

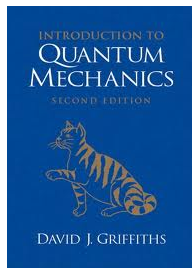
PHYS 406 - Fundamentals of Quantum Theory II

Term: Spring 2013
Meetings: Monday & Wednesday 15:15-16:30
Location: 106 Stuart Building

Instructor: Carlo Segre
Office: 166A Life Sciences
Phone: 312.567.3498
email: segre@iit.edu

Book: *Introduction to Quantum Mechanics, 2nd ed.*,
D. Griffiths (Pearson, 2005)

Web Site: <http://phys.iit.edu/~segre/phys406/13S>



Course Objectives

- 1 Understand time-independent perturbation theory.

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- ① Understand time-independent perturbation theory.
- ② Understand the variational method.

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- ② Understand the variational method.
- ③ Understand the WKB and adiabatic approximations.
- ④ Understand time-dependent perturbation theory.
- ⑤ Understand scattering theory.
- ⑥ Be able to solve quantum mechanics problems using the approximation method appropriate to the situation.

Course Grading

15% – Homework assignments

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Weekly or bi-weekly

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Due at beginning of class

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Grading scale

A – 88% to 100%

B – 75% to 88%

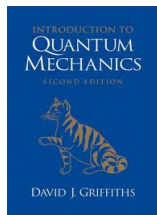
C – 62% to 75%

D – 50% to 62%

E – 0% to 50%

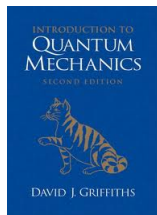
Topics to be Covered (Chapter titles)

- 1 Time-independent perturbation theory



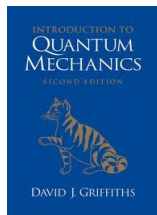
Topics to be Covered (Chapter titles)

- 1 Time-independent perturbation theory
- 2 Variational method



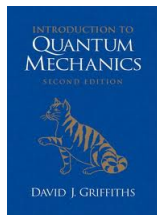
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- 1 Time-independent perturbation theory
- 2 Variational method
- 3 WKB approximation



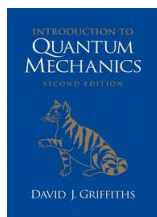
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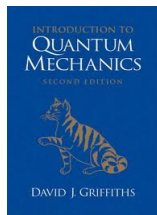
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- 3 WKB approximation
- 4 Time-dependent perturbation theory
- 5 Adiabatic approximation



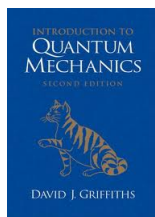
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- 6 Scattering



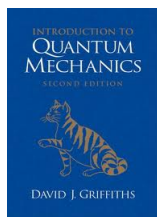
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- 7 Quantum paradoxes



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- 1 Time-independent perturbation theory
- 2 Variational method
- 3 WKB approximation
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- 6 Scattering
- 7 Quantum paradoxes
- 8 Other topics as appropriate



Course Schedule

Up-to-date schedule at

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29 class sessions

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Focus on applications of quantum mechanics this semester.

Today's Outline - January 14, 2013

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- Tips for success

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Reading Assignment: Chapter 5.3–5.4, 6.1

Tips for success

- 1 Do the reading assignments before lecture, you will understand them better.

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- ⑥ Come to office hours with questions, I'll be less lonely and it will help you too!

Free electron gas

Solids are a particular example of a system of identical particles

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The simplest model of a solid is the free electron gas

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$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{l_x l_y l_z}} \sin\left(\frac{n_x \pi}{l_x} x\right) \sin\left(\frac{n_y \pi}{l_y} y\right) \sin\left(\frac{n_z \pi}{l_z} z\right)$$

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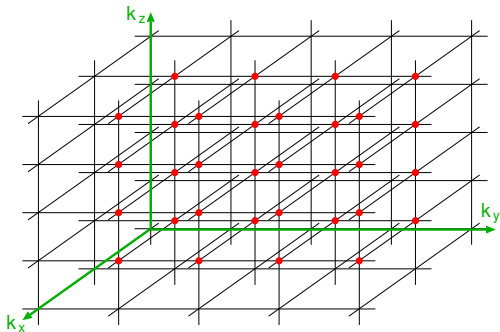
these discrete values of k_x , k_y , k_z form a lattice called the reciprocal lattice.

