Physics 215B- Quantum Mechanics, Winter 2014
Final Exam

Instructions: Answer four of the five questions.

[1.] The "one-dimensional Ising Model in a transverse field" is

$$\hat{H} = -J/\hbar^2 \sum_{l=1}^{N} \hat{S}_l^z \hat{S}_{l+1}^z - B/\hbar \sum_l \hat{S}_l^x$$

Here $\hat{S}_l^x$ and $\hat{S}_l^z$ are spin-1/2 operators. There are more than one of them, hence the label l. In all the questions below, consider a small chain of $N = 4$ spins. Assume there are periodic boundary conditions so that the spin at site $l = 4$ couples to the spin at site $l = 1$.
(a) What are the eigenvalues of $\hat{H}$ for $J = 0$?
(b) What are the eigenvalues of $\hat{H}$ for $B = 0$?
Do either (c) or (d) but not both:
(c) Compute the eigenvalues of $\hat{H}$ for B nonzero treating J as a perturbation.
(d) Compute the eigenvalues of $\hat{H}$ for J nonzero treating B as a perturbation.
(e) To solve for the *exact* eigenvalues of the model we need to diagonalize a big matrix. Compute two of the rows of the matrix by telling me how $\hat{H}$ acts on the two basis states $|\, S_1^z\, S_2^z\, S_3^z\, S_4^z\,\rangle = |++++\rangle$ and $|\, S_1^z\, S_2^z\, S_3^z\, S_4^z\,\rangle = |+++-\rangle$.

[2.] A Hydrogen atom is placed in a time dependent homogeneous electric field

$$\vec{\mathcal{E}}(t) = \frac{A\tau}{e\pi} \frac{1}{\tau^2 + t^2}\, \hat{z}$$

where A and τ are constants. If, at $t = -\infty$, the atom is in its ground state, calculate the probability that it will be in a $2p$ state at $t = +\infty$. The $n = 1, 2$ hydrogenic wavefunctions are:

$$\phi_{100} = \frac{1}{\sqrt{\pi a^3}}\, e^{-r/a} \qquad \phi_{200} = \frac{1}{4\sqrt{2\pi a^3}}\, (2 - \frac{r}{a})\, e^{-r/2a}$$

$$\phi_{21\pm1} = \frac{1}{4\sqrt{4\pi a^3}}\, \frac{r}{a}\, e^{-r/2a} \sin\theta\, e^{\pm i\phi} \qquad \phi_{210} = \frac{1}{4\sqrt{4\pi a^3}}\, \frac{r}{a}\, e^{-r/2a} \cos\theta$$

A possibly useful integral is $\int_0^\infty r^n e^{-ur} dr = n!/u^{n+1}$.

[3.] Compute $d\sigma/d\Omega$ and $\sigma_{\rm tot}$ for $V(r) = V_0 \exp(-r^2/2r_0^2)$ within the Born approximation. *Hint:* Do the r integration by completing the square. What is $\sigma_{\rm tot}$ in the low energy limit?

[4.] Consider the three site Heisenberg model (with "open boundary conditions"):

$$\hat{H} = J/\hbar^2\, (\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3)$$

Here $\vec{S}_1, \vec{S}_2, \vec{S}_3$ are spin-1/2 operators.
(a) Find one of the two (degenerate) ground state wave functions $|\psi_0\rangle$.
(b) What is the associated density matrix $\hat{\rho}$?
(c) What is the reduced density matrix $\hat{\rho}_A$ if region A consists of site 1 and region B consists of sites 2 and 3?
(d) What is the second Renyi entropy S_2?

Problem [5.] on reverse side!!

[5.] Consider s-wave ($l = 0$) scattering of a particle of mass m from a delta function spherical-shell potential of radius a and strength $U > 0$, that is $V(r) = U\delta(r - a)$.
(a) Write down the $l = 0$ radial Schroedinger equation for the function $u(r) = r\psi(r)$ and an energy $E = \hbar^2 k^2/2m$.
(b) Formulate the boundary conditions on u and du/dr at $r = 0$ and at $r = a$ using the abbreviation $\gamma = 2mU/\hbar^2$.
(c) Show that $u(r)$ has the following form

$$\begin{aligned} u(r) &= A\sin(kr) & \qquad r \leq a \\ u(r) &= B\sin(kr + \delta_0) & \qquad r \geq a \end{aligned}$$

(d) Derive a transcendental equation for δ_0.
(e) What is the total cross section σ_{tot}?

