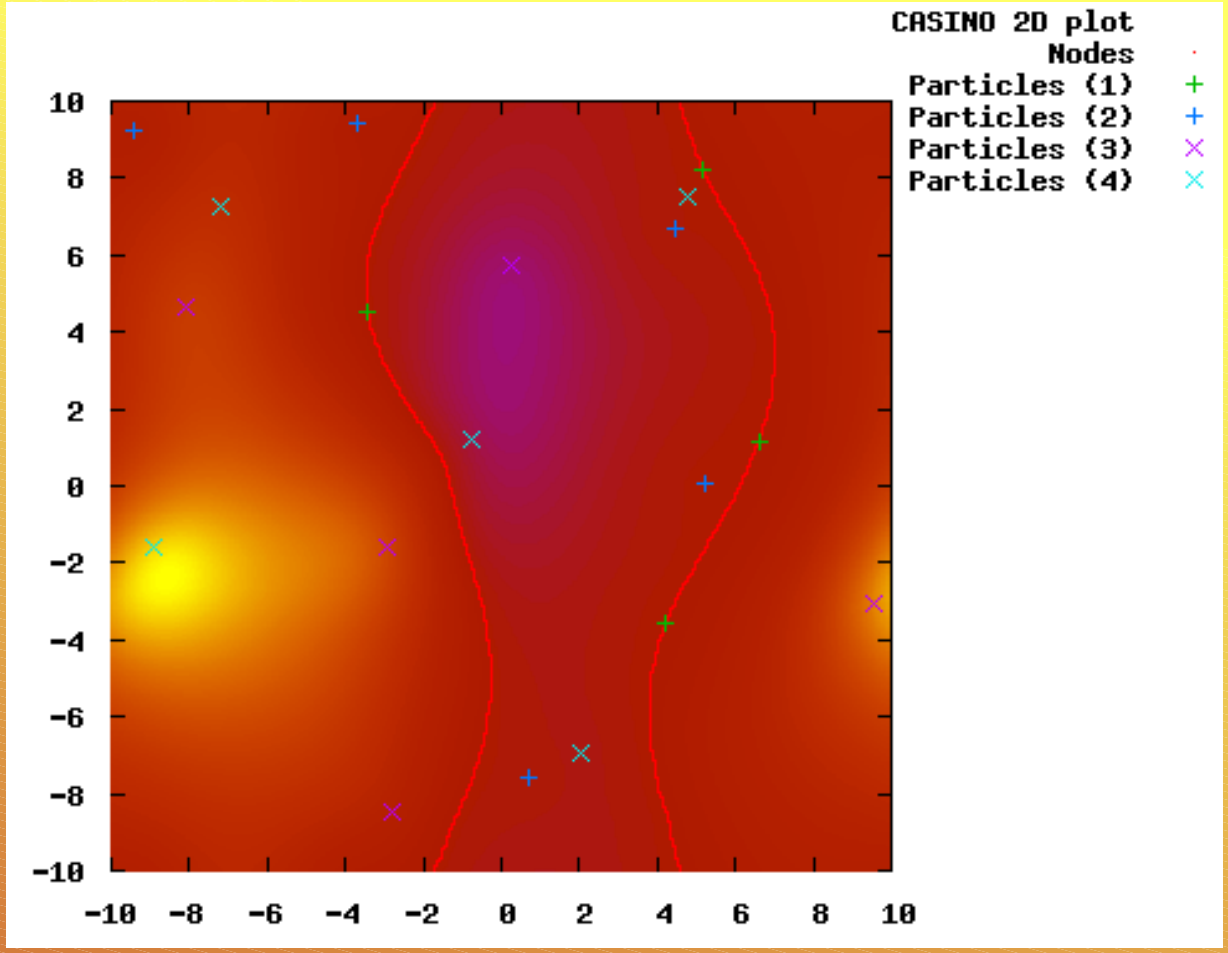


SJ wfn, $c_F/c_P = 80$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$



SJ wfn, $c_F/c_P = 100$

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P \left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow} \right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

* Positive ratios seem wrong. Solution: use negative ratios here.

