2D Schrodinger Equation

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In this assignment, we have found the first four energy states and plotted the probability distribution by solving the shcrodinger equation with a 2D potential numerically. Here in this project, we applied two methods- Variational methord and Lanczos method. Also, we compared the results got from these two methods.

Variational calculation

While using variational method, we tried different wavefunction basis, where the wavefunctions are the eigenfunctions of 2D ifinite potential well. Fig.1 shows how the ground state energy convergies slowly as we increase the basis number $n_x * n_y$, where n_x and n_y stands for $\phi(n_x)$ and $\phi(n_y)$ respectively.
The expressions for $\phi(n_x) and\ \phi(n_y)$ are:

$$\phi_{n_x} = \sqrt{\frac{2}{L_x}} sin(n_x \pi x / L_x),$$

$$\phi_{n_y} = \sqrt{\frac{2}{L_y}} sin(n_y \pi y / L_y),$$

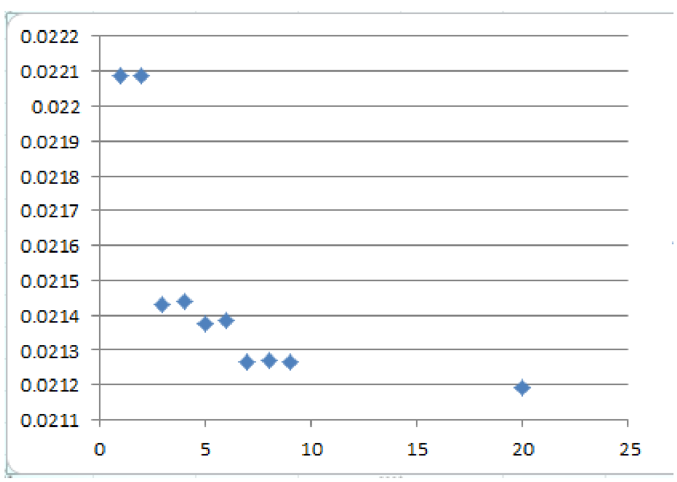

FIG. 1: Ground energy converges with increasing n_x

Here are the results I get when n_x=20 and n_y=20, which means the basis number is 400. The first 4 energy values are: E_1=0.0211937 ev, E_2=0.03624195 ev, E_3=0.053122 ev, E_4=0.06436071 ev.

Fig.2 shows the picture of probability distribution for each state.

Lanczos Calculation

While using Lanczos method, I tried different combinations of Δ (0.2, 0.1, 0.05 and 0.25) and iteration time m, and I found that for certain Δ, as m increases, the ground energy converges rapidly, as shown in Fig.3.

Also, I found that as Δ becomes smaller, the iteration times m becomes larger to enable energy converges, and the converged energy becomes lower with smaller Δ. For example, when Δ=0.2, m=200 and the converged ground energy E_1=0.0158127 ev, when Δ=0.1, m=300 and E_1=0.0155445 ev , when Δ=0.05, m=400,and E_1=0.0147747 ev , when Δ=0.025, m=600, and E_1=0.0143 ev.

Here are the results I got when Δ=0.1 and m=300.

The first 4 energy values are: E_1=0.01554453 ev, E_2=0.023493175 ev, E_3=0.446647 ev, E_4=0.0636476 ev.

Fig.4 shows the probability distribution for each state.

In conclusion, from the probability distribution of 4 energy states, we can find that the results I got from both methods concide with each other. However, I got different energy values for the first 4 states. Systematically, the energy I got from Lanczos method is lower than the energy I got while using Variational method. I think probably the wavefunction basis I used, which is 400, is not enough to get a very accurate energy value. With increasing number of wavefunction basis, we can get lower energy from Variational method, which has already shown this trend in Fig.1.

