Introduction to Quantum Mechanics 2014/15
Solution to the Exam

1. Energy quantisation for the finite square well potential

(seen in class)

(a) The solutions of the time-independent Schrödinger equation in the separate regions are of the form $ae^{ikx}+be^{-ikx}$ with $k=\sqrt{2m(E-V_j)}/\hbar$, where V_j is the value of the constant potential in region j. For values $E > V_j$, $k \in \mathbb{R}$ this can be equivalently written as $\tilde{a}\cos(kx)+\tilde{b}\sin(kx)$, while for $E < V_j$ we have $\kappa = \sqrt{2m(V_j-E)}/\hbar \in \mathbb{R}$, and the solutions take the form $ae^{-\kappa x}+be^{\kappa x}$.

Here we are looking for *bound states*, that is $\phi(x \to \pm\infty) \to 0$. From the general form of the solution we deduce that this is only possible for $E < V_0$, and the solutions are of the form

$$\phi_E(x) = \begin{cases} Ce^{\kappa x}, & x \leq -L \\ A\cos(kx) + B\sin(kx), & -L < x \leq L \\ De^{-\kappa x}, & x > L, \end{cases} \tag{1}$$

with $k = \frac{\sqrt{2mE}}{\hbar}$ and $\kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$. The wave function $\phi_E(x)$ and its first derivative with respect to x have to be continuous everywhere. This is automatically fulfilled in the separate regions, but it imposes boundary conditions between the different regions. Before we deduce these conditions, we use the symmetry to simplify the problem.

(5 points)

(b) In class we have learned that the bound state eigenfunctions of a Hamiltonian of the form $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ with $V(-x) = V(x)$ are either even or odd. Let us know consider even and odd solutions separately. For the functions (1) to be even, i.e. $\phi_E(-x) = \phi_E(x)$ it needs to hold $B = 0$ and $C = D$. For odd functions $\phi_E(-x) = -\phi_E(x)$ we need $A = 0$ and $D = -C$.

(3 points)

(c) For even states the continuity of the wave function and its first derivative for this case yield

$$Ce^{-\kappa L} = A\cos(kL) \tag{2}$$
$$\kappa Ce^{-\kappa L} = kA\sin(kL). \tag{3}$$

Dividing condition (3) by condition (2) this yields the quantisation condition

$$\kappa = k\tan(kL) \tag{4}$$

for even eigenfunctions.

(5 points)

For odd states the continuity of the wave function and its first derivative yields

$$Ce^{-\kappa L} = -B\sin(kL) \tag{5}$$
$$\kappa Ce^{-\kappa L} = kB\cos(kL), \tag{6}$$

Dividing (6) by (5) we find the quantisation condition for odd eigenfunctions as

$$\kappa = -k\cot(kL). \tag{7}$$

(5 points)

We can rewrite these in terms of the energy using the identities

$$k = \sqrt{2mE}/\hbar, \quad \text{and}$$
$$\kappa/k = \sqrt{\frac{V_0}{E} - 1} \tag{8}$$

to find

$$\tan\left(\frac{\sqrt{2mE}L}{\hbar}\right) = \sqrt{\frac{V_0}{E} - 1}\,, \tag{9}$$

and

$$-\cot\left(\frac{\sqrt{2mE}L}{\hbar}\right) = \sqrt{\frac{V_0}{E} - 1}\,, \tag{10}$$

for even and odd eigenfunctions, respectively.

(2 points)

2. The principles of quantum mechanics

(Seen similar - however, details of the question are quite different. The similarity might be confusing rather than helpful.)

(a) From the characteristic polynomial of $\hat{H}$ we find for the eigenvalues λ of $\hat{H}$

$$-\lambda^3 + E^2\lambda = 0,$$

and thus $\lambda_0 = 0$ and $\lambda_\pm = \pm E$. For the components of the eigenvector ϕ_0 we find from $\hat{H}|\phi_0\rangle = 0$

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & E & 0 \\ E & 0 & E \\ 0 & E & 0 \end{pmatrix}\begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

that is,

$$y_0 = 0, \text{ and } x_0 = -z_0.$$

Together with the normalisation condition that yields

$$\phi_0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},$$

up to an arbitrary phase factor $e^{i\varphi}$. Similarly we find the remaining eigenvectors

$$\phi_+ = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}, \quad \text{and} \quad \phi_- = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}.$$

(5 points - for results *and* calculations)

(b) The probability to measure an eigenvalue of an observable is given by the modulus square of the coefficient of the wave function in the basis of the eigenvectors of the observable.
Since the eigenvectors of $\hat{A}$ are just the basis vectors, we can directly read off the probabilities for the different eigenvalues from the wave function as

$$P(a) = \frac{9}{11}, \quad P(0) = \frac{1}{11}, \quad \text{and} \quad P(-a) = \frac{1}{11}.$$

