

UNIVERSITY OF OSLO

Faculty of Mathematics and Natural Sciences

Solution to exam in: FYS3110, Quantum mechanics

Day of exam: Dec. 12., 2017 (4 hours)

Permitted material: Approved calculator, D.J. Griffiths: “Introduction to Quantum Mechanics”, the printed notes: “Time evolution of states in quantum mechanics” and “Symmetry and degeneracy”, one handwritten A4-sheet(2 pages) with your own notes, and K. Rottmann: “Matematisk formelsamling”.

Problem 1

1.1 The hermitian conjugate $\hat{A}^\dagger$ of an operator $\hat{A}$ satisfies

$$|\beta\rangle = \hat{A}|\alpha\rangle, \quad \langle\beta| = \langle\alpha|\hat{A}^\dagger, \quad \forall|\alpha\rangle$$

In terms of matrix elements this is equivalent to

$$\langle m|\hat{A}^\dagger|n\rangle = \langle n|\hat{A}|m\rangle^*, \quad \forall n, m$$

A hermitian operator is an operator which is equal to its hermitian conjugate

$$\underline{\hat{A}^\dagger = \hat{A}}$$

Properties of hermitian operators (see Griffiths, chapter 3):

- Real eigenvalues. Eigenvalues correspond to measurement values, they should be real.
- Eigenstates with different eigenvalues are orthogonal. Eigenstates are states for which the measurement value is the corresponding eigenvalue with 100% certainty. Physical states that for sure give different measurement values must be orthogonal.
- Eigenstates span the Hilbert space¹. It must be possible to assign probabilities for getting a particular measurement value for *any* state. This means that it must be possible to write any state as a superposition of eigenstates. This is the spanning or completeness property.

¹ The last property is not automatic for hermitian operators in an ∞ -dimensional Hilbert space.

1.2 The perturbation is

$$\hat{H}' = g(|1\rangle\langle 2| + |2\rangle\langle 1|)$$

For $1 < a < 2$ we can use non-degenerate perturbation theory. The first order energy correction to the ground state energy is then

$$E_1^1(1 < a < 2) = \langle 1|\hat{H}'|1\rangle = 0$$

For $a = 1$, both states $|1\rangle$ and $|2\rangle$ have the same energy so we must use degenerate perturbation theory. Alternatively we can find the good states which diagonalizes the perturbation. These are the eigenstates of $\hat{H}'$

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|1\rangle \pm |2\rangle)$$

which have eigenvalues ± 1 . Using non-degenerate perturbation theory with the good states gives

$$E_1^1(a = 1) = \langle \pm|\hat{H}'|\pm\rangle = \pm g.$$

Alternatively one can compute the W-matrix in the basis $\{|1\rangle, |2\rangle\}$.

1.3 The variational principle states

$$E_{trial} \equiv \frac{\langle \psi|\hat{H}|\psi\rangle}{\langle \psi|\psi\rangle} \geq E_0$$

With $|\psi\rangle = |1\rangle + b|2\rangle$ we get

$$\begin{aligned}\langle \psi|\hat{H}|\psi\rangle &= (\langle 1| + b\langle 2|)\hat{H}(|1\rangle + b|2\rangle) = (\langle 1| + b\langle 2|)(|1\rangle + ab|2\rangle + g|2\rangle + gb|1\rangle) \\ &= 1 + gb + ab^2 + gb = ab^2 + 2gb + 1 \\ \langle \psi|\psi\rangle &= 1 + b^2\end{aligned}$$

Therefore

$$E_{trial} = \frac{ab^2 + 2gb + 1}{1 + b^2}$$

The lowest upper bound is found by differentiating with respect to b . This gives

$$\begin{aligned}\frac{(2ab + 2g)(1 + b^2) - 2b(ab^2 + 2gb + 1)}{(1 + b^2)^2} = 0 &\implies 2ab + 2g + 2ab^3 + 2gb^2 - 2ab^3 - 4gb^2 - 2b = 0 \\ &\implies ab + g - gb^2 - b = 0\end{aligned}$$

Setting $a = 1$ we get $g(1 - b^2) = 0 \implies b = \pm 1$. Thus the lowest upper bound when $a = 1$ is

$$E_{trial} = \frac{1 \pm 2g + 1}{2} = 1 \pm g \implies \underline{E_{trial_{min}} = 1 - |g|}$$

which occurs for $b = \pm 1$. Note that for $g > 0$ ($g < 0$) it is the state with $b = -1$ ($b = +1$) which gives the lowest energy.