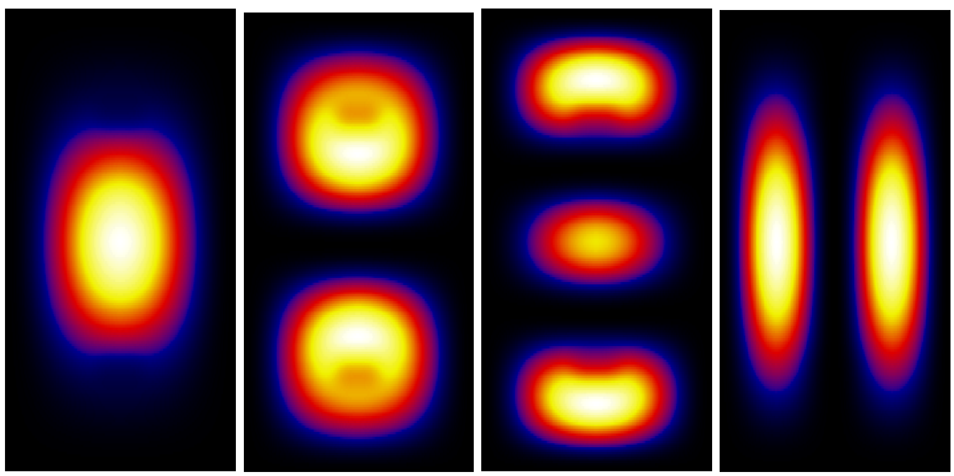

FIG. 2: Probability distribution for the first four energy states(variational method).

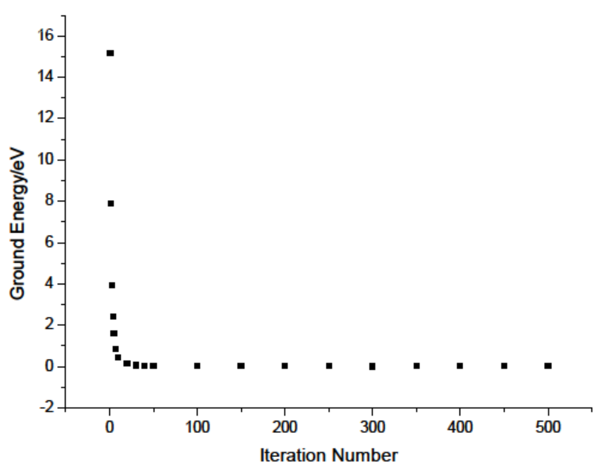

FIG. 3: Ground energy converges rapidly with increasing iteration number.

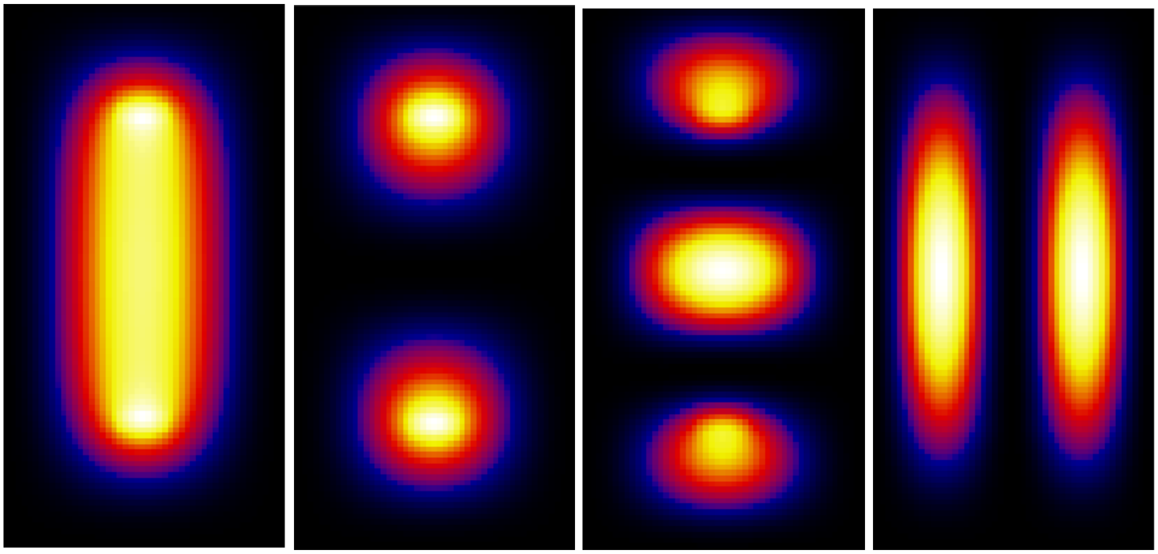

FIG. 4: Probability distribution for the first four energy states(lanczos method).