Homework #1

Due Sunday, February 16, 2025, at 11:59 PM CST, by electronic upload of a single PDF

Problem 1: Calculate the matrix elements in both the coordinate representation and the momentum representation for the following quantum-mechanical operators:

a) Position

b) Momentum

c) Kinetic energy (remember, this operator is quadratic in momentum)

d) Potential energy (which can presumably be written purely as a function of position)

e)* Angular momentum — look this up. *(Note: This one has to be done in 3D)*

f)* Velocity — look this up. Velocity operator is not momentum over mass, but rather the time derivative of position, and calculating the time derivative of an operator involves using its commutator with the Hamiltonian. Assume the Hamiltonian consists of kinetic energy (quadratic in momentum) and potential energy (a function of position only). In this, it will be helpful to use the commutation relationship between position and momentum. $[\hat{x}, \hat{p}] = i\hbar$.

For simplicity, assume unbounded space and 1D. Also remember:

$A(x, x') = \langle x|\hat{A}|x'\rangle$ is the matrix element of an operator in coordinate representation

$A(k, k') = \langle k|\hat{A}|k'\rangle$ is the matrix element of an operator in the momentum representation (technically, the wave-vector representation)

The fundamental operators in terms of which all others can be expressed are the position and momentum operators, and for them it holds:

$$\hat{x}|x\rangle = x|x\rangle \,;\, \langle x|\hat{x}|\Psi\rangle = \Psi(x)$$

$$\hat{p}|k\rangle = \hbar k|k\rangle \,;\, \langle x|\hat{p}|\Psi\rangle = -i\hbar\frac{\partial\Psi(x)}{\partial x}$$

$$\langle x|k\rangle = \frac{e^{ikx}}{\sqrt{2\pi}}$$

Operators are diagonal in the representation that uses their eigenvectors. For example, an operator that is a function of position only will have a matrix element in the coordinate representation of the form $A(x, x') = A(x)\delta(x - x')$, while an operator that is a function of

momentum only will have a matrix element in the momentum representation of the form $A(k, k') = \delta(k - k')$. (In case of finite volume, Kronecker delta symbol is involved instead $A(k, k') = \delta_{k,k'}$.)

Problem 2: Derive (as we did in class) the density of states per spin for a free particle of mass m moving in

a) 3D

b) 2D

c) 1D

d)* In general, the density of states depends on energy as E^m , where m depends on dimension. Derive the full expression for the density of states of arbitrary dimension greater than 3.

e) In 0D, the density of states can be written simply as

$$g_{0D}(E) = \sum_n \delta(E - E_n)$$

where n denotes the relevant quantum numbers enumerating the bound states.

Show (by explicit integration and comparison to the results in a through c above) that the density of states from 0D to 3D can be written as

$$g_{dim}(E) = \frac{1}{V_{dim}} \sum_n \delta(E - E_n)$$

where n denotes all relevant quantum numbers. In 1D-3D, the role of n is played by the quasicontinuous quantum number known as the wave vector **k**. (V_{dim} can be thought of as length to the power of dimension, so $V_{0D}=1$).

Problem 3: A particle of spin ½ and mass $m=0.067m_0$, where m_0 is the free-electron mass, moves in 3D. If its motion is restricted in the z-direction to a well of width W by very high

potential walls, then the quantum numbers describing a stationary state in the so-called envelope

function approximation (look it up) are **k** (2D wave vector perpendicular to the confinement

direction), $\sigma = \pm 1/2$ (spin up or down), and, the discrete quantum number n characterizing particle in a box states. This system is referred to as a *quasi-2D system* (unconfined motion in

2D, confined in1D), n is referred to as the subband index, and the energy dispersion of the confined particle is given by

$$E_{\sigma,n,k} = \frac{\hbar^2 \pi^2}{2mW^2} n^2 + \frac{\hbar^2 k^2}{2m}$$

a) Plot the density of states per unit area of the unconfined 2D plane for the quasi-2D electron of mass m for a given width W, as well as $10W$ and $100W$ (all on the same graph). For comparison, also on the same graph, plot the 3D density of states for the unconfined electron (clearly, the 3D DOS is per unit volume, so you will need to multiply it by W in order to put it on the same graph as the quasi-2D DOS). Which one among the thicknesses – W, $10W$, or $100W$ – gives the quasi-2D DOS closest to that of a completely free particle in 3D?

b) Plot the constant-energy surfaces in the 2D k-space.

Problem 4: Some quantum mechanical particle of spin ½ is able to move in 3D and has the following dispersion

$$E_{\sigma,k} = \frac{\hbar^2 \left(k_x^2 + k_y^2 \right)}{2m_{xy}} + \frac{\hbar^2 k_z^2}{2m_z}$$

where m_{xy}=0.98m_0 and m_z=0.19m_0, m_0 being the free-electron mass.

a) Graph a few constant-energy surfaces in the 3D k-space.

b) Derive the expression for the density of states per unit volume (hint: a simple map will transform the constant energy surface into a sphere).

c) Derive the dispersion in case the particle is confined to a well of width W in the z-direction (as in problem 3).

d) Derive the dispersion in case the particle is confined to a well of width W in either x or y-direction.

e) On the same graph, plot the density of states per unit area for confinement types in c and d. What do you notice? How are the two densities of states the same and how are they different?