PHY 304, II-Semester 2023/24, Assignment 2 solution

(1) Symmetries: [8 pts]

(a) First, supply some of the unproven arguments in our section on symmetries. (i) Show that the eigenvalue z of a unitary operator must have unit modulus $|z| = 1$. (ii) Show that the parity operator is Hermitian. (iii) Show that the rotation operator around the z axis is:

$$\hat{R}_z(\alpha) = e^{-i\frac{\alpha}{\hbar}\hat{L}_z}. \tag{1}$$

using similar arguments as those that led to Eq. (6.3). [4 pts]
Solution: (i) Since the operator $\hat{U}$ is unitary, we know that $\hat{U}^\dagger = \hat{U}^{-1}$. Suppose we found an eigenstate of it with eigenvalue z

$$\hat{U}|\,\phi\,\rangle = z|\,\phi\,\rangle. \tag{2}$$

Since $\hat{U}$ is not necessarily Hermitian, the eigenvalue does not need to be real, but can be complex, $z \in \mathbb{C}$. If we do the adjoint operation on both sides of (2), we reach

$$\langle\,\phi\,|\hat{U}^\dagger = \langle\,\phi\,|z^*. \tag{3}$$

Now define $|\,\phi_U\,\rangle \equiv \hat{U}|\,\phi\,\rangle$ and inspect

$$\langle\,\phi_U\,|\,\phi_U\,\rangle = \underbrace{\langle\,\phi\,|\underbrace{\hat{U}^\dagger\hat{U}}_{=\mathbb{1}}|\,\phi\,\rangle}_{=1} = \langle\,\phi\,|z^*z|\,\phi\,\rangle, \qquad \Leftrightarrow |z|^2 = 1. \tag{4}$$

On the left we have first used that $\hat{U}$ is unitary and then that $|\,\phi\,\rangle$ is normalised.
(ii) Let $f(x)$ and $g(x)$ be two functions in the Hilbertspace, then

$$\int_{-\infty}^{\infty} dx f^*(x)[\hat{\Pi}g(x)] = \int_{-\infty}^{\infty} dx f^*(x)g(-x) \overset{z=-x}{=} -\int_{\infty}^{-\infty} dz f^*(-z)g(z)$$
$$\overset{rename\ z=x}{=} \int_{-\infty}^{\infty} dx f^*(-x)g(x) = \int_{-\infty}^{\infty} dx[f(x)\hat{\Pi}(x)]^* g(x). \tag{5}$$

According to the first definition of a Hermitian operator that we had seen in Eq. (1.24), this implies that $\hat{\Pi}$ is Hermitian.

(iii) We follow the same steps used to show the form $\hat{T}(a) = e^{-i\frac{a}{\hbar}\hat{p}}$ for the 1D translation operator, but now using 2 dimensional polar coordinates. Let a wavefunction in terms of those be $\Psi(r,\phi)$, then the action of the rotation operator by an angle α is

$$\hat{R}_z(\alpha)\Psi(r,\phi) = \Psi(r,\phi-\alpha) \tag{6}$$

[compare Eq. (6.20)]. We can now Taylor expand the function $\Psi(r, \phi - \alpha)$ only in its angular dimension around the angle ϕ which gives

$$\Psi(r,\phi-\alpha) = \sum_{n=0}^{\infty} \frac{(-\alpha)^n}{n!} \frac{d^n}{d\phi^n} \Psi(r,\phi) \tag{7}$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\alpha \frac{d}{d\phi}\right)^n \Psi(r,\phi) \overset{Eq.(4.53)}{=} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i\alpha}{\hbar} \hat{L}_z\right)^n \Psi(r,\phi)$$

$$\overset{e^z = \sum_{n=0}^{\infty} z^n/n!}{=} e^{-i\frac{\alpha}{\hbar}\hat{L}_z} \Psi(r,\phi). \tag{8}$$

Comparing with Eq. (6), we read of what was to be shown.

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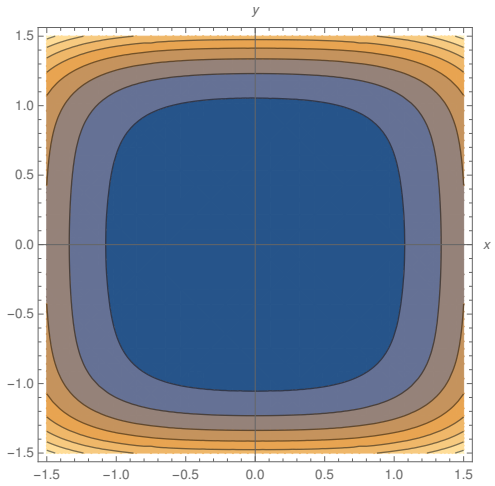

Figure 1: Potential from Eq. (9).

