QLab App - Use Manual

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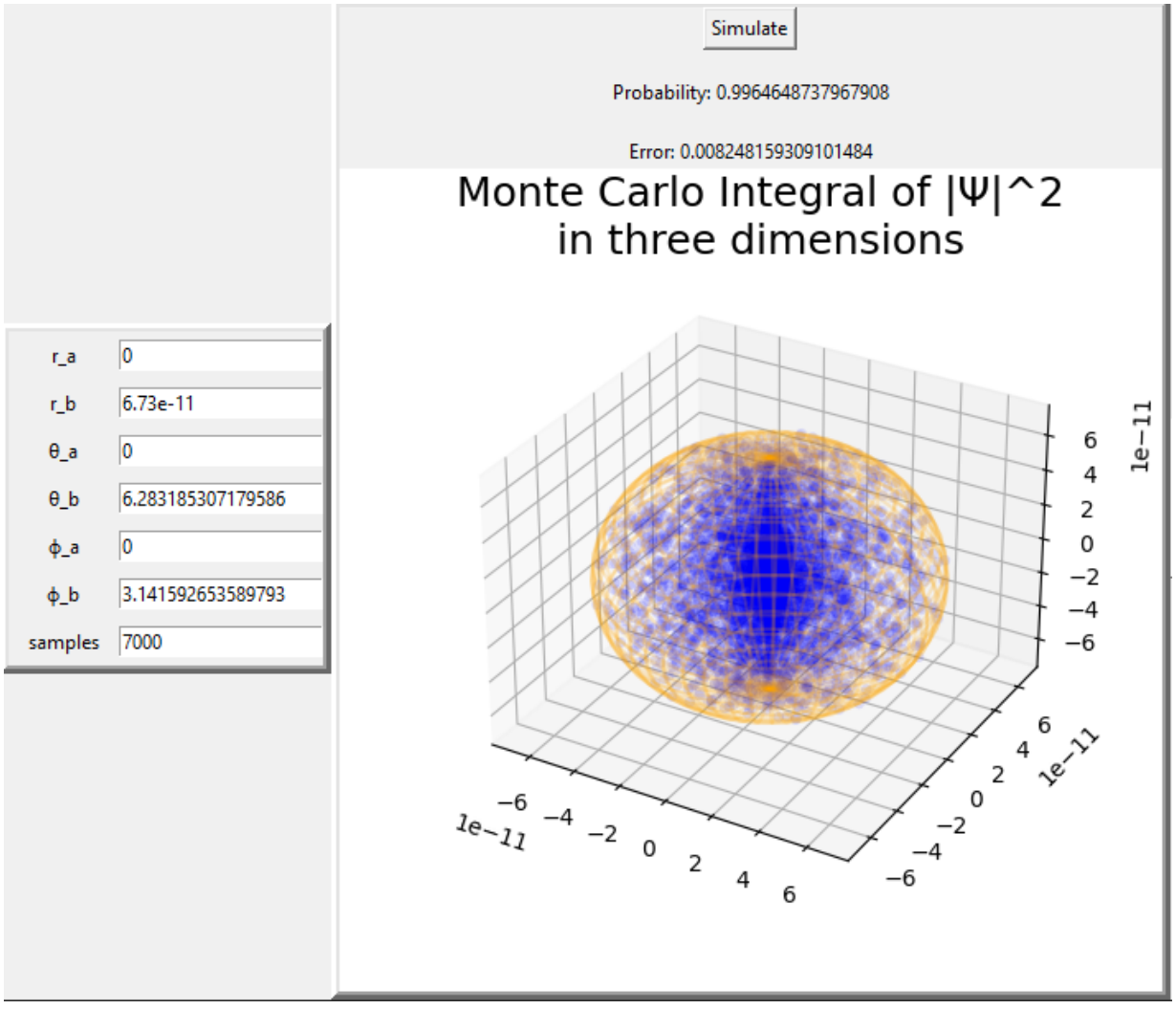
EXECUTING THE APPLICATION

Open the CMD and put the following commands

```
> cd [full path to where you have tha QLab app folder]
> python qlab.py
```

That will start the program. Now, for Windows, Linux and Mac users it is the same procedure, go to the folder “QLab app” and put python qlab.py, It will work if you installed all the modules required.

