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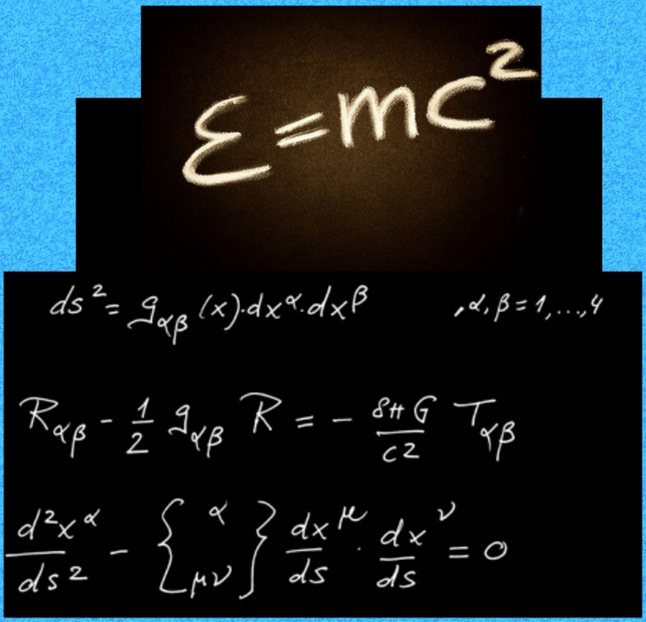

O`ZBEKISTON RESPUBLIKASI OLIY VA O`RTA MAXSUS TA'LIM VAZIRLIGI

AL-XORAZMIY NOMLI URGANCH DAVLAT UNIVERSITETI

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KVANT MEXANIKASIDAN MASALALAR

O`quv- uslubiy qo`llanma

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Ushbu o`quv uslubiy qo`llanma fizika bakalavr yo`nalishi talabalari uchun tasdiqlangan na'munaviy dastur asosida tuzilgan bo`lib, unda kvant mexanikasining asosiy bo`limlariga oid masalalar va ularning batafsil yechimlari keltirilgan. Mualliflar kvant mexanikasinining talabalar tomonidan o`zlashtirilishi murakkabligini hisobga olib yechimlarining to`liq bayonini keltirganlar. O`quv qo`llanma Urganch davlat universitetining 2013 йил 4 сентябрdagi Ilmiy-uslubiy Kengashi tomonidan muhokama qilinib, nashr qilishga tavsiya qilingan.

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So`z boshi

Keyingi yillarda oliy ta’limda bakalavr yo`nalishlari talabalarga mo`ljallangan ko`plab yangi o`quv qo`llanmalari va darsliklar Respublikamizning universitetlari olimlari va professor-o`qituvchilar tomonidan yaratildi va yaratilmoqda. Shuni ta’kidlash kerakki, ushbu o`quv qo`llanmalar va darsliklar ko`pincha lotin grafikasida yaratilmagan.

“Kvant mexanikasi” nazariy fizikaning talabalar tomonidan o`zlashtirilishi murakkab bo`lgan bo`limlaridan biri hisoblanadi. Bu fanni o`zlashtirishda amaliy mashgulotlarning ahamiyati juda kattadir.

Taqdim qilinayotgan ushbu o`quv-uslubiy qo`llanma Urganch Davlat universiteti Fizika kafedrasi professor o`qituvchilar tomonidan yozilgan bo`lib, ushbu ta’lim yo`nalishi talabalariga “Kvant mexanikasi” fanidan amaliy mashg`ulotlar darslarida o`zlashtirilishi zarur bo`lgan masala va mashqlarni o`z ichiga olgan.

Qo`llanmani masalalarini tanlashda nazariy kurs bilan uzviy bog`liqlik, ketma-ketlik va matematik apparatning tushunarliligi kabi jihatlarga e’tibor qaratilgan. Har bir paragraf boshida qisqacha nazariy ma’lumotlar va asosiy formulalar keltirilgan.

Qo`llanmadagi ko`pgina masalalar mavjud qo`llanmalardan olindi hamda avtorlar tomonidan tuzilib, yechimlari ham keltirildi.

Ushbu o`quv-uslubiy qo`llanma 2012 yil 14-martda O`zbekiston Respublikasi Oliy va o`rta maxsus ta’lim vazirligi tomonidan BD 5140200-3.09 raqami bilan tasdiqlangan namunaviy dasturga mos keladi.

Qo`llanma haqidagi fikr-mulohazalaringizni UrDU Fizika kafedrasiga yo`llashingizni so`raymiz. Mualliflar ularni mamnuniyat bilan qabul qiladilar va oldindan o`z minnatdorchiliklarini bildiradilar.

Mualliflar

1-mavzu. Kvant mexanikasining paydo bo`lishi. Kvant mexanikasining fizik asoslari

Kvant mexanikasi mikroolamga tegishli bo`lgan zarralarning hatti-harakati qonuniyatlarini va bu olamda ro`y beradigan fizikaviy hodisalar va jarayonlarni o`rganadigan fandir. Mikroolamga mansub bo`lgan zarralarning o`lchami nihoyatda kichik bo`lib, ularni mikrozarralar deb atashadi. O`lchami $\sim 10^{-10}$ $m$ ga teng bo`lgan yoki undan kichik bo`lgan zarralar ***mikrozarralar*** deyiladi. Masalan, foton, elektron, neytron, proton, mezon kabi zarralar mikrozarralardir.

Kvant mexanikasisi jumlasidagi "kvant" so`zi uzluklilik tushunchasini xarakterlab, u o`zbekchada bo`lak, parcha yoki qism degan ma'noni anglatadi, ilmiy til bilan aytganda kvant so`zi ob'ektni diskretligini, ya'ni shu bo`laklardan tashkil topganligini bildiradi. Masalan, O`zbekiston Respublikasining puli fizikaviy kattalik bo`lib, u kvantlangan, ya'ni mazkur pul bo`laklardan iborat bo`lib, uning eng kichik kvanti bir tiyindir.

Mikrozarralar oddiy (makroskopik) zarralardan mutlaqo farq qilib, ular bir vaqtning o`zida ham korpuskulyar, ham to`lqin tabiatga ega. Mikrozarralarning bu ikkiyoqlama xususiyati ***zarralarning dualizmi*** deyiladi. To`lqin xossalar ayniqsa mikrozarralarning tarqalishida namoyon bo`ladi. Korpuskulyar xossa esa zarralarning o`zaro ta'sir jarayoniga ta'aluqlidir. Masalan, yorug`lik dualistik xarakterga ega, u ham to`lqin, ham zarradir. Mikrozarralar xuddi to`lqin kabi birdaniga fazoning hamma nuqtalarida mavjud. Shuning uchun mikrozarralar harakatini traektoriya tushunchasi bilan tavsiflash mumkin emas. Aksincha, klassik mexanikada esa, zarralarning asosiy xossasi uning traektoriyasi mavjudligidir. Elektron, foton, proton kabi zarralar uchun traektoriya tushunchasini umuman qo`llab bo`lmaydi. Shu sababga ko`ra mikrozarralar harakatini va u bilan bo`ladigan jarayonlarni tavsiflash uchun mutlaqo yangi tasavvur, zarrani dualistik xususiyatini inobatga oladigan mexanika va uning yangicha matematik apparatini yaratish lozim.

Oddiy mexanikaning negizini Isaak Nyuton mexanikasi tashkil qiladi, relyativistik tezliklar uchun esa Albert Eynshteyn mexanikasi ishlatiladi. Bu mexanikalarning tenglamalarida asosiy tushuncha traektoriyadan foydalaniladi.

Kvant mexanikasini asosida elementar zarralarning ikkiyoqlama xususiyatini e'tiborga oluvchi tenglama yotishi kerak. Xuddi shunday tenglama 1926 yilda shveytsariyalik fizik Ervin Shryodinger tomonidan birinchi bo`lib taklif qilindi. Uning relyativistik varianti esa elektronlar uchun ingliz fizigi Pol Dirak tomonidan berildi. Shryodinger va Dirak tenglamalari g`alati ko`rinishdagi to`lqin tenglamalaridir. Bu tenglamalar shunday tuzilganki, ularning yechimi elementar zarralarning xossalarini hisobga olgan holda ularning dualistik xarakterini ham nazardan qochirmaydi. Kvant mexanik to`lqin tenglamalarining yechimi oddiy ko`rinishdagi to`lqin tenglamalar yechimi kabi to`lqin funktsiyalar ko`rinishda bo`ladi. Kvant mexanikasida bu funktsiyalarni ψ ***-funktsiya*** (***psi-funktsiya***) deb atashadi. Kvant mexanikasining to`lqin tenglamasi ***Shryodinger tenglamasi*** deyiladi va Nyutonning ikkinchi qonuni klassik mexanikada qanday o`rin tutsa, Shryodinger tenglamasi kvant mexanikasida shunday o`rin tutadi.

ψ -funktsiya mikrozarraning to`lqin tabiatini aks ettiradi. Uning yordamida, masalan, elektronlarning difraktsiyasi hodisasini yoki $K^0$-mezonlarning interferentsiyasi hodisalarini tavsiflash mumkin. Biroq Jeyms Klerk Maksvell tenglamalari yechimidan farq qilib, u kompleks ko`rinishga ega va uni aniq talqin qilib bo`lmaydi. Chunki u tarqalayotgan yorug`lik yoki tovush ko`rinishidagi yugurma to`lqin ham emas, shuningdek interferentsiya manzarasini hosil qiluvchi turg`un to`lqin ham emas, balki u yoki bu natijani ob'ekti mavjud bo`lgan imkoniyatini bajarilishini tavsiflovchi to`lqin ehtimolidir. Shu jihatdan qaraganda ψ -funktsiyaning fizik ma'nosi yo`qdir. To`lqin funktsiya modulining kvadrati $|\psi|^2$ esa fizik ma'noga ega bo`lib, berilgan vaqt momentida fazoning berilgan nuqtasida zarraning qayd qilinishi ehtimolligiga teng. To`lqin tenglama va to`lqin funktsiyaning ana shu xossasi mikrozarraning korpuskulyar xususiyatini aks ettiradi.

Kvant mexanikasi 1926 – 28 yillarda nemis fizigi Verner Geyzenberg, shveytsariyalik olim Ervin Shryodinger, ingliz fizik nazariyotchisi Pol Dirak tomonidan yaratildi.

1925 yilda V.Geyzenberg kvant mexanikasining matritsali ko`rinishdagi birinchi variantini yaratdi. 1932 yilda kvant mexanikasini yaratishdagi xizmatlari uchun unga Nobel mukofoti berildi. 1926 yilda Lui de Broyl g`oyalaridan ruhlangan E.Shryodinger to`lqin mexanikani yaratdi. Klassik mexanikada Nyuton qonunlari qanday rol o`ynasa, Shryodinger tenglamasida atom jarayonlarini tushuntirishda shunday rol o`ynaydi. 1933 yilda Shryodinger bilan Dirak birgalikda yangi mexanika yaratganligi munosabati bilan Nobel mukofotiga sazovor bo`ldi.

1927 yilda 25 yoshli Pol Dirak kvant mexanikasining relyativistik matematik apparatini yaratdi va birinchi bo`lib bu apparatni elektromagnit maydonga qo`lladi. Natijada u yangi kvant elektrodinamika fanini paydo bo`lishiga asos soldi.

1.1. Klassik elektrodinamika qonunlariga asosan vodorod atomida proton atrofida harakat qilayotgan elektron

$$\frac{dE}{dt} = -\frac{2}{3}\frac{e_0^2}{4\pi\varepsilon_0 c^3}\ddot{\vec{r}}^{\,2}$$

qonun bo`yicha energiya nurlantiradi deb hisoblab uning yadrosi qulab tushish vaqtini baholang. Bunda yadro atrofida harakat orbitasi $0{,}53 \cdot 10^{-10}$ m deb olinsin. ($\ddot{\vec{r}}$ − elektron tezlanish vektori)

Yechish: elektronning yadro atrofida harakatida uning nurlanish hisobiga energiya yo`qotishi shu daraja kichikki uning harakat davomida uning tezlanishi

$$\omega = \frac{\upsilon^2}{2} = \frac{e^2}{4\pi\varepsilon_0 m_0 r^2}$$

ga teng. U holda elektron to`la energiyasi quydagicha aniqlanadi.

$$E = \frac{m_0\upsilon^2}{2} - \frac{e^2\omega^2}{4\pi\varepsilon_0 r} = -\frac{m_0\upsilon^2}{2}$$

Elektronning nurlanishi hisobiga energiyasi kamayishi

$$\frac{dE}{dt} = -\frac{e^2\omega^2}{6\pi\varepsilon_0 c^3} = \frac{128\pi\varepsilon_0}{3m_0^2 e^2 c^3}E^2$$

ga teng. Bundan

$$\frac{1}{E^3} = \frac{1}{E_0^3} + \frac{128\pi\varepsilon_0}{3m_0^2 e^2 c^3}\cdot t\,; \quad E_0 = -\frac{e^2}{8\pi\varepsilon_0 r_0}, \qquad r_0 = 0{,}53\cdot 10^{-10}\ m.$$

Elektron harakat radiusi r_0 dan $\upsilon_1 = 0{,}1c = 3\cdot 10^7\,\frac{m}{s}$ tezlik bilan harakatlanuvchi r_1 radiusli orbitagacha kamayishi uchun ketgan τ vaqt quydagicha aniqlanadi

$$\tau = \frac{4\pi^2\varepsilon_0^2 e^3 m_0}{e^4}\left(r_0^3 - r_1^3\right) \approx 1{,}4\cdot 10^{-11}\,s\,.$$

1.2. Vodorodsimon atomlarda elektronning $n+1$ orbitadan n orbitaga o`tishida chiqargan nurlanish chastotasi uning $n$-orbitada aylanish chastotasiga teng ekanligini ko`rsating. Bunda $n>>1$ deb hisoblang.

Yechish: $\nu = cRZ^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$ chastotalar qoidasidan $n+1$ *va* n holatlarga o`tilsa

$$\nu_{n,n+1} = cRZ^2\left(\frac{1}{n^2} - \frac{1}{(n+1)^2}\right), \quad \upsilon = \omega\cdot r = 2\pi f\cdot r\,,$$

$$k = \frac{1}{2}m\upsilon^2 = \frac{1}{8\pi\varepsilon_0}\frac{e^2}{r}$$

$$\upsilon^2 = \frac{e^2}{4\pi\varepsilon_0 rm}; \qquad r_n = \frac{4\pi\varepsilon_0 n^2\hbar^2}{me^2} \to f_k = \frac{me^4}{64\pi^2\varepsilon_0^2\hbar^2}\cdot\frac{2}{n^3}\,.$$

Bor nazaryasidan

$$\nu = \frac{me^4}{64\pi^3\varepsilon_0^2\hbar^3}\cdot\left(\frac{1}{n_j^2} - \frac{1}{n_i^2}\right) = \frac{me^4}{64\pi^3\varepsilon_0^2\hbar^3}\cdot\left(\frac{n_j^2 - n_i^2}{n_j^2\cdot n_i^2}\right)$$

n_i va n_j bir-biriga yaqin bo`lsa n_i-n_j=Δn , n_i+n_j=2n_i=2n , $n_i^2 - n_j^2 = n^4$ desak,

$$\nu = \frac{me^4}{64\pi^3\varepsilon_0^2\hbar^3}\cdot\left(\frac{\Delta n\cdot 2n}{n^4}\right) = \frac{me^4}{64\pi^3\varepsilon_0^2\hbar^3}\cdot\left(\frac{2\Delta n}{n^3}\right);\ \Delta n\text{=1 bo`lsa,}$$

$$\nu = \frac{me^4}{64\pi^3\varepsilon_0^2\hbar^3}\cdot\left(\frac{2}{n^3}\right)$$

1.3. Vodorod atomida elektron asosiy holatga qaytishida to`lqin uzunliklari $\lambda_1$=65630 nm va $\lambda_2$=12160 nm bo`lgan ikkita foton chiqargan bo`lsa bu uyg`ongan holat uchun n – kvant sonini aniqlang.

1.4. He^{+} va Li^{++} ionlari uchun ionizatsiya potensiali va birinchi uyg`ongan holat potensialini hisoblang.

1.5. Atom radiusidagi ($r \approx 10^{-15}$ m) nuklon energiyasini baholang.

1.6. Noaniqlik munosabatidan foydalanib vodorod atomidagi elektron energiyasini baholang (vodorod atomi radiusi $5\cdot 10^{-11}$ m).

2-mavzu: Fotoeffekt va Kompton effektlari. Fotoeffekt qonunlari

Fotonlar haqidagi gipotezani tasdiqlovchi hodisalaridan biri fotoelektrik effekt hisoblanadi. Yorug`lik ta’sirida moddadan elektronlar chiqarilish hodisasi fotoelektrikeffekt yoki ***fotoeffekt*** deyiladi. Fotoeffekt sodir bo`lishi uchun asosiy shart yorug`likni yoritilayotgan moddani sirtida yutilishidir. Fotoelektrik effekt faqat ultrabinafsha nurlar ta’siridagina hosil bo`lmasdan, balki ishqoriy metallar –litiy Li, natriy Na, kaliy K, rubidiy Rb, seziy Ce kabi moddalarda spektrning ko`rinadigan sohasida ham kuzatiladi.

Fotoeffekt hodisasini rus fizigi A.G.Stoletov mukammal o`rgandi va qator muhim qonuniyatlarni aniqladi:

1. To`yinish toki tushayotgan yorug`likni intesivligiga to`gri proporsional.

2. Moddadan chiqarilayotgan fotoelektronlarning maksimal tezligi yorug`lik chastotasiga bogliq bo`lib, uning intensivligiga bogliq emasdir.

3. Fotoeffekt har bir modda uchun shunday minimal ν_0 chastota mavjudki, bu chastotadan past nurlanish chastotalarida fotoeffekt sodir bo`lmaydi. Bu chastotaga ***fotoeffektning qizil chegarasi*** deyiladi.

