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TENTAMEN I KVANTMEKANIK FÖRDJUPNINGSKURS
EXAMINATION IN ADVANCED QUANTUM MECHANICS

Kvantmekanik fördjupningskurs 5A1385/5A1329 för F4
Tuesday June 5 2007, kl. 08.00-13.00

Write on each page:	Name, study program and year, problem number
Motivate in detail!	Insufficient motivation leads reduction of points
Allowed material:	Summary of lectures, BETA, pocket calculator
Grading system:	Max 3 points per problem
Examiner:	Mats Wallin tel 5537 8475

1. Spin $\frac{1}{2}$ particle

A spin $\frac{1}{2}$ particle is in the normalized spin state

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

where α, β are constants. Determine the probabilities for the different possible outcomes of a measurement of S_y and the expectation value $\langle S_y \rangle$.

2. Particle in a harmonic oscillator potential

Consider a particle with mass m in a simple harmonic oscillator potential. Calculate the first order shift in the ground state energy to due to a weak perturbation

$$H^1 = cp^2$$

where p is the momentum operator and c is a constant. Compare the result with the exact solution.

3. Orbital angular momentum

The wave function of a particle in a spherically symmetric potential is

$$\psi(\mathbf{r}) = (x + y + 3z)f(r)$$

What are the possible values for L^2 and for L_z that can be obtained in a measurement, and what are the corresponding probabilities?

SEE NEXT PAGE!

4. Variational calculation

Estimate the ground state energy of a simple harmonic oscillator using the variational trial wave function

$$\psi(x) = e^{-\lambda|x|}$$

where λ is to be varied.

5. Identical fermions

Two noninteracting identical spin $\frac{1}{2}$ fermions move in one dimension in an infinite square well potential:

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

What is the ground state energy and wave function in the following cases:

(a) The two particles are constrained to a singlet spin state?

(b) The two particles are constrained to a triplet spin state?

6. One dimensional scattering

Use the Lippmann-Schwinger equation

$$|\psi^{\pm}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{\pm}\rangle$$

to determine the transmission and reflection coefficients for one-dimensional scattering off an attractive delta function potential

$$V(x) = -c\delta(x)$$

where $c > 0$ is a constant.

GOOD LUCK!

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Examination in Quantum Mechanics 070605 Solutions

1. Set $|\chi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ and assume without loss of generality that α is purely real, and that $\beta = \beta' + i\beta''$. Normalization:

$$\langle\chi|\chi\rangle = (\alpha, \beta' - i\beta'') \begin{pmatrix} \alpha \\ \beta' + i\beta'' \end{pmatrix} = \alpha^2 + \beta'^2 + \beta''^2 = 1$$

From this we get that $|\alpha\beta''| \leq \frac{1}{2}$ which is needed below. Probabilities:

$$P(S_y = \pm\frac{\hbar}{2}) = \left|\langle S_y = \pm\frac{\hbar}{2}|\chi\rangle\right|^2 = \left|\frac{1}{\sqrt{2}}(1, \mp i) \begin{pmatrix} \alpha \\ \beta' + i\beta'' \end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{2}}(\alpha \pm \beta'' \mp i\beta')\right|^2 =$$

$$= \frac{1}{2}[(\alpha \pm \beta'')^2 + \beta'^2] = \frac{1}{2}(\alpha^2 + \beta''^2 + \beta'^2 \pm 2\alpha\beta'') = \frac{1}{2} \pm \alpha\beta''$$

where we used the normalization requirement in the last step. Note that the probabilities obey

$$0 \leq P(S_y = \pm\frac{\hbar}{2}) \leq 1, \quad P(S_y = +\frac{\hbar}{2}) + P(S_y = -\frac{\hbar}{2}) = 1$$

as they should. Expectation value:

$$\langle S_y\rangle = +\frac{\hbar}{2}P(S_y = +\frac{\hbar}{2}) - \frac{\hbar}{2}P(S_y = -\frac{\hbar}{2}) = \hbar\alpha\beta''$$

Note that $|\langle S_y\rangle| \leq \hbar/2$. OK!