(b) Consider a particle of mass m in the potential

$$V(x,z) = \kappa(\hat{x}^2 + \hat{y}^2) + \bar{\eta}(\hat{x}^4 + \hat{y}^6), \tag{9}$$

for $\kappa > \bar{\eta} > 0$. Make a meaningful 2D plot of this potential with a computer (or by hand).

Find all symmetries of the Hamiltonian. Based on that discuss whether or not you expect the spectrum to show degeneracies. [4 pts]
Solution: See the plot in Fig. 1 for $\eta = 1$ and $\kappa = 1$.

We can see that the rotation symmetry that would be present for $\eta = 0$ is broken, and The system thus has only two symmetries, Π_x and Π_y. But these commute, as we can show by application onto a testfunction:

$$(\Pi_x\Pi_y - \Pi_y\Pi_x)f(x,y) = \Pi_x f(x,-y) - \Pi_y f(-x,y) = f(-x,-y) - f(-x,-y) = 0. \tag{10}$$

Thus there is no reason to expect degeneracies, according to section 6.6.5.

(2) Perturbed square well potential: **[8 pts]** A particle is subject to the infinite square well potential (confined within $x = 0$ and $x = a$, see e.g. Eq. (2.10) of QM-1), with an additional potential of

$$W(x) = W_0 x/a. \tag{11}$$

(a) Make a drawing of the complete potential, and discuss under which conditions we can handle it in perturbation theory. [2 pts].

(b) Then find the energy corrections to the lowest two states of the original square well potential to first order perturbation theory. [6 pts]
Solution
(a)Unperturbed part:
$V(x) = \begin{cases} 0 & 0 \leqslant x \leqslant a \\ \infty & otherwise \end{cases}$
The energy eigenvalues: $E_n^0 = \frac{n^2\pi^2\hbar^2}{2ma^2}$*; The eigenfunctions:* $\Psi_n^0 = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$ *with* $n = 1, 2, 3, ...$
Perturbed part: $W(x) = \frac{W_0 x}{a}$*;*

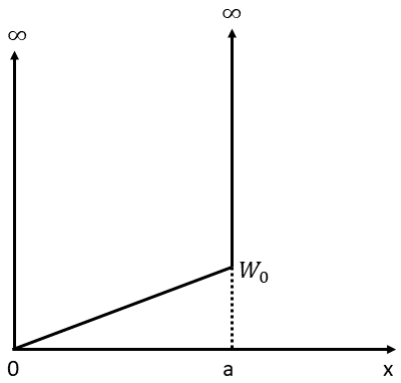

Figure 2: Diagram of complete potential

Condition: *W_0 has to be small enough, such that the matrix elements $\mathcal{M}_{mn} = \langle m|W_o x/a|n\rangle$ are small compared to energy differences $E_m^{(0)} - E_n^{(0)}$.*
(b)Energy correction to state n=1

$$E_1^{(1)} = \langle\, \Psi_1^0 \,|\frac{W_0 x}{a}|\, \Psi_1^0 \,\rangle \tag{12}$$

$$= \frac{W_0}{a}\frac{2}{a}\int_0^a x\sin^2\frac{\pi x}{a}dx \tag{13}$$

$$= \frac{2W_0}{a^2}\int_0^a \frac{x}{2}(1 - \cos\frac{2\pi x}{a})dx \tag{14}$$

$$= \frac{W_0}{2} \tag{15}$$

Energy correction to state n=2

$$E_1^{(2)} = \langle \Psi_2^0 | \frac{W_0 x}{a} | \Psi_2^0 \rangle \tag{16}$$

$$= \frac{W_0}{a}\frac{2}{a}\int_0^a x \sin^2 \frac{2\pi x}{a} dx \tag{17}$$

$$= \frac{2W_0}{a^2}\int_0^a \frac{x}{2}(1 - \cos\frac{4\pi x}{a})dx \tag{18}$$

$$= \frac{W_0}{2} \tag{19}$$

(3) Charged oscillator: [14pts] Consider a particle of mass m and charge q in a harmonic potential with frequency ω subject to a constant electric field of strength $\mathcal{E}$. The Hamiltonian is hence

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - q\mathcal{E}\hat{x}, \tag{20}$$

(a) Define a suitable splitting of the Hamiltonian for the use of perturbation theory, if the field is sufficiently weak. What constitutes "sufficiently weak"? [2 pts]

(b) Find all the matrix elements $\mathcal{M}_{nm} = \langle n | \hat{H}' | m \rangle$ of whatever you choose as perturbation above. Then use the special case $\langle n | \hat{H}' | n \rangle$ to evaluate the first order correction $E_n^{(1)}$ to the energies. *Hint: Use the ladder operators from Eq. (2.43, QM-I)* [2 pts]