1.4 The two-particle fermion state must be antisymmetric under the interchange of the labels on the two fermions. A spin-1 state, the triplet, is symmetric under the interchange of spin labels, so the spatial part needs to be antisymmetric under the change of particle labels. For $1 < a < 2$ and $g = 0$ this minimum energy state is

$$\frac{1}{\sqrt{2}} (|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle)$$

with energy $E = 1 + a$. Combining this with the triplet spin states we get the three states

$$\begin{aligned} |\psi_1\rangle &= \frac{1}{\sqrt{2}} (|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle) \otimes |\uparrow\rangle \otimes |\uparrow\rangle \\ |\psi_2\rangle &= \frac{1}{2} (|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle) \otimes (|\uparrow\rangle \otimes |\downarrow\rangle + |\downarrow\rangle \otimes |\uparrow\rangle) \\ |\psi_3\rangle &= \frac{1}{\sqrt{2}} (|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle) \otimes |\downarrow\rangle \otimes |\downarrow\rangle \end{aligned}$$

where $|\uparrow\rangle$ ($|\downarrow\rangle$) is the spin-1/2 state with $m_s = +\frac{1}{2}$ ($-\frac{1}{2}$). The energy of these state(s) depend only on the spatial part, and is $\underline{E = 1 + a}$.

Problem 2

2.1 a) The scattering amplitude in terms of phase shifts for an azimuthally symmetric target (for which a spherical symmetric target is a special case) is

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) \frac{e^{i\delta_l}}{k} \sin \delta_l.$$

b) The total scattering cross section is

$$\sigma = \int d\Omega |f(\theta)|^2 = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

2.2 The general form of the wave function expressed in terms of partial waves can be found in Griffiths Eqs. [11.29] and [11.46]

$$\psi(r, \theta) = A \sum_{l=0}^{\infty} i^l (2l+1) \left(j_l(kr) + i e^{i\delta_l} \sin \delta_l h_l^{(1)}(kr) \right) P_l(\cos \theta)$$

We will keep only the s-wave term ($l = 0$) and take the long wavelength limit $kR_0 \ll 1$ and compare the result to the expression given just outside R_0 . Using $h_0^{(1)}(kr) = -i \frac{e^{ikr}}{kr}$ and $j_0(kr) = \frac{\sin kr}{kr}$ we get when expanding in terms of small kr which can be justified as $r \sim R_0$ (just outside the potential) and $kR_0 \ll 1$:

$$\begin{aligned} \psi_s(r, \theta) &= A \left(\frac{\sin kr}{kr} + e^{i\delta_0} \sin \delta_0 \frac{e^{ikr}}{kr} \right) \approx \frac{A}{kr} (kr + e^{i\delta_0} \sin \delta_0 (1 + ikr)) \\ &= A \left(\underbrace{(1 + i e^{i\delta_0} \sin \delta_0)}_{e^{i\delta_0} \cos \delta_0} + e^{i\delta_0} \sin \delta_0 \frac{1}{kr} \right) = A e^{i\delta_0} \cos \delta_0 \left(1 + \frac{\tan \delta_0}{kr} \right) \end{aligned}$$

Comparing this with the wave function expression given in the problem text:

$$\psi(r, \theta) = D \left(1 - \frac{c_0}{r} \right)$$

we get $D = A e^{i\delta_0} \cos \delta_0$ and

$$\frac{\tan \delta_0}{k} = -c_0 \implies \tan \delta_0 = -k c_0 \quad \left(\text{or} \quad k \cot \delta_0 = -\frac{1}{c_0} \right)$$

To obtain the s-wave contribution to the total cross section we can use

$$\sin^2 \delta_0 = \frac{\tan^2 \delta_0}{1 + \tan^2 \delta_0} = \frac{k^2 c_0^2}{1 + (k c_0)^2}$$

thus the s-wave contribution to the total cross section in the long wavelength limit is

$$\sigma_s = 4\pi \frac{c_0^2}{1 + (k c_0)^2}$$

This is maximal for $c_0 \rightarrow \infty$ where it becomes $4\pi/k^2$ which is the same as the threshold contribution for s-wave scattering. Note that c_0 can very well be infinite even with R_0

finite. For an infinite or big c_0 one cannot automatically assume $kc_0 \ll 1$.