Bu holda elektronning kinetik energiyasi metallning sirt qatlamida ta’sir qiluvchi kuchni yengishga ya’ni chiqish ishiga sarf bo`ladi. Faraz qilaylik, bitta foton modda ichidan bitta elektron chiqarayotgan bo`lsin, u holda fotoelektronlar ega bo`ladigan maksimal kinetik energiya quyidagi formuladan aniqlanadi:

$$\frac{1}{2}m_e v_{\max}^2 = h\nu - A_{ch}$$

yoki

$$h\nu = A_{ch} + \frac{1}{2}m_e v_{ch}^2$$

bu erda, $h\nu$ – moddaga tushayotgan foton energiyasi, A_{chiq} – moddadan elektronlarning chiqish ishi, $\frac{1}{2}m_e v_{\max}^2$ – fotoelektronlarning maksimal kinetik energiyasi. Yuqoridagi ifoda fotoeffekt uchun ***Eynshteyn tenglamasi*** deyiladi.

XIX asr oxiri va XX asr boshlarida klassik fizika doirasida turib tushuntirib bo`lmaydigan bir qator tajriba ma'lumotlari to`plandi. Ularni olishda o`rganilgan hodisalarni bir qarashda go`yo o`zaro bog`liq bo`lmagan ikki guruhga ajratish mumkin edi. Birinchi guruh hodisalardan (absolyut qora jism nurlanishi, fotoeffekt, Kompton effekti, sekin elektronlar dastasida difraktsiyasi) yorug`lik va mikrozarralar oqimining ikki yoqlamalik – dualistik tabiati kelib chiqsa, ikkinchisi esa (atomlarni murakkab tuzilganligini tasdiqlovchi tajribalar, atomlarning nurlanish va yutilish chiziqli spektrlari) klassik tasavvurlarga tayanib turg`un atomlar mavjudligini va ularning optik spektrlaridagi qonuniyatlarni asoslab bo`lmasligi bilan bog`liq edi. Ana shu ikki guruh hodisalar o`rtasidagi bog`lanishni topishga va ularni yagona nuqtai nazardan tushuntira oladigan nazariya yaratishga bo`lgan urinishlar oxir-oqibatda kvant mexanikasining tug`ilishiga sabab bo`ldi.

Kompton effekti uchun ushbu qonuniyat o`rinli:

$$\lambda' - \lambda = \lambda_K(1 - \cos\vartheta) = 2\lambda_K \sin^2\left(\frac{\vartheta}{2}\right)$$

bu yerda

$$\lambda_K = \frac{h}{m_e c} = 2{,}4263096^{-10}\ sm,$$

bu ifodadan ko`rinadiki, Kompton siljishi sochuvchi moddaga bogliq emas. Bunda formuladagi λ_K – elektron uchun ***Kompton uzunligi*** deyiladi

2.1. Agar oltin uchun chiqish ishi A=4,58 eV va alyuminiy uchun A=3,7 eV bo`lsa: a) fotoeffektning qizil chegara to`lqin uzunligini toping; b) nurlanishning to`lqin uzunligi 270 *nm* bo`lsa, oltin va alyuminiy sirtidan chiqayotgan elektronlrning maksimal kinetik energiyasi va tezligini toping.

2.2. To`lqin uzunligi $\lambda_1$=0,1849·10$^{-6}$ $m$ bo`lgan simob spektrini ultrabinafsha nuri ta'sirida rux metalldan chiqayotgan elektronni to`xtatuvchi potensial 2,42 V ga teng. Shu spektrning λ_2=0,2537·10^{-10} m

to`lqin uzunlikka ega bo`lgan fotoelektronlari uchun to`xtatuvchi potensial nimaga teng?

2.3. Natriy metalli sirtidan fotoelektronlarni urib chiqarish uchun kerak bo`lgan maksimal to`lqin uzunlik $0{,}5450 \cdot 10^{-6}$ *m*: a) agar tushayotgan nurlanishning to`lqin uzunligi $0{,}2000 \cdot 10^{-6}$ *m* bo`lsa, chiqayotgan elektronlarning maksimal tezligini toping; b) tushayotgan nurning to`lqin uzunligi $0{,}2000 \cdot 10^{-6}$ *m* bo`lsa, natriy sirtidan chiqayotgan fotoelektronlar uchun to`xtatuvchi potensialni toping.

2.4. Ikki fotonli fotoeffektda berilgan metall uchun qizil chegara to`lqin uzunligi $\lambda_0$=580 *nm*. $\lambda$=650 *nm* to`lqin uzunlikda uch fotonli fotoeffektda metall sirtidan chiqayotgan elektronlarning maksimal kinetik energiyasini toping.

Kompton effekti

2.5. Kompton siljishining maksimal qiymati qanday burchakka to`g`ri keladi? Elektron va proton uchun $\Delta\lambda_{\max}$ ni toping.

2.6. Elektronning Kompton to`lqin uzunligi $\lambda_K$ ga teng bo`lgan nurlanishi kvanti to`lqin uzunligiga mos kelgan energiyani toping.

2.7. Foton tinch turgan erkin elektronda Kompton sochilishda $\theta = \dfrac{\pi}{2}$ burchakka burilishida uning to`lqin uzunligi ikki marta ortishi uchun energiyasi qanday bo`lishi kerak?

2.8. To`lqin uzunligi $\lambda$=3,64 *pm* bo`lgan foton tinch turgan erkin elektronda sochildi. Sochilish jarayonida tepki elektronning kinetik energiyasi tushayotgan fotonning energiyasini η=25% ni tashkil qilsa: a) sochilgan fotonning Kompton siljishi to`lqin uzunligini; b) sochilgan fotonning hosil qilgan θ burchagini toping.

2.9. λ to`lqin uzunlikka ega bo`lgan rentgen nurlari bilan modda nurlantirilganda maksimal energiyasi 0,44 *MeV* Kompton elektronlarining chiqishi kuzatildi. λ ni toping.

2.10. Foton bilan relyativistik elektronni to`qnashishi natijasida foton $\theta$=60° burchakka sochildi, elektron esa to`xtab qoldi. Sochilgan foton uchun to`lqin uzunlikning Kompton siljishini toping. Agar tushayotgan foton energiyasi tinch turgan elektron energiyasining η=1,0 ulishini tashkil qilsa, tushayotgan fotonning energiyasini toping.

2.11. Norelyativistik v tezlik bilan harakat qilayotgan uyg`ongan atom $\theta$ burchak ostida foton chiqardi (o`zining dastlabki yo`nalishiga nisbatan). Saqlanish qonunlaridan foydalangan holda atomning tepkisi tufayli vujudga kelgan fotonning chastotasini nisbiy siljishini toping.

2.12. Fotonning tinch turgan elektronda θ=60º sochilishi tufayli elektron K=450 keV energiya olgan bo`lsa, tushayotgan fotonning energiyasini toping.

2.13. To`lqin uzunligi 0,024·10$^{-10}$ $m$ bo`lgan fotonlar yordamida antikatod bombardimon qilindi. Natijada 60º ostida sochilgan fotonlar kuzatildi. Sochilgan fotonning to`lqin uzunligi va tepki elektronning sochilish burchagini toping.

3-mavzu: Bor-Zommerfeld formulasi

Avstriyalik fizik Arnold Zommerfeld daniyalik fizik Nils Borning kvant nazariyasini rivojlantirishda navbatdagi muhim qadamni qo`ydi. O`sha vaqtda Borning dastlabki **nazariyasidagiga o`xshash** faqat doiraviy orbitalar qaralardi, Zommerfeld klassik mexanikadagi Kepler masalasining umumiy yechimidan foydalandi, ya’ni elliptik orbitalarni ham e’tiborga oldi. Buning uchun kvantlash shartini kengaytirish zarur bo`ldi. Haqiqatan ham, biz elektronning faqat doiraviy harakatini qarayotganimizda, bizga bitta erkinlik darajasi uchun kvantlash qoidasi yetarlidir. Agar elliptik orbitalarni ham e’tiborga olishni xoxlasak, bu holda elektronning orbitadagi vaziyati ikkita parametr: $\vec{r}$ radius-vektor va qutbiy burchak (azimut) φ bilan aniqlanishligi sababli, bizga ikkita erkinlik darajali sistema uchun kvantlash qoidasi kerak bo`ladi.

Oddiy holda **sharli-davriy** harakat ikkita oddiy garmonik tebranishlarga keltiriladi:

$$\oint P_x dx = n_x h, \qquad \oint p_y dy = n_y h$$

n_x, n_y=1, 2, 3, … – butun sonlar. Bir necha erkinlik darajali sistema uchun kvantlash sharti

$$\oint P_1 dq_1 = n_1 h \qquad \oint P_2 dq_2 = n_2 h, \qquad \oint P_f dq_f = n_f h$$

kabi yoziladi.

3.1. $\oint p_i dq_i = \hbar n_i$ Bor-Zommerfeld kvantlash qoidasidan foydalanib ω chastotali bir o`lchovli garmonik ossilyatorning energiya sathlarini aniqlang.

Yechish: Ma’lumki garmonik otsilyator harakat tenglamasi $x = A\cos\omega t$, impulsi esa $p = -m_0\omega A \cdot \sin\omega t$.

Garmonik otsilyator energiyasini uning xususiy chastotasi ω va amplitudasi A orqali ifodalaymiz

$$E = \frac{p^2}{2m_0} + \frac{m_0\omega^2 x^2}{2} = \frac{m_0\omega^2 A^2}{2}.$$

Yuqoridagi kvantlash qoidasidan foydalanib, amplitudaning ruxsat etilgan qiymatlarini aniqlaymiz:

$$\oint pdq = m_0 A\omega \int \sqrt{1 - \frac{x^2}{A^2}} dx = m_0 \omega A^2 \pi = nh$$

$$A_n^2 = \frac{2\hbar}{m_0\omega} n, \qquad n = 0,\ 1,\ 2,\ 3, \ldots.$$

A_n^2 ni energiyaning ifodasiga qo`yib, energiya ruxsat etilgan qiymatlarini aniqlaymiz:

$$E_n = n\hbar\omega.$$

3.2. Zarra kengligi a ga teng bo`lgan chuqurda impulsi $\vec{p}$ va $-\vec{p}$ impulslarga ega bo`lgan intervalida harakatlansa, uning energiyasini kvantlang.

Yechish: $\oint Pdx = nh$ Bor-Zommerfeld kvantlash shartidan

$$\oint Pdx = \int_0^a 2pdx = nh \quad \Rightarrow P_n = \frac{nh}{2a}, \qquad E_n = \frac{P_n^2}{2m} \text{ dan}$$

$$E_n = \frac{1}{2m}\left(\frac{nh}{2a}\right)^2 = \frac{1}{2m}\frac{h^2 n^2}{4a^2} = \frac{h^2}{8ma^2} n^2$$

ekanini olamiz.

3.3. m_0 massali zarra $U = \frac{1}{2}kr^2$ maydonda doiraviy orbita bo`ylab harakatlanayapdi. Uning energiyasini kvantlang.

Yechish: $F = -\frac{\partial U}{\partial r} = -kr$

bundan

$$m\ddot{r} = -kr, \quad m\ddot{\vec{r}} + k\vec{r} = 0$$

$$\ddot{r} + \omega^2 r = 0, \quad \omega = \sqrt{\frac{k}{m}}$$

$$r = A\cos\omega t, \qquad P = -m_0\omega A \sin\omega t$$

bir o`lchovli holga o`tsak

$$x = A\cos\omega t \qquad P_x = -m_o\omega \sin\omega t$$

$$\oint pdq = \oint p_x dx = \int \sqrt{1 - \frac{x^2}{A^2}} dx = m_0 \omega A^2 \pi = nh$$

$$A_n = \frac{2\hbar}{m_0 \omega} \cdot n, \qquad n = 0,\ 1,\ 2, \ldots$$

$$E_n = n\hbar\omega .$$

3.4. Kvaziklassik maydonni qo`llab, $U(x) = -U_0\left(1 - \frac{|x|}{a}\right)$ maydonda harakatlanayotgan m_0 massali zarra uchun energetik spektrini $E<0$ hol uchun aniqlang.

Yechish: Bor-Zommerfeld kvantlash sharti

$$\oint pdx = 2\pi\hbar\left(n + \frac{1}{2}\right) \quad \text{va} \quad P = \sqrt{2m_0\left(U_0 + E - \frac{U_0}{a}x\right)}$$

ekanini hisobga olib energetik spektrni aniqlaymiz

$$E_n = -U_0 + \alpha\left(n + \frac{1}{2}\right)^{2/3}, \text{ bunda } \quad n = 0,\ 1,\ 2,\ \ldots, N.$$

$$\alpha = \left(\frac{3\pi\hbar U_0}{4\sqrt{2}a\sqrt{m_0}}\right)^{\frac{2}{3}};$$

N ning maksimal qiymati $E_N = 0$ shartdan topiladi

$$N = \left(\frac{U_0}{\alpha}\right)^{\frac{3}{2}} - \frac{1}{2}.$$

3.5. Cheksiz baland devorlari $x=0$ va $x=a$ nuqtalarda joylashgan bir o`lchamli potensial chuqurlikdagi zarrachaning energiya sathlarini Bor-Zommerfeld kvantlash shartidan foydalanib aniqlang.

4-mavzu: Mikrozarralar to`lqin xususiyatlari. Noaniqlik munosabatlari. De-Broyl to`qini

Geyzenberg 1927 yilda kvant mexanikasi tenglamalarining fizik ma’nosini yoritib beruvchi ***noaniqliklar munosabatini*** topdi. Bu munosabatga ko`ra, jumladan, mikrozarra koordinatasini aniq o`lchashga urinish uning impulsini noaniq bo`lib qolishiga olib keladi yoki aksincha va demak, klassik trayektoriya tushunchasidan mikrozarra harakatini o`rganishda foydalanish mumkin emas. N.Bor Geyzenbergning bu ishlarini rivojlantirib to`ldiruvchanlikning umumiy printsipini ilgari surdi va mikrodunyo xossalarini ehtimolli tavsiflash zarurligini ko`rsatdi. Fizikada birinchi marta makroskopik sistemadagi hodisalarnigina emas, balki alohida olingan mikrozarra harakatini ham statistik xarakterda o`rganish metodi yuzaga keldi.

Bir qator atom hodisalarni, birinchi navbatda, atomlar nurlanish spektrlarini sinchiklab o`rganish elektron xossalarini to`liq ifodalash uchun uni elektr zaryad va massadan tashqari ichki (xususiy) impuls momenti – spin bilan ham xarakterlash zarurligiga olib keldi. Elektron $h/2$ – xususiy mexanik moment va $e_0\hbar/(2m_0c)$ ($\hbar = \dfrac{h}{2\pi}$, e_0, m – mos holda, elektron zaryadi va massasi) xususiy magnit momentga egaligi to`g`risidagi gipoteza 1925 yilda amerikalik fiziklar Semyuel Gaudsmit va Jorj Ulenbeklar tomonidan o`rtaga tashlangan edi. Elektronning spin nazariyasi shveytsariyalik fizik Volfgang Pauli ishlarida keng rivojlantirildi. U elektron spinni hisobga olish natijasida atomlar, molekulalar, atom yadrolari va qattiq jismlar nazariyalarida hal qiluvchi ahamiyat kasb etgan o`zining taqiqlanish printsipini (Pauli printsipi, 1925 yil) kashf etishga muvaffaq bo`ldi. Pauli printsipiga muvofiq ixtiyoriy atom sistemada ayni bir kvant holatda bo`lgan bittadan ortiq elektron bo`lishi mumkin emas. Elektron spinining mavjudligi atomlar spektrining multiplet (nozik) strukturasini, Zeeman effektini, atomlar elektron qobiqlarining to`lib borish tartibini, ferromagnetizm va boshqa juda ko`p hodisalarni to`g`ri tushuntirib berdi. Bu yerda shuni qayd qilmoq kerakki, agar norelyativistik kvant mexanikasining matematik apparatiga spin tushunchasi Pauli tomonidan fenomenologik ravishda kiritilgan bo`lsa, Dirakning relyativistik to`lqin tenglamasidan elektron spinga va spin magnit momentga ega bo`lishi bevosita kelib chiqadi.

Agar qaytish, sinish, difraktsiya kabi jarayonlarda zarrachalarni butunligi saqlansa, u holda ikki muhitning chegara sirtiga tushgan zarracha yo qaytadi, yoki ikkinchi muhitga o`tadi. Ammo bunday holda to`lqinlar va zarrachalar orasidagi boglanish faqat **statistik talqin** qilinadi: To`lqin intensivligining o`lchovi bo`lgan amplituda kvadratining ma’lum joydagi qiymati zarrachaning shu joyda **topilish ehtimolligining o`lchovi** bo`ladi. Shu nuqtai nazardan, de Broyl to`lqinlarini talqin qilishda to`lqin paketlarni saqlab qolish mumkin. Elektronni fazoning biror nuqtasidagi to`lqin paket desak, u holda uning keyingi t vaqtdagi shaklini topsak, unda uning amplitudasi kvadrati elektronni shu joyda topish ehtimolligiga proportsional bo`ladi. Shu kabi difraktsion manzaradagi yorug` joylarda elektronlarni topish ehtimolligi maksimal, qorong`i joylarda esa nolga teng bo`ladi. Klassik mexanikada makroskopik zarralarning muhim xususiyati shundan iboratki, bir vaqtning o`zida ularning koordinata va tezligini aniq belgilab olish mumkin. Mikrozarrachalarda to`lqin xususiyatining namoyon bo`lishi esa ular holatini bunday aniqlashga imkon bermaydi. Agar mikrozarralarning $x$ o`qidagi o`rni biror $\Delta x$ noaniqlik bilan ma’lum bo`lsa, zarracha x_0 va $x_0 + \Delta x$ oraliqda turadi deyish mumkin. To`lqin manzarada buni to`lqin funktsiyasi amplitudasi Δx kesmada noldan farqli desak bo`ladi. Bunday to`lqin funktsiyasi garmonik to`lqinlar qo`shilishidan hosil bo`lsa ham uni o`zi garmonik funktsiya emas. Bunday fazoda cheklangan to`lqin funktsiya ***to`lqin paket*** deyilishi mumkin. Paketning to`lqin kenligi $\Delta x$ va unga mos to`lqin vektori farqi $\Delta\vec{k}$ uchun

$$\Delta x \Delta k_x \geq 1$$

tengsizlikni yozishimiz mumkin, bundan $\Delta x \Delta p_x \geq h$ kelib chiqadi.

Bu munosabatdan x va p_x bir vaqtda aniq qiymatlarga ega bo`la olmasligi kelib chiqadi. Boshqa koordinatalar uchun ham shu munosabatlarni yozish mumkin:

$$\Delta x \Delta p_x \geq h,$$

$$\Delta x \Delta p_y \geq h,$$

$$\Delta x \Delta p_z \geq h.$$

Bu tengsizliklar ***Geyzenbergning noaniqlik munosabatlari*** deyiladi. Xuddi shuningdek energiya va vaqt uchun

$$\Delta E \cdot \Delta t \geq h$$

kabi aniqlanadi.