(4 points)

The expectation value can be either deduced from $\langle\psi|\hat{A}|\psi\rangle$ via vector and matrix multiplications, or we calculate

$$\langle\hat{A}\rangle = \sum_j P(\lambda_j)\lambda_j = aP(a) - aP(-a) = a\left(\frac{9}{11} - \frac{1}{11}\right) = \frac{8}{11}a.$$

(3 points)

(c) A measurement of the value a at time $t = 0$ projects the system onto the corresponding eigenstate of $\hat{A}$, the first basis vector,

$$|\psi(t=0)\rangle = |\phi_a\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

(2 points)

which is not an eigenstate of $\hat{H}$. The time-dependent wave function is then given by

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle.$$

(1 point)

We can use the method of stationary states to find $|\psi(t)\rangle$. For this purpose we need to represent $|\psi(0)\rangle$ as a linear superposition of the eigenstates of $\hat{H}$,

$$|\psi(t=0)\rangle = \psi_+|\phi_+\rangle + \psi_-|\phi_-\rangle + \psi_0|\phi_0\rangle,$$

the coefficients of which we need to deduce via the projection of $|\psi\rangle$ onto the eigenvectors of $\hat{H}$:

$$\psi_j = \langle\phi_j|\psi\rangle.$$

In this case, these are just the first components of the eigenvectors of $\hat{H}$ deduced in part (a):

$$\psi_+ = \frac{1}{2}, \qquad \psi_- = \frac{1}{2}, \qquad \psi_0 = \frac{1}{\sqrt{2}}.$$

Therefore the state at time t is given by

$$|\psi(t)\rangle = \frac{1}{2}e^{-iEt/\hbar}|\phi_+\rangle + \frac{1}{2}e^{iEt/\hbar}|\phi_-\rangle + \frac{1}{\sqrt{2}}|\phi_0\rangle,$$

(3 points)

The probability to measure the result a again is given by

$$\begin{aligned} P(a) = |\langle\phi_a|\psi(t)\rangle|^2 &= \left|\frac{1}{2}e^{-iEt/\hbar}\cdot\frac{1}{2} + \frac{1}{2}e^{iEt/\hbar}\cdot\frac{1}{2} + \frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}\right|^2 \\ &= \left|\frac{1}{2}\left(1+\cos(Et/\hbar)\right)\right|^2 \\ &= \frac{1}{4}\left(1+\cos(Et/\hbar)\right)^2, \end{aligned}$$

which oscillates between zero and one.

(2 points)

3. The variational method for the approximate calculation of eigenfunctions

(Part (a) and variational method for harmonic oscillator seen in the lecture notes, part (b) unseen)

(a) Consider the basis of normalised eigenstates of the Hamiltonian $|\phi_n\rangle$, with $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$, where the states are numbered according to increasing energy. We can expand an arbitrary state $|\psi\rangle$ as

$$|\psi\rangle = \sum_j \psi_j|\phi_j\rangle.$$

Thus, the expectation value of $\hat{H}$ in the state $|\psi\rangle$ is given by

$$\langle\hat{H}\rangle := \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{jk}\bar{\psi}_j\psi_k\langle\phi_j|\hat{H}|\phi_k\rangle}{\sum_{jk}\bar{\psi}_j\psi_k\langle\phi_j|\phi_k\rangle} = \frac{\sum_{jk}E_k\bar{\psi}_j\psi_k\langle\phi_j|\phi_k\rangle}{\sum_{jk}\bar{\psi}_j\psi_k\langle\phi_j|\phi_k\rangle}.$$

The eigenstates are orthonormal, i.e. $\langle\phi_j|\phi_k\rangle = \delta_{jk}$, that is we have

$$\langle\hat{H}\rangle = \frac{\sum_k E_k|\psi_k|^2}{\sum_k|\psi_k|^2}.$$

By definition we have $E_j \geq E_0$, and thus

$$\langle\hat{H}\rangle \geq \frac{E_0\sum_k|\psi_k|^2}{\sum_k|\psi_k|^2} = E_0. \quad \square$$

(5 points)

(b) We calculate the expectation value of the Hamiltonian in the trial wave function and minimise the result with respect to λ. We have

$$\begin{aligned}\hat{H}\phi(x) &= \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^4\right)\phi(x)\\ &= \frac{1}{2}\left(\lambda - \lambda^2x^2 + x^4\right)\phi(x).\end{aligned}$$

(4 points)