Physics 215B Winter 2014
Final Exam Solutions

$\boxed{1}$ a) For $J=0$ we have four completely independent spin 1/2 operators, $\hat{S}_\ell^x$. Each has eigenvalues $\pm\hbar/2$. Thus the 16 eigenvalues are

	deg	
$E = -2B$	1	$\leftarrow$ all $S_\ell^x = +\hbar/2$
$E = -B$	4	$\leftarrow$ three $S_\ell^x = +\hbar/2$ and one $-\hbar/2$
$E = 0$	6	$\leftarrow$ two $S_\ell^x = +\hbar/2$ and two $-\hbar/2$
$E = +B$	4	"
$E = +2B$	1	..etc...

b) For $B=0$ we work in basis $|S_1^z S_2^z S_3^z S_4^z\rangle$ and note these are eigenstates of $\hat{H}$.

$|++++\rangle$ $\qquad E = -J$

$|+++-\rangle, |++-+\rangle, |+-++\rangle, |-+++\rangle$ $\qquad E = \phi$

$|++--\rangle, |+--+\rangle, |--++\rangle, |-++-\rangle$ $\qquad E = \phi$

$|+-+-\rangle, |-+-+\rangle$ $\qquad E = +J$

$|---+\rangle, |--+-\rangle, |-+--\rangle, |+---\rangle$ $\qquad E = \phi$

$|----\rangle$ $\qquad E = -J$

c) Ground state for $B \neq 0$ and $J = 0$ is

$$|\psi_0\rangle = |S_1^x\ S_2^x\ S_3^x\ S_4^x\rangle = |+\ +\ +\ +\rangle$$

If we work in the "usual" basis of eigenstates of S^z

$$|S_1^x = +\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$ since $\hat{S}_e^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ in the S_e^z basis.

meaning $S_e^z = +$

So $|\psi_0\rangle$ is actually a linear combination of all 16 $|S_1^z\ S_2^z\ S_3^z\ S_4^z\rangle$ states with each coefficient $\left(\frac{1}{\sqrt{2}}\right)^4 = \frac{1}{4}$

What we need to compute is

$$\Delta E^{(1)} = \langle \psi_0 | -\frac{J}{\hbar^2} \sum_e \hat{S}_e^z \hat{S}_{e+1}^z | \psi_0 \rangle$$

But from part (b) we know the matrix elements of each of the 16 components of $|\psi_0\rangle$ (Note $\hat{S}_e^z \hat{S}_{e+1}^z$ does <u>not</u> mix them.) we get

$$\Delta E^{(1)} = \frac{1}{16}\left\{-J + 12(\phi) - J + J + J\right\} = \phi$$

as we might have guessed by symmetry

1-3

(d) For J nonzero the two degenerate ground states are

$$|++++\rangle \quad \text{and} \quad |----\rangle$$

We compute

$$\langle ++++| -\frac{B}{\hbar}(S_1^x + S_2^x + S_3^x + S_4^x)|++++\rangle$$

which vanishes since $S_1^x|++++\rangle = \frac{\hbar}{2}|-+++\rangle$ etc

So again here $\Delta E' = \phi$,

(e) Working in S_e^z basis

$$\hat{H}|++++\rangle = -J|++++\rangle - B/2|-+++\rangle - B/2|+-++\rangle - B/2|++-+\rangle - B/2|+++-\rangle$$

$$\hat{H}|+++-\rangle = \phi|+++-\rangle - B/2|++++\rangle - B/2|-++-\rangle - B/2|+-+-\rangle - B/2|++--\rangle$$

etc.

1-4

The first two rows of the matrix for $\hat{H}$ are therefore

	$\vert{++++}\rangle$	$\vert{+++-}\rangle$	$\vert{++-+}\rangle$	$\vert{+-++}\rangle$	$\vert{-+++}\rangle$	$\vert{++--}\rangle$	$\vert{+-+-}\rangle$	$\vert{+--+}\rangle$	$\vert{-++-}\rangle$	$\vert{-+-+}\rangle$	$\vert{--++}\rangle$	$\vert{---+}\rangle$	$\vert{--+-}\rangle$	$\vert{-+--}\rangle$	$\vert{+---}\rangle$	$\vert{----}\rangle$
$\vert{++++}\rangle$	$-J$	$-\frac{B}{2}$	$-\frac{B}{2}$	$-\frac{B}{2}$	$-\frac{B}{2}$	ϕ	ϕ	ϕ	ϕ	ϕ	ϕ	ϕ	ϕ	ϕ	ϕ	ϕ
$\vert{+++-}\rangle$	$-\frac{B}{2}$	ϕ	ϕ	ϕ	ϕ	$-\frac{B}{2}$	$-\frac{B}{2}$	ϕ	$-\frac{B}{2}$	ϕ	ϕ	ϕ	ϕ	ϕ	ϕ	ϕ

