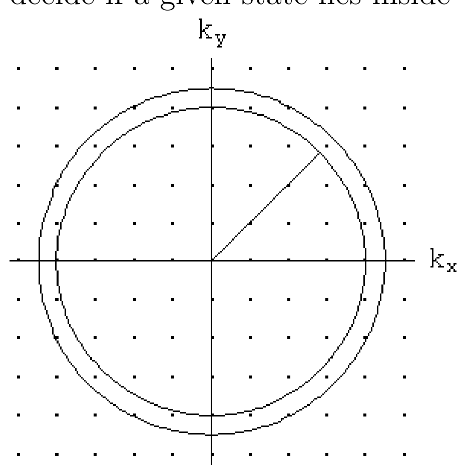
Physics 4P70: Programming Assignment 2
Due: Friday Nov. 17, 2017

1. Consider a free electron gas inside a two dimensional box of side L. We know that if one assumes periodic boundary conditions the allowed k vectors are:
$$\vec{k} = \frac{2\pi}{L}(n_x\hat{x} + n_y\hat{y})$$
This makes the allowed energy states equal to:
$$E = E_o(n_x^2 + n_y^2)$$
where $n_i \in I$ and $E_o = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2$

During class, the concept of the "density of states" $g(E)$ was defined which means the number of states per unit energy range. A way to calculate $g(E)$ using the computer would be to count the number of states in a given energy range. This involves "binning" states into energy ranges and a decision as to which "bin" a state is. In 2D, the allowed k values lie on a square grid as shown in the diagram below. Each allowed $\vec{k}$ corresponds to an ordered (n_x, n_y) pair. All states inside the ring lie in the energy range $E_{mid} \pm \Delta E/2$ where ΔE is the "bin size". Your program will have to sample possible states and then decide if a given state lies inside the ring or not.



Write a well-commented program that

(a) Creates two vectors g_{2D} and E where the energy (E) is the mid-point value for each range. Using units of E_o, E=[250, 750, 1250,...,9750] . etc.

(b) Determines the total degeneracy (density of states=g_{2D}) in the energy ranges: $(n_x^2 + n_y^2) < 499, 500 < (n_x^2 + n_y^2) < 999, ..., 9500 < (n_x^2 + n_y^2) < 10000$

(c) Assumes that $g_{2D}(E) = CE^{\alpha}$, and finds α and C using curve fitting routines.

(d) Plots g_{2D} vs E as well as the curve of best fit on a single graph.

(e) Calculate $g_{2D}(E)$ theoretically using the technique used in class and compare to your computer calculation.

2. Consider a free electron gas inside a three dimensional box of side L. This time, the energy states are

$$E = E_o(n_x^2 + n_y^2 + n_z^2)$$

where $n_i \in I$. Write a well-commented program that

(a) Creates two vectors g_{3D} and E where the energy (E) is the mid-point value for each range, that is when using units of E_o, E=[250, 750, 1250,...,9750] . etc.

(b) Determines the total degeneracy (density of states=g_{3D}) in the energy ranges: $(n_x^2 + n_y^2 + n_z^2) < 499, 500 < (n_x^2 + n_y^2 + n_z^2) < 999, ..., 9500 < (n_x^2 + n_y^2 + n_z^2) < 10000$

(c) Assumes that $g_{3D}(E) = CE^{\alpha}$ and finds α and C.

(d) Plots g_{3D} vs E as well as the curve of best fit on a single graph.

(e) Calculate $g_{3D}(E)$ theoretically using the technique used in class and compare to your computer calculation.