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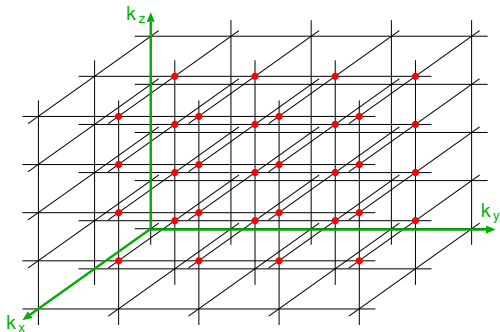
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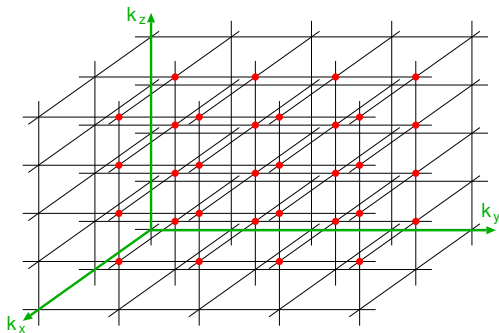
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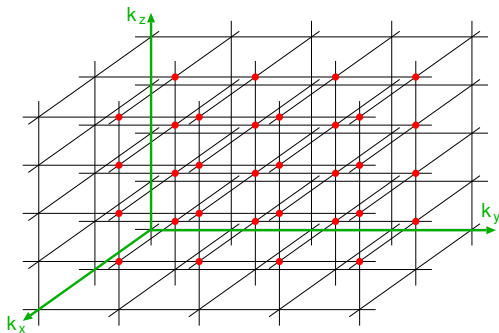
each point is a discrete single particle state



Volume of reciprocal lattice point

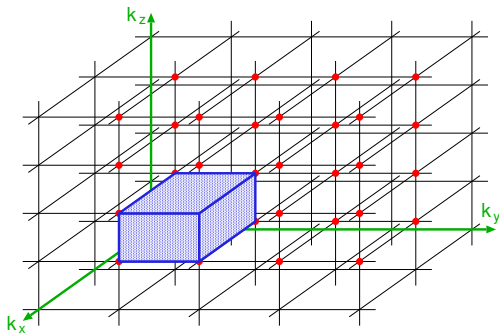


Volume of reciprocal lattice point



What is the volume, in reciprocal space, occupied by each of these states?

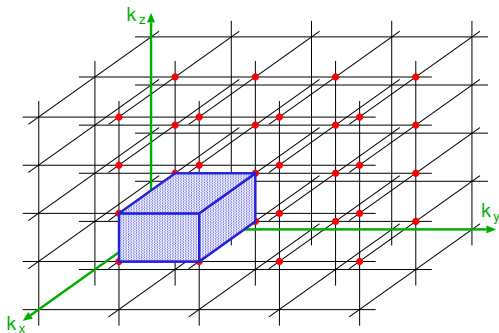
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start by drawing a rectangular box with a point at each corner

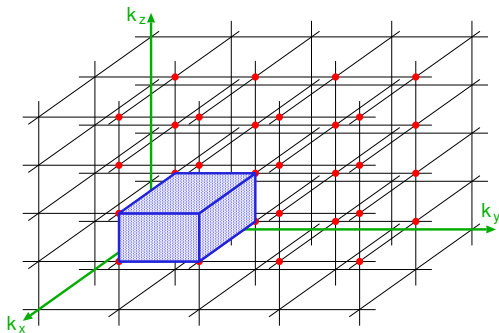
Volume of reciprocal lattice point



What is the volume, in reciprocal space, occupied by each of these states?

start by drawing a rectangular box with a point at each corner which represents the volume occupied by one point

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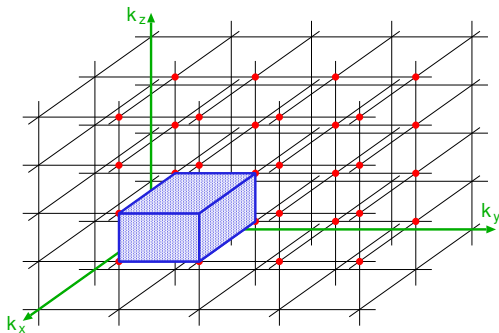


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$$\Delta k_x \cdot \Delta k_y \cdot \Delta k_z = \frac{\pi}{l_x} \cdot \frac{\pi}{l_y} \cdot \frac{\pi}{l_z}$$

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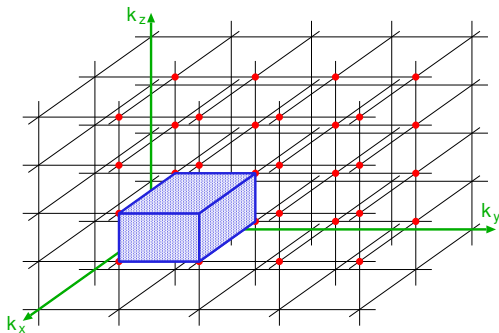


