

# Physics 215B- Quantum Mechanics, Winter 2014

## Midterm Exam

**Instructions:** Answer three of the five questions.

[1.] Solve the two site 'spin-1' Heisenberg model

$$\hat{H} = J\hat{S}_1 \cdot \hat{S}_2$$

where  $\hat{S}_1$  and  $\hat{S}_2$  are spin-1 operators instead of the spin-1/2 operators we (mainly) did in class and on homework. There are two rather different ways to do the problem. With one of those methods you may want to use the formula  $L_{\pm}|lm\rangle = \hbar\sqrt{(l \mp m)(l \pm m + 1)}|l, m \pm 1\rangle$  where  $L_{\pm} = L_x \pm iL_y$ .

[2.] Consider the quantum harmonic oscillator, and perturbation

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 \qquad \hat{V} = \delta\hat{x}^2$$

Compute the first and second order shifts in the energy levels of  $\hat{H}_0$  due to  $\hat{V}$ . If you have time, solve the problem exactly and expand your result in a Taylor series in  $\delta$  to check the perturbation calculation. You may find the identity  $\hat{x} = \sqrt{\hbar/(2m\omega_0)}(a + a^\dagger)$  useful.

[3.] Outline the steps in the solution of the 3D Schroedinger equation for a potential  $V(r)$  which is independent of  $\theta, \phi$ . Provide equations if you can, most mostly I expect the conceptual steps and their consequences. What are the energy levels that you ultimately get for the Hydrogen atom case  $V(r) = -e^2/r$ ? (It would be nice if you recall what a Rydberg is in terms of  $\hbar, e, m$ , but don't worry if you do not.) What extra feature does the particular Hydrogen atom form have that is not true for other  $V(r)$ ? How do the energy levels of the Hydrogen atom, and their degeneracy, explain the structure of the periodic table?

[4.] What are the eigenvalues and eigenvectors of a 'quinti-diagonal' matrix, ie which has five diagonals of nonzeros, with appropriate periodic boundary conditions:

$$\hat{H} = \begin{pmatrix} A & B & C & 0 & 0 & \dots & 0 & 0 & C & B \\ B & A & B & C & 0 & \dots & 0 & 0 & 0 & C \\ C & B & A & B & C & \dots & 0 & 0 & 0 & 0 \\ 0 & C & B & A & B & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ C & 0 & 0 & 0 & 0 & \dots & C & B & A & B \\ B & C & 0 & 0 & 0 & \dots & 0 & C & B & A \end{pmatrix}$$

[5.] What is a pure state? When you make a measurement on a pure state, are you assured of getting precise values for observables (ie there is only one possible outcome for the measurement, with probability unity)? What is a mixed state? What is a density matrix? What properties does the density matrix have for a pure state? What is a reduced density matrix? How would you compute the second Rényi entropy (which I have, a bit sloppily, been calling the entanglement entropy in class) from the reduced density matrix?

R215B W2014

MIDTERM EXAM SOLUTIONS

1. There are two ways to do this problem, The easier method is to rewrite

$$\hat{H} = \frac{1}{2} \frac{J}{\hbar^2} \left[ (S_1 + S_2)^2 - S_1^2 - S_2^2 \right]$$

Then for spin 1  $S_1^2 = S_2^2 = 1(1+1)\hbar^2 = 2\hbar^2$

$$\begin{aligned} \text{and } (S_1 + S_2)^2 &= 0(0+1)\hbar^2 = 0 & (S_{TOT} = 0) \\ &= 1(1+1)\hbar^2 = 2\hbar^2 & (S_{TOT} = 1) \\ &= 2(2+1)\hbar^2 = 6\hbar^2 & (S_{TOT} = 2) \end{aligned}$$

$$\begin{aligned} \text{Thus } \hat{H} &= \frac{1}{2} J \{ 0 - 2 - 2 \} = -2J & S_{TOT} = 0 \\ &= \frac{1}{2} J \{ 2 - 2 - 2 \} = -J & S_{TOT} = 1 \\ &= \frac{1}{2} J \{ 6 - 2 - 2 \} = +J & S_{TOT} = 2 \end{aligned}$$