2-1

We know that to first order in $\hat{V}$

$$a^{(1)}_{2\ell m}(t) = \underbrace{1/i\hbar \; e^{i(E_m - E_0)t/\hbar} \langle \phi_{2\ell m} | \hat{V} | \phi_{100} \rangle}_{\text{see class notes}}$$

see class notes

all objects on RHS are unperturbed eigenvalues + eigenvectors

$$a^{(1)}_{2\ell m}(+\infty) = \int_{-\infty}^{\infty} \frac{1}{i\hbar} e^{i(E_m^0 - E_0)t/\hbar} \langle \phi_{2\ell m} | \hat{V} | \phi_{100} \rangle$$

In our problem $\hat{V} = -\frac{A\tau}{\pi} \frac{1}{\tau^2 + t^2} z$

$r\cos\theta$

It is pretty clear that $\langle \phi_{2\ell m} | \hat{V} | \phi_{100} \rangle$ will vanish unless we consider $\langle \phi_{2\ell m} | = \langle \phi_{210} |$ because of the $\int_0^{2\pi} d\phi$ vanishing in the case of $\langle \phi_{21\pm1} |$ and $\int_0^{\pi} \sin\theta \, d\theta$ vanishing in the case of $\langle \phi_{200} |$

So we have a time and a space integral to do.

2-2

Time: Define $\omega = (E_m - E_0)/\hbar$

$$\int_{-\infty}^{\infty} e^{i\omega t} \frac{1}{t^2+\tau^2} dt = \int_{\infty} e^{i\omega t} \frac{1}{(t+i\tau)(t-i\tau)} dt$$

This is best done by noting $1/t^2+\tau^2$ has poles at $t = \pm i\tau$

so the Residue theorem gives $\quad 2\pi i \frac{e^{i\omega(i\tau)}}{2i\tau} = \frac{\pi}{\tau} e^{-\omega\tau}$

$$\text{Space: } \int_0^{\infty} r^2 dr \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \; \underbrace{r\cos\theta}_{z} \; \underbrace{\frac{1}{\sqrt{\pi a^3}} e^{-r/a}}_{|\phi_{100}\rangle}$$

$$\vdots \qquad \cdot \underbrace{\frac{1}{4\sqrt{4\pi a^3}} \frac{r}{a} e^{-r/2a} \cos\theta}_{\langle \phi_{210}|}$$

$$= 2\pi \frac{1}{8} \frac{1}{\pi a^3} \frac{1}{a} \underbrace{\int_0^{\pi} \sin\theta \cos^2\theta \, d\theta}_{2/3} \int_0 r^4 dr \, e^{-3r/2a}$$

Consider $\quad \int_0^{\infty} e^{-ur} dr = 1/u$

differentiate wrt u $\quad \int_0^{\infty} r e^{-ur} dr = 1/u^2$

again $\quad \int_0^{\infty} r^2 e^{-ur} dr = 2/u^3$

So in general $\int_0^\infty r^n e^{-ur}\,dr = n!/u^{n+1}$

Thus $$a^{(1)}_{2lm}(+\infty) = \frac{1}{i\hbar}\left(\frac{-A\tau}{\pi}\right)\frac{2\pi}{\tau} e^{-\omega\tau} \frac{1}{6a^4}\frac{4!}{(3/2a)^5}$$

$$= \frac{4A}{\hbar} e^{-\omega\tau}\, a\, \frac{1}{6}\,\frac{24\ 32}{3^5}$$

$$= \frac{4Aa}{\hbar} e^{-\omega\tau}\, \frac{2^7}{3^5}$$

$$P^{(1)}_{2lm}(+\infty) = \left| a^{(1)}_{2lm}(+\infty)\right|^2$$

$$= \frac{A^2 a^2}{\hbar^2}\,\frac{2^{14}}{3^{10}}\, e^{-2\omega\tau}$$

In the Born Approximation, for a spherically symmetric potential

$$f(\theta) = \frac{-2m}{\hbar^2 q} \int_0^\infty r\,dr\, V(r) \sin qr \qquad q = 2k\sin\frac{\theta}{2}$$

$$V(r) = V_0 e^{-r^2/2r_0^2}$$

This is an even function of r so we can write it as

$$= \frac{-m}{\hbar^2 q} \int_{-\infty}^{\infty} r\,dr\, V_0 e^{-r^2/2r_0^2} \sin qr$$