2.3 The s-wave radial equation for $r < R_0$ is

$$\frac{d^2 u}{dr^2} = - \underbrace{\left(k^2 - \frac{2mV_0}{\hbar^2} \right)}_{k'^2} u$$

which have solution $u(r) = B \sin k'r$. Note that the boundary condition at $r = 0$ requires $u(0) = 0$ so the $\cos(k'r)$ term must vanish. We can compare this to the expression for the outside wavefunction deduced from the problem text, $\psi(r, \theta, \phi) = Y_0^0(\theta, \phi)u(r)/r = \frac{1}{\sqrt{4\pi}}u(r)/r = D(1 - \frac{c_0}{r})$, which gives $u(r > r_0) = \sqrt{4\pi}D(r - c_0)$. Continuity of $u(r)$ and its derivative $u'(r)$ at $r = R_0$ gives

$$B \sin(k'R_0) = \sqrt{4\pi}D(R_0 - c_0) \quad (1)$$

$$Bk' \cos(k'R_0) = \sqrt{4\pi}D \quad (2)$$

Dividing Eq. (1) by Eq. (2) and solving for c_0 one gets

$$c_0 = R_0 - \frac{\tan(k'R_0)}{k'} = R_0 \left(1 - \frac{\tan(k'R_0)}{k'R_0} \right)$$

Note that k' is not necessarily small even though k is, this depends on the magnitude of V_0 .

We also see that $c_0 \rightarrow \pm\infty$ when $k'R_0 = (n + \frac{1}{2})\pi$ which implies that

$$k'^2 \equiv k^2 - \frac{2mV_0}{\hbar^2} = \left[\left(n + \frac{1}{2} \right) \frac{\pi}{R_0} \right]^2 \implies V_0 = \frac{\hbar^2}{2mR_0^2} \left((kR_0)^2 - \pi^2 \left(n + \frac{1}{2} \right)^2 \right) \approx - \frac{\hbar^2 \pi^2}{2mR_0^2} \left(n + \frac{1}{2} \right)^2$$

Problem 3

3.1

$$\begin{aligned} P(\theta < \pi/3) &= \int_0^{2\pi} d\phi \int_0^{\pi/3} d\theta \sin \theta \langle \theta, \phi | 1, 0 \rangle \langle 1, 0 | \theta, \phi \rangle = \int_0^{2\pi} d\phi \int_0^{\pi/3} d\theta \sin \theta |Y_1^0|^2 \\ &= \int_0^{2\pi} d\phi \int_0^{\pi/3} d\theta \sin \theta \frac{3}{4\pi} \cos^2 \theta = \frac{3}{4\pi} 2\pi \int_{\frac{1}{2}}^1 dx x^2 = \frac{3}{2} \cdot \frac{1}{3} \left(1 - \frac{1}{2^3} \right) \\ &= \frac{7}{16} \end{aligned}$$

3.2 Since the z -coordinate has no ϕ -dependence the perturbation can only excite $m = 0$ states. The first excited state is therefore $|1, 0\rangle$ which has energy $2J$ above the ground state. The probability amplitude to find the system in this state after the pulse has passed is

$$\begin{aligned} a_{1,0} &= \frac{1}{i\hbar} \int_0^\tau dt g \langle 1, 0 | z | 0, 0 \rangle e^{i2Jt/\hbar} = \frac{1}{i\hbar} g \langle 1, 0 | z | 0, 0 \rangle \int_0^\tau dt e^{i2Jt/\hbar} \\ &= \frac{1}{i\hbar} g \langle 1, 0 | z | 0, 0 \rangle \frac{\hbar}{J} \left(\frac{e^{i2J\tau/\hbar} - 1}{2i} \right) \\ &= \frac{1}{iJ} g \langle 1, 0 | z | 0, 0 \rangle e^{iJ\tau/\hbar} \sin(J\tau/\hbar) \end{aligned}$$