The degeneracies are 1, 3, 5 for  $S_{TOT} = 0, 1, 2$  respectively

The total # of eigenvalues is  $1+3+5=9$  which makes

sense since the Hilbert space has  $\dim 3 \times 3 = 9$

since  $S_{1z}$  and  $S_{2z}$  both have 3 values  $m = -1, 0, 1$ .

1/cont'd. The slower method explicitly constructs

a matrix for  $\hat{H}$  by looking at basis vectors  $|\uparrow_1 \uparrow_2 \uparrow_3\rangle$

$$\hat{H} = \frac{J}{\hbar^2} \left\{ S_1^z S_2^z + \frac{1}{2} (S_1^+ S_2^- + S_1^- S_2^+) \right\}$$

$$\hat{H} |11\rangle = J |11\rangle$$

Eigenvalue  $J$

$$\hat{H} |10\rangle = J \sqrt{2} \sqrt{2} \frac{1}{2} |00\rangle$$

$$\hat{H} |00\rangle = J \sqrt{2} \sqrt{2} \frac{1}{2} |10\rangle$$

$$\rightarrow J \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Eigenvalues  
 $\pm J$

By symmetry  $|1-1\rangle$  and  $|0-1\rangle$  have same eigenvalues  
 $\uparrow$   $\uparrow$   
 $J$   $\pm J$

Our list so far:  $J, J, J, J, -J, -J$

Last case is

$$\hat{H} |1-1\rangle = J \sqrt{2} \sqrt{2} \frac{1}{2} |00\rangle$$

$-J |1-1\rangle$

$$\hat{H} |00\rangle = J \sqrt{2} \sqrt{2} \frac{1}{2} |1-1\rangle + J \sqrt{2} \sqrt{2} \frac{1}{2} |11\rangle$$

$$\hat{H} |11\rangle = J \sqrt{2} \sqrt{2} \frac{1}{2} |00\rangle$$

$-J |11\rangle$

$$\hookrightarrow J \begin{pmatrix} -1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix}$$

1/cont'd

Eigenvalues of this  $3 \times 3$  matrix are (dropping  $J$ )

$$(-1-\lambda) \{ -\lambda(-1-\lambda) - 1 \} - 1 \{ 1(-1-\lambda) \} = 0$$

$$(\lambda+1) [\lambda^2 + \lambda - 1 - 1] = 0$$

$$\lambda = -1 \quad (\lambda^2 + \lambda - 2) = 0$$

$$(\lambda+2)(\lambda-1) = 0$$

$$\lambda = -2 \quad \lambda = 1$$

So complete list is  $\underbrace{J, J, J, J, J}_{, , , , ,} -J, -J, -J, -2J$

In agreement with method #1  $\square$

$$\boxed{2} \quad \hat{H} = \hat{P}^2 / 2m + \frac{1}{2} m \omega_0^2 \hat{X}^2 + \delta \hat{X}^2$$

The exact soln is obtained via

$$\frac{1}{2} m \omega_0^2 \hat{X}^2 + \delta \hat{X}^2 = \frac{1}{2} m \left( \omega_0^2 + \frac{2\delta}{m} \right) \hat{X}^2$$

$$\text{so } \omega^2 = \omega_0^2 + \frac{2\delta}{m}$$

$$\omega = \sqrt{\omega_0^2 + 2\delta/m}$$

$$E = \hbar \omega \left( n + \frac{1}{2} \right) = \hbar \sqrt{\omega_0^2 + \frac{2\delta}{m}} \left( n + \frac{1}{2} \right)$$