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2. Shift in the ground state energy from first order perturbation theory:

$$\Delta E = \langle H^1\rangle = c\langle 0|p^2|0\rangle = c\langle 0\left|\left(i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a)\right)^2\right|0\rangle =$$

$$= -c\frac{m\omega\hbar}{2}\langle 0|(a^\dagger)^2 - a^\dagger a - aa^\dagger + a^2|0\rangle = c\frac{m\omega\hbar}{2}$$

where we used that $\langle 0|(a^\dagger)^2|0\rangle = \langle 0|a^\dagger a|0\rangle = \langle 0|a^2|0\rangle = 0$ and $[a, a^\dagger] = 1 \Rightarrow \langle 0|aa^\dagger|0\rangle = \langle 0|1 + a^\dagger a|0\rangle = 1$.

Exact solution:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 + cp^2 = \frac{p^2}{2m'} + \frac{1}{2}kx^2$$

with $m' = m/(1 + 2mc)$. Exact new ground state energy:

$$E = \frac{1}{2}\hbar\omega' = \frac{1}{2}\hbar\sqrt{\frac{k}{m'}} = \frac{1}{2}\hbar\sqrt{\frac{k}{m}(1 + 2mc)} \approx \frac{1}{2}\hbar\sqrt{\frac{k}{m}}(1 + mc) = \frac{1}{2}\hbar\omega + \frac{m\omega\hbar c}{2}$$

in agreement with the result from perturbation theory.

3. Rewrite the angular part of the state in terms of spherical harmonics:

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta, Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta(\cos\phi \pm i\sin\phi)$$

$$\Rightarrow \cos\theta = \sqrt{\frac{4\pi}{3}}Y_1^0, \sin\theta\cos\phi = \sqrt{\frac{4\pi}{3}}\frac{1}{\sqrt{2}}(-Y_1^1 + Y_1^{-1}), \sin\theta\sin\phi = \sqrt{\frac{4\pi}{3}}\frac{i}{\sqrt{2}}(Y_1^1 + Y_1^{-1})$$

Use these results to rewrite the angular part of the wave function:

$$\psi(\theta,\phi) = \frac{x+y+3z}{r} = \sin\theta\cos\phi + \sin\theta\sin\phi + 3\cos\theta =$$

$$= \sqrt{\frac{4\pi}{3}}\left(\frac{1}{\sqrt{2}}(-Y_1^1 + Y_1^{-1}) + \frac{i}{\sqrt{2}}(Y_1^1 + Y_1^{-1}) + 3Y_1^0\right)$$

$$= \sqrt{\frac{4\pi}{3}}\left(\frac{-1+i}{\sqrt{2}}Y_1^1 + \frac{1+i}{\sqrt{2}}Y_1^{-1} + 3Y_1^0\right)$$

Normalize using $\langle Y_l^m | Y_{l'}^{m'}\rangle = \delta_{l,l'}\delta_{m,m'}$:

$$\langle\psi|\psi\rangle = \frac{4\pi}{3}(1+1+3^2) = 11\frac{4\pi}{3}$$

$$\Rightarrow \psi(\theta,\phi) = \frac{1}{\sqrt{11}}\left(\frac{-1+i}{\sqrt{2}}Y_1^1 + \frac{1+i}{\sqrt{2}}Y_1^{-1} + 3Y_1^0\right)$$

We therefore get $l = 1$ with certainty, and $m = +1$ with probability $P = 1/11$, $m = -1$ with probability $P = 1/11$, and $m = 0$ with probability $P = 9/11$.