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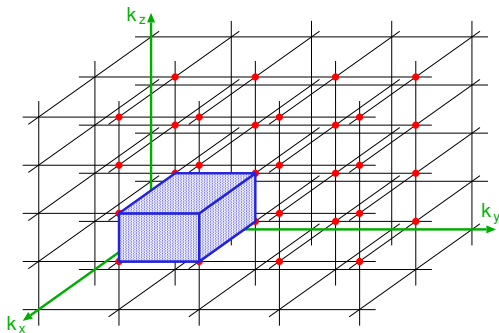


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What is the volume, in reciprocal space, occupied by each of these states?

start by drawing a rectangular box with a point at each corner which represents the volume occupied by one point

$$\Delta k_x \cdot \Delta k_y \cdot \Delta k_z = \frac{\pi}{l_x} \cdot \frac{\pi}{l_y} \cdot \frac{\pi}{l_z} = \frac{\pi^3}{l_x l_y l_z} = \frac{\pi^3}{V}$$

if the solid contains N atoms and each atom contributes q free electrons to the electron gas, we can begin to see how the states in reciprocal space are populated

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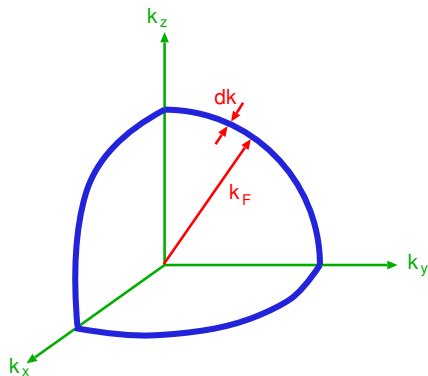
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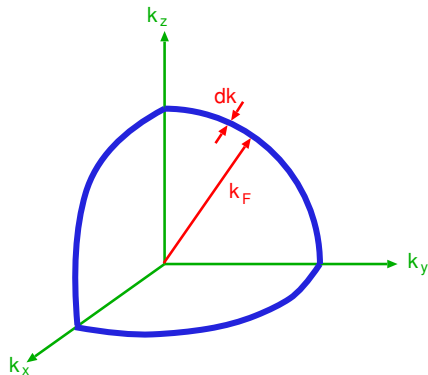


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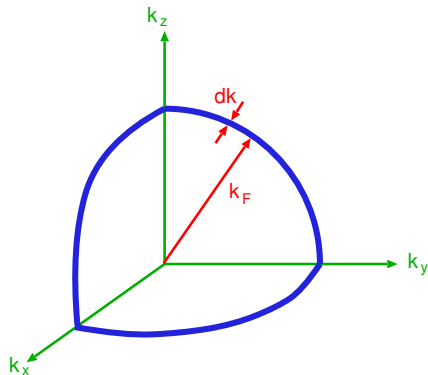
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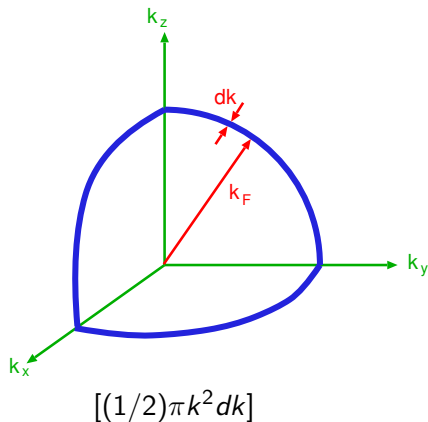
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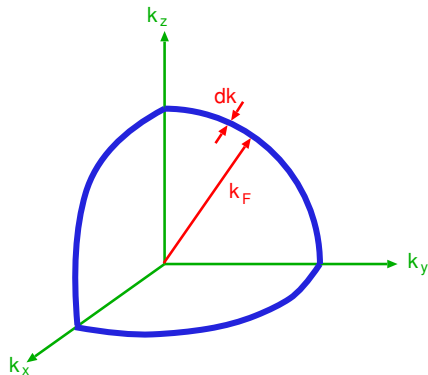
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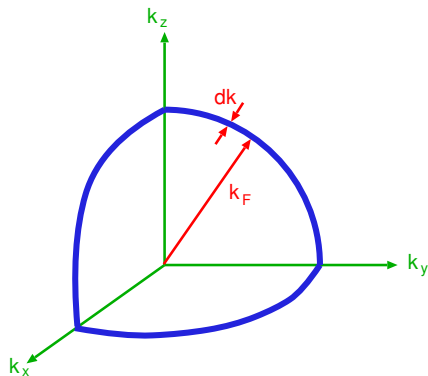
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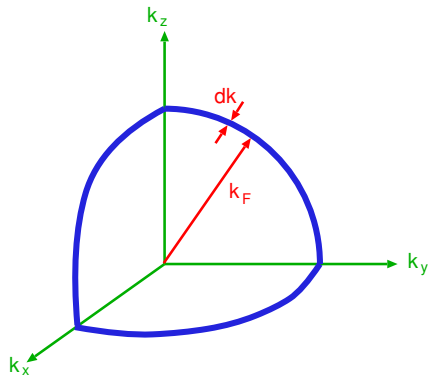
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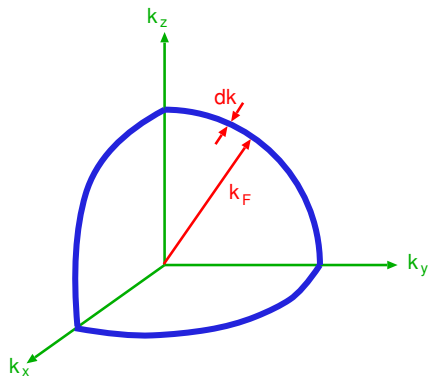
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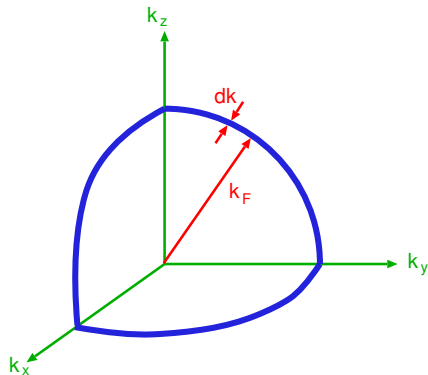
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Band theory