To make contact with perturbation theory, expand

$$\left( \omega_0^2 + \frac{2\delta}{m} \right)^{1/2} = \omega_0 \left( 1 + \frac{2\delta}{m\omega_0^2} \right)^{1/2}$$

$$= \omega_0 \left\{ 1 + \frac{\delta}{m\omega_0^2} - \frac{\delta^2}{2m^2\omega_0^4} \right\}$$

$$= \omega_0 + \frac{\delta}{m\omega_0} - \frac{\delta^2}{2m^2\omega_0^3}$$

$$\textcircled{1} \quad \frac{\hbar \delta}{m\omega_0} \left( n + \frac{1}{2} \right)$$

$$\textcircled{2} \quad -\frac{\hbar \delta^2}{2m^2\omega_0^3} \left( n + \frac{1}{2} \right)$$

5,

2 / cont'd Now solve by perturbation theory

$$\hat{x}^2 = \frac{\hbar}{2m\omega_0} (q + q^\dagger)^2 = \frac{\hbar}{2m\omega_0} (aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)$$

$$E_{n1} = \langle n | \delta \hat{x}^2 | n \rangle$$

$$= \frac{\hbar \delta}{2m\omega_0} (\emptyset + (n+1) + n + \emptyset) = \frac{\hbar \delta}{m\omega_0} (n + \frac{1}{2})$$

Matches ① on page 4

$$\text{To second order } E_{n2} = \sum_{m \neq n} \frac{|\langle n | \delta \hat{x}^2 | m \rangle|^2}{E_{n0} - E_{m0}}$$

 $\hat{x}^2$  connects  $|n\rangle$  to  $|n \pm 2\rangle = |m\rangle$ 

$$E_{n2} = \delta^2 \left( \frac{\hbar}{2m\omega_0} \right)^2 \left\{ \frac{(\sqrt{n+2}\sqrt{n+1})^2}{-2\hbar\omega_0} + \frac{(\sqrt{n-1}\sqrt{n})^2}{+2\hbar\omega_0} \right\}$$

$$\uparrow$$

$$|m\rangle = |n+2\rangle$$

$$\uparrow$$

$$|m\rangle = |n-2\rangle$$

$$= -\delta^2 \frac{\hbar^2}{4m^2\omega_0^2} \frac{1}{2\hbar\omega_0} \{ n^2 + 3n + 2 - n^2 + n \}$$

$$\uparrow$$

$$4n + 2 = 4(n + \frac{1}{2})$$

$$= -\delta^2 \frac{\hbar}{2m^2\omega_0^3} (n + \frac{1}{2})$$

$$\uparrow$$
 matches ② on page 4

$$\boxed{3} \quad \text{If } \hat{H} = \hat{p}^2/2m + V(r)$$

↑  
no  $\theta, \phi$

$$\text{Then } [\hat{H}, \hat{L}^2] = [\hat{H}, \hat{L}_z] = 0$$

So observation #1 is that eigenstates of  $\hat{H}$  are also

eigenstates of  $\hat{L}^2$  and  $\hat{L}_z$  i.e.  $\psi(r, \theta, \phi) = R(r)Y_{\ell m}(\theta, \phi)$

The next element is rewriting  $\hat{p}^2 = -\frac{\hbar^2}{2m} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right)$

in terms of  $d/dr$  and  $\hat{L}^2$ . According to the clue

in the problem, the result is  $-\frac{\hbar^2}{2m} \frac{1}{r} \frac{d^2}{dr^2} r + \frac{\hat{L}^2}{2mr^2}$

Acting with this on  $R(r)Y_{\ell m}(\theta, \phi)$  gives an eqn for  $R(r)$ :

$$\left( -\frac{\hbar^2}{2m} \frac{1}{r} \frac{d^2}{dr^2} r + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r) \right) R(r) = ER(r)$$

So the second observation is that we have to solve the

above radial eqn. For each  $\ell$  there will be a set

of solutions labeled by  $n$ :  $R_{n\ell}(r)$

7.