* Problem: if we swap around up/down spin holes, the relative sign of the determinants changes, but the coeffs don't.

* Hence some configurations are going to have this problem. VarMin won't like this. Need symmetrizing determinant.

* Such term also describes biexcitons, which should be taken into account.

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P \left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow} \right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

Even with that term, there are more problems:

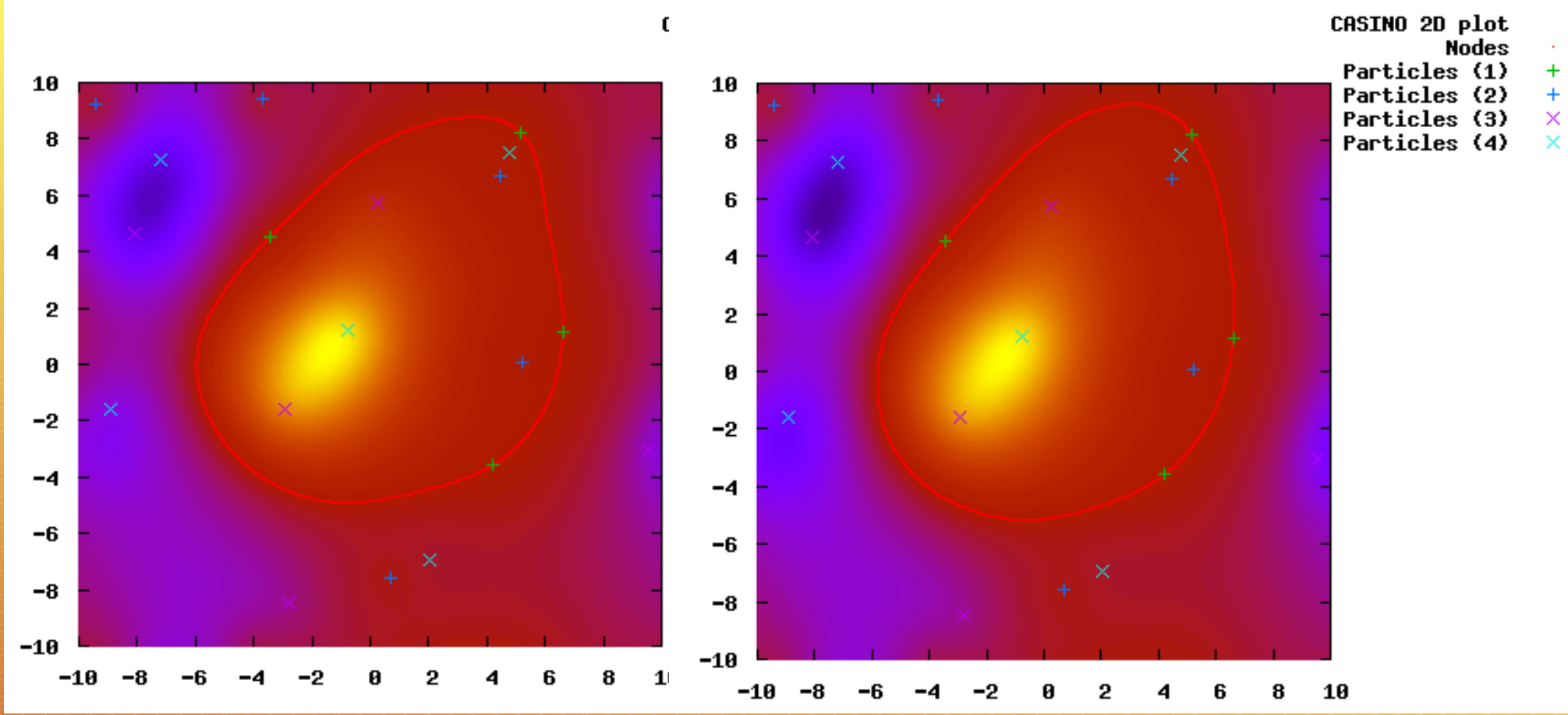
* Pairing alone gives lower energy and larger variance than plane waves. Hence plane waves are (unphysically?) favoured over pairing by VarMin.