Thus we find

$$\begin{aligned}\langle\hat{H}\rangle &= \frac{1}{2}\lambda\sqrt{\frac{\lambda}{\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-\lambda x^2}\mathrm{d}x - \frac{1}{2}\lambda^2\sqrt{\frac{\lambda}{\pi}}\int_{-\infty}^{\infty}x^2\mathrm{e}^{-\lambda x^2}\mathrm{d}x + \frac{1}{2}\sqrt{\frac{\lambda}{\pi}}\int_{-\infty}^{\infty}x^4\mathrm{e}^{-\lambda x^2}\mathrm{d}x\\ &= \frac{\lambda}{2} - \frac{\lambda^2}{2}\frac{1}{2\lambda} + \frac{3}{8\lambda^2}\\ &= \frac{\lambda}{4} + \frac{3}{8\lambda^2}.\end{aligned}$$

(4 points)

Now we need to find the value of λ for which this is minimal. Thus, we first identify the zeros of the first derivative of $\langle\hat{H}\rangle$ with respect to λ:

$$\frac{\partial\langle\hat{H}\rangle}{\partial\lambda} = \frac{1}{4} - \frac{3}{4\lambda^3} = 0,$$

from which we find

$$\lambda^3 = 3.$$

As we assume λ to be real and positive the only relevant solution is $\lambda = 3^{1/3}$. This is indeed a minimum of $\langle \hat{H} \rangle$, which is easily verified by considering the second derivative

$$\frac{\partial^2 \langle \hat{H} \rangle}{\partial \lambda^2} = \frac{9}{4\lambda^4},$$

which is indeed positive for all real λ.

(4 points)

The approximation of the ground state energy is then given by

$$\langle \hat{H} \rangle_{min} = \frac{3^{1/3}}{4} + \frac{3}{8 \cdot 3^{2/3}} = \frac{3}{8} 3^{1/3}.$$

Using the numerical value $3^{1/3} = 1.4422\ldots$, a quick calculation yields

$$\langle \hat{H} \rangle_{min} = 0.5408\ldots$$

Which is close to, but slightly larger than, the exact value E_0.

(3 points)

4. Orbital angular momentum.

(Sketch of idea seen in class, details unseen)

(a) We have by definition

$$[\hat{L}_1, \hat{L}_3] = [\hat{q}_2\hat{p}_3 - \hat{q}_3\hat{p}_2, \hat{q}_1\hat{p}_2 - \hat{q}_2\hat{p}_1]$$

Recalling that the commutator is linear in both elements, and that $[\hat{A}\hat{B}.\hat{C}] = \hat{A}[\hat{B}.\hat{C}] + [\hat{A},\hat{C}]\hat{B}$, we expand this to yield

$$\begin{aligned}[\hat{L}_1, \hat{L}_3] &= [\hat{q}_2\hat{p}_3, \hat{q}_1\hat{p}_2 - \hat{q}_2\hat{p}_1] - [\hat{q}_3\hat{p}_2, \hat{q}_1\hat{p}_2 - \hat{q}_2\hat{p}_1] \\ &= [\hat{q}_2\hat{p}_3, \hat{q}_1\hat{p}_2] - [\hat{q}_2\hat{p}_3, \hat{q}_2\hat{p}_1] - [\hat{q}_3\hat{p}_2, \hat{q}_1\hat{p}_2] + [\hat{q}_3\hat{p}_2, \hat{q}_2\hat{p}_1]\end{aligned}$$

The two middle terms vanish and we partially expand the remaining terms to find

$$\begin{aligned}[\hat{L}_1, \hat{L}_3] &= [\hat{q}_2\hat{p}_3, \hat{q}_1\hat{p}_2] + [\hat{q}_3\hat{p}_2, \hat{q}_2\hat{p}_1] \\ &= \hat{q}_2[\hat{p}_3, \hat{q}_1\hat{p}_2] + [\hat{q}_2, \hat{q}_1\hat{p}_2]\hat{p}_3 + \hat{q}_3[\hat{p}_2, \hat{q}_2\hat{p}_1] + [\hat{q}_3, \hat{q}_2\hat{p}_1]\hat{p}_2\end{aligned}$$

Here the first and the last term vanish. Expanding the remaining terms yields

$$\begin{aligned}[\hat{L}_1, \hat{L}_3] &= \hat{q}_1[\hat{q}_2, \hat{p}_2]\hat{p}_3 + [\hat{q}_2, \hat{q}_1]\hat{p}_2\hat{p}_3 + \hat{q}_3\hat{q}_2[\hat{p}_2, \hat{p}_1] + \hat{q}_3[\hat{p}_2, \hat{q}_2]\hat{p}_1 \\ &= \mathrm{i}\hbar\hat{q}_1\hat{p}_3 - \mathrm{i}\hbar\hat{q}_3\hat{p}_1 \\ &= -\mathrm{i}\hbar\hat{L}_2.\end{aligned}$$

(3 points)

(b) $\hat{L}_1$ and $\hat{L}_3$ cannot be measured simultaneously, as they do not commute (their commutator is non-zero).