$$= \frac{-mV_0}{\hbar^2 q i}\, \mathrm{Im} \int_{-\infty}^{\infty} r e^{-r^2/2r_0^2} e^{iqr}\, dr$$

$$= \frac{-mV_0}{\hbar^2 q i}\, iqr_0^2 e^{-q^2 r_0^2/2} \sqrt{2\pi r_0^2}$$

(see page 3-1A)

$$\frac{d\sigma}{d\Omega} = |f|^2 = \left(\frac{mV_0 r_0^3}{\hbar^2}\right)^2 e^{-q^2 r_0^2}\, 2\pi$$

where $q = 2k\sin\theta/2$

3-1A

Complete the square

$$-\frac{r^2}{2r_0^2} + iqr = -\frac{1}{2r_0^2}\left\{r^2 - iqr2r_0^2\right\}$$

$$= -\frac{1}{2r_0^2}\left\{r - iqr_0^2\right\}^2 - \frac{q^2 r_0^2}{2}$$

$$\int_{-\infty}^{\infty} r\,dr\; e^{-1/2r_0^2 (r - iqr_0^2)^2 - q^2 r_0^2/2}$$

$$u = r - iqr_0^2$$

$$\int_{-\infty}^{\infty} (u + iqr_0^2)\,du\; e^{-u^2/2r_0^2}\; e^{-q^2 r_0^2/2}$$

ODD $\rightarrow \phi$

$$= iqr_0^2\, e^{-q^2 r_0^2/2}\sqrt{\pi 2 r_0^2}$$

3-2

The total cross section

$$\sigma = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \; \frac{d\sigma}{d\Omega}$$

$$= (2\pi)^2 \int_0^{\pi} \sin\theta \, d\theta \left(\frac{m V_0 r_0^3}{\hbar^2}\right)^2 e^{-4k^2 r_0^2 \sin^2 \frac{\theta}{2}}$$

$2 \sin \theta/2 \cos \theta/2$

Let $x = \sin \theta/2$ $\quad dx = \frac{1}{2} \cos \theta/2 \; d$

$$\sigma = (2\pi)^2 \left(\frac{m V_0 r_0^3}{\hbar^2}\right)^2 \int_0^1 2x \, 2dx \; e^{-4k^2 r_0^2 x^2}$$

$$= (2\pi)^2 \left(\frac{m V_0 r_0^3}{\hbar^2}\right)^2 4 \; \frac{-e^{-4k^2 r_0^2 x^2}}{8k^2 r_0^2}\Bigg|_0^1$$

$$= (2\pi)^2 \left(\frac{m V_0 r_0^3}{\hbar^2}\right)^2 \frac{1}{2k^2 r_0^2} \left\{1 - e^{-4k^2 r_0^2}\right\}$$

If K is really small (low E) this simplifies

$4k^2 r_0^2$

$$\sigma = (2\pi)^2 \left(\frac{m V_0 r_0^3}{\hbar^2}\right)^2 2.$$

4-1

8 dim Hilbert space

$$\hat{H} = J/\hbar^2 \{ S_1^z S_2^z + S_2^z S_3^z + 1/2 (S_1^+ S_2^- + S_1^- S_2^+ + S_2^+ S_3^- + S_2^- S_3^+) \}$$

$$\hat{H} |+++\rangle = J/2 \, |+++\rangle$$

$$\hat{H} |---\rangle = J/2 \, |---\rangle$$

$$\hat{H} |++-\rangle = J/2 \, |+-+\rangle$$

$$\hat{H} |+-+\rangle = -J/2 \, |+-+\rangle + J/2 \, |++-\rangle + J/2 \, |-++\rangle$$

$$\hat{H} |-++\rangle = J/2 \, |+-+\rangle$$

$|--+\rangle$
$|-+-\rangle$
$|+--\rangle$
same by symmetry

Matrix of $\hat{H}$ is $J/2 \begin{pmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

Eigenvalues $-\lambda \left[(-1-\lambda)(-\lambda) - 1 \right] - 1 \left(1(-\lambda) - 0 \right)$

$$= -\lambda \left[\lambda^2 + \lambda - 1 \right] + \lambda = 0$$

$$\Rightarrow \lambda \left[\lambda^2 + \lambda - 2 \right] = 0$$

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

$$\lambda = 0 \qquad \lambda = 1 \qquad \lambda = -2$$

$$E = 0 \qquad J/2 \qquad -J$$

Ground state $E = -J$

Wave vector
$$\begin{pmatrix} 2 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 2 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

check: these rows linearly dependent: $-2 \times \text{row } 2 + \text{row } 1 = -\text{row } 3$

$$\begin{aligned} 2x + y &= 0 \\ 2z + y &= 0 \end{aligned} \quad \Rightarrow \quad \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$

$$|\psi_0\rangle = 1/\sqrt{6} \left\{ |++-\rangle - 2|+-+\rangle + |-++\rangle \right\}$$

$$\hat{\rho} = |\psi_0\rangle\langle\psi_0| = \frac{1}{6}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & -2 & 1 \end{pmatrix}$$

$$= 1/6 \begin{pmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{pmatrix} \quad \leftarrow \text{NB } Tr\,\hat{\rho} = 1 \; \checkmark\checkmark$$