* Parametrization of pairing orbitals seems important. Might solve the issue to use gaussians rather than exp(-r/Rex).

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P\left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow}\right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$



Gaussians fit to exp(-r/Rex)

Free gaussians

The electron-hole system and QMC

4. Correct approach #1

$$\Psi_S = c_P \left[D^P_{e\uparrow h\downarrow} D^P_{e\downarrow h\uparrow} + D^P_{e\uparrow h\uparrow} D^P_{e\downarrow h\downarrow} \right] + c_F D^F_{e\uparrow} D^F_{e\downarrow} D^F_{h\uparrow} D^F_{h\downarrow}$$

Problems in approach #1:

* Determinant coeffs need careful optimization if using VarMin. Would benefit from energy optimization?

* Choice of parametrization important.

The electron-hole system and QMC

4. Correct approach #2

$$\Psi_S = D^G_{e\uparrow h\downarrow} D^G_{e\downarrow h\uparrow} + D^G_{e\uparrow h\uparrow} D^G_{e\downarrow h\downarrow}$$

where G stands for “geminal”.

Geminal orbitals:

$$\phi_G(\boldsymbol{e}_i, \boldsymbol{h}_j) = \sum_{\alpha,\beta=1}^{n} c_{\alpha\beta} f_\alpha(\boldsymbol{e}_i) f_\beta(\boldsymbol{h}_j)$$

The electron-hole system and QMC

4. Correct approach #2

$$\Psi_S = D^G_{e\uparrow h\downarrow} D^G_{e\downarrow h\uparrow} + D^G_{e\uparrow h\uparrow} D^G_{e\downarrow h\downarrow}$$

where G stands for “geminal”.

Geminal orbitals:

$$\phi_G(\boldsymbol{e}_i, \boldsymbol{h}_j) = \sum_{\alpha,\beta=1}^{n} c_{\alpha\beta} f_\alpha(\boldsymbol{e}_i) f_\beta(\boldsymbol{h}_j)$$

These are hard-ish to differenciate when in a determinant, as we need separate derivatives for $\mathbf{e}_i$ and $\mathbf{h}_j$.

The electron-hole system and QMC

4. Correct approach #2

$$\Psi_S = D^G_{e\uparrow h\downarrow} D^G_{e\downarrow h\uparrow} + D^G_{e\uparrow h\uparrow} D^G_{e\downarrow h\downarrow}$$

A particular case of the former (disregarding the crystal) is:

$$\phi_G(\boldsymbol{e}_i - \boldsymbol{h}_j) = \sum_{\alpha=1}^{n} c_\alpha e^{i\boldsymbol{k}_\alpha(\boldsymbol{e}_i - \boldsymbol{h}_j)} + \phi_P(\boldsymbol{e}_i - \boldsymbol{h}_j)$$

* This form of wave function also includes the right limits in it.

* Haven't tried it.

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4. Correct approach #2

Possible problems of geminals:

* Geminals require some work on determinant handling. And I'm lazy.
* What basis functions to choose? Must minimize number of parameters.

Possible problems of particular form:

* Wigner Crystals require (almost) the same treatment as geminals.
  And I'm still lazy.

Possible problems of both:

* Larger number of parameters than approach #1.
* Perhaps optimization problems?
* Untested.

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5. Conclusions

* Previous way of analyzing phase diagram must be discarded in favour of global wave functions + density matrices.

* Two forms of global trial wave function proposed. Which to choose?

* Optimization issues. Must be careful.

* Analysis of phases using density matrices never performed before on this system. What kind of transitions are we going to encounter? What objects to analyze?

* Extrapolation to infinite size:
    * Can it be performed with the resulting energies?
    * Can it be performed on the density matrices?
    * May it be possible to extrapolate the phase diagram itself?