(2 points)

(c) (i) We find for the commutators of the new operators

$$[\hat{x}, \hat{y}] = 0 = [\hat{p}_x, \hat{p}_y],$$

$$\begin{aligned}[\hat{x}, \hat{p}_x] &= \frac{1}{2}[\hat{q}_1 + \hat{p}_2, \hat{p}_1 - \hat{q}_2] \\ &= \frac{1}{2}\left([\hat{q}_1, \hat{p}_1] - [\hat{p}_2, \hat{q}_2]\right) \\ &= \mathrm{i}\hbar,\end{aligned}$$

$$\begin{aligned}[\hat{x}, \hat{p}_y] &= \frac{1}{2}[\hat{q}_1 + \hat{p}_2, \hat{p}_1 + \hat{q}_2] \\ &= \frac{1}{2}\left([\hat{q}_1, \hat{p}_1] + [\hat{p}_2, \hat{q}_2]\right) \\ &= 0,\end{aligned}$$

$$\begin{aligned}[\hat{y}, \hat{p}_x] &= \frac{1}{2}[\hat{q}_1 - \hat{p}_2, \hat{p}_1 - \hat{q}_2] \\ &= \frac{1}{2}\left([\hat{q}_1, \hat{p}_1] + [\hat{p}_2, \hat{q}_2]\right) \\ &= 0,\end{aligned}$$

and

$$\begin{aligned}[\hat{y}, \hat{p}_y] &= \frac{1}{2}[\hat{q}_1 - \hat{p}_2, \hat{p}_1 + \hat{q}_2] \\ &= \frac{1}{2}\left([\hat{q}_1, \hat{p}_1] - [\hat{p}_2, \hat{q}_2]\right) \\ &= \mathrm{i}\hbar.\end{aligned}$$

(4 points)

That is, also the new operators fulfil the fundamental commutation relation of position and momenta.

(1 point)

To rewrite $\hat{L}_3$ in terms of $\hat{x}$, $\hat{y}$, $\hat{p}_x$, and $\hat{p}_y$ we substitute

$$\hat{q}_1 = \frac{1}{\sqrt{2}}(\hat{x} + \hat{y}), \qquad \hat{q}_2 = \frac{1}{\sqrt{2}}(\hat{p}_y - \hat{p}_x)$$
$$\hat{p}_1 = \frac{1}{\sqrt{2}}(\hat{p}_x + \hat{p}_y), \qquad \hat{p}_2 = \frac{1}{\sqrt{2}}(\hat{x} - \hat{y}),$$

into the expression for $\hat{L}_3$ to find

$$\begin{aligned}\hat{L}_3 &= \frac{1}{2}\left(\hat{x} + \hat{y}\right)\left(\hat{x} - \hat{y}\right) - \frac{1}{2}\left(\hat{p}_y - \hat{p}_x\right)\left(\hat{p}_x + \hat{p}_y\right) \\ &= \frac{1}{2}\left(\hat{x}^2 - \hat{y}^2\right) - \frac{1}{2}\left(\hat{p}_y^2 - \hat{p}_x^2\right) \\ &= \frac{1}{2}\left(\hat{p}_x^2 + \hat{x}^2\right) - \frac{1}{2}\left(\hat{p}_y^2 + \hat{y}^2\right)\end{aligned}$$

(4 points)

(ii) We see that $\hat{L}_3$ can be written as the difference of two harmonic oscillators $\hat{H}_x$ and $\hat{H}_y$, with masses $m = 1$ and frequencies $\omega = 1$:

$$\hat{L}_3 = \hat{H}_x - \hat{H}_y.$$

From the spectra of $\hat{H}_x$ and $\hat{H}_y$ we thus deduce that the eigenvalues of $\hat{L}_3$ are given by

$$\lambda_n = \hbar(n_x + \frac{1}{2}) - \hbar(n_y + \frac{1}{2}) = \hbar(n_x - n_y),$$

where n_j are non-negative integers. Thus, the eigenvalues of $\hat{L}_3$ are integer multiples of $\hbar$.

(4 points)

(d) The same argument as above can be used to deduce the eigenvalues of $\hat{L}_1$ (and $\hat{L}_2$), which are also integer multiples of $\hbar$.

(2 points)