De-Broyl moddiy zarrachalar to`lqin xossali bo`ladi degan fikrni aytdi. Korpuskulyar manzarada zarrachalar E – energiya va p – impuls bilan, to`lqin manzarada $\nu$ – chastota va $\lambda$ – to`lqin uzunliklik bilan xarakterlanadi. Agar bitta ob’ektning turli jihatlari bo`lsa, ularni xarakterlovchi chastotalar orasidagi bog`lanish quyidagicha bo`ladi:

$$E = h\nu, \qquad p = \frac{h}{\lambda}.$$

Optik hodisalarni tekshirganda fotonning impulsini aniqlash uchun bu ifodadan foydalanilanishadi. De-Broyl fikricha o`sha ifoda moddiy zarrachalar uchun shu zarrachalarga to`gri keltiriluvchi yassi monoxromatik to`lqinlarning to`lqin uzunliklarini aniqlaydi:

$$\lambda = \frac{h}{p} \qquad \text{yoki} \qquad \lambda = \frac{h}{m\vartheta}$$

4.1. U $=10^3$ V potensiallar farqidan o`tib tezlashtirilgan elektronning de-Broyl to`lqin uzunligi topilsin.

4.2. Kinetik energiyasi bir atomli gazlarning xona haroratidagi kinetik energiyasiga teng bo`lgan proton va elektronning de-Broyl to`lqin uzunligini aniqlang.

4.3. Kinetik energiyasi 24,6 eV bo`lgan elektronning de-Broyl to`lqin uzunligini aniqlang.

4.4. Esterman-Shtern tajribasida LiF kristaliga tushayotgan geliy atomlarining difraksiyasi o`rganilgan. Kinetik energiyasi $(2/3)kT$ formula bilan $T$=290 $K$ haroratdagi geliy atomlarining de-Broyl to`lqin uzunligi qanday?

4.5. Noaniqlik munosabatidan foydalanib vodorod atomidagi elektron energiyasi baholansin (vodorod atomi radiusi $5\cdot10^{-11}$ m).

4.6. Maksvell taqsimotidan foydalanib molekulalarning de-Broyl to`lqin uzunligi bo`yicha taqsimotini aniqlang. 300 K haroratdagi vodorod molekulasi uchun eng ehtimolli de-Broyl to`lqin uzunligini aniqlang.

Yechish: Maksvell taqsimotini ushbu ko`rinishda yozamiz.

$$f(\upsilon) = 4\pi\left(\frac{m_0}{2\pi k_0 T}\right)^{\frac{3}{2}} e^{-\frac{m_0\upsilon^2}{2\pi k_0 T}}\upsilon^2$$

Yana $f(\lambda) = f(\upsilon)\dfrac{d\upsilon}{d\lambda}$, $\lambda = \dfrac{h}{m_0\upsilon}$ ekanligini hisobga olib, to`lqin uzunligi bo`yicha taqsimot funksiyasini yozamiz:

$$f(\lambda) = 4\pi h^3 (2\pi m_0 k_0 T)^{-\frac{3}{2}} \lambda^{-4} e^{-\frac{h^2}{2k_0 T m_0 \lambda^2}}$$

Bundan foydalanib qidirilayotgan eng ehtimolli to`lqin uzunligini aniqlaymiz.

$$\frac{df(\lambda)}{d\lambda} = 0, \quad \frac{df(\lambda)}{d\lambda} = 0, \qquad \lambda_b = \frac{h}{2\sqrt{m_0 k_0 T}} = 0{,}09\ nm.$$

4.7. Elektron chiziqli o`lchami 0,1 $nm$ bo`lgan sohaga qamalgan. Bu elektron impulsining noaniqligi qanday? Bu impulsga qanday energiya mos keladi?

4.8. Vodorod atomi diametri d=10^{-8} sm deb hisoblab, atomdagi elektron tezligining noaniqligini toping. Bu tezlik qiymatini birinchi Bor orbitasida harakatlanayotgan elektron tezligi bilan taqqoslang.

4.9. Noaniqlik munosabatlaridan foydalanib elektronning atom yadrosi ichida bo`la olmasligini ko`rsating.

5-mavzu: Kvant mexanikasining matematik apparati. Chiziqli va Ermit operatorlari

Biror funktsiyaga mos ravishda boshqa funktsiyani hosil qilish qoidasi ***operator*** deyiladi. Kvant mexanikasida operatorlar harf tepasiga ^ - belgi qo`yish bilan yoziladi. Masalan:

$$f = \hat{L}\varphi . \qquad (1)$$

bunda $\hat{L}$ – operator φ – funktsiyaga ta'sir qilib f – funktsiyani hosil qilgan.

Biroq kvant mexanikasida haqiqiy operatorlar barchasi ham ishlatavermaydi. Kvant mexanikasida qo`llaniladigan operatorlar faqat ikkita xossaga – chiziqli va Ermit operatorlar bo`lishi kerak.

$\hat{L}$ operator ***chiziqli*** bo`lishi uchun quyidagi shartga bo`ysunishga majbur:

$$\hat{L}(c_1\varphi_1 + c_2\varphi_2) = \hat{L}c_1\varphi_1 + \hat{L}c_2\varphi_2 = c_1\hat{L}\varphi_1 + c_2\hat{L}\varphi_2 = c_1 f_1 + c_2 f_2 . \qquad (2)$$

bunda φ_1 va φ_2 – erkli funktsiyalar, c_1 va c_2 – erkli o`zgarmas sonlar (doimiy sonlarni operator belgisidan tashqariga chiqarib yozish mumkin). (2) xossadan ko`rinib turibdiki ildiz chiziqli operator bo`la olmaydi, aksincha $\frac{d}{dx}$ esa chiziqli operatorlardir. Kvant fizikasida operatorlarni chiziqli bo`lishi xossasi holatlarning superpozitsiya printsipinda aks etadi.

Chiziqli operator o`ziga qo`shma yoki ***Ermit operatori*** bo`lishi uchun quyidagi integral tenglik bajarilishi kerak.

$$\int \varphi_1^*(x)\hat{L}\varphi_2(x)dx = \int \varphi_2(x)\hat{L}\varphi_1^*(x)dx . \qquad (3)$$

(3) tenglikdagi harflar tepasidagi "*" belgisi bu harflar o`ziga qo`shma ekanligini xarakterlaydi. Integral x – o`zgaruvchilarni barcha sohasiga nisbatan olinadi. $\varphi_1^*$ va $\varphi_2$ – ikkita erkli funktsiya (ular integrallash xususiyatga ega bo`lishi va integrallash chegarasida hosilasi nolga teng bo`lishi kerak). Agar o`zgaruvchilar ko`p bo`lsa, u holda dx deganda $dxdydz$ … ni tushunish kerak.

Operatorlarni Ermit xossasi bevosita fizikaviy kattaliklarni haqiqiy kattalik ekanligini aks ettiradi.

5.1. $\frac{d^2}{dx^2}x^2$ va $\left(\frac{d}{dx}x\right)^2$ operatorlarining ushbu funksiyalarga ta'sirini toping: a) $\sin x$; b) e^{2x}.

Yechish: a)

$$\frac{d^2}{dx^2}\left(x^2\sin x\right) = \frac{d}{dx}\left(2x\sin x + x^2\cos x\right) = 2\frac{d}{dx}\left(x\sin x\right) + \frac{d}{dx}\left(x^2\cos x\right) =$$
$$= 2\left(\sin x + x\cos x\right) + \left(2x\cos x - x^2\sin x\right) = 2\sin x + 4x\cos x - x^2\sin x$$

b) $\frac{d^2}{dx^2}\left(x^2e^{2x}\right) = \frac{d}{dx}\left(2xe^{2x} + 2x^2e^{2x}\right) = 2\frac{d}{dx}\left(xe^{2x}\right) + 2\frac{d}{dx}\left(x^2e^{2x}\right) =$

$$= 2\left(e^{2x} + 2xe^{2x}\right) + 2\left(2xe^{2x} + 2x^2e^{2x}\right) = 2e^{2x} + 4xe^{2x} + 4xe^{2x} + 4x^2e^{2x} =$$
$$= e^{2x}\left(2 + 8x + 4x^2\right) = 2e^{2x}\left(1 + 4x + 2x^2\right)$$

5.2. $\hat{A} = \dfrac{\partial}{\partial x}$ operator uchun $e^{\alpha \hat{A}} = \sum\limits_{n=0}^{\infty} \dfrac{\alpha^n}{n!} \dfrac{\partial^n}{\partial x^n}$ operator tenglik o\`rinli ekanligini ko\`rsating, bunda α – o\`zgarmas son.

Yechish: Operatorga bog\`liq funksiyaning qatorga yoyish qoidasiga asosan:

$$f\left(\hat{A}\right) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \hat{A}^n$$

buni $\hat{A} = \dfrac{\partial}{\partial x}$ operator uchun eksponentaning qatorga yoyilishidan foydalansak

$$e^{\alpha \hat{A}} = 1 + \alpha \hat{A} + \frac{\alpha^2}{2!} \hat{A}^2 + \ldots + \frac{\alpha^n}{n!} \hat{A}^n = 1 + \alpha \frac{\partial}{\partial x} + \frac{\alpha^2}{2!} \frac{\partial}{\partial x} + \ldots = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \frac{\partial^n}{\partial x^n}.$$

5.3. Kvadrati birga teng bo\`lgan har qanday $\hat{\sigma}$ operator uchun ($\hat{\sigma}^2=1$) ushbu tenglik o\`rinliligi ko\`rsatilsin.

Yechish: Trigonometik funksiyalar sin va cos ning qatorga yoyish ifodalaridan foydalanamiz.

$$\sin\theta = \sum_{n=0}^{\infty} (-1)^n \frac{\theta^{2n+1}}{(2n+1)!}, \qquad \cos\theta = \sum_{n=0}^{\infty} (-1)^n \frac{\theta^{2n}}{(2n)!}.$$

Bularni e^x funksiyaning qatori uchun ham yozib chiqsak

$$e^{i\theta\hat{\sigma}} = \cos\theta + i\hat{\sigma}\sin\theta$$

munosabatni olamiz.

5.4. Parallel ko\`chirish operatori $T_a\psi(\vec{r}) = \psi(\vec{r} + \vec{a})$ operatorni impuls operatori orqali ifodalang.

Yechish: $\psi\ (\vec{r}\ +\ \vec{a}\ )$ operatorni Teylor qatoriga yoyamiz

$$\psi(\vec{r} + \vec{a}) = \psi(\vec{r}) + \vec{a}\frac{\partial}{\partial\vec{r}}\psi(\vec{r}) + \frac{a^2}{2}\frac{\partial^2}{\partial r^2}\psi(\vec{r}) + ... = (1 + \vec{a}\frac{\partial}{\partial\vec{r}} + \frac{\vec{a}^2}{2!}\frac{\partial^2}{\partial\vec{r}^2} + ...)\psi(\vec{r})$$
.

Impuls operatorining ko\`rinishi $\hat{p} = \dfrac{\hbar}{i}\dfrac{\partial}{\partial\vec{r}}$ ekanini esga olsak,

$$T\vec{a} = 1 + \frac{i}{\hbar}\left(\vec{a}\cdot\hat{\vec{p}}\right) + \frac{1}{2!}\frac{\left(i\vec{a}\,\hat{\vec{p}}\right)^2}{\hbar^2} + \ldots = e^{\frac{i}{\hbar}\vec{a}\,\hat{\vec{p}}}$$

ekanini olamiz.

5.5. $e^{kx\frac{\partial}{\partial x}}$ operatorning $\psi(x)$ funsiyaga tasirini aniqlang.

Yechish: $e^{kx\frac{\partial}{\partial x}}\psi(x)=e^{\frac{i}{\hbar}kxP_x}\psi(x)=\psi((k+1)x)$.

5.6. $\hat{A}$ va $\hat{B}$ operator chiziqli bo`lsa, ularning yig`indisi $\hat{A}+\hat{B}$, ko`paytmasi $\hat{A}\cdot\hat{B}$ dan tashkil topgan operator ham chizqli ekanini ko`rsating.

Yechish: malumki operatorlarning chiziqlilik sharti

$$\hat{A}(C_1\psi_1+C_2\psi_2)=C_1\hat{A}\psi_1+C_2\hat{A}\psi_2$$

kabi ifodalanadi va $\hat{B}$ operator uchun ham ushbu munosabat o`rinli.

$$\left(\hat{A}+\hat{B}\right)(C_1\psi_1+C_2\psi_2)=\left(\hat{A}+\hat{B}\right)C_1\psi_1+\left(\hat{A}+\hat{B}\right)C_2\psi_2=C_1\left(\hat{A}+\hat{B}\right)\psi_1+C_2\left(\hat{A}+\hat{B}\right)\psi_2$$

,

demak, $\hat{A}+\hat{B}$ ham chiziqli ekan. $\hat{A}\cdot\hat{B}$ operator uchun ham chiziqlilik shunday ko`rsatiladi.

5.7. Kompleks qo`shmaga aylantiruvchi $\hat{M}\psi=\psi^*$ operator chiziqli operator bo`la oladimi?

Yechish: Agar $\hat{A}\psi=\psi^*$ va $\hat{A}C\psi=C^*\psi^*$ bo`lsa, unda

$$\hat{A}(C_1\psi_1+C_2\psi_2)=C_1^*\psi_1^*+C_2^*\psi_2^*=C_1\hat{A}\psi_1+C_2\hat{A}\psi_2.$$

demak, kompleks qo`shmaga aylantiruvchi $\hat{M}$ operator umuman aytganda chiziqli emas, chunki $C_1\neq C_1^*$ va $C_2\neq C_2^*$.

5.8 Kompleks qo`shmaga aylantiruvchi operator Ermit operatormi?

Yechish: $\hat{B}$ operatorga ***kompleks qo`shma operator*** deb, $\left(\hat{B}^*\psi^*\right)=\hat{B}\psi$ shartni qanoatlaniruvchi $\hat{B}^*$ operatorga aytiladi. Kompleks qo`shmaga aylantiruvchi $\left(\hat{A}\psi=\psi^*\right)$ operator uchun bu shart quyidagicha yoziladi. $\left(\hat{A}^*\psi^*\right)=\hat{A}\psi=\psi^*$, shuning uchun $\hat{A}^*\psi^*=\psi$. Lekin, biz bilamizki $\hat{A}\psi^*=\psi$. Demak, $\hat{A}^*$ operator $\hat{A}$ operator o`ziga teng.

$$\int\psi_1^*\hat{A}\psi_2d\tau=\int\psi_1^*\psi_2^*d\tau\neq\int\psi_2\hat{A}\psi_1^*d\tau=\int\psi_2\psi_2d\tau,$$

demak, kompleks qo`shmaga aylantiruvchi $\hat{A}$ operator ermit operator emas.

5.9. Ixtiyoriy $\hat{A}$ operator va uning $\hat{A}^{+}$ qo`shma operatorlarining yig`indisi $\left(\hat{A}+\hat{A}^{+}\right)$ ermit operatori ekanini ko`rsating.

Yechish: A ga qo`shma $A^{+}$ ning orasidagi munosabat quyidagicha: $\int \psi_1^* \hat{A}\psi_2 d\tau = \int \psi_2 \left(\hat{A}^{+}\psi_1\right)^* d\tau$ bundan va ermitlik shartdan foydalanib, $\hat{A}+\hat{A}^{+}$ ning ermitligini ko`rsatamiz.

$$\int \psi_1^* \left(\hat{A}+\hat{A}^{+}\right)\psi_2 d\tau = \int \psi_2 \left(\hat{A}^{+}\psi_1\right)^* d\tau + \int \psi_2 \left(\hat{A}\psi_1\right)^* d\tau = \int \psi_2 \left(\hat{A}+\hat{A}^{+}\right)^* \psi_1^* d\tau$$

,

demak, $\hat{A}+\hat{A}^{+}$ yig`indi operator Ermit operatori ekan.

5.10. Ushbu operatorlarning ermit ekanligini ko`rsating: a) p_x, b) L_z, d) p_x^2, e) H.

5.11. Quyidagi operator ifodalarda qavslarni oching: a) $\left(\frac{d}{dx}+x\right)^2$, b) $\left(\frac{d}{dx}+\frac{1}{x}\right)^3$, v) $\left(\frac{d}{dx}x\right)^2$.

5.12. Differensiallash operatori $\hat{A}=\frac{\partial}{\partial x}$ Ermit operatorimi?

5.13. Agar $\hat{A}$ va $\hat{B}$ operatorlar Ermit operatori bo`lsa, ularning yigindi operatori $\hat{A}+\hat{B}$ ham Ermit ekanligini ko`rsating.

5.14. Funksiyani kompleks qo`shmasiga aylantiruvchi $\hat{M}\psi=\psi^*$ operator chiziqli operator bo`la oladimi?

6-mavzu: Operatorlar kommutatsiyasi

Bizga bir nechta operatorlar berilgan bo`lsa, ular orqali boshqa murakkab operatorlarni yasash mumkin. Oddiy operatorlar yordamida boshqa murakkab operator tuzish yo`lini bir nechta algebraik qoidalar orqali ifodalash mumkin.

Ikkita chiziqli va Ermit bo`lgan $\hat{A}$ va $\hat{B}$ operatori bilan berilgan bo`lsin. Bu operatorlarni yig`indisi $\hat{C}$ ni quyidagicha topamiz:

$$\hat{C}\psi = \hat{A}\psi + \hat{B}\psi \,. \tag{1}$$

Misol uchun, agar $\hat{A} = i\dfrac{\partial}{\partial x}$ va $\hat{B} = x$ bo`lsa, u holda

$$\hat{C} = i\frac{\partial}{\partial x} + x \,. \tag{2}$$

Endi operatorlarni bir-biriga ko`paytirish amalini ko`raylik. $\hat{A}$ operatorni $\hat{B}$ operatorga ko`paytirganda $\hat{C}$ operatorni hosil bo`lishi

$$\hat{C}\psi = \hat{A}\left(\hat{B}\psi\right) \tag{3}$$

ko`rinishida ifodalanadi. (3) ga ko`ra, y funktsiyaga avval $\hat{B}$ operatorini ta'sir ettirib, so`ng hosil bo`lgan natijaga $\hat{A}$ operatorni ta'sir ettirish kerak. Simvolik jihatdan bu

$$\hat{C} = \hat{A}\cdot\hat{B} \tag{4}$$

ko`rinishda bo`ladi.