More precisely
$$\hat{\rho} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & & & & 0 & 0 & 0 & 0 \\ 0 & & & & & & & \\ 0 & & & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & & \vdots & & \vdots & & \vdots & \end{pmatrix}$$

4-3

$$\hat{\rho}_A = \underset{B}{\mathrm{tr}}\, \hat{\rho}$$

sites 2,3 $\in$ B

$$\langle + | \hat{\rho}_A | + \rangle = \langle + \underbrace{++} | \hat{\rho} | + \underbrace{++} \rangle \qquad \phi$$

$$+ \langle + + - | \hat{\rho} | + + - \rangle \qquad 1/6$$

$$+ \langle + - + | \hat{\rho} | + - + \rangle \qquad 4/6$$

$$+ \langle + - - | \hat{\rho} | + - - \rangle \qquad \phi$$

$$\langle + | \hat{\rho}_A | - \rangle = \langle + + + | \hat{\rho} | - + + \rangle + \ldots = \phi$$

$$\langle - | \hat{\rho}_A | + \rangle = \langle - + + | \hat{\rho} | + + + \rangle + \ldots = \phi$$

$$\langle - | \hat{\rho}_A | - \rangle = 1/6 + \phi + \phi + \phi = 1/6$$

$$\hat{\rho}_A = \begin{pmatrix} 5/6 & 0 \\ 0 & 1/6 \end{pmatrix} \Leftarrow \text{ check } \mathrm{Tr}\, \hat{\rho}_A = 1 \ \checkmark\checkmark$$

$$S_2 = -\ln \mathrm{Tr}\, \hat{\rho}_A^2 = -\ln\left(\frac{25+1}{36}\right) = \ln\left(\frac{36}{26}\right) = \ln\left(\frac{18}{13}\right).$$

$\boxed{5}$ a) The radial Schroedinger eqn is

$$\left\{ -\hbar^2/2m \, d^2/dr^2 + V(r) + \hbar^2/2m \, \ell(\ell+1)/r^2 \right\} u(r) = E u(r)$$

For $\ell = 0$, $V(r) = U \delta(r-a)$, and $E = \hbar^2 k^2/2m$

$$\left\{ d^2/dr^2 - \underbrace{2mU/\hbar^2}_{\gamma} \delta(r-a) + k^2 \right\} u(r) = 0$$

b) at $r=0$ $u(r)$ must vanish because otherwise

$\psi(r) = u(r)/r$ would blow up.

at $r=a$ $u(r)$ must be continuous.

at $r=a$, integrating

$$\int_{a-\epsilon}^{a+\epsilon} \left\{ \frac{d^2}{dr^2} - \gamma \delta(r-a) + k^2 \right\} u(r) = \phi$$

$$\left. \frac{du}{dr} \right|_{a-\epsilon}^{a+\epsilon} - \gamma u(a) + \phi = \phi$$

c) For $\ell = 0$ $\left\{ d^2/dr^2 + k^2 \right\} u(r) = 0$

so $u(r)$ is $\sin(kr + \phi)$

For $r<a$ must have $\phi = 0$ because $u(r=0) = 0$

Thus $u(r) = A \sin kr \quad r \le a$

$= B \sin(kr + \delta_0) \quad r \geq a$

(d) $A \sin ka = B \sin(ka + \delta_0)$ continuity of u

$kB\cos(ka+\delta_0) - kA\cos ka - \gamma A \sin ka = \phi$ condition on du/dr

Eliminating B

$$\frac{kA\sin ka}{\sin(ka+\delta_0)}\cos(ka+\delta_0) - kA\cos ka - \gamma A \sin ka = 0$$

A cancels leaving (after $\div$ by $k\sin ka$)

$$\cot(ka+\delta_0) - \cot ka - \gamma = 0$$

$$\cot(ka+\delta_0) = \cot ka + \gamma$$

$$\delta_0 = \cot^{-1}\{\cot ka + \gamma\} - ka$$

(e) $\sigma_{tot} = \frac{4\pi}{k^2}\sin^2\delta_0$