(c) Use the $\mathcal{M}_{nm}$ to also find an expression for the second order correction $E_n^{(2)}$ to the energy and the first order correction to the states $|\psi_n^{(1)}\rangle$. [4 pts]

(d) Trying to analytically evaluate $E_n^{(2)}$ and $|\psi_n^{(1)}\rangle$ is not going to be very illuminating, instead let us explore their use on a computer. `Assignment2_program_draft_v1.nb` is set up to help you compare all your results above with those provided by a numerical solution of the complete problem. For that adjust the script at the places with XXXXX: (i) Complete the definition of `TISELHSpert`, which should contain the left hand side of the TISE with the perturbation. (ii) Execute the solution of the unperturbed oscillator numerically in the line below, and verify eigenvalues are as expected. (iii) In the definition of `Energyfirstorder`, insert your first order result from (b). In the definition of `Matrixelement` insert $\mathcal{M}_{nm}$ from (c). (iv) Also use this and `Energy[n]` to complete the definitions of second order energies, first order states and normalisation of the perturbed state. Then run all the commands for comparison of energy eigenvalues and wavefunctions. Discuss and compare with your expectations from (c). [4 pts]

(e) Why could we have guessed the change under this perturbation of all energy eigenvalues directly from the start, without doing perturbation theory? [2 pts]

Solution: (Note: All a and $a^\dagger$ represent ladder operators)

(a) A suitable splitting is:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - q\mathcal{E}\hat{x} = \hat{H}^{(0)} + \hat{H}'$$

where, $\hat{H}' = -q\mathcal{E}\hat{x}$ represents the perturbed part of Hamiltonian.

From the discussion in section 7.3.1 of lecture notes (specifically Eq. (7.35) there), it is clear that a sufficiently weak field is one for which all matrix elements $\mathcal{M}_{nm} = \langle\, n \,|\, -q\mathcal{E}\hat{x} |\, m \,\rangle$ are much less than $E_n^{(0)} - E_m^{(0)}$.

(b) Using position operator expressed in terms of ladder operators:

$$\hat{x} = \sigma(a + a^\dagger), \text{ with } \sigma = \sqrt{\frac{\hbar}{2m\omega}}$$

the perturbation in Hamiltonian takes the form :

$$H' = -q\mathcal{E}\sigma(a + a^\dagger) \tag{21}$$

The matrix elements $\mathcal{M}_{nm} = \langle\, n \,|\hat{H}'|\, m \,\rangle$ can be found as:

$$\begin{aligned}
\mathcal{M}_{nm} &= \langle n|\hat{H}'|m\rangle && (22)\\
&= -q\mathcal{E}\sigma\langle n|(a + a^\dagger)|m\rangle && (23)\\
&= -q\mathcal{E}\sigma(\sqrt{m}\langle\, n \,|\, m-1 \,\rangle + \sqrt{m+1}\langle\, n \,|\, m+1 \,\rangle) && (24)\\
&= -q\mathcal{E}\sigma\left(\sqrt{m}\ \delta_{n,m-1} + \sqrt{m+1}\ \delta_{n,m+1}\right) && (25)
\end{aligned}$$

Now, to find out first order correction to energies we put $m = n$ to get:

$$\begin{aligned}
E_n^{(1)} &= \langle n|\hat{H}'|n\rangle && (26)\\
&= -q\mathcal{E}\left(\sqrt{n}\delta_{n,n-1} + \sqrt{n+1}\delta_{n,n+1}\right) && (27)\\
&= 0 && (28)
\end{aligned}$$

We see that the first order correction to the energies is zero.

(c) The $\mathcal{M}_{nm}$ also enable you to calculate the second order correction $E_n^{(2)}$ to the energy

and the first order correction to the states as follows:

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\mathcal{M}_{nm}|^2}{E_n^{(0)} - E_m^{(0)}} \tag{29}$$

$$= \sum_{m\neq n} \frac{|-q\mathcal{E}\sigma\left(\sqrt{m}\ \delta_{n,m-1} + \sqrt{m+1}\ \delta_{n,m+1}\right)|^2}{E_n^{(0)} - E_m^{(0)}} \tag{30}$$

$$= q^2\mathcal{E}^2\sigma^2 \sum_{m\neq n} \frac{|\left(\sqrt{m}\ \delta_{n,m-1} + \sqrt{m+1}\ \delta_{n,m+1}\right)|^2}{E_n^{(0)} - E_m^{(0)}} \tag{31}$$

$$= q^2\mathcal{E}^2\sigma^2 \left(\frac{n+1}{E_n^{(0)} - E_{n+1}^{(0)}} + \frac{n}{E_n^{(0)} - E_{n-1}^{(0)}}\right) \tag{32}$$

$$= q^2\mathcal{E}^2\sigma^2 \left(\frac{n+1}{(-\hbar\omega)} + \frac{n}{(\hbar\omega)}\right) \tag{33}$$

$$= -\frac{q^2\mathcal{E}^2\sigma^2}{\hbar\omega} = -\frac{q^2\mathcal{E}^2}{2m\omega^2} \tag{34}$$