MONTE CARLO INTEGRATION



As is showed in the image, the Monte Carlo integral has the parameters You can fill the parameters taking into consider

Application parameter	Equivalent Variable	Default Value
@r_a	r_a	0,E+0
@r_b	r_b	6,73E-11
@θ_a	θ_b	0,E+0
@θ_b	θ_b	2π
@ϕ_a	ϕ_a	0,E+0
@ϕ_b	ϕ_b	π
@samples	N	100

Table 1. Values and Parameters - Monte Carlo Integral

the following graph which shows how spherical coordinates works:

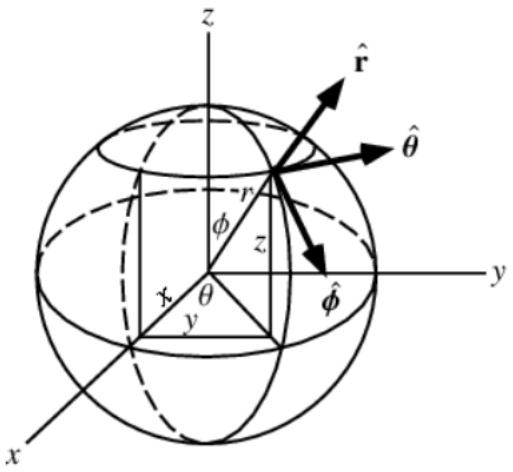


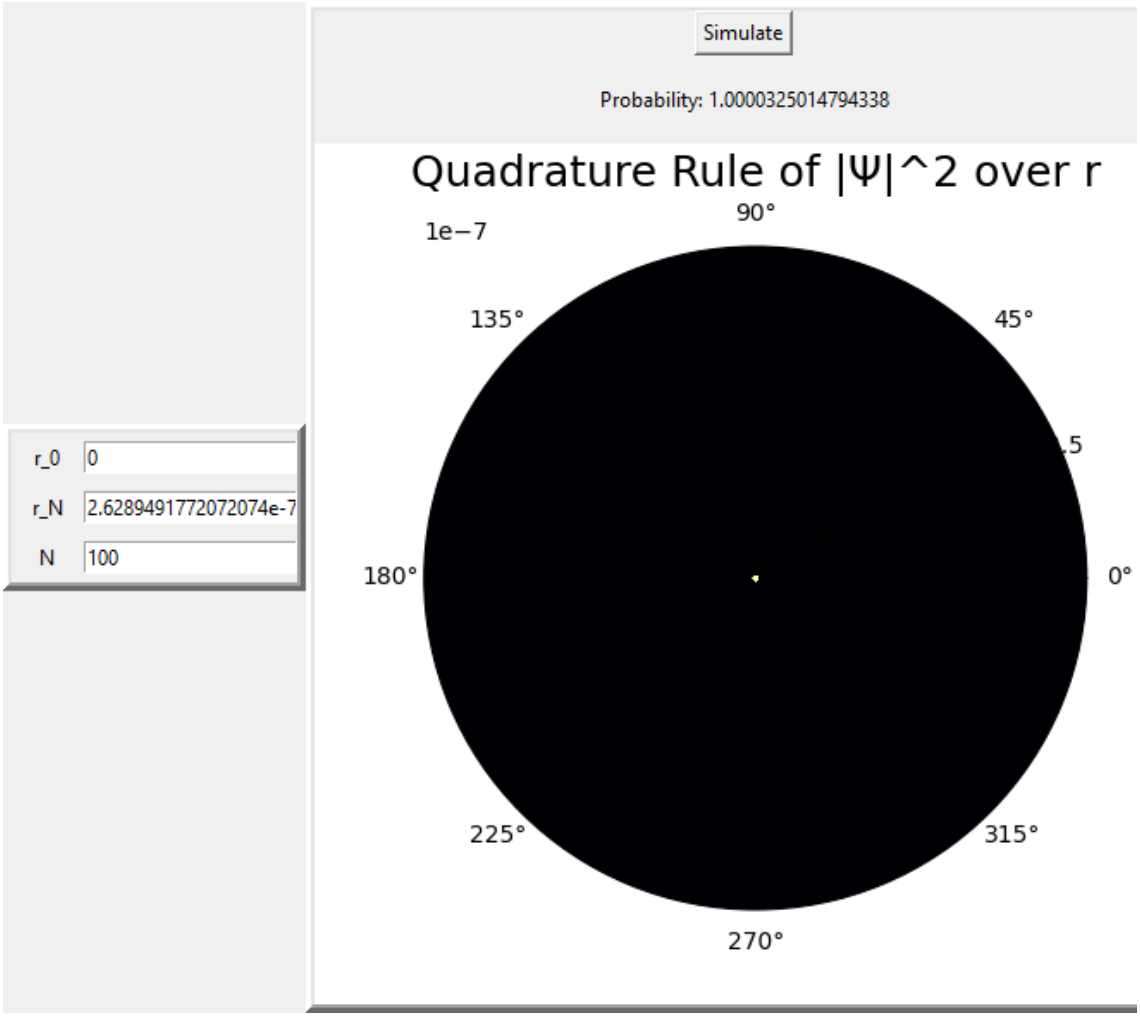
Figure 1. Source: https://mathworld.wolfram.com/SphericalCoordinates.html

Now, as to how was done the conversion from spherical coordinates to cartesian coordinates, it was done using the following equalities:

$$x = r\sin\theta\cos\phi \tag{1}$$
$$y = r\sin\theta\sin\phi \tag{2}$$
$$z = r\cos\theta \tag{3}$$

