Edlisefnafrædi 1

Midannarpróf, 25. október 2005, 8:15-9:30.

Leyfileg hjálpargögn: Reiknivélar og stærdfrædihandbækur
Prófid samanstendur af 2 spurningum og er á 3 bladsídum. Aftast er tafla yfir jöfnur. Mikilvægt er ad rökstydja öll svör.

Spurning 1: (50 pts)

In English:

Consider an electron in a delocalized molecular orbital that can be approximated by a particle-in-a-box with hard walls at $x = 0$ and $x = a$. The system is prepared in such a way that the wavefunction is

$$\psi(x) = N\left(3\sin\left(\frac{\pi x}{a}\right) - 4\sin\left(\frac{2\pi x}{a}\right)\right)$$

inside the box $0 < x < a$. Here, N is a constant.

(a) Sketch the wavefunction and the probability density for the location of the electron.

(b) Find the value of the normalization constant, N.

(c) What is the probability that a measurement of the total energy of the system will give the value corresponding to the first excited state energy?

(d) What is the expectation value of the total energy in the state $\psi(x)$?

(e) Assume the wavefunction $\psi(x)$ describes the state of the system at an initial time t=0. Write an expression for the time dependent wavefunction $\Psi(x, t)$.

(f) What does the frequency of electromagnetic radiation need to be in order to excite the system from the ground state to the first excited state?

Á Íslensku:

Rafeind í löngu sameindasvigrúmi sem líkja má vid ögn-í-kassa med veggi í $x = 0$ og $x = a$ er í ástandi sem lýsa má med bylgjufallinu

$$\psi(x) = N\left(3\sin\left(\frac{\pi x}{a}\right) - 4\sin\left(\frac{2\pi x}{a}\right)\right) \ .$$

N er normunarfasti.

(a) Teiknadu mynd af fallinu og líkindadreifingunni fyrir stadsetningu rafeindarinnar.

(b) Finndu gildi normunarfastans, N.

(c) Hverjar eru líkurnar á ad mæling á orkunni gefi orku fyrsta örvada ástandsins?

(d) Hvad er væntigildi orkunnar í ástandinu $\psi(x)$?

(e) Gerdu rád fyrir ad bylgjufallid $\psi(x)$ lýsi ástandi kerfisins vid upphafstíma t=0. Skrifadu líkingu fyrir tímaháda bylgjufallid $\Psi(x,t)$.

(f) Hver verdur tídni rafsegulbylgju ad vera til ad örva kerfid úr grunnástandinu í fyrsta örvada ástandid?

Spurning 2: (10 punktar)

In English:

(a) Calculate the commutator for the operators corresponding to momentum and position.

(b) How does the commutator relate to the possibility of knowing momentum and position of a quantum mechanical particle?

Á Íslensku:

(a) Reiknadu út víxlunarvirkjann fyrir skridpunga og stadsetningu.

(b) Hvernig tengist hann möguleikanum á því ad vita skridpunga og stadsetningu skammtafrædilegrar agnar?

Spurning 3: (40 punktar)

In English:

A simple function that is frequently used to describe the potential energy of diatomic molecules, such as HF, is the Morse potential

$$U(r) \;=\; D\left(e^{-2\beta(r-r_b)} - 2e^{-\beta(r-r_b)}\right)$$

where r is the distance between the two atoms. The parameters D, β and r_b depend on which atoms are involved. In each one of the questions (b-e) below you should give an expression that contains the parameters of the potential function and possibly also the mass of the two atoms, m_1 and m_2.

(a) What is the bond length and bond energy of the molecule?

(b) Expand $U(r)$ in a Taylor series about $r = r_b$ up to second order and give an expression for the force constant, k, of the harmonic oscillator approximation to $U(r)$.

(c) Assuming the Harmonic Oscillator approximation is good enough for the ground state, what is the dissociation energy of a molecule described by a Morse potential (that is, what is the minimum energy required to break the molecule apart)?

(d) A molecule initially in the ground state can get excited to the first excited state by absorption of a photon. What is the frequency of the radiation that can excite the molecule from the ground vibrational state to the first vibrational excited state assuming the harmonic oscillator approximation is valid?

(e) Sketch the absorption spectrum for the molecule: (i) first by assuming the molecule is a harmonic oscillator, and (ii) recognizing that the harmonic oscillator is just a good approximation for the lowest energy levels of HF.

Á Íslensku:

Morse fallid

$$U(r) \;=\; D\left(e^{-2\beta(r-r_b)} - 2e^{-\beta(r-r_b)}\right)$$

er mættisfall sem oft er notad til ad lýsa stöduorku tvíatóma sameinda, til dæmis HF. Hér er r fjarlægdin milli atómanna og studlarnir D, β og r_b einkenna sameindina. Í lidunum (b-e) hér ad nedan á ad gefa líkingu sem inniheldur studlana og e.t.v. massa atómanna, m_1 og m_2.

(a) Vid hvada fjarlægd, r_b, er orka sameindarinnar í lágmarki (tengjalengdin) og hver samsvarandi stöduorka (tengjaorkan)?

(b) Lidadu $U(r)$ í annarrar grádu Taylorröd um $r = r_b$ og skrifadu líkingu fyrir gormafastann, k, í kjörsveifilsnálgunni fyrir $U(r)$.

(c) Hver er sundrunarorka sameindarinnar ef gert er rád fyrir ad kjörsveifilsnálgunin er nógu gód (hver er lágmarksorkan til ad rjúfa sameindina)?

(d) Hægt er ad örva sameindina úr grunn ástandinu í fyrsta örvada ástandid med upptöku ljóseindar. Hver á tídni rafsegulbylgjunnar ad vera fyrir slíka örvun ef gert er rád fyrir ad kjörsveifilsnálgunin gildi?

(e) Skissadu gleypniróf sameindarinnar, (i) Í fyrsta lagi gerandi rád fyrir ad sameindinni megi lýsa sem kjörsveifli, og (ii) gerandi rád fyrir ad kjörsveifillinn sé bara gód nálgun fyrir HF.