The matrix element is

$$\langle 1, 0 | z | 0, 0 \rangle = \frac{\sqrt{3}}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta \cos^2\theta = \frac{\sqrt{3}}{2} \underbrace{\int_{-1}^1 dx x^2}_{2/3} = \frac{1}{\sqrt{3}}$$

The probability is thus

$$P_{1,0} = \frac{g^2}{3J^2} \sin^2(J\tau/\hbar)$$

3.3 The Hamiltonian can be rewritten in terms of the total angular momentum operator $\vec{L} = \vec{L}_1 + \vec{L}_2$ using

$$L^2 = \vec{L} \cdot \vec{L} = \vec{L}_1^2 + \vec{L}_2^2 + 2\vec{L}_1 \cdot \vec{L}_2$$

so that

$$H = \left(\frac{L_1^2}{\hbar^2} + \frac{L_2^2}{\hbar^2} \right) \left(J - \frac{K}{2} \right) + \frac{K}{2\hbar^2} L^2$$

So let's write the state $|\psi\rangle$ in terms of states $|l, m\rangle$ with total angular momentum quantum number l and z -component m . We use the Clebsch-Gordan tables to find

$$\begin{aligned} |1, 0\rangle \otimes |2, 0\rangle &= \sqrt{\frac{3}{5}} |3, 0\rangle - \sqrt{\frac{2}{5}} |1, 0\rangle \\ |2, -1\rangle \otimes |1, +1\rangle &= \sqrt{\frac{1}{5}} |3, 0\rangle - \sqrt{\frac{1}{2}} |2, 0\rangle + \sqrt{\frac{3}{10}} |1, 0\rangle \end{aligned}$$

Thus the state $|\psi\rangle$ can be written in terms of total angular momentum states as

$$|\psi\rangle = \left(\sqrt{\frac{3}{20}} - \sqrt{\frac{1}{5}} \right) |1, 0\rangle - \frac{1}{2} |2, 0\rangle + \left(\sqrt{\frac{3}{10}} + \sqrt{\frac{1}{10}} \right) |3, 0\rangle$$

which means that the total angular momentum takes the values 1, 2, or 3. The state $|\psi\rangle$ is an eigenstate of the non-interacting part of the Hamiltonian

$$\left(\frac{L_1^2}{\hbar^2} + \frac{L_2^2}{\hbar^2}\right) |\psi\rangle = (1(1+1) + 2(2+1)) |\psi\rangle = 8|\psi\rangle$$

while it is not an eigenstate for the interaction as the energy there also depends on the value of the total angular momentum. The three possible energies are

$$8\left(J - \frac{K}{2}\right) + \frac{K}{2}3 \cdot (3+1) = 8J + 2K, \quad l = 3$$

$$8\left(J - \frac{K}{2}\right) + \frac{K}{2}2 \cdot (2+1) = 8J - K, \quad l = 2$$

$$8\left(J - \frac{K}{2}\right) + \frac{K}{2}1 \cdot (1+1) = 8J - 3K, \quad l = 1$$

For $K > 0$ the $l = 1$ state has the lowest energy. It has probability $P_1 = |\sqrt{\frac{3}{20}} - \sqrt{\frac{1}{5}}|^2 = \frac{3}{20} + \frac{1}{5} - 2\sqrt{\frac{3}{100}} = \frac{7-4\sqrt{3}}{20}$. For $K < 0$ the $l = 3$ state has the lowest energy. It has probability $P_3 = |\sqrt{\frac{3}{10}} + \sqrt{\frac{1}{10}}|^2 = \frac{3}{10} + \frac{1}{10} + 2\sqrt{\frac{3}{100}} = \frac{2+\sqrt{3}}{5}$.

– THE END –