A better model is one which includes the periodic potential of the positive ions in a solid.

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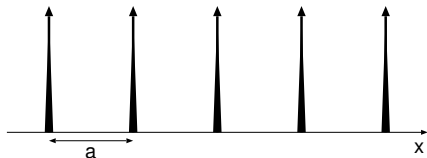
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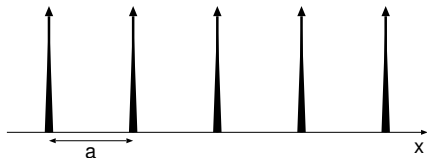


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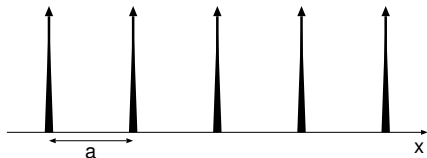


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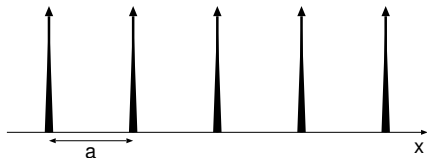
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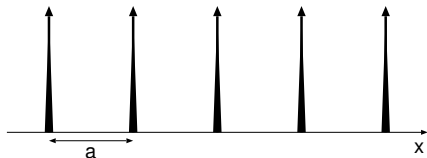
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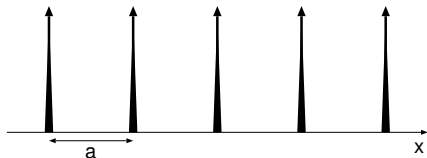
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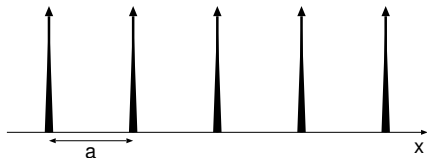
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To determine this, let's compute the commutator of D and H ,

$$[D, H] = DH - HD$$

$$\begin{aligned}[D, H] f(x) &= D\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right]f(x) - \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right]Df(x) \\ &= D\left[-\frac{\hbar^2}{2m} f''(x) + V(x)f(x)\right] - \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right]f(x+a) \\ &= \left[-\frac{\hbar^2}{2m} f''(x+a) + V(x+a)f(x+a)\right] \\ &\quad - \left[-\frac{\hbar^2}{2m} f''(x+a) + V(x+a)f(x+a)\right] = 0\end{aligned}$$

but since $V(x+a) = V(x)$, H and D commute and we can have simultaneous eigenfunctions of both operators

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by assuming that the edges of the solid are always far away, and applying periodic boundary conditions, Bloch's theorem can be made applicable to the Dirac comb and other models of solids

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$$K = \frac{2\pi n}{Na}, \quad (n = 0, \pm 1, \pm 2, \dots)$$