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4. Normalization:

$$\int_{-\infty}^{\infty}|\psi|^2 dx = 2|c|^2\int_0^{\infty} e^{-2\alpha x}dx = \frac{|c|^2}{\alpha} = 1 \Rightarrow |c|^2 = \alpha$$

Kinetic energy:

$$\langle T\rangle = \frac{1}{2m}\int_{-\infty}^{\infty}\psi^* p^2\psi dx = \frac{1}{2m}\int_{-\infty}^{\infty}(p\psi)^*(p\psi)dx = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\frac{d\psi}{dx}\right)^2 dx$$

Since $\left(\frac{d\psi}{dx}\right)^2$ is an even function we have

$$\langle T\rangle = \frac{\hbar^2}{m}\int_0^{\infty}\left(\frac{d\psi}{dx}\right)^2 dx = \frac{\alpha\hbar^2}{m}\int_0^{\infty}\left(-\alpha e^{-\alpha x}\right)^2 dx = \frac{\alpha^3\hbar^2}{m}\frac{1}{2\alpha} = \frac{\hbar^2\alpha^2}{2m}$$

Potential energy:

$$\langle V\rangle = \frac{1}{2}m\omega^2\int_{-\infty}^{\infty}x^2\psi^2 dx = \alpha m\omega^2\int_0^{\infty}x^2 e^{-2\alpha x}dx = \alpha m\omega^2\frac{2}{(2\alpha)^3} = \frac{m\omega^2}{4\alpha^2}$$

Total energy:

$$E = \langle T\rangle + \langle V\rangle = \frac{\hbar^2\alpha^2}{2m} + \frac{m\omega^2}{4\alpha^2}$$

Optimize:

$$\frac{dE}{d\alpha^2} = \frac{\hbar^2}{2m} - \frac{m\omega^2}{4\alpha^4} = 0 \Rightarrow \alpha^2 = \frac{m\omega}{\sqrt{2}\hbar}$$

Minimum energy:

$$E = \frac{\hbar^2}{2m}\frac{m\omega}{\sqrt{2}\hbar} + \frac{m\omega^2}{4}\frac{\sqrt{2}\hbar}{m\omega} = \frac{\hbar\omega}{\sqrt{2}}$$

5. Single particle energy eigenstates:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}, n = 1, 2, 3, \ldots$$

(a) The singlet spin state, $S = 0$, is anti-symmetric with respect to spin exchange. To make the overall state antisymmetric with respect to exchange the spatial part of the state must be symmetric. The lowest energy is therefore obtained by having both particles in the single particle ground states. The ground state is non degenerate:

$$\psi_0(x_1, x_2, S, m) = \psi_1(x_1)\psi_1(x_2)|S = 0, m = 0\rangle = \psi_0(x_1)\psi_0(x_2)\frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$$

The ground state energy is

$$E_0 = 2\frac{\hbar^2\pi^2}{2mL^2} = \frac{\hbar^2\pi^2}{mL^2}$$

(b) The triplet spin state $S = 1$ is symmetric with respect to exchange, so the spatial part must be antisymmetric with respect to exchange to make the state overall antisymmetric. This state is three fold degenerate:

$$\psi_0(x_1, x_2, S, m) = \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)\right)|S = 1, m = 0, \pm 1\rangle$$

Ground state energy:

$$E_0 = (1 + 2^2)\frac{\hbar^2\pi^2}{2mL^2} = \frac{5\hbar^2\pi^2}{2mL^2}$$

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6. In the position representation the Lippmann-Schwinger equation becomes

$$\psi^\pm(x) = \phi(x) + \int_{-\infty}^{\infty} dx' \langle x|\frac{1}{E - H_0 \pm i\epsilon}|x'\rangle V(x')\psi^\pm(x') =$$

$$= \phi(x) + \frac{2m}{\hbar^2}\int_{-\infty}^{\infty} dx' G^\pm(x, x')V(x')\psi^\pm(x')$$

