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Quantenmechanik, Herbstsemester 2021

Blatt 9

Abgabe: 23.11.21, 12:00H (Treppenhaus 4. Stock)
Tutor: Gaomin Tang, Zi.: 4.48

(1) **Matrix elements of z** (2 Punkte)
In the discussion of the Stark effect in the lecture we used some properties of the matrix elements of z with the H-atom states $|nlm\rangle$ that we want to prove now.

(a) Show that $[L_z, z] = 0$ and conclude that $\langle n'l'm'|z|nlm\rangle = 0$ unless $m' = m$.

(b) Use a symmetry argument to prove that $\langle n'lm'|z|nlm\rangle = 0$ (same l!).

(c) Show that $\langle 200|z|210\rangle = -3a_0$ where $a_0 = 4\pi\epsilon_0\hbar^2/(me^2)$ is the Bohr radius.
Hint: the H-atom wave functions are $\psi_{nlm}(r,\theta,\phi) = \langle r,\theta,\phi|nlm\rangle = R_{nl}(r)Y_{lm}(\theta,\phi)$.
In particular, $R_{20}(r) = 2\left(\frac{1}{2a_0}\right)^{3/2}(1-\frac{r}{2a_0})e^{-\frac{r}{2a_0}}$ and $R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\frac{r}{a_0}e^{-\frac{r}{2a_0}}$

(2) **Perturbed two-dimensional harmonic oscillator** (4 Punkte)
Consider the two-dimensional harmonic oscillator with a perturbed potential energy of the form

$$V(x,y) = \frac{1}{2}m\omega^2(x^2 + y^2 + \lambda xy)\,. \tag{1}$$

(a) Calculate the energy eigenvalues for the unperturbed case ($\lambda = 0$) and discuss their degeneracies.
Hint: Use creation (annihilation) operators for each of the two degrees of freedom x, y, i.e.,

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a_1 + a_1^\dagger), \qquad p_x = i\sqrt{\frac{m\hbar\omega}{2}}(a_1^\dagger - a_1)\,,$$

and similarly for y, p_y, and a_2, $a_2^\dagger$.

(b) Compute the ground-state energy of the system ($\lambda \neq 0$) up to second order in λ and the ground-state wave function up to first order in λ.

(c) The first excited state of the unperturbed system ($\lambda = 0$) is doubly degenerate. Calculate the energy splitting up to first order in λ. What are the corresponding eigenstates in zeroth order?

(d) * Compare with the exact result.
Hint: express (1) as a sum of two harmonic potentials.

(3) **Numerically solving the Schrödinger equation** (4 Punkte + 1 Bonuspunkt)
One way to solve quantum problems numerically is to turn the Schrödinger equation into a matrix equation by discretizing the variable x. The goal of this problem is to apply this procedure to the one-dimensional Hamiltonian $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$.

(a) Slice the relevant interval in evenly spaced points x_j with $\Delta x := x_{j+1} - x_j$, and let $\psi_j := \psi(x_j)$ and $V_j := V(x_j)$. Show that the discretized Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m}\left(\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}\right) + V_j\psi_j = E\psi_j$$

or

$$-\lambda\psi_{j+1} + (2\lambda + V_j)\psi_j - \lambda\psi_{j-1} = E\psi_j \quad \text{where} \quad \lambda = \frac{\hbar^2}{2m(\Delta x)^2}\,.$$

In matrix form, $\mathsf{H}\psi = E\psi$, where H is a tridiagonal matrix and

$$\psi = \begin{pmatrix} \cdot \\ \cdot \\ \psi_{j-1} \\ \psi_j \\ \psi_{j+1} \\ \cdot \\ \cdot \end{pmatrix}.$$

Write down the matrix H. What goes in the upper left and lower right corners of H depends on the boundary conditions. The allowed energies are the eigenvalues of the matrix H if the discretization is fine enough, $\Delta x \to 0$.

(b) Apply this method to the harmonic oscillator, $V(x) = \frac{1}{2}m\omega^2x^2$.
Chop the interval [-5:5] into $N+1$ equal segments, i.e., $\Delta x = 10/(N+1)$, $x_0 = -5$, $x_{N+1} = 5$. Choose the boundary condition $\psi_0 = \psi_{N+1} = 0$ (what does that mean?), leaving $\psi = (\psi_1, \ldots \psi_N)$. Construct the tridiagonal $N \times N$ matrix H.

(c) Choose e.g. $N = 100$ and use a computer to find the 10 lowest eigenvalues numerically. Compare with the exact result.
Hint: We support Julia, but you are free to use any programming language.
In Julia, a symmetric tridiagonal $N \times N$ matrix can be created using
$\mathsf{H} = \mathrm{SymTridiagonal}(d, od)$ where the N-dimensional vector d contains the diagonal elements and the $(N-1)$-dimensional vector od contains the off-diagonal elements.
$e, ev = \mathrm{eigen}(\mathsf{H})$ will create a vector e containing the eigenvalues and a matrix ev containing the eigenvectors.

(d) Repeat (c) for $V(x) = kx^4$ and confirm the value of the ground-state energy mentioned in problem 4 on Blatt 8, viz., $E_0 = 0.66798626\ldots(\hbar^4k/m^2)^{1/3}$.

(e) Bonus point: plot the lowest five eigenstates, both for (b) and (d).

Please submit your code in electronic form or print it out.