PHY 308/578 **QUANTUM PHYSICS** **Spring 2006**

Homework #9 with Solutions

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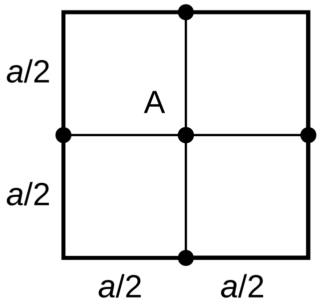
Problem 9.1

Use the finite difference method with step $h = a/2$ to find eigenenergies of a free particle confined to the interior of:

(i) a square with side a;

(ii) a cube with side a.

Compare the results with the exact formulas.



Solutions:

(i) For the square (see Fig.), the 2D finite difference equation is

$$-\frac{\hbar^2}{2m}\left(\frac{0-2u_A+0}{h^2}+\frac{0-2u_A+0}{h^2}\right)=Eu_A,$$

where the first fraction is the parentheses is an approximation for $\partial^2 u/\partial x^2$, and the second for $\partial^2 u/\partial y^2$. (Zeros present the values of *u* at the boundary points marked on the Figure.) Canceling u_A and plugging in *h* = *a*/2, we get $E = 8\frac{\hbar^2}{ma^2}$, the value to be compared with the exact result $E_{1,1}=\pi^2\frac{\hbar^2}{2ma^2}(1^2+1^2)=\pi^2\frac{\hbar^2}{ma^2}$. We see that the error is about 20% ($8 \leftrightarrow \pi^2 = 9.87...$).

(iii) In 3D, the calculation is similar, besides there is an additional similar term in parentheses, presenting $\partial^2 u/\partial z^2$. The result, $E = 12\frac{\hbar^2}{ma^2}$, is similarly far from the exact value $E_{1,1,1}=\frac{3\pi^2}{2}\frac{\hbar^2}{ma^2}\approx 14.8\frac{\hbar^2}{ma^2}$.

Problem 9.2

Repeat the calculations for the square, using a finer step: $h = a/3$. Compare the results with:

- the exact formula, and
- the result of Problem 9.1 (i).

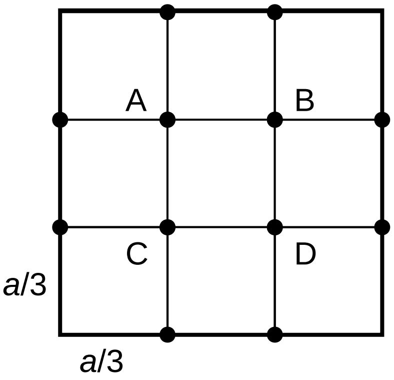
What is the order of degeneracy of each eigenvalue you have found?

Hint: exploit the symmetry of the problem.

Solution:

Due to the obvious symmetry of the problem, we may distinguish 4 significantly different "modes" (wavefunction types) which cannot be reduced to each other via the trivial multiplication by a scalar:

(1,1): $u_A = u_B = u_C = u_D$
(1,2): $u_A = u_B = -u_C = -u_D$
(2,1): $u_A = -u_B = u_C = -u_D$
(2,2): $u_A = -u_B = -u_C = u_D$



(The notation in parentheses corresponds to the values of k_x and k_y (in the units of π / a) in the analytical solution of the problem.)

The symmetry enables us to write, for each mode, the finite difference equations for just one point, e.g., A. For example, for the lowest (1,1) mode we have:

$$-\frac{\hbar^2}{2m}\left(\frac{0-2u_A+u_B}{h^2}+\frac{u_C-2u_A+0}{h^2}\right)=-\frac{\hbar^2}{2m}\left(\frac{0-2u_A+u_A}{h^2}+\frac{u_A-2u_A+0}{h^2}\right)=E_{1,1}u_A.$$

From here (with $h = a/3$): $E_{1,1} = 9\frac{\hbar^2}{ma^2}$. This is a better approximation of the exact result $E_{1,1} \approx 9.87\frac{\hbar^2}{ma^2}$ than what we had with $h = a/2$ (see Problem 9.1 (i) above).

In the same way, for the (1,2) mode we get

$$-\frac{\hbar^2}{2m}\left(\frac{0-2u_A+u_B}{h^2}+\frac{u_C-2u_A+0}{h^2}\right)=-\frac{\hbar^2}{2m}\left(\frac{0-2u_A+u_A}{h^2}+\frac{-u_A-2u_A+0}{h^2}\right)=E_{1,2}u_A,$$

giving $E_{1,2} = 18\frac{\hbar^2}{ma^2}$, to be compared with the exact result $E_{1,2} = \frac{\pi^2\hbar^2}{2ma^2}\left(1^2+2^2\right) \approx 24.6\frac{\hbar^2}{ma^2}$.

For mode (2,1), we evidently get the same result ($E_{2,1} = E_{2,1}$), indicating that this energy level is doubly degenerate.

Finally, for the highest mode (2,2) which we can describe with the step so coarse:

$$-\frac{\hbar^2}{2m}\left(\frac{0-2u_A+u_B}{h^2}+\frac{u_C-2u_A+0}{h^2}\right)=-\frac{\hbar^2}{2m}\left(\frac{0-2u_A-u_A}{h^2}+\frac{-u_A-2u_A+0}{h^2}\right)=E_{2,2}u_A,$$

resulting in $E_{1,2} = 27\frac{\hbar^2}{ma^2}$, a rather mediocre approximation to the exact result $E_{2,2} = \frac{\pi^2\hbar^2}{2ma^2}\left(2^2+2^2\right) \approx 39.5\frac{\hbar^2}{ma^2}$.

So, we clearly see the general trend: a finite-difference scheme with *n* internal points allows us to find *n* eigenstates, with better accuracy achieved for states with the lower energies.