For 1st order correction to the states, we do the same steps as above (noting $\mathcal{M}_{nm}$ is real):

$$|\,\psi_n^{(1)}\,\rangle = \sum_{m\neq n} \frac{\mathcal{M}_{nm}}{E_n^{(0)} - E_m^{(0)}} |\,\psi_m^{(0)}\,\rangle \tag{35}$$

$$= (-q\mathcal{E}\sigma) \sum_{m\neq n} \frac{\left(\sqrt{m}\ \delta_{n,m-1} + \sqrt{m+1}\ \delta_{n,m+1}\right)}{E_n^{(0)} - E_m^{(0)}} |\,\psi_m^{(0)}\,\rangle \tag{36}$$

$$= (-q\mathcal{E}\sigma) \left(\frac{\sqrt{n+1}}{E_n^{(0)} - E_{n+1}^{(0)}} |\,\psi_{n+1}^{(0)}\,\rangle + \frac{\sqrt{n}}{E_n^{(0)} - E_{n-1}^{(0)}} |\,\psi_{n-1}^{(0)}\,\rangle\right) \tag{37}$$

Solution: See **`Assignment2_program_solution_v1.nb`** *line. From that mathematica file, for the parameters inserted there*

1. *The true energy-eigenvalues of the total Hamiltonian are:*
   [0.875, 2.875, 4.87501, 6.87502, 8.87502, 10.8751]

2. *The first order corrected energy values are found to be:*
   [1.05625, 3.28125, 5.73125, 8.40625, 11.3063, 14.4312]

3. *And the second-order corrected energy values are found to be:*
   [0.875, 2.875, 4.875, 6.875, 8.875, 10.875]

The deviations calculated also in the script, show that the second order values are much more closer to the real values than first order ones.

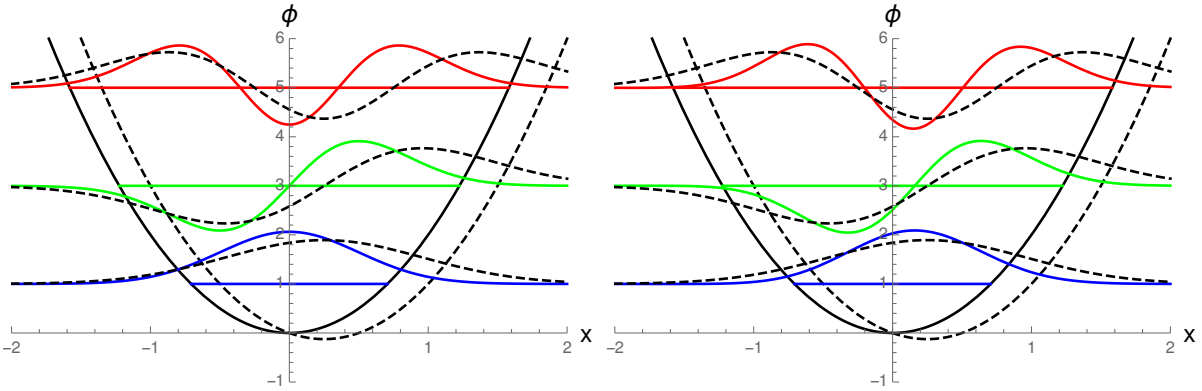

Figure 3: [left] Unperturbed states (color) and perturbed ones (black dashed). [right] analytical perturbed states to second order (color) and numerically obtained perturbed ones (dashed).

(e) We can rewrite the potential by completing the square into

$$V_{tot} = \frac{1}{2}m\omega^2(x - \frac{q\mathcal{E}}{m\omega^2})^2 - \frac{(q\mathcal{E})^2}{2m\omega^2} \tag{38}$$

through which we realize that this is just a shifted harmonic oscillator potential, with new centre at $x_0 = \frac{q\mathcal{E}}{m\omega^2}$ *and minimum energy* $-V_0$ *Logic (or more formally a redefinition of lengths and energies) then tells us that the solutions are simply* $\phi_n(x')$*from (2.65 in lecture's note) with energies* $\tilde{E}_n = E_n - V_0$.