At this point it is often useful to figure out the behavior at small  $r$  and large  $r$ . I will refer you to the notes for details, but isolating the small  $r$  and large  $r$  asymptotics can lead to a more simple radial eqn for some redefined  $u(r)$ . Note also the introduction of a dimensionless variable  $\xi = r/a_0$  where  $a_0 = \frac{\hbar^2}{me^2}$  is the Bohr radius is useful.

What happens now is that one solves the radial eqn with a power series guess and discovers the power series causes  $R(r)$  to diverge at  $r = \infty$  unless it terminates. This termination condition results in quantized energy levels. (As is often the case in QM, boundary conditions  $\rightarrow$  quantization)



8.

In the end we get energy levels  $E_n = -\frac{e^2}{2a_0} \frac{1}{n^2}$

if we do all this for  $V(r) = -\frac{e^2}{r}$ .

What is different about this from other  $V(r)$  is

that the levels do not depend on  $l$ ! This is

surprising because the radial eqn does depend on  $l$ ,

so naively one would expect so should its eigenvalues.

The allowed  $l$  values for a given  $n$  are  $l = 0, 1, \dots, n-1$

and of course  $m = -l, -l+1, \dots, +l$ , so for

$n=0 \rightarrow l=0, m=0, s=\pm\frac{1}{2} \leftarrow 2 \text{ states}$

$n=1 \rightarrow l=0, m=0, s=\pm\frac{1}{2} \leftarrow 2 \text{ states}$   
 $+ l=1, m=\pm 1, 0, s=\pm\frac{1}{2} \leftarrow 6 \text{ states}$

The first row of the periodic table has 2 elements,

the second has 8 and so on,

9.

4 Writing  $\hat{H} |\psi\rangle = E |\psi\rangle$  out in

component form:

$$* \quad C \psi_{n-2} + B \psi_{n-1} + A \psi_n + B \psi_{n+1} + C \psi_{n+2} = E \psi_n$$

Guessing  $\psi_n = \alpha e^{ikn}$  yields

$$C e^{-2ik} + B e^{-ik} + A + B e^{ik} + C e^{2ik} = E$$

So  $E = A + 2B \cos k + 2C \cos 2k$ .

The  $k$  are quantized as usual to be  $\frac{2\pi}{N} \{1, 2, \dots, N\}$

because the eqn  $*$  is valid for all  $n$  only

if we insist  $\psi_{-1} = \psi_{N-1}$

$$\psi_0 = \psi_N$$

$$\psi_{N+1} = \psi_1$$

$$\psi_{N+2} = \psi_2$$

5 A pure state is one in which a QM system is described by a single ket  $|\psi\rangle$ .

A measurement on a pure state will in general not result in a unique possible result because, typically  $|\psi\rangle$  will have a nontrivial expansion

$$|\psi\rangle = \sum c_n |\phi_n\rangle$$

in terms of the eigenfunctions  $|\phi_n\rangle$  of the operator corresponding to the observable to be measured.

A mixed state is a QM system which has a probability  $p_i$  of being in the ket  $|\psi_i\rangle$

The density matrix for a pure state

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

and for a mixed state

$$\hat{\rho} = \sum p_i |\psi_i\rangle\langle\psi_i|$$

15 / cont'd

For a pure state  $\hat{\rho}^2 = |\psi\rangle\langle\psi| \psi\rangle\langle\psi|$   
 $= |\psi\rangle\langle\psi| = \hat{\rho}$

A "reduced density matrix" is obtained by

dividing a system into several pieces (eg

two different sets of sites in the Heisenberg model) A, B.

Then  $\hat{\rho}_A = \text{Tr}_B \hat{\rho}$ .

The entanglement entropy (actually the 2nd Renyi entropy)

is  $S_A = -\ln \text{Tr} \hat{\rho}_A^2$ .