

QM-08 Question Bank

Canonical Quantization

Using Commutators *

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Abstract

Finding matrix element between harmonic oscillator states, Ladder operators and eigenfunctions of angular momentum, Constructing matrices for angular momentum operators, Zero point energy, Allowed values of j, m

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Zero point energy The potential energy of two protons in hydrogen molecule ion in a model is given below

$$V(x) = |E_1|f(x) \quad (1)$$

$$f(x) = -1 + \frac{2}{x} \left[\frac{(1 - (2/3)x^2)e^{-x} + (1+x)e^{-2x}}{1 + (1+x+x^2/3)e^{-x}} \right], \quad x = R/a \quad (2)$$

$E_1 = 13.6$ eV is the ground state energy of H atom and a is the Bohr radius \hbar^2/me^2 . The graph of this function $f(x)$ is reproduced below. Find numerical values of the bond length in Å , the zero point energy and spacing of vibrational spectrum, both energies in electron volts.

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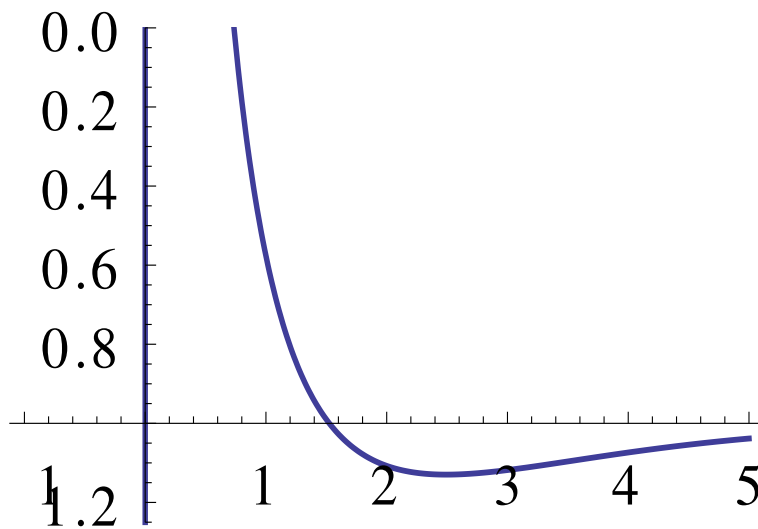


Fig. 1

⚡ The expression for $V(x)$ is taken from an approximate variational calculation of energy of the H molecule ion in Born Oppenheimer approximation

⊗ qm-que-08002

State if the combinations of j, m values, in the table given below, are allowed or not. Complete the table by writing ALLOWED/NOT ALLOWED in the second column and specifying a reason in support of your answer selecting a reason from the list, (R1) – (R5), given below. In case you do not find a valid or appropriate reason listed below, feel free to select option (R6) and specify your reason.¹

List of Possible Reasons:

- (R1) All values of jm are allowed.
- (R2) Not allowed because m is not an integer
- (R3) Allowed because all vales of m in the range $-j$ to $+j$ are allowed
- (R4) Not allowed because j, m must be an integers
- (R5) Not allowed because both j, m must be integers, or half integers.
- (R6) Any other reason, please specify for each case separately

⊗ qm-que-08003

¹This question requires knowledge of angular momentum eigenvalues.

Compute average value $\langle n|q^4|n\rangle$ of q^4 in the n^{th} energy state of harmonic oscillator.

⊙ **qm-que-08004**

Let $|n\rangle$ denote the n^{th} excited state of a harmonic oscillator. Show that

$$\langle n|x|m\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n+1}\delta_{m,n+1} + \sqrt{n}\delta_{m,n-1} \right)$$

⊙ **qm-que-08005**

The the exact zero point energy of a several coupled oscillators is given to be $3.1415\hbar\omega_0$. What is the energy of first excited state?

⊙ **qm-que-08006**

- (a) What are the eigenvalues of $L^2 + \alpha L_x + \beta L_y + \gamma L_z$ for $\ell = 2$. Give a full explanation for your answer.
- (b) Construct matrices for L_x, L_y, L_z for $\ell = 1$ case and verify that L^2 is a multiple of identity.

⊙ **qm-que-08007**

Let $Y_{\ell m}(\theta, \phi)$ denote the simultaneous normalized eigenfunctions of L^2 and L_z operators. Use the properties of the ladder operators, L_{\pm} , and construct the expressions for $Y_{\ell m}(\theta, \phi)$ for $\ell = 2$ and $m = 2, 1, 0, -1, -2$.

Hint: $Y_{\ell\ell}(\theta, \phi)$ satisfies

$$L_z Y_{\ell\ell}(\theta, \phi) = \ell\hbar Y_{\ell\ell}(\theta, \phi) \quad (3)$$

$$L_+ Y_{\ell\ell}(\theta, \phi) = 0. \quad (4)$$

Set up these differential equations and solve to find (normalized) Y_{22} . Next apply L_- repeatedly and use

$$L_- Y_{\ell m} = \sqrt{\ell(\ell+1) - m(m+1)} \hbar Y_{\ell(m-1)}$$

to successively construct Y_{2m} for other values $m = 1, 0, -1, -2$.