Misol: agar $\hat{A} = i\dfrac{\partial}{\partial x}$, $\hat{B} = x$ bo`lsa, u holda

$$\hat{C}\psi = \hat{A}\left(\hat{B}\psi\right) = i\frac{\partial}{\partial x}(x\psi) = i\psi + ix\frac{\partial\psi}{\partial x},$$

Bundan:

$$\hat{C} = i + ix\frac{\partial}{\partial x} = i\left(1 + x\frac{\partial}{\partial x}\right).$$

Qizig`i shundaki, operatorlarning ko`paytirish amali ularni qanday tartibda ko`paytirishga bog`liq. Masalan,

$$\hat{C}'\psi = \hat{B}\left(\hat{A}\psi\right) = ix\frac{\partial\psi}{\partial x},$$

ya'ni

$$\hat{C}' = ix\frac{\partial}{\partial x}.$$

Shuning uchun, agar $\hat{A}$ va $\hat{B}$ operatorlar berilgan bo`lsa, $\hat{C}$ ko`rinishidagi ko`paytmadan boshqa

$$\hat{C}' = \hat{B}\,\hat{A} \tag{5}$$

ko`paytmani hosil qilish mumkin.

Yuqorida qayd qilingan qoidalar yordamida operatorlar ustida qo`shish, ayirish, ko`paytirish va bo`lish amallarini bajarish mumkin. Bu amallar xuddi oddiy algebradagi amallarga o`xshab amalga oshiriladi, biroq bir narsani unutmaslik kerak, operatorlar bilan ish ko`ganda ko`paytiruvchilarni joylashish tartibini o`zgartirmaslik kerak.

Masalan: $\hat{C} = \left(\hat{A} - \hat{B}\right)\left(\hat{A} + \hat{B}\right) = \hat{A}^2 + \hat{A}\hat{B} - \hat{B}\hat{A} + \hat{B}^2$. Lekin $\hat{C} \neq \hat{A}^2 - \hat{B}^2$ deb yozish o`rinli bo`lmaydi.

Ko`paytiruvchilarni joylashish tartibini o`zgartirmasdan amallar bajaradigan algebra nokommutativ kattaliklar algebrasi deyiladi.

Agar $\hat{C}$ va $\hat{C}'$ ko`paytmalar teng bo`lsa, u holda

$$\hat{A}\hat{B} - \hat{B}\hat{A} = 0. \tag{6}$$

Bu holda $\hat{A}$ va $\hat{B}$ operatorlar ***kommutativ operatorlar***, aksincha ***nokommutativ operatorlar*** deyiladi.
Masalan,

$$\hat{A}\hat{B} - \hat{B}\hat{A} = \hat{F} \tag{7}$$

nokommutativ bo`lgani bo`lgani uchun, $\hat{A}$ va $\hat{B}$ operatorlar ***nokommutativ*** yoki ***antikommutativ operatorlar*** deyiladi.

Demak, (7) ni

$$\hat{A}\hat{B} \neq \hat{B}\hat{A} \tag{8}$$

ko`rinishda ham yozish mumkin.

Odatda $\hat{A}$ va $\hat{B}$ operatorlar ***kommutativ*** bo`lsa, ularning kommutatorlarini

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0 \tag{9}$$

ko`rinishida ham beriladi.

Keyingi boblarda kvant mexanik operatorlarining ba'zi birlarining kommutativlik va nokommutativlik xossalari bilan tanishamiz.

6.1. Agar $\hat{A}$ va $\hat{B}$ operatorlar kommutativ bo`lsa, ushbu ayniyatlarni isbotlang: a) $\left(\hat{A} + \hat{B}\right)^2 = \hat{A}^2 + 2\hat{A}\hat{B} + \hat{B}^2$, b) $\left(\hat{A} + \hat{B}\right)\left(\hat{A} - \hat{B}\right) = \hat{A}^2 - \hat{B}^2$, v) $\left[\left(\hat{A} + \hat{B}\right)\left(\hat{A} - \hat{B}\right)\right] = 0$.

Yechish: kommutativlikdan $\hat{A}\hat{B} = \hat{B}\hat{A}$ ekanini bilamiz. v)

$$\left[\left(\hat{A}+\hat{B}\right),\left(\hat{A}-\hat{B}\right)\right]=\left(\hat{A}+\hat{B}\right)\left(\hat{A}-\hat{B}\right)-\left(\hat{A}-\hat{B}\right)\left(\hat{A}+\hat{B}\right)=$$

$$=\hat{A}^2-\hat{A}\hat{B}+\hat{B}\hat{A}-\hat{B}^2-\left(\hat{A}^2+\hat{A}\hat{B}-\hat{B}\hat{A}-\hat{B}^2\right)=0$$

a) va b) lar ham shunday yechiladi.

6.2. Agar $\hat{A}_i$ operator $\hat{B}$ operator bilan kommutativ bo`lsa, u bilan $\hat{A}=\sum_i A_i^2$ operator ham komutativ ekanini ko`rsating.

Yechish: $\hat{A}_i\hat{B}=\hat{B}\hat{A}_i$ ekanligi berilgan, $\hat{A}\hat{B}=\hat{B}\hat{A}$ ekanini talab qilinadi. $\hat{A}\hat{B}=\sum_i \hat{A}_i\hat{B}=\left(\hat{A}_1^1+\hat{A}_1^2+...\right)\hat{B}=\hat{B}\hat{A}_1^2+\hat{B}\hat{A}_2^2+...=\hat{B}\sum_i \hat{A}_i$ isbotlandi.

6.3. Agar $\left[\hat{A},\hat{B}\right]=1$ tenglik o`rinli bo`lsa, ushbu munosabatlarni tekshiring: a) $\left[\hat{A},\hat{B}^2\right]=2\hat{B}$, b) $\left[\hat{A},\hat{B}^3\right]=3\hat{B}^2$, c) $\left[\hat{A}^2,\hat{B}^2\right]=2\left(\hat{A}\hat{B}+\hat{B}\hat{A}\right)$.

Yechish: Kommutator ta’rifidan foydalanib hamda davriy almashtirishlar bajarib

$$\left[\hat{A}^2,\hat{B}^2\right]=A^2B^2-B^2A^2=A^2B^2-BBAA=A^2B^2-B(AB-1)A=$$

$$=A^2B^2-BABA+BA=A^2B^2-(AB-1)BA+BA=A^2B^2ABBA+BA+BA=$$

$$=A^2B^2-AB(AB-1)+2BA=A^2B^2-ABAB+AB+2BA=A^2B^2-A(AB-1)B+$$

$$+AB+2BA=A^2B^2-A^2B^2+AB+AB+2AB=2AB+2BA=2(AB+BA)$$

6.4. Quyidagi operatorlar komutatorlarini aniqlang: a) x va $\frac{d}{dx}$; b) $i\hbar\nabla$ va $\hat{A}(r)$; c) $\frac{d}{d\varphi}$ va $f(r,\sigma,\varphi)$.

6.5. $U(x)$ potensial maydondagi $\hat{H}$ gamilton operatori uchun ushbu kommutatsiya qoidalarini tekshiring: a) $\left[\hat{H}, y\right] = i\frac{\hbar}{m_0}\hat{P}_y$; b) $\left[\hat{H}, \hat{P}_x\right]_- = i\hbar\frac{\partial U}{\partial x}$; c) $\left[\hat{H}, \hat{P}_x^2\right]_- = 2i\hbar\frac{\partial U}{\partial x}\hat{P}_x + \hbar^2\frac{d^2U}{dx^2}$.

Yechish: Kommutator ifodasidan va to`lqin funksiyasi ψ ga ta'sirini qarab:

a) $\left[\hat{H}, y\right] = \hat{H}(y\psi(x,y,z)) - y\hat{H}\psi(x,y,z) =$

$$= -\frac{\hbar^2}{2m_0}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)(y\cdot\psi) - y\left(-\frac{\hbar^2}{2m_0}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\right)\psi =$$

$$= -\frac{\hbar^2}{2m_0}\left(y\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2(y\psi)}{\partial y^2} + y\frac{\partial^2\psi}{\partial z^2}\right) + y\frac{\hbar^2}{2m_0}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) =$$

$$= -\frac{\hbar^2}{2m_0}\cdot\frac{\partial^2(y\psi)}{\partial y^2} + \frac{\hbar^2}{2m_0}\cdot y\frac{\partial^2\psi}{\partial y^2} = -\frac{\hbar^2}{2m_0}\left(\frac{\partial^2(y\psi)}{\partial y^2} - y\frac{\partial^2\psi}{\partial y^2}\right) =$$

$$= -\frac{\hbar^2}{2m_0}\left(\frac{\partial}{\partial y}\left(\psi + y\frac{\partial\psi}{\partial y}\right) - y\frac{\partial^2\psi}{\partial y^2}\right) = -\frac{\hbar^2}{2m_0}\left(\frac{\partial\psi}{\partial y} + \frac{\partial}{\partial y}\left(y\frac{\partial\psi}{\partial y}\right) - y\frac{\partial^2\psi}{\partial y^2}\right) =$$

$$= -\frac{\hbar^2}{2m_0}\left(\frac{\partial\psi}{\partial y} + \frac{\partial\psi}{\partial y} + y\frac{\partial^2\psi}{\partial y^2} - y\frac{\partial^2\psi}{\partial y^2}\right) = -\frac{\hbar^2}{2m_0}\cdot 2\frac{\partial\psi}{\partial y} =$$

$$= -\frac{\hbar^2}{m_0}\cdot\frac{\partial\psi}{\partial y} = i\frac{\hbar}{m_0}\hat{P}_y.$$

b) va c) kommutatsiya qoidalarini mustaqil isbotlang.

6.6. $\hat{A}$ operator $\hat{B}$ va $\hat{C}$ operatorlar bilan kommutatsiya qiladi. Bundan $\hat{B}$ va $\hat{C}$ larning o`zaro kommutativ ekanligi kelib chiqadimi?

Yechish: Umumiy holda bunday xulosa kelib chiqmaydi. Masalan, $\hat{p}_x$ operator y va $\hat{p}_y$ operatorlar bilan kommutatsiya qiladi. Lekin y va $\hat{p}_y$ lar o`zaro kommutativ ekan.

6.7. Ushbu kvadrat integrallanuvchi funksiyaning $(0,a)$ kesmada chekliligini tekshiring.

Yechish: Ushbu $\psi(x) = C\sin\frac{\pi x}{a}$ funksiyaning chekliligini tekshirish uchun uni $0x$ o`qida $(0, a)$ kesmada integrallaymiz:

$$\int_0^a C^2 \sin^2\frac{\pi x}{a}dx = \frac{a}{2}C^2$$

Demak, funksiya chekli ekan.

Normallashtirish shartidan C doimiyning qiymatini aniqlaymiz

$$\int_0^a C^2 \sin^2\frac{\pi x}{a}2x = 1, \qquad C^2 = \sqrt{\frac{2}{a}}.$$

6.8. $\left[x, \hat{L}_x\right] = 0$, $\left[y, \hat{L}_x\right] = -i\hbar z$ va $\left[z, \hat{L}_x\right] = -i\hbar y$ ***kommutatsiya qoidalarini tekshiring.***

6.9. $\left[\hat{L}_x, \hat{p}_x\right] = 0$, $\left[\hat{L}_x, \hat{p}_x\right] = -i\hbar\,\hat{p}_z$, $\left[\hat{L}_x, \hat{p}_x\right] = -i\hbar\,\hat{p}_y$ ***kombinatsiyalarni tekshiring.***

6.10. $\left[\hat{L}_x, \hat{p}_x^2\right] = 0$, $\left[\hat{L}_x, \hat{p}^2\right] = 0$ ***va*** $\left[\hat{L}_x^2, \hat{p}^2\right] = 0$ ***ekanligini ko`rsating.***

6.11. $\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\,\hat{L}_z$, $\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\,\hat{L}_x$, $\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\,\hat{L}_y$ ***ekanligini ko`rsating.***

6.12. x ***va Laplas operatori*** $\vec{\nabla}^2$ ***larning kommutatorini hisoblang.***

6.13. $\hat{L}^2$ operator va kinetik energiya operatori $\hat{T}$ ning kommutativ ekanligini ko`rsating.

7-mavzu: Operatorlarning xususiy qiymat va xususiy funktsiyalari. Diskret va tutash spektrlar

Oldingi mavzudagi $<\hat{L}>$ – o`rtacha qiymat va $\left\langle (L)^2 \right\rangle$ o`rtacha kvadratik og`ishish formulalari alohida o`lchangan fizikaviy kattaliklarni qanday qiymatga ega bo`lishi haqida hech qanday ma'lumot bermaydi. Fizikaviy kattaliklarni xarakterlovchi $L$ kattalik qachon bitta qiymatga ega bo`ladi? Endi ana shu hol haqida ma'lumot beramiz. L kattalik aniq bir qiymatga ega bo`lganda dispersiya $\left\langle (L)^2 \right\rangle = 0$. Shu bois yuqoridagi formulaga asosan bu holatlar uchun

$$\int \left| \Delta \hat{L} \psi_L \right|^2 dx = 0$$

integral ostidagi ifoda doimo musbat bo`lgani uchun

$$\left| \Delta \hat{L} \psi_L \right|^2 = 0$$

ekanligi kelib chiqadi. Agar soning o`zi nolga teng bo`lsa, u holda kompleks sonning moduli ham nolga teng. Demak,

$$\Delta \hat{L} \psi_L = 0$$

yoki oldingi formuladagi $\Delta \hat{L}$ operatorning qiymatini nazarda tutsak, va qaralayotgan holat uchun $< L >= L$ bo`lsa, u holda

$$\hat{L} \psi_L(x) = L \psi_L(x)$$

ko`rinishdagi ifoda hosil bo`ladi. Bu tenglama chiziqli bo`lganligi uchun $\hat{L}$ operator bilan tasvirlanuvchi kattalik $L$ yagona qiymatga ega bo`ladi. Ko`p hollarda $\hat{L}$ operator differentsial operator bo`ladi. Shuning uchun bu ifoda chiziqli bir jinsli differentsial tenglamadir. Differentsial tenglamalarni yechimi bo`lishi uchun chegaraviy shartlar bo`lishi kerak.

Berilgan chegaraviy shartlarda chiziqli differentsial tenglamalar ($\hat{L}\psi = L\psi$) notrivial (noldan farqli) yechimga ega. umuman olganda L parametrning barcha qiymatlarida emas, balki tanlangan ayrim qiymatlarida, ya'ni $L = L_1$, L_2, $L_3, \ldots$, $L_n, \ldots$ yechimga ega bo`lishi mumkin. Unga mos kelgan yechimlar y_1, y_2, y_3, $\ldots$, $y_n, \ldots$ – ***xususiy funktsiyalar***, L_1, L_2, $L_3, \ldots$, $L_n, \ldots$ – qiymatlar esa ***xususiy qiymatlar*** deyiladi.

Endi Ermit operatorlarining xususiy funktsiyalarini asosiy alomatlariga tadbiq qilib ko`ramiz. Avval diskret spektr uchun ko`raylik. Fizikaviy kattalikni diskret spektr uchun xususiy qiymatlar va xususiy funktsiyalar tenglamasi quyidagicha yoziladi:

$$\hat{L} \psi_n = L_n \psi_n . \tag{1}$$

Bu formuladagi n indeks $\hat{L}$ operatorning xususiy qiymatlar va xususiy funktsiyalarini ketma-ketligini xarakterlaydi. Matematikadan yaxshi bilamizki erkli φ_1 va φ_2 funktsiyalar ortogonal bo`lishi uchun

$$\int \varphi_1^*(x) \varphi_2(x) dx = 0 \tag{2}$$

shart bajarilishi kerak.

L_n va L_m – xususiy qiymatlarga tegishli bo`lgan $\hat{L}$ operatorni $y_n$ va $y_m$ – xususiy funktsiyalari ham o`zaro ortogonaldir:

$$\int \psi_n^*(x)\psi_m(x)dx = 0. \tag{3}$$

Bunda $m \neq n$, y_n va y_m funktsiyalar xususiy bo`lgani uchun, ular

$$\hat{L}\psi_n = L_n\psi_n \tag{4}$$

va

$$\hat{L}\psi_m = L_m\psi_m \tag{5}$$

tengliklarning yechimidir.

(4) tenglamanining kompleks qo`shmasi

$$\hat{L}\psi_n^* = L_n\psi_n^*. \tag{6}$$

Eslatamizki, $L_m = L_m^*$.

(5) ni chapdan ψ_n^* ga, (6) ni esa chapdan ψ_n ga ko`paytiramiz, so`ngra birinchidan ikkinchisini ayiramiz:

$$\psi_n^*\hat{L}\psi_m - \psi_n\hat{L}^*\psi_m^* = (L_m - L_n)\psi_n^*\psi_m dx. \tag{7}$$

Barcha o`zgaruvchilar sohasida (7) formuladagi ikkala tomonni ham integrallasak

$$\int \psi_n^*\hat{L}\psi_m dx - \int \psi_m^*\hat{L}^*\psi_n dx = (L_m - L_n)\int \psi_n^*\psi_m dx \tag{8}$$

hosil bo`ladi. $\hat{L}$ operator Ermit bo`lgani sababli (8) tengliknitp chap qismi nolga teng (bunga ishonch hosil qilish uchun formulada $\varphi_1 = \psi_n$ va $\varphi_2 = \psi_m$ deb o`zgartirishlar kiritish kerak).

Demak,

$$(L_m - L_n)\int \psi_n^*\psi_m dx = 0. \tag{9}$$

Bundan chiqadiki, $L_m \neq L_n$ bo`lgani uchun ham usbu shart o`rinlidir.