As a warning, try to not exceed the default values for the upper limits for this integral, being those @θ_a, @θ_b, @ϕ_a, @ϕ_b. That because the application was not programmed to normalize the angles (put them values into its initial value ranges). So, do not exeed for θ the value of 2π and for ϕ the value of π

QUADRATURE RULE

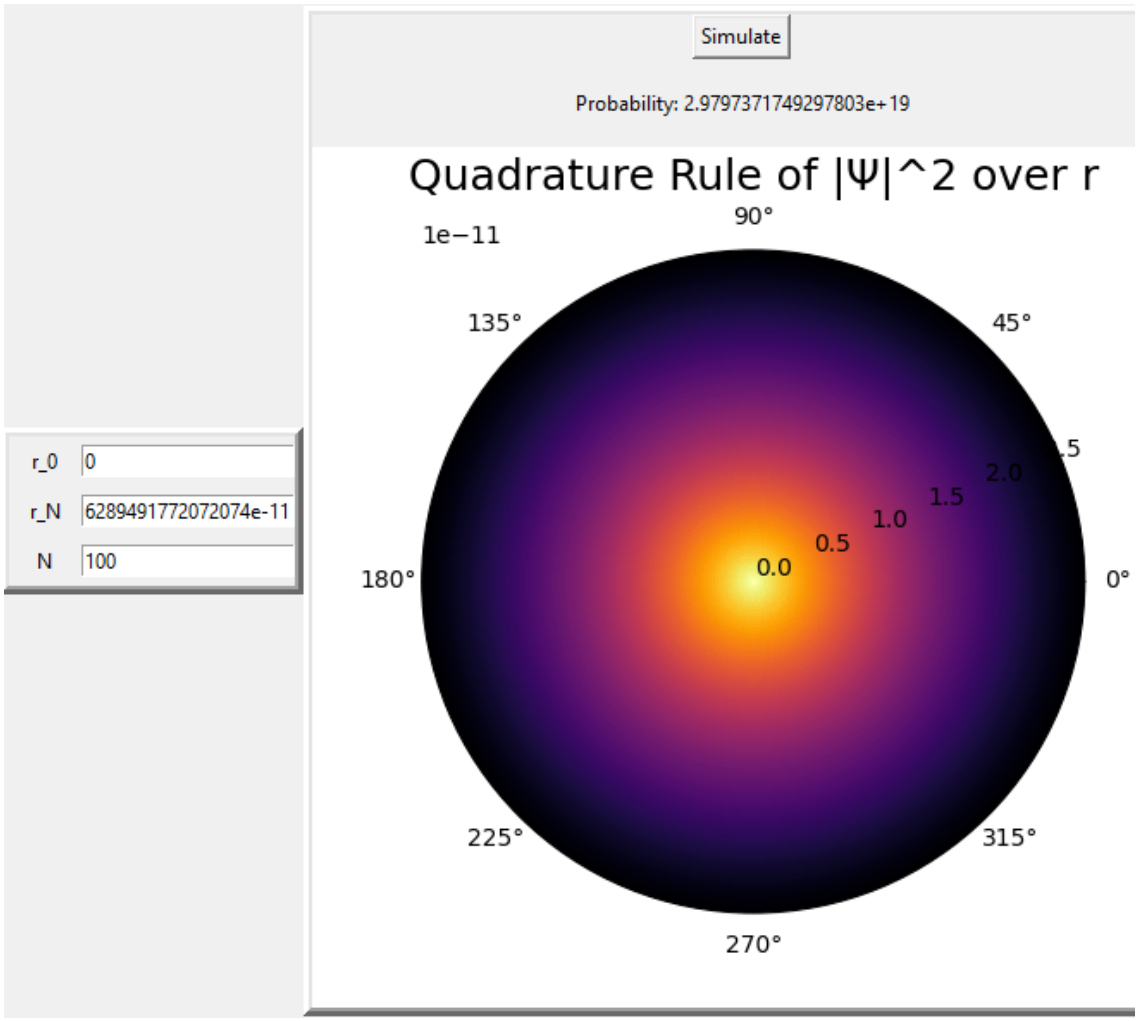


Application parameter	Equivalent Variable	Default Value
@r_0	r_0	0,E+0
@r_N	r_N	2,629029177212380E-07
@N	N	100

Table 2. Values and Parameters - Quadrature Rule

This sumulation works smoothly for @N, if you increase the number of sub-intervals then it can take more time or directly stop working. For this simulation the value obtained is deterministic (is in **P**, opposite to the Monte Carlo integral which is in the **NP** domain) the value will be the same for every simulation with same parameters (again, unlike in the Monte Carlo Integral).

It is recommended to play only with the parameters @r_0 and @r_N and let quiet @N. An example of how the result changes is shown in the following image:



Here @r_N has the value of 2,629029177212380E-11 and we can visualize better the distribution of the probability density in the absolute squared wave function $|\psi_{1,0,0}|^2$ we talked about before.