Calculate the Green functions, using $E = \frac{\hbar^2 k^2}{2m}$

$$G^\pm(x, x') = \frac{2m}{\hbar^2}\langle x|\frac{1}{E - H_0 \pm i\epsilon}|x'\rangle =$$

$$= \frac{2m}{\hbar^2}\int dk' \int dk'' \langle x|k'\rangle\langle k'|\frac{1}{E - H_0 \pm i\epsilon}|k''\rangle\langle k''|x'\rangle =$$

$$= \frac{2m}{\hbar^2}\int dk' \int dk'' \frac{e^{ik'x}}{\sqrt{2\pi}} \frac{\delta(k' - k'')}{\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k'^2}{2m} \pm i\epsilon} \frac{e^{-ik''x'}}{\sqrt{2\pi}} =$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk' \frac{e^{ik'(x-x')}}{k^2 - k'^2 \pm i\epsilon}$$

where $\epsilon > 0$ means a different constant on the last line. Evaluate using residue integration. There are two poles in the complex plane: $k' = \pm k\sqrt{1 \pm \frac{i\epsilon}{k^2}} \rightarrow \pm k \pm i\epsilon$ (where again the last ϵ is a different constant) which gives

$$G^\pm(x, x') = \frac{1}{2\pi} \times 2\pi i \mathrm{Res}\left[\frac{e^{ik'(x-x')}}{k^2 - k'^2 \pm i\epsilon}\right]$$

We need to distinguish two cases to make the semicircle contour integral vanish:
1. For $x - x' > 0$ we must close the integral above the real axis and thus take $k' = k + \epsilon$

$$G^+(x,x') = i \left. \frac{e^{ik'(x-x')}}{\frac{d}{dk'}(k^2 - k'^2 + i\epsilon)} \right|_{k'=+k+i\epsilon} = -\frac{i}{2k} e^{+ik(x-x')}$$

2. For $x - x' < 0$ we must close the integral below the real axis and thus take $k' = -k - \epsilon$, and in this case we get a minus sign in front since we circulate the pole in the clockwise direction:

$$G^-(x,x') = -i \left. \frac{e^{ik'(x-x')}}{\frac{d}{dk'}(k^2 - k'^2 - i\epsilon)} \right|_{k'=-k-i\epsilon} = -\frac{i}{2k} e^{-ik(x-x')}$$

With $\phi(x) = e^{ikx}$ (unnormalized) and $V(x) = -c\delta(x) = -\frac{d\hbar^2}{2m}\delta(x)$ we now get

$$\psi^\pm(x) = e^{ikx} - dG^\pm(x,0)\psi^\pm(0)$$

Determine the constant $\psi^\pm(0)$:

$$\psi^\pm(0) = 1 + \frac{id}{2k}\psi^\pm(0) \Rightarrow \psi^\pm(0) = \frac{1}{1 - \frac{id}{2k}}$$

From this we find

$$\psi^\pm(x) = e^{ikx} + \frac{id/2k}{1 - id/2k} e^{\pm ikx}$$

This gives for $x > 0$:

$$\psi^+(x) = e^{ikx} + \frac{id/2k}{1 - id/2k} e^{ikx} = \left[1 + \frac{id/2k}{1 - id/2k}\right] e^{ikx}$$

and the transmission coefficient is

$$T = \left|1 + \frac{id/2k}{1 - id/2k}\right|^2 = \left|\frac{1}{1 - id/2k}\right|^2 = \frac{1}{1 + (d/2k)^2} = \frac{1}{1 + (mc/\hbar^2 k)^2}$$

Similarly we find for $x < 0$:

$$\psi^-(x) = e^{ikx} + \frac{id/2k}{1 - id/2k} e^{-ikx}$$

and the reflection coefficient is

$$R = \left|\frac{id/2k}{1 - id/2k}\right|^2 = \frac{(d/2k)^2}{1 + (d/2k)^2} = \frac{(mc/\hbar^2 k)^2}{1 + (mc/\hbar^2 k)^2}$$

Note that both T and R are independent of the sign of the delta function potential.

(Test:

$$T + R = \frac{1}{1 + (d/2k)^2} + \frac{(d/2k)^2}{1 + (d/2k)^2} = 1$$

OK!)