**To`lqin funktsiyani normalash.** Odatda xususiy to`lqin funktsiyalar erkin ko`paytma ko`rinishdagi aniqlikda topiladi. Bu ko`paytmani aniqlab olish uchun xususiy to`lqin funktsiyalar birga normallanadi, ya'ni

$$\int \psi_n(x)dx = \int \psi_n^*(x)\psi_n dx = 1 \tag{10}$$

(3) va (10) xossalarni bitta yagona formula ko`rinishida yozish mumkin:

$$\int \psi_n^*(x)\psi_m dx = \delta_{nm}. \tag{11}$$

Bunda δ_{nm} – ***Kronekerning delta-simvoli*** deyiladi:

$$\delta_{nm} = \begin{cases} 1, & \text{agar } n = m \text{ bo`lsa,} \\ 0, & \text{agar } n \neq m \text{ bo`lsa.} \end{cases} \tag{12}$$

(11) shartni qanoatlantiruvchi funktsiyaga ortogonal va ***normallangan funktsiya*** yoki ***qisqacha ortonormallangan funktsiya*** deyiladi.

Xususiy qiymatlarning uzluksiz (tutash) spektri. Agar $\hat{L}$ operatorni xususiy qiymatlari uzluksiz bo`lsa, u holda yuqoridagi teoremani bu hol uchun bevosita ishlatib bo`lmaydi. Ammo bu holda ham Ermit operatorining xususiy qiymatlari haqiqiy bo`ladi. Shuning xususiy funktsiyalar va xususiy qiymatlar uchun

$$\hat{L}\psi_L(x) = L\psi_L(x) \tag{13}$$

tenglamani yozsak bo`ladi. Bunda $\psi_L(x)$ funktsiya $L$ parametrga bog`liq. Uzluksiz spektr uchun (3) ortogonallik sharti o`rinli, ya'ni

$$\int \psi_L^*(x)\psi_{L'}(x)dx = 0, \qquad L \neq L'. \tag{14}$$

Biroq, yuqorida aytganimizdek, uzluksiz spektrning xususiy funktsiyalarini diskret spektrdagi kabi birga normallab bo`lmaydi, chunki uzluksiz spektr uchun xususiy funktsiya modulining kvadrati cheksizlikka teng bo`lib qoladi:

$$\int \psi_L^*(x)\psi_{L'}(x)dx = \infty, \qquad L = L'. \tag{15}$$

Shuning uchun uzluksiz spektrni normallash uchun Dirakning delta-funktsiyasidan foydalaniladi.

$$\delta(L) = \begin{cases} 0, & \text{agar } L \neq 0 \text{ bo`lsa,} \\ \infty, & \text{agar } L = 0 \text{ bo`lsa.} \end{cases} \tag{16}$$

**Xususiy funktsiyalar sistemasining to`laligi.** Matematikada operatorlarni xususiy funktsiyalar sistemasi to`la sistema hosil qilishi bilan hosil qilinadi. Bu degani istalgan $y(x)$ ni berilgan o`zgaruvchilar sohasida xususiy funktsiyalari bo`yicha qatorga yoyish mumkin ekanligini bildiradi:

$$\psi(x) = \sum_n c_n\psi_n(x). \tag{17}$$

Bunda c_n – doimiy, umumiy holda kompleks bo`lib, yoyilish koeffitsientlari, ya'ni xususiy holatlarning amplitudalari deb qarasa bo`ladi.

y_n funktsiyani (11) xossadan foydalanib, yoyilish koeffitsienti c_n ni topish mumkin. Shu maqsadda (17) ifodani ψ_m^* ga ko`paytiramiz va barcha o`zgaruvchilar sohasida integrallaymiz:

$$\int \psi_m^*(x)\psi(x)dx = \sum_n c_n \int \psi_m^*(x)\psi_n(x)dx. \tag{18}$$

y_n funktsiyani ortonormallash xossasiga binoan o`ng tomonidagi integral $\delta_{nm}$ delta simvoliga teng. (12) ga ko`ra

$$\int \psi_m^*(x)\psi(x)dx = \sum_n c_n\delta_{nm} = c_m.$$

Bu ifodadagi m indekslarni p indekslarga almashtirsak

$$c_n = \int \psi_m^*(x)\psi(x)dx$$

natijaga kelamiz.

7.1. Quyidagi operatorlarning xususiy funksiya ψ va xususiy qiymatlarini aniqlang: a) $-i\frac{d}{dx}$, agar $\psi(x)=\psi(x+a)$ bo`lsa; b) $-i\frac{d^2}{dx^2}$, agar $\psi$ =0 bo`lsa, x =0 va $x=l$ qiymatlarida.

Yechish: a) $-\frac{d}{dx}\psi(x)=\lambda\psi(x)$, $\frac{d\psi}{dx}=i\lambda dx$

Bundan

$$\psi(x)=Ce^{i\lambda x}$$

kelib chiqadi.

$$\psi(x)=\psi(x+a)$$

shartdan

$$\lambda a=i2\pi n \text{ va } \lambda_n=\frac{2\pi}{a}n, \text{ bunda } (n=0,\pm1,\pm2,....).$$

b) $-\frac{d^2x}{dx^2}=\lambda\psi(x)$ yechimni quyidagicha ko`rinishda yozamiz:

$$\psi=C_1\sin\sqrt{\lambda}x+C_2\cos\sqrt{\lambda}x.$$

Chegaraviy shartlardan foydalanib,

$$\psi(0)=C_2=0, \qquad \psi(l)=C_1\sin\sqrt{\lambda}l=0$$

bundan

$$\sqrt{\lambda}l=\pi n, \qquad (n=0, \pm1, \pm2, \ldots)$$

Demak xususiy funksiya

$$\psi(x)=C_2\sin\sqrt{\lambda}x.$$

Xususiy funksiyalar esa

$$\lambda_n=\frac{\pi^2n^2}{l^2}, \qquad (n=0, \pm1, \pm2, \ldots).$$

7.2. Ushbu operatorlarning xususiy funksiyasi va xususiy qiymatlari topilsin: a) $\hat{L}_z=-i\hbar\frac{\partial}{\partial\varphi}$; b) $\hat{L}_z^2=-\hbar^2\frac{\partial^2}{\partial\varphi^2}$; c) $\hat{A}=-i\hbar\frac{\partial}{\partial\varphi}+a\sin\varphi$ (bu yerda φ – azimutal burchak).

Yechish: a) $-i\hbar\frac{\partial\psi}{\partial\varphi}=L_z\psi$

yechimni

$$\psi(\varphi)=Ae^{i\frac{L_z}{\hbar}\varphi}$$

$\psi(\varphi)=\psi(\varphi+2a)$ bir qiymatlili shartidan

$$L_z=m\hbar, \quad (m=0, \pm1, \pm2, \ldots).$$

aniqlaymiz. Normallashtirish shartidan

$$\int_0^{2\pi}\psi(\varphi)\psi^*(\varphi)d\varphi=1, \quad A=\frac{\lambda}{\sqrt{2\pi}}.$$

Shuning uchun normallashgan xususiy funksiyalar quyidagi ko`rinishga ega bo`ladi.

$$\psi_m(\varphi)=(2\pi)^{-\frac{1}{2}}e^{i\varphi m}.$$

b) $L_z^2=m^2\hbar^2$, (m=0, ±1, ±2, …)

$$\psi_m(\varphi)=(2\pi)^{-\frac{1}{2}}e^{i\varphi m}.$$

c) $-i\hbar\frac{\partial\psi}{\partial\varphi}+a\sin\varphi\psi=\lambda\psi$ bu tenglamani yechish uchun ψ funksiyaning

$$\psi(\varphi)=Ae^{\frac{i}{\hbar}(\lambda\varphi+a\cos\varphi)}$$

bir qiymatlilik shartidan:

$$\lambda=m\hbar.$$

xususiy qiymatlarini aniqlaymiz

Normallashtirish shartidan $A=(2\pi)^{-\frac{1}{2}}$ kelib chiqadi. Shuning uchun

$$\psi(\varphi)=\frac{1}{\sqrt{2\pi}}e^{i\left(m\varphi+\frac{a}{\hbar}\cos\varphi\right)}.$$

7.3. $\hat{L}^2$ operatorning $\psi(\theta,\varphi)=A(\cos\theta+2\sin\theta\cos\varphi)$ xususiy funksiyasiga mos keluvchi xususiy qiymatinianiqlang.

Yechish: $\hat{L}^2\psi(\theta,\varphi)=L^2\psi(\theta,\varphi)$

$$\hat{L}^2=-\left(\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\cdot\frac{\partial}{\partial\varphi^2}\right)\hbar^2$$

$$\hat{L}^2\psi=\left(\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}(A\cos\theta+2\sin\theta\cos\varphi)\right)+\frac{1}{\sin^2\theta}\cdot\frac{\partial}{\partial\varphi^2}(A\cos\theta+2\sin\theta\cos\varphi)\right)=$$

$$=\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}(\sin\theta(-A\sin\theta+2\cos\theta\cos\varphi))+\frac{1}{\sin^2\theta}\cdot\frac{\partial}{\partial\varphi}(-2\sin\theta\sin\varphi)=$$

$$=\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(-A\sin^2\theta+\sin 2\theta\cos\varphi)+\frac{1}{\sin^2\theta}(-2\sin\theta\cos\varphi)=$$

$$=\frac{1}{\sin\theta}(-A2\sin\theta\cos\theta-2\cos 2\theta\cos\varphi)-2\frac{\cos\varphi}{\sin\theta}=$$

$$=-2A\cos\theta-2\frac{\cos 2\theta\cos\varphi}{\sin\theta}-2\frac{\cos\varphi}{\sin\theta}=$$

$$= 2\hbar^2\left(A\cos\theta - \frac{\cos 2\theta\cos\varphi}{\sin\theta} - \frac{\cos\varphi}{\sin\theta}\right) = 2\hbar^2\left(A\cos\theta - \left(\frac{\cos 2\theta}{\sin\theta} + \frac{1}{\sin\theta}\right)\cos\varphi\right) =$$

$$= 2\hbar^2\left(A\cos\theta - (\cos 2\theta - 1)\frac{\cos\varphi}{\sin\theta}\right) = 2\hbar^2(\cos\theta + 2\sin\theta\cos\varphi).$$

Demak, $\hat{L} = 2\hbar^2$ ekanini topamiz.

7.4. Impuls tasavvurida $\hat{x}$ operatorning xususiy funksiya va xususiy qiymatlarini aniqlang.

Yechish: Impuls tasavvurida koordinata operatori $\hat{x} = i\hbar\frac{\partial}{\partial p_x}$ kabi yoziladi. Unda xususiy funksiya va xususiy qiymati uchun tenglama quyidagicha yoziladi:

$$i\hbar\frac{\partial\varphi(p_x)}{\partial p_x} = x\varphi(p_x).$$

Bu tenglamaning barcha shartlarini qanoatlantiruvchi yechim quyidagicha aniqlanadi.

$$\varphi(p_x) = Ce^{-\frac{i}{\hbar}xp_x}$$

bunda x – ixtiyoriy son. Shuning uchun $\hat{x}$ ning xususiy qiymatlari uzluksizdir.

7.5. Zarra cheksiz chuqur potensial o`rada ($0 \le x \le a$) $\psi(x) = A\sin\frac{2\pi}{a}x$ funksiya bilan aniqlanuvchi holatda joylashgan. Uning impulslar bo`yicha taqsimotini aniqlang.

Yechish: Normallashtirish shartidan $A = \sqrt{\frac{2}{a}}$ ekanini topamiz. Bu to`lqin funksiyani impuls tasavvurida quyidagicha ko`rinishga ega.

$$\varphi(p) = (a\pi\hbar)^{-1/2}\int_0^a \sin\frac{2\pi x}{a}\cdot e^{-\frac{ixp}{\hbar}}dx = -2\hbar(a\pi\hbar)^{1/2}\cdot\frac{e^{-\frac{iap}{\hbar}} - 1}{4\pi^2\hbar^2 - a^2p^2}.$$

Shuning uchun zarrachani p va dp impulslar intervalida topish ehtimolligi

$$dW(p) = |\psi(p)|^2 dp = \frac{16\pi a\hbar^3\sin^2\frac{ap}{2\hbar}}{\left(a^2p^2 - 4\pi^2\hbar^2\right)^2}dp.$$

7.6. Bir o`lchovli potensial o`rada ($0 \le x \le a$) zarra $\psi(x) = A\cdot x(a - x)$ funksiya bilan ifodalanuvchi holatda joylashgan. To`lqin funksiyani energiya tasavvurida yozing va energiyaning o`rtacha qiymatini aniqlang.

Yechish: Normallashtirish shartidan foydalanib $A^2 = \frac{30}{a^5}$ ekanini topamiz. Energiya operatorining xususiy qiymatlari uchun tenglama

$$\frac{d^2\psi(x)}{ax^2} + \frac{2m_0}{\hbar^2}E\psi = 0$$

kabi energiya xususiy qiymatlari esa

$$E_n = \frac{\pi^2\hbar^2 n^2}{2m_0 a^2}.$$

7.7. $\frac{\partial}{\partial x}$ va $i\frac{d}{dx}$ operatorlarning xususiy funksiya va xususiy qiymatlarnini toping.

7.8. Quyidagi operatorlarning xususiy funksiya va xususiy qiymatini toping: a) $\left(x + \frac{d}{dx}\right)$; b) $d/d\varphi$; v) $\sin\frac{d}{d\varphi}$; g) $i\frac{d}{d\varphi}$.

7.9. $\frac{d^2}{dx^2} + \frac{2}{x}\frac{d}{dx}$ operatorlarning xususiy funksiya va xususiy qiymatini toping.

7.10. Erkin zarra kinetik energisi operatori $T = -\frac{\hbar^2}{2m}\Delta$ ning xususiy funksiya va xususiy qiymatlarini aniqlang.

8-mavzu: Fizik kattaliklar operatorlari, ularning hususiy qiymat va hususiy funksiyalari

Koordinata va impulsning operatorlari. To`lqin funktsiya zarra koordinatasining funktsiyasi bo`lgani uchun zarra koordinatasining operatori $\hat{x}$, x soniga teng, ya’ni

$$\hat{x} = x,\ \hat{y} = y,\ \hat{z} = z.$$

Odatda koordinata operatorlarini belgisi “$\wedge$” ni qo`yilamaydi. Impuls operatorining proektsiyalari

$$\hat{P}_x = -i\hbar\frac{\partial}{\partial x},\ \hat{P}_y = -i\hbar\frac{\partial}{\partial y},\ \hat{P}_z = -i\hbar\frac{\partial}{\partial z}$$

vektor ko`rinishi esa

$$\hat{P} = -i\hbar\vec{\nabla}.$$

Mikrozarraning harakat miqdori momenti. Yuqorida aytganimizdek, impuls momenti va uning operatori:

$$\vec{L} = [\vec{r}\vec{p}], \qquad \hat{\vec{L}} = \left[\hat{\vec{r}}\,\hat{\vec{p}}\right].$$

Bundan

$$\hat{L}_x = \hat{P}_z\, y - \hat{P}_y\, z = i\hbar\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right),$$

$$\hat{L}_y = \hat{P}_x\, z - \hat{P}_z\, x = i\hbar\left(x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}\right),$$

$$\hat{L}_z = \hat{P}_y\, z - \hat{P}_x\, y = i\hbar\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right).$$

va

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2\left\{\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right)^2 + \left(x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}\right)^2 + \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)^2\right\}.$$

8.1. Ushbu kommutatsiya qoidalarini tekshiring: a) $\left[\hat{L}_z \cdot \hat{L}_y\right] = i\hbar\,\hat{L}_z$; b) $\left[\hat{L}_y \cdot \hat{L}_z\right] = i\hbar\,\hat{L}_x$; c) $\left[\hat{L}_z \cdot \hat{L}_x\right] = i\hbar\,\hat{L}_y$.

Yechish: a) $\left[\hat{L}_z \cdot \hat{L}_y\right]_- = \hat{L}_z\,\hat{L}_y - \hat{L}_y\,\hat{L}_z =$

$$= \left(x\hat{P}_y - y\hat{P}_x\right)\cdot\left(z\hat{P}_x - x\hat{P}_z\right) - \left(zP_x - xP_z\right)\cdot\left(xP_y - yP_x\right) =$$

$$= xP_y \cdot zP_x - x\hat{P}_y \cdot x\hat{P}_z - yP_x \cdot zP_x + yP_x \cdot xP_z - (z\hat{P}_x \cdot x\hat{P}_y - zP_x \cdot yP_x -$$

$$- xP_z \cdot xP_y + xP_z \cdot yP_x = x \cdot zP_yP_x - x^2\,\hat{P}_y\,\hat{P}_z - y\cdot z\,\hat{P}_x + yP_x \cdot xP_z -$$

$$- zP_x \cdot xP_y + z \cdot yP_x^{\;2} - x^2 P_z P_y + xyP_zP_x =$$

$$= xzP_yP_x + xyP_zP_x + yP_xxP_z - zP_xxP_y =$$

$$= xP_x(zP_y + yP_z) + xP_x(yP_z - zP_y) = xP_x(yP_z) + xP_x(yP_z) =$$

$$= xP_x(yP_z) + \left(-i\hbar\frac{\partial}{\partial x}(x(yP_z))\right) = xP_x(yP_z) - i\hbar\left(yP_z + x\frac{\partial}{\partial x}(yP_z)\right) = i\hbar\,\hat{L}_z\,.$$

8.2. Ushbu kommutatsiya qoidalarini tekshiring: a) $\left[\hat{L}_x, \hat{P}_x\right]_- = 0$; b) $\left[\hat{L}_x, \hat{P}_y\right] = i\hbar\,\hat{P}_z$; c) $\left[\hat{L}_x, \hat{P}_z\right] = -i\hbar\,\hat{L}_x\,\hat{P}_y$

8.3. Sferik koordinatalar sistemasidan foydalanib impuls momenti kvadrati operatori $\hat{L}^2$ ning Laplas operatori va T – kinetik energiya operatori orasidagi bog`lanishni toping.

Yechish: $T = -\frac{\hbar^2}{2m_0}\nabla^2 = \hat{T}_2 + \frac{\hat{L}^2}{2m_0 r^2}$, bunda $T_2 = -\frac{\hbar^2}{2m_0}\cdot\frac{\hat{\lambda}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)$.

8.4 Diskret spektrning statsionar holatida zarra impulsining o`rtacha qiymati nolga tengligini ko`rsating.

Yechish: Ma'lumki, $\left[\hat{H}, x\right]_- = -\frac{i\hbar}{m_0}\hat{P}_x$.

Shuning uchun zarracha impulsining o`rtacha qiymati quyidagicha topiladi.

$$\overline{P_x} = \int\psi^*\hat{P}_x\psi dx = \int\psi^*\frac{im_0}{\hbar}\left(\hat{H}x - x\hat{H}\right)\psi dx.$$

Gamilton operatori $\hat{H}$ ning ermit operatori ekanligidan foydalansak

$$\overline{P_x} = \frac{im_0}{\hbar}\int\left(x\psi\hat{H}\psi^* - x\psi^*\hat{H}\psi\right)dx = \frac{im_0}{\hbar}\int E(x\psi\psi^* - x\psi^*\psi)dx = 0,$$

bunda $\hat{H}\psi = E\psi$ ekanligi hisobga olindi.

8.5. $\hat{L}_z$ operatorning xususiy qiymatiga mos keluvchi ψ holatda L_x va L_z o`rtacha qiymatlarining nolga tengligi ko`rsatilsin.

Yechish: Ma'limki $\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x$, shuning uchun

$$\overline{L_x} = \frac{1}{i\hbar}\int\psi^*\left[\hat{L}_y\hat{L}_z - \hat{L}_z\hat{L}_y\right]\psi d\tau.$$

Endi $\hat{L}_z$ operatorning ermit ekanligidan foydalansak va $\hat{L}_z$ ning xususiy funksiyasi ψ ekanligini inobatga olsak, ya'ni

$$\hat{L}_z\psi = L_z\psi,$$

$$\overline{L_x} = \frac{1}{i\hbar}\int\left(L_z\psi^*\hat{L}_y\psi - \left(\hat{L}_y\psi\right)\hat{L}_z^*\psi^*\right)d\tau = \frac{1}{i\hbar}\int\psi^*\left(L_z - L_z^*\right)\left(\hat{L}_y\psi\right)d\tau = 0,$$

chunki $L_z = L_z^*$, xuddi shuningdek $\overline{L_y} = 0$ ekanini ko`rsatish mumkin emas.

8.6. p tasavvuridagi zarra radius vektori operatori $\hat{r} = i\hbar\frac{\partial}{\partial\vec{p}}$ ekanini ko`rsating.

Yechish: Koordinata tasavvurida $\hat{\vec{r}} = \vec{r}$, p-tasavvurga o`tish uchun radius vektorning o`rttacha qiymatidan foydalanamiz.

$$< \vec{r} >= \int \varphi^*(\vec{p})\vec{r}\varphi(\vec{p})d^3 p$$

bunda

$$\varphi(\vec{p}) = (2\pi\hbar)^{-3/2}\int \psi(\vec{r})e^{-\frac{i}{\hbar}\vec{p}\vec{r}} d\tau .$$

$\psi(\vec{r})$ funksiyaning $\psi_{\vec{p}}$ funksiya bo`yicha yoyilmasining koeffitsientlari

$$\psi(\vec{r}) = (2\pi\hbar)^{-3/2}\int \varphi(\vec{p})e^{\frac{i}{\hbar}\vec{p}\vec{r}} d^3 p ,$$

ikkinchi tomondan

$$< \vec{r} >= \int \psi^*(\vec{r})\vec{r}\psi(\vec{r})d\tau .$$

Yuqoridagilari e'tiborga olib va bo`laklab integrallab $\vec{r}\psi(\vec{r})$ni quyidagicha yozish mumkin:

$$< \vec{r} >= (2\pi\hbar)^{-3/2}\iint \psi^*(\vec{r})e^{\frac{i}{\hbar}\vec{p}\vec{r}} i\hbar\frac{\partial\varphi(\vec{p})}{\partial\vec{p}}d^3 p d\tau = \int \varphi^*(\vec{p})i\hbar\frac{\partial\varphi(\vec{p})}{\partial\vec{p}}d^3 p .$$

Bu ifodani eng yuqorida keltirilgan ifoda bilan taqqoslab

$$\hat{\vec{r}} = i\hbar\frac{\partial}{\partial\vec{p}}$$

ekanini olamiz.

8.7. Chiziqli garmonik ossilyator uchun $\bar{x}^2$ ning o`rtacha qiymatini toping.

Yechish: Ma'lumki chiziqli garmonik ossilyator to`lqin funksiyasi Ermit polinomlari orqali ifodalanar edi

$$\psi_n(\xi) = \left[n!\cdot 2^n\sqrt{\pi}\right]^{-1/2} H_n(\xi)\cdot\exp\left(-\frac{\xi^2}{2}\right).$$

Energiyasi spektri esa

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

kabi aniqlanadi.

Bu to`lqin funksiyaning xossalaridan foydalanib $\bar{x}^2$ ni hisoblash mumkin.

Buning uchun dastlab $\xi = x\sqrt{\frac{m_0\omega}{\hbar}}$ kattalikni $\psi_n(\xi)$ dagi o`rtacha kvadratik og`ishini hisoblaymiz. Uning o`rtacha qiymati

$$\langle\xi\rangle = \int_{-\infty}^{+\infty}\psi_n{}^2(\xi)\cdot\xi\cdot d\xi = 0 ,$$

chunki integral ostida ξ ning tok funksiyasi turibdi. Shuning uchun

$$\langle \Delta\xi^2 \rangle_n = \langle \xi^2 \rangle_n = \int_{-\infty}^{+\infty} \psi_n \xi^2 d\xi . \qquad (1)$$

Ermit polinominit

$$\xi \cdot H_n(\xi) = nH_{n-1}(\xi) + \frac{1}{2} H_{n+1}(\xi)$$

xossasidan foydalanib

$$\xi \cdot \psi_n = \sqrt{\frac{n}{2}}\psi_{n-1} + \sqrt{\frac{n+1}{2}}\psi_{n+1}$$

ekanini topamiz. Bu tenglikni yana bir marta qo`llab

$$\xi^2 \cdot \psi_n(\xi) = \frac{1}{2}\sqrt{n(n-1)}\psi_{n-2} + \left(n + \frac{1}{2}\right)\psi_n + \frac{1}{2}\sqrt{(n+1)(n+2)}\psi_{n+2} \qquad (2)$$

ekanini aniqlaymiz. (2) ni (1) ga qo`yib va $\Psi_n(\xi)$ funksiyalarning ortonormalligidan foydalanib

$$\langle \xi \rangle^2 = n + \frac{1}{2} \qquad \text{yoki} \quad \vec{x}_n^2 = \left(n + \frac{1}{2}\right)\frac{\hbar}{m_0 \omega}$$

ekanini topamiz.

8.8. Impuls momenti kvadrati operatori $\hat{L}^2$ ning xususiy funksiya va xususiy qiymatlari topilsin.

Yechish: $\hat{L}^2$ operator xususiy qiymat va funksiyalarini topish uchun $\hat{L}^2 \psi = L^2 \psi$ tenglamani yechish kerak. Buning uchun $\hat{L}^2$ operatorning sferik koordinatalar sistemasidagi ko`rinishidan foydalanamiz

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{L^2}{\hbar^2}\right)\psi(\theta,\varphi) = 0 .$$

Bu tenglamani sferik funksiyalar uchun yozilgan tenglamasi

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + l(l+1)\right)Y_{l,m}(\theta,\varphi) = 0$$

bilan taqqoslab

$$L^2 = \hbar^2 l(l+1), \qquad l = 0,\ 1,\ 2,\ \ldots$$

qidirilayotgan xususiy qiymatlarni topamiz har bir l va $2l+1$ ta $Y_{lm}(\theta,\varphi)$ funksiya mos keladi, m=0, ±1, ±2,…. – magnit kvant soni.

$$Y_{lm}(\theta,\varphi) = \theta_{lm}(\theta)\frac{\exp(im\varphi)}{\sqrt{2\pi}}$$

Bunda

$$\theta_{lm}(\theta) = \frac{(-1)^{l+m}}{2^l l!}\sqrt{\frac{(2l+1)(l-m)!}{2(l+m)!}}(\sin\theta)^m \frac{d^{l+m}(\sin\theta)^{2l}}{(d\cos\theta)^{l+m}} .$$

Bu funksiyani Lemandr polinomlari orqali ham ifodalash mumkin:

$$\theta_{lm}(\theta)=(-1)^m\left[\frac{(2l+1)(l-m)!}{2(l+m)!}\right]^{1/2}\sin^m\theta\frac{\partial^m}{(\partial\cos\theta)^m}p_l(\cos\theta)$$

Shuni ham hisoblash mumkinki sferik funksiyalar o`z navbatida $\hat{L}_z=-i\hbar\frac{\partial}{\partial\varphi}$ – impuls momenti yig`indisi proyeksiyasi operatorining ham xususiy funksiyalari hisoblanadi, ya'ni:

$$-i\hbar\frac{\partial}{\partial\varphi}Y_{lm}(\theta,\varphi)=\hbar mY_{lm}(\theta,\varphi)$$

o`rinli.

8.9. Energiyasi $\frac{5}{2}\hbar\omega$ teng bo`lgan garmonik ossilyator uchun o`rtacha kinetik energiyani hisoblang.

8.10. $\hat{L}_z$ va $\hat{L}_z^2$ - operatorlarning xususiy funktsiyalarini toping.

8.11. $\psi(\varphi)=A(1+\cos\varphi)^2$ to`lqin funksiya bilan xarakterlanuvchi kvant holatda $L_z$ operatorning xususiy qiymatlarini va shu holatda bo`lish ehtimolini aniqlang.

9-mavzu: Shryodinger tenglamasi. Statsionar holatlar

Shryodingerning vaqtga bog`liq tenglamasini bir o`lchamli fazo uchun

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\hat{H}\psi(x,t) \tag{1}$$

ko`rinishda yoziladi, bunda $\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x,t)$ – Gamilton operatori.

Tashqi o`zgaruvchan maydonlar bo`lmaganda, $\hat{H}$ – gamiltanian vaqtga bog`liq bo`lmaydi va u $\hat{H}(x)$ to`la energiya operatori bilan mos tushadi. Bu tenglamaning yechimi

$$\psi(x,t)=A\exp\left[-\frac{i}{\hbar}(Et-px)\right]$$

ko`rinishdagi to`lqin funktsiyaga ega.

x va t o`zgaruvchilarga ajratish usulini qo`llab ushbu funktsiyani

$$\psi(x,t)=\psi(x)f(t)$$

shaklga keltiramiz. Bunda

$$\psi(x)=Ae^{-\frac{i}{\hbar}px} \qquad \text{va} \qquad f(t)=e^{-\frac{i}{\hbar}Et}.$$

Yuqoridagi ifodani

$$\psi(x,t)=\psi(x)e^{-\frac{iEt}{\hbar}} \tag{2}$$

ko`rinishda yozish mumkin.

Bundan vaqt bo`yicha birinchi tartibli hosila olsak:

$$\frac{\partial\psi(x,t)}{\partial t}=-\frac{i}{\hbar}E\psi(x)e^{-\frac{i}{\hbar}Et}, \tag{3}$$

x koordinata bo`yicha ikkinchi tartibli

$$\frac{\partial^2\psi(x,t)}{\partial x^2}=\frac{\partial^2\psi(x)}{\partial x^2}e^{-\frac{i}{\hbar}Et} \tag{4}$$

ko`rinishdagi munosabatga olib keladi.

(1), (2) va (3) larni (4) tenglamaga qo`yamiz va natijada

$$i\hbar\left(-\frac{i}{\hbar}E\psi(x)\right)e^{-\frac{i}{\hbar}Et}=-\frac{\hbar^2}{2m}\frac{\partial\psi(x,t)}{\partial x^2}e^{-\frac{i}{\hbar}Et}+U\psi(x)e^{-\frac{i}{\hbar}Et}$$

tenglik kelib chiqadi. Bu tenglikni ikkala tomonini $\exp\left[-\frac{iEt}{\hbar}\right]$ ko`paytuvchiga qisqartirib va $\frac{\partial^2}{\partial x^2}$ ni $\frac{d^2}{dx^2}$ ga almashtirib

$$E\psi(x)=-\frac{\hbar^2}{2m}\frac{\partial\psi(x,t)}{\partial x^2}+U\psi(x) \tag{5}$$

tenglamani hosil qilamiz. Ushbu tenglamaga ***Shryodingerning vaqtga bog`liq bo`lmagan*** yoki ***statsionar tenglama*** deb ataladi. Bu tenglamadagi $\psi(x)$ funktsiyani ham ***to`lqin funktsiya*** deb atashadi.

(5) tenglamani kanonik (standart) shaklda yozamiz, ya’ni

$$\frac{d\psi(x,t)}{dx^2}+\frac{2m}{\hbar^2}(E-U)\psi(x)=0. \tag{6}$$

Bu tenglamada $U(x)$ – potentsial funktsiya oshkor ravishda vaqtga bog`liq emas deb hisoblanadi. (6) tenglamani o`lchamli fazoga ham juda oson ifodalash mumkin:

$$\nabla^2\psi(r)+\frac{2m}{\hbar^2}(E-U)\psi(r)=0.$$

9.1. t=0 paytda yassi rotatorning to`lqin funksiyasi kabi $\psi=A\sin^2\varphi$ bo`lsa, uning keyingi vaqt momentlari uchun to`lqin funksiyasini aniqlang.

Yechish: Masalada vaqtga bogliq Shryodinger tenglamasi

$$\hat{H}\psi(\varphi,t)=i\hbar\frac{\partial\psi(\varphi,t)}{\partial t}$$

ni yuoridagi boshlangich shartlar asosida yechish talab etiladi. Buning uchun o`zgaruvchilar t va φ ni ajratish usuli bilan bu tenglamaning xususiy yechimini topamiz.

$$\psi_m(\varphi,t)=e^{im\varphi-\frac{i\hbar m^2}{2I}t}, \qquad (m=0,\pm1,\pm2,\ldots)$$

Bu tenglamaning umumiy yechimi

$$\psi_m(\varphi,t)=\sum_m c_m\psi_m(\varphi,t)$$

kabi bo`lib, c koeffitsientlar boshlangich shartdan topiladi

$$\psi(\varphi,0)=\sum_m c_m e^{im\varphi}=A\sin^2\varphi.$$

Bundan c koeffitsientlarni aniqlab, umumiy yechimni aniqlaymiz.

$$\psi(\varphi,t)=\frac{A}{2}\left(1-\cos 2\varphi\cdot e^{-\frac{2i\hbar}{I}t}\right).$$

Normallashtirish shartidan $\int\limits_0^{2\pi}|\psi(\varphi,t)|^2 d\varphi=1$ foydalanib, $\frac{A}{2}=\frac{1}{\sqrt{3\pi}}$ ekanini aniqlaymiz.

9.2. Erkin zarra uchun Shryodingerning vaqtga bogliq tenglamasi umumiy yechimini toping.

9.3. $t=0$ vaqtda erkin zarraning to`lqin funksiyasi quyidagicha bo`lsa , uning keyingi vaqt momentlari uchun to`lqin funksiyasini aniqlang:

a) $\psi(x,0)=\sqrt{\frac{2}{\pi\hbar}}\sin\left(\frac{xp_0}{\hbar}\right)$; b) $\psi(x,0)=(2\pi\hbar)^{-\frac{1}{2}}e^{i\frac{xp_0}{\hbar}}$.

9.4. Erkin zarraning energiyasi spektri uzluksiz ekanligini ko`rsating.

9.5. Statsionar holatda fizik kattalikning biror qiymatga ega bo`lish ehtimolligi vaqtga bog`liq emasligini ko`rsating.

9.6. $H\psi=i\hbar\frac{\partial\psi}{\partial t}$ tenglamaning E_1 va E_2 energiyali holatlarga mos yechimlari mos ravishda ψ_1 va ψ_2 bo`lsa, ularning chiziqli kombinatsiyasi $\psi=C_1\psi_1+C_2\psi_2$ ham shu tenglamaning yechimi bo`la olishini ko`rsating.

10-mavzu: Turli operatorlarning hosilasini hisoblash. Harakat integrallari

Dinamik o`zgaruvchilarning o`rtacha qiymati vaqt o`tishi bilan o`zgaradi. Kvant mexanikasida fizikaviy kattalikning o`rtacha qiymati

$$<L>=\int\psi^*(x,t)\hat{L}\psi(x,t)dx \qquad (1)$$

ifoda bilan aniqlanadi. (1) ifodaning ikkala qismidan vaqt bo`yicha differentsial olamiz. U holda

$$\frac{d}{dt}<L>=\int\psi^*(x,t)\frac{d\hat{L}}{dt}\psi(x,t)dx+\int\frac{\partial\psi^*(x,t)}{\partial t}\hat{L}\psi(x,t)dx+ \\ +\int\psi^*(x,t)\hat{L}\frac{\partial\psi(x,t)}{\partial t}dx \qquad (2)$$

ifoda o`rinli bo`ladi. (2) ifodadagi birinchi had $\frac{\partial L}{\partial t}$ ning o`rtacha qiymati va nolga teng.

Shryodinger tenglamasidan foydalangan holda, (2) ifodadagi ikkinchi va uchinchi hadlarni soddalashtirib yozamiz. Shryodinger tenglamasi

$$i\hbar\frac{\partial\psi}{dt}=\hat{H}\psi$$

cheksiz kichik vaqt oralig`ida o`rtacha qiymatning o`zgarishini hisoblaydi. Bu tenglamani quyidagicha yozamiz:

$$\frac{\partial\psi}{dt}=\frac{1}{i\hbar}\hat{H}\psi, \qquad \frac{\partial\psi^*}{dt}=-\frac{1}{i\hbar}\hat{H}^*\psi^*. \qquad (3)$$

(3) tenglamalarni e'tiborga olgan holda (2) ifodani quyidagi ko`rinishga keltiramiz:

$$\frac{d}{dt}\langle L\rangle=\left\langle\frac{\partial L}{\partial t}\right\rangle-\frac{1}{i\hbar}\int\left(\hat{H}^*\psi^*\right)\left(\hat{L}\psi\right)dx+\frac{1}{i\hbar}\int\psi^*\left(\hat{L}\hat{H}\psi\right)dx. \qquad (4)$$

$\hat{H}$ operatorni ermitligidan foydalanib, (4) ifodadagi birinchi integralni quyidagicha yozamiz:

$$\int\hat{H}^*\psi^*\left(\hat{L}\psi\right)dx=\int\psi^*\left(\hat{H}^*\hat{L}\psi\right)dx. \qquad (5)$$

(5) ni (4) ga qo`ysak

$$\frac{d}{dt}\langle L\rangle=\left\langle\frac{\partial L}{\partial t}\right\rangle+\frac{1}{i\hbar}\int\psi^*\left(\hat{L}\hat{H}-\hat{H}\hat{L}\right)\psi dx \qquad (6)$$

ifoda hosil bo`ladi.

Quyidagicha belgilash kiritamiz:

$$\left[\hat{H},\hat{L}\right]=\frac{1}{i\hbar}\left(\hat{L}\hat{H}-\hat{H}\hat{L}\right). \qquad (7)$$

(7) belgini (6) ga qo`ysak, u ixcham ko`rinishga keladi, ya'ni

$$\frac{d}{dt}\langle L\rangle=\left\langle\frac{\partial L}{\partial t}\right\rangle+\left\langle\left[\hat{H},\hat{L}\right]\right\rangle. \qquad (8)$$

va

$$\frac{d\hat{L}}{dt}=\frac{\partial\hat{L}}{\partial t}+\left[\hat{H},\hat{L}\right]. \qquad (9)$$

$\left[\hat{H},\hat{L}\right]$ – kommutatorni ***Puassonning kvant qavslari*** deb atashadi.

Puassonning kvant qavslari klassik fizikadagi Puassonning qavslariga o`xshash. Klassik fizikada $L$ dinamik o`zgaruvchidan vaqt bo`yicha olingan to`la hosila

$$\frac{dL}{dt}=\frac{\partial L}{\partial t}+\sum_i\left(\frac{\partial L}{\partial x_i}\frac{\partial x_i}{\partial t}+\frac{\partial L}{\partial p_i}\frac{\partial p_i}{\partial t}\right) \tag{10}$$

formula bilan beriladi. Bunda x_i – koordinatalar, p_i – impulslar.

Gamilton tenglamalari

$$\frac{dx_i}{dt}=\frac{\partial H}{\partial p_i},\quad \frac{dp_i}{dt}=\frac{\partial H}{\partial x_i}$$

dan foydalanib (10) ni quyidagicha yozamiz:

$$\frac{dL}{dt}=\frac{\partial L}{\partial t}+\sum_i\left(\frac{\partial H}{\partial p_i}\frac{\partial L}{\partial x_i}+\frac{\partial L}{\partial p_i}\frac{\partial H}{\partial x_i}\right)=\frac{\partial L}{\partial t}+[H,L]. \tag{11}$$

Bunda H – Gamilton funktsiyasi.

Klassik fizikada

$$[H,L]=\sum_i\left(\frac{\partial H}{\partial p_i}\frac{\partial L}{\partial x_i}+\frac{\partial L}{\partial p_i}\frac{\partial H}{\partial x_i}\right)$$

kattalikka ***Puassonning qavslari*** deyiladi.

Agar $\hat{L}$ operator yoki L kattalik vaqtga oshkor ravishda bog`liq bo`lmasa, u holda (9) va (11) formulalar quyidagi ko`rinishga keladi:

$$\frac{d\hat{L}}{dt}=\left[\hat{H},\hat{L}\right],$$

$$\frac{dL}{dt}=[H,L].$$

Kvant mexanikasida L kattalik harakat integrali bo`lishi uchun ikkita shartni qanoatlantirishi kerak: 1) vaqtga oshkor bog`liq bo`lmasligi; b) gamiltonion bilan kommutativ, ya’ni $\left[\hat{H},\hat{L}\right]$=0 bo`lishi zarur.

Shunday qilib, kvant mexanikasida L kattalik harakat integrali bo`lishi uchun

$$\frac{d\hat{L}}{dt}=\frac{\partial}{\partial t}\hat{L}+\left[\hat{H},\hat{L}\right]=0$$

munosabat bajarilishi kerak. Agar L kattalik t ga oshkor ravishda bog`liq bo`lmasa

$$\frac{d\hat{L}}{dt}=\left[\hat{H},\hat{L}\right]=0$$

10.1. Agar zarra $U(x)$ potensial maydonda harakatlanayotgan bo`lsa, quyidagi operatorlar hosilasi to`griligini tekshiring: a) $\frac{\partial}{\partial t}\left(x^2\right)=\frac{1}{m_0}\left(x\hat{p}_x-p_x x\right)$; b) $\frac{\partial}{\partial t}\left(xp_x\right)=\left(\frac{p_x^2}{m_0}-x\frac{\partial U}{\partial x}\right)$; c) $\frac{\partial}{\partial t}\left(p_x{}^2\right)=-\left(\hat{p}_x\frac{\partial U}{\partial x}+\frac{\partial U}{\partial x}p_x\right)$.

10.2. Agar zarra $U(x)$ potensial maydonda xaraktlanaetgan bulsa, quyidagi operatorlar tenglamalar to`g`riligini tekshiring: a) $\frac{\partial}{\partial t}(x)=\frac{p_x}{m_0}$; b) $\frac{\partial p_x}{\partial t}=\frac{\partial U}{\partial x}$.

10.3. Kvant mexanikasida xam energiya, impuls va impuls momentlarining harakat integrali ekanini ko`rsating.

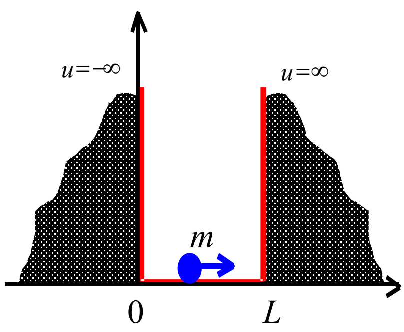
10.4. Kvant mexanikasida biror L kattalikning xarkat integrali bo`la olish shartini yozing.

10.5. Gamiltonian qachon to`la energiya operatoriga mos keladi?

10.6. Operatorlar uchun ushbu qoida urinli bo`lishini tekshiring: $\frac{d}{dt}(AB)=\frac{dA}{dt}B+A\frac{dB}{dt}$

11-mavzu: Shryodinger tenglamasini turli potentsiallar uchun yechish. O`tish va qaytish koeffisientlari

Bir o`lchovli potentsial o`ra. Shryodinger teglamasini bir necha oddiy masalalarni yechishga qo`llaymiz. Bu xil oddiy masalalarni yechishdan maqsad Shryodinger tenglamasining matematik apparatini egallashdir.



1-rasm. Cheksiz potensial o`radagi zarra

Cheksiz potentsial chuqurlikga ega bo`lgan potentsial o`rada yotgan mikrozarra uchun Shryodingerning bir o`lchovli statsionar teglamasini tadbiq etaylik. Bu masalani yechishdan asosiy maqsad – xususiy funktsiyalar va xususiy qiymatlarni topishdir. 1-rasmda ikki tomoni cheksiz baland potentsial devor bilan o`ralgan va x o`qida $(0, L)$ soha bilan chegaralangan potentsial o`ra tasvirlangan.

Zarraning potentsial energiyasi x o`qining $0 \le x \le L$ oralig`ida nolga, x<0 va x>0 sohalarda cheksiz katta qiymatga ega.

Matematika nuqtai nazaridan qaraganda bir o`lchovli harakat uchun bu masalada potentsial energiya quyidagi chegaraviy shartlarni qanoatlantirishi kerak:

$$U(x) = \begin{cases} \infty, & \text{agar } -\infty < x < 0 \text{ bo`lsa,} \\ 0, & \text{agar } 0 < x < \mathrm{L} \text{ bo`lsa,} \\ \infty, & \text{agar } L < x < \infty \text{ bo`lsa.} \end{cases} \quad (1)$$

Potentsialning bunday chegaralanishi o`z navbatida, to`lqin funktsiyani ham quyidagi shartlarni bajarishga majbur qiladi

$$\psi(x) = 0 \text{, agar} \begin{cases} x \le 0, \\ x \ge L \end{cases} \text{ bo`lsa}$$

va

$$\int_0^L \psi^*(x)\psi(x)dx = 1 \text{, agar } 0 < x < L \text{ bo`lsa.} \quad (2)$$

Zarra har bir vaqt paytida o`raning qayerida bo`lishini aniq bilmaymiz, shuning uchun Shryodingerning vaqtga bog`liq bo`lgan tenglamasini bu masalaga qo`llab bo`lmaydi, demak Shryodingerning statsionar teglamasini ishlatamiz.

(1) shartdagi $U(x) = 0$ ni e’tiborga olgan holda

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \quad (3)$$

ni yozamiz va

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad (4)$$

belgilash kiritib, (3) ni quyidagicha yozamiz:

$$\frac{d^2\psi(x)}{dx^2} + \alpha^2\psi = 0. \quad (5)$$

(5) tenglama mikrozarraning o`ra ichidagi holatini xarakterlaydi va bu tenglamaning yechimi umumiy holda

$$\psi(x) = Ae^{i\alpha x} + Be^{-i\alpha x} \quad (6)$$

ko`rinishga ega. Bu yechim o`ra ichida x o`qi buylab bir-biriga qarama-qarshi yo`nalishda harakatlanayotgan to`lqinlarning superpozitsiyasini tasvirlaydi. O`raning devorlari mutlaq qattiq deb hisoblanganligi sababli o`ra ichida turg`un to`lqinlar hosil bo`ladi.

Zarraning to`la energiyasi $E \le U$ dan kichik bo`lganligi sababli, u potentsial o`radan tashqariga chiqib keta olmaydi. Shuning uchun potentsial o`ra chekkasiga yetgan zarra potentsial o`ra devoridan qaytadi, so`ngra, teskari yo`nalishda harakatlanadi, o`raning ikkinchi devoriga o`rilib yana orqaga qaytadi va h.k. Natijada qarama-qarshi zarralarning qo`shilishi tufayli, (6) ko`rinishdagi turg`un to`lqin hosil bo`ladi.

Matematik nuqtai nazardan (6) funktsiyani (5) Shryodinger tenglamasining haqiqatan yechimi ekanligini tekshirish foydalidir.

(6) tenglamadagi A va B doimiylarni aniqlash uchun, (2) chegaraviy shartdan foydalanamiz. x=0 hol uchun $\psi(x)=0$ va (6) tenglama, $0=A+B$ ko`rinishga keladi, bundan $A=-B$.

Demak,

$$\psi(x)=A(e^{i\alpha x}-e^{-i\alpha x}). \tag{7}$$

Eyler formulasi yordamida bu funktsiyani

$$\psi(x)=2iA\sin\alpha x \tag{8}$$

ko`rinishga keltiramiz.

Endi ikkinchi chegaraviy shartni qo`llaymiz, yangi $x=L$ hol uchun $\psi(x)=0$ va

$$0=2iA\sin\alpha x \tag{9}$$

shartga ko`ra, $A\neq 0$, u holda $\sin\alpha L=0$ bo`lishi kerak, bundan

$$\alpha L=\pi n,\ n=1,\ 2,\ 3,\ ... \tag{10}$$

ekanligi kelib chiqadi. (10) dan:

$$\alpha=\frac{\pi n}{L},\ n=1,\ 2,\ 3,\ ... \tag{11}$$

(11) ni (4) ga qo`yib energiya uchun quyidagi formulani olamiz

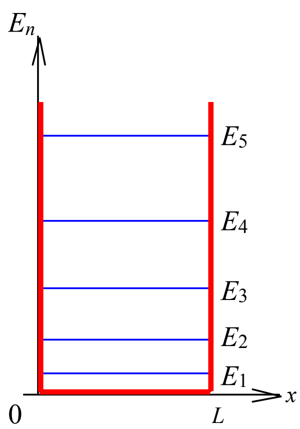
$$E_n=\frac{\hbar^2\alpha^2}{2m}=\frac{\pi^2\hbar^2}{2mL^2}n^2,\ n=1,\ 2,\ 3,\ .... \tag{12}$$

Agar mikrozarra potentsial o`ra ichida yotgan bo`lsa, uning energiyasi (12) tenglamaning ma’lum diskret xususiy qiymatlarigagina teng bo`lgan qiymatlar qabul qila olar ekan. Bu vaziyatda energiya diskret qiymatlarga kvantlanadi va zarra bu diskret holatlardan birida yotishi mumkin. Zarra energiyasining bu qiymatlari ***energetik sathlar*** deb ataladi. Shuni qayd qilamizki zarraning energiyasi nolga teng bo`lmaydi. (12) tenglamaga ko`ra, zarraning eng kichik energiyasini n=1 da olamiz, ya’ni

$$E_1=\frac{\pi^2\hbar^2}{2mL^2}. \tag{13}$$

Xuddi shuningdek n=2, 3, 4, ... lar uchun $4E_1$, $9E_1$, $16E_1$ larni mos ravishda olish mumkin.

(13) munosabat bilan topilgan energiya ***nolinchi energiya*** deb ataladi. Boshqacha aytganda zarraning energiyasi hech qachon nolga teng bo`lmaydi. Bu xulosa noaniqlik munosabatidan kelib chiqib, klassik mexanika qarashiga ziddir. Buni quyidagi mulohazadan ham bilish mumkin. Zarra potentsiali chegarada cheksiz bo`lgan devor orasida joylashgani uchun, uning holati $\Delta x\approx L$ noaniqlik bilan ma’lumdir. Geyzenbergning noaniqlik munosabatiga ko`ra



2-rasm.

impulsni aniqlashdagi noaniqlik $\Delta p \geq \hbar / L$ ga bo`ysunadi. Shunday qilib, energiya hech qachon nolga teng bo`lmaydi, chunki u holda $\Delta p = 0$ shart bajarish talab qilingan bo`lardi.

(12) munosabatdan impulsni ham kvantlanishi kelib chiqadi, ya'ni

$$E_n = \frac{\pi^2 \hbar^2}{2mL^2} n^2 = \frac{p_n^2}{2m}.$$

Bundan

$$p_n = \frac{\pi\hbar}{L} n^2 \text{, bunda } n = 1, 2, 3, ... \tag{14}$$

Shunday qilib, zarra potentsial o`rada "qamoqda" bo`lsa, Shryodingerning statsionar tenglamasining yechimi diskret xususiy qiymatlarga ega bo`lar ekan va energiyaning xususiy qiymatlari (12) formula yordamida topiladi. (13) formula bilan hisoblangan energiya spektrini qiymatlari 1-jadvalda keltirilgan, bu sathlar chizmasi esa 2-rasmda tasvirlangan. Qo`shni sathlar orasidagi masofani chamalaylik va uni masalaning m va L parametrlariga qanday bog`liq ekanligini tahlil qilamiz. Ikki qo`shni sath orasidagi energiya farqi

$$\Delta E_n = E_{n+1} - E_n = \frac{\pi^2\hbar^2}{2mL^2}(2n+1) \approx \frac{\pi^2\hbar^2}{2mL^2} n \text{, } (n >> 1 \text{ uchun}).$$

Olingan ushbu natijadan ko`ramizki ikkita qo`shni energiya sathi orasidagi masofa n ni ortishiga mos ravishda chiziqli o`sadi. Zarra massasini yoki o`raning kengligini ortishi qo`shni sathlar orasidagi masofani kichraytiradi (2-rasm).

Endi potentsial o`ra ichida xususiy funktsiyalar ko`rinishini izlaymiz. (8) to`lqin funktsiyani quyidagi ko`rinishda yozib olamiz.

$$\psi = 2i\alpha \sin\left(\frac{\pi n}{L} x\right). \tag{15}$$

(15) ga qo`shma funktsiya

$$\psi' = -2iA \sin\left(\frac{\pi n}{L} x\right) \tag{16}$$

bo`ladi. Ehtimollik zichligi

$$\psi^* \psi = 4A^2 \sin^2\left(\frac{\pi n}{L} x\right) \tag{17}$$

formula bilan topiladi.

Potentsial o`ra ichida zarrani qayd qilinishi aniq bo`lgani uchun, normallash sharti (2) ga ko`ra

$$\int_0^L \psi^*(x)\psi(x)dx = \int 4A^2 \sin^2\left(\frac{\pi n}{L} x\right) dx = 1.$$

Bu funktsiyani integrallasak

$$4A^2 \int_0^L \sin^2\left(\frac{\pi n}{L} x\right) dx = 2A^2 \left[x - \frac{L}{2\pi n} \sin\left(\frac{\pi n}{L} x\right) \right]\Bigg|_0^L = 2A^2 L,$$

bundan

$$2A^2L = 1 \text{ yoki } A = \frac{1}{\sqrt{2L}}$$

ni olamiz.

Shunday qilib, normallangan to`lqin funktsiyalar quyidagi ko`rinishga keladi:

$$\psi_n(x) = \frac{2i}{\sqrt{2L}}\sin\left(\frac{\pi nx}{L}\right) = i\sqrt{\frac{2}{L}}\sin^2\left(\frac{\pi nx}{L}\right), \tag{18}$$

bunda n=1, 2, 3,...

(18) funktsiyani ***xususiy funktsiyalar*** deb ataladi, chunki n ning har bir qiymatiga mos ravishda yagona funktsiya ko`rinishi to`g`ri keladi.

Endi cheksiz potentsial o`ra ichida zarraning qayd qilinishi ehtimolligini topamiz $x_1 = a$ va $x_2 = b$ interval bilan chegaralangan sohada zarrani o`rnini qayd qilinishi ehtimolligini

$$\int_a^b \psi^*\psi dx = \int_a^b \frac{2}{L}\sin^2\left(\frac{\pi n}{L}x\right)dx \tag{19}$$

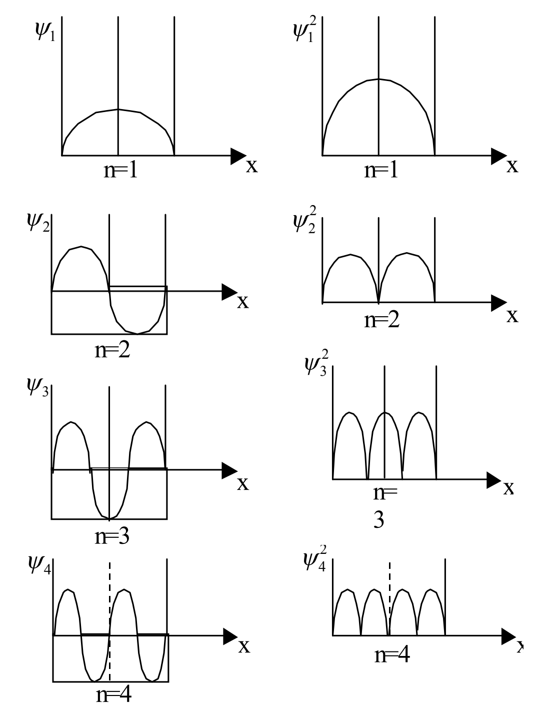
formula bilan aniqlanadi.

Cheksiz potentsial o`ra ichida yotgan zarra uchun qo`yilgan masalaning yechimlari 1-jadvalda umumlashtirilgan.

1-jadval

n	Xususiy funktsiya $\psi(x)$	Ehtimollik zichligi, $\psi^*(x)\psi(x)$	Energiyaning xususiy qiymatlari, E_n
1	$i\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}$	$\frac{2}{L}\sin^2\frac{\pi x}{L}$	$\frac{\pi^2\hbar^2}{2mL^2}$
2	$i\sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L}$	$\frac{2}{L}\sin^2\frac{2\pi x}{L}$	$\frac{4\pi^2\hbar^2}{2mL^2}$
3	$i\sqrt{\frac{2}{L}}\sin\frac{3\pi x}{L}$	$\frac{2}{L}\sin^2\frac{3\pi x}{L}$	$\frac{9\pi^2\hbar^2}{2mL^2}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	$i\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}$	$\frac{2}{L}\sin^2\frac{n\pi x}{L}$	$\frac{n^2\pi^2\hbar^2}{2mL^2}$

n=1, 2, 3,... hollar uchun to`lqin funktsiya va ehtimollik zichligini taqsimlanishi 3-rasmda keltirilgan. Bu grafiklar $n$ nomerli holatlarni fizik ma'nosini ochadi. 3-rasmdan ko`rinadiki n soni o`radagi to`lqin funktsiyalar ko`rinishini belgilaydi. Harakat cheklangan bo`lsa, sistemani hamma holatlarini va unga mos ravishda energetik sathlarni tartib bilan belgilab chiqish mumkin. $(n-1)$ son $\psi_n(x)$ to`lqin funktsiyaning tugunlar sonini (nollarini) beradi. Potentsial chuqurlik chegarasiga tegishli nollar bundan mustasno. Zarraning (o`ra ichida) har qanday nuqtada qayd qilinish ehtimolligi $|\psi|^2$ ga proportsional va 3.b-rasmda n=1, 2, 3,... uchun $|\psi|^2$ larning ko`rinishlari keltirilgan. Rasmdan ko`ramizki, asosiy energetik sathda, ya'ni n=1 holda zarrani eng katta ehtimollik bilan potentsial o`ra o`rtasida $\left(x=\frac{L}{2}\right)$ topamiz, potentsial o`raning chekkalarida esa zarraning qayd qilish ehtimolligi aksincha nolga teng. $n$=2 uchun esa xususiy funktsiyani ko`rinishi 3.a-rasmdagi kabi bo`lib, $x=\frac{L}{2}$ nuqtada (ya'ni o`ra o`rtasida) zarraning qayd qilinishi ehtimolligi esa nolga teng. Shunday qilib, zarraning energetik sathi $E_2$ bo`lsa, u holda uni $x=\frac{L}{4}$ nuqtada bo`lishi ehtimolligi kattadir.

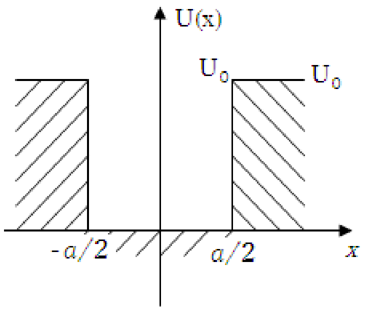


3-rasm.

Demak, potentsial o`ra ichida ma'lum nuqtalarda zarraning qayd qilinishi ehtimolligi $n$ ning qiymatiga bog`liq bo`lib, uning o`zgarishi bilan ehtimollik ham keskin o`zgaradi. 3-rasmdan ko`ramizki n ning qiymati kattalashgan sari, ya'ni energiya kattalashgani bilan $|\psi_n|^2$ ning maksimumlari bir-biriga yaqinlashib boradi va n ning katta qiymatlarida $|\psi_n|^2$ taqsimoti klassik fizikaning taqsimoti bilan br xil bo`lib qoladi. Boshqacha aytganda Borning moslik printsipi bu masala uchun ham o`rinlidir. Shunday qilib, bu masalada ham to`lqin funktsiyaning o`zi emas, balki modulining kvadrati fizik ma'noga egadir. Energetik sathlar orasidagi oraliq

$$\frac{\Delta E_n}{E_n}=\frac{2\Delta n}{n+1}$$

ko`rinishga ega.



4-rasm.

11.1. 4-rasmda ko`rsatilgan shakldagi potensial o`radan m_0 massali zarra energiyasi diskret qiymatlarini aniqlash uchun tenglamani oling. $E < U_0$ sohada energiya qiymatlari diskretligini asoslang.

$$U(x) = \begin{cases} U_0, & \text{agar } x < -a/2, \\ 0, & \text{agar } -a/2 < x < a/2, \\ U_0, & \text{agar } x > a/2. \end{cases}$$

Yechish: Bir o`lchovli Shryodinger tenglamasini yozamiz:

$$\left[\frac{d^2}{dx^2} + \frac{2m_0}{\hbar^2}\left(E - U(x)\right)\right]\psi(x) = 0. \tag{1}$$

Potensial simmetriyasi masalani yechishni osonlashtiradi. Yechimni x ning musbat qiymatlari sohasi uchun topishning o`zi yetarli.

Biz shartda berilganidek, $E < U_0$ energiya qiymatlarida masalani yechamiz. Buning uchun quyidagicha belgilashlar kiritamiz

$$k^2 = \frac{2m_0 E}{\hbar^2}, \qquad \chi^2 = \frac{2m_0}{\hbar^2}\left(U_0 - E\right) \tag{2}$$

Unda (1) ning shakli ushbu ko`rinishga keladi:

$$\left(\frac{d^2}{dx^2} + k^2\right)\cdot\psi_{\mathrm{I}} = 0, \qquad 0 \le x \le \frac{a}{2},$$

$$\left(\frac{d^2}{dx^2} - \chi^2\right)\cdot\psi_{\mathrm{II}} = 0, \qquad x \ge \frac{a}{2}.$$

$x \to \infty$ dagi ψ_{II} ning chekli yechimini

$$\psi_{II} = A \cdot e^{-\chi\cdot x},$$

ψ_I ning yechimi esa

$$\psi_I^{(+)} = B\cos kx$$

shaklda qidirami.

Bu funksiyaning o`zlari va birinchi tartibli hosilalari uzluksizligidan $x = a/2$ nuqtada A, B larni aniqlash uchun quyidagi tenglamalarni olamiz

$$\begin{cases} B\cos\dfrac{ka}{2} = A \cdot e^{-\frac{\chi a}{2}} \\ B\sin\dfrac{ka}{2} = \dfrac{\chi}{k} A \cdot e^{-\frac{\chi a}{2}} \end{cases} \tag{3}$$

Bu sistema faqat ushbu shart bajarilgandagina noldan farqli yechimga ega

$$k \cdot tg\frac{ka}{2} = \chi = \sqrt{\frac{2m_0U_0}{\hbar^2} - k^2}\ ,$$

tangens davri π ga teng davriy funksiya bo`lgani uchun bu tenglama quyidagicha yoziladi:

$$ka = \pi n - 2\arcsin\frac{\hbar k}{\sqrt{2m_0U_0}}; \qquad n = 1,\ 2,\ 3,\ \ldots.$$

Ushbu tenglama zarraning energiya spektrini aniqlovchi transindent tenglamadir.
Arksinus qiymati birdan kichikligi sababli

$$0 \le k \le \frac{\sqrt{2m_0U_0}}{\hbar}$$

intervalda o`zgaradi.

11.2. Oldingi masaladan foydalanib zarraning asosiy holatini energiyasi $E_1 = \frac{3}{4}U_0$ qiymatni qabul qilgan bo`lsa, a^2U_0 ning qiymatini toping.

Yechish: Masala shartiga asosan $E_1 = \frac{3}{4}U_0$ energiya diskret spektri esa $E_n = \frac{\hbar^2 k_n^2}{2m_0}$ ifodadan topilar edi. Bu ikki tenglamadan:

$$E_1 = \frac{\hbar^2 k_1^2}{2m_0} = \frac{3}{4}U_0\,,$$

bundan

$$k_1 = \sqrt{\frac{3}{2} \cdot \frac{m_0U_0}{\hbar^2}}$$

ekanini topamiz.

Buni oldingi masaladagi k qiymatlarini aniqlovchi tenglamaga qo`ysak

$$k_1 \cdot a = \pi - 2\arcsin\frac{\hbar k_1}{\sqrt{2m_0U_0}}$$

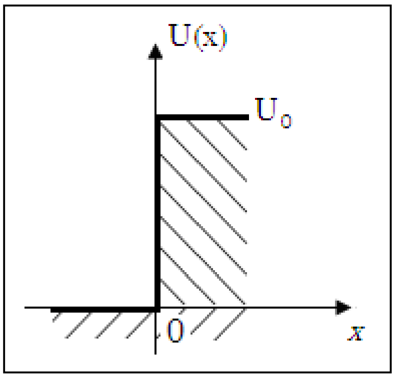
$$\sqrt{\frac{3}{2} \cdot \frac{m_0U_0}{\hbar^2}} \cdot a = \pi - 2\arcsin\frac{\hbar\sqrt{\frac{3}{2} \cdot \frac{m_0U_0}{\hbar^2}}}{\sqrt{2m_0U_0}} = \pi - 2\arcsin\frac{\sqrt{3}}{2} = \pi - \frac{2\pi}{3} = \frac{\pi}{3};$$

$$\sqrt{\frac{3}{2} \cdot \frac{m_0U_0}{\hbar^2}} \cdot a = \frac{\pi}{3}$$

bundan

$$a^2U_0 = \frac{2\pi^2}{27} \cdot \frac{\hbar^2}{m_0}$$

ekanini topish qiyin emas.



11.3. m_0 massali zarra

$$U(x)=\begin{cases} U_0, & \text{agar } x>0, \\ 0, & \text{agar } x>0. \end{cases}$$

potensial maydonda harakatlanganda $E>U_0$ energiyali hol uchun to`lqin funksiyani aniqlang. O`tish koeffitsienti D va qaytish koeffitsienti R larni aniqlang.

Yechish: Shryodinger tenglamasining ichki $U(x)$ sohadagi umumiy yechimlari quyidagicha: $E>U_0$.

$$\psi_I = A_1\cdot e^{ik_1x}+B_1\cdot e^{-ik_1x}, \qquad x<0,$$
$$\psi_{II} = A_2\cdot e^{ik_2x}+B_2\cdot e^{-ik_2x}, \qquad x>0.$$

Bunda

$$k_1=\frac{1}{\hbar}\sqrt{2m_0E}\,; \qquad k_2=\frac{1}{\hbar}\sqrt{2m_0(E-U_0)}$$

va A_1 – tushayotgan to`lqin amplitudasi, $B_1$ – qaytgan to`lqin amplitudasiga mos keladi. x>0 sohada faqat o`tgan to`lqin mavjud bo`lishidan B_2=0 ekanini aniqlash qiyin emas.

Qaytish koeffitsienti qaytgan to`lqin intensivligining tushgan nur intensivligiga nisbati bilan aniqlanadi

$$R=\frac{|B_1|^2}{|A_1|^2}.$$

ψ va ψ' larning uzluksizligidan (x=0 nuqtada) $A_1+B_1=A_2$,

$$A_1-B_1=\frac{k_2}{k_1}A_2 .$$

Bundan

$$R=\left(\frac{k_1-k_2}{k_1+k_2}\right)^2$$

ni olamiz. O`tish koeffitsienti esa o`tgan to`lqin intensivligining tushgan nur intensivligiga nisbatiga teng

$$D=\left(\frac{A_2}{A_1}\right)^2=\frac{4\cdot k_1\cdot k_2}{(k_1+k_2)^2}$$

kabi aniqlanadi.

11.4 Ushbu $\psi(x)=C\sin\dfrac{\pi x}{a}$ kvadrat integrallanuvchi funksiyaning $(0,a)$ kesmada chekliligini tekshiring.

Yechish:

$$\psi(x) = C\sin\frac{\pi x}{a}.$$

Bu funksiyaning chekliligini tekshirish uchun uni OX o`qida $(0, a)$ kesmada integrallaymiz

$$\int_0^a C^2 \sin^2\frac{\pi x}{a}dx = \frac{a}{2}C^2.$$

Demak, funksiya chekli ekan. Normallashtirish shartidan C doimiyning qiymatini aniqlaymiz

$$\int_0^a C^2 \sin^2\frac{\pi x}{a}2x = 1, \qquad C^2 = \sqrt{\frac{2}{a}}$$

11.5. Erkin zarra uchun ehtimollik oqim zichligini hisoblang.

Yechish: Erkin zarra to`lqiniga mos keluvchi

$$\psi(x, y, z, t) = Ce^{\frac{i}{\hbar}(\vec{p}\vec{r} - Et)}$$

dan va ehtimollik oqim zichligi ifodasidan

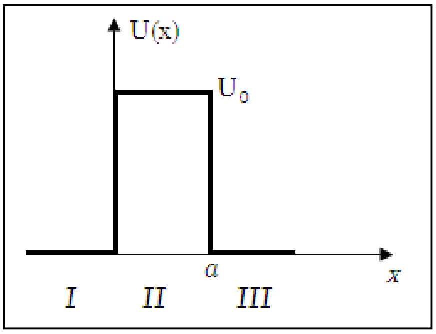
$$\vec{j} = \frac{\hbar R^2}{m}\mathrm{grad}\,\alpha$$

dan foydalanib

$$j = \frac{\hbar}{m}|C|^2\mathrm{grad}\left(\vec{k}\vec{r}\right) = \frac{\hbar k}{m}|C|^2 = \frac{P}{m}|C|^2$$

Biz C ni shunday tanlaymizki j sirt birlik yuzasini vaqt birligida kesib o`tuvchi zarralar soniga teng bo`lsin. $j = n\vec{v}$ deb olib, $|C|^2 = n$ ekanini aniqlaymiz, bu yerda n – zarralar konsentratsiyasi.

11.6 Mikrozarraning



$$U(x) = \begin{cases} U_0, & \text{agar } x \le 0, \\ 0, & \text{agar } 0 < x < 0, \\ U_0, & \text{agar } a \ge a. \end{cases}$$

potensial to`siqdan qaytishi va o`tish ehtimolliklarini (koeffitsienlarini) aniqlang.

Yechish: Potensial to`siq to`g`ri burchakli bo`lib, o`tish uchun uch sohada Shryodinger tenglamasi quyidagicha

$$\left.\begin{aligned} &\frac{d^2\psi_1}{dx^2} + k^2\psi_1 = 0, \qquad k^2 = \frac{2mE}{\hbar^2}, \\ &\frac{d^2\psi_2}{dx^2} + q^2\psi_2 = 0, \qquad q^2 = \frac{2m}{\hbar^2}(E - U), \\ &\frac{d^2\psi_3}{dx^2} + k^2\psi_3 = 0, \qquad k^2 = \frac{2mE}{\hbar^2}. \end{aligned}\right\} \qquad (1)$$

Chegaraviy shartlarni yozamiz:

$$\left.\begin{array}{ll}\psi_1(0)=\psi_2(0) & \psi_2(a)=\psi_3(a)\\ \psi_1'(0)=\psi_2'(0) & \psi_2'(a)=\psi_3'(a)\end{array}\right\} \tag{2}$$

(1) sistemaning tenglamalari umumiy yechimlari

$$\left.\begin{array}{l}\psi_1=Ae^{ikx}+Be^{-ikx}\\ \psi_2=Ce^{i\xi x}+De^{-i\xi x}\\ \psi_3=Fe^{ikx}+Ge^{-ikx}\end{array}\right\}. \tag{3}$$

Bu yechimdagi koeffitsientlar (2) chegaraviy shartlardan foydalanib topiladi.

I va III sohada zarralar erkin harakat qiladi shuning uchun ularga mos to`lqinlar tahlilidan $G=0$.

Endi o`tish koeffitsientlarini ehtimollik oqim zichliklarini topamiz

$$j_{tush}=\frac{\hbar k}{m}|A|^2$$

$$j_{qayt}=\frac{\hbar k}{m}|B|^2$$

$$j_{o't}=\frac{\hbar k}{m}|F|^2$$

Bundan

$$P=\frac{j_{o't}}{j_{tush}}=\frac{|F|^2}{|A|^2}\ ;\quad R=\frac{j_{qayt}}{j_{tush}}=\frac{|B|^2}{|A|^2}$$

o`tish va qaytish koeffitsientlarini aniqlash mumkin: $j_{tush}=j_{qayt}+j_{o't}$.

(1) chegaraviy shartdan foydalanib mos koeffitsientlarni topamiz

$$\frac{F}{A}=\frac{4kqe^{-ika}}{(k+q)^2e^{-iqa}-(k-q)^2e^{iqa}}$$ yoki

$$\frac{F}{A}=\frac{2qke^{-ika}}{2qk\cos qa-i(k^2+q^2)\sin qa}.$$

Endi mos o`tish va qaytish koeffitsientlarini topamiz:

$$P=\frac{4qk^2}{4q^2k^2\cos^2 qa+(k^2+q^2)^2\sin^2 qa}$$

$$R=1-P=\frac{(k^2-q^2)^2}{(k^2+q^2)^2+4k^2q^2\mathrm{ctg}qa}.$$

11.7. Erkin zarra uchun ehtimolli oqim zichligini hisoblang.

Yechish: Erkin zarra to`lqiniga mos keluvchi $\psi(x,y,z,t) = Ce^{\frac{i}{\hbar}(\vec{p}\vec{r}-Et)}$ dan va ehtimolli oqim zichligi ifodasi $\vec{j} = \frac{\hbar R^2}{m}\mathrm{grad}\alpha$ dan foydalanib

$$j = \frac{\hbar}{m}|C|^2 \mathrm{grad}(\vec{k}\vec{r}) = \frac{\hbar k}{m}|C|^2 = \frac{P}{m}|C|^2.$$

Biz C ni shunday tanlaymizki j sirt birlik yuzasini vaqt birligida kesib o`tuvchi zarralar soniga teng bo`lsin.

$$j = n\vec{v}$$

deb olib

$$|C|^2 = n$$

ekanini aniqlaymiz, bunda n – zarralar konsentratsiyasi.

11.8. Chiziqli garmonik ossillyator uchun Shryodinger tenglamasining xususiy funksiya va xususiy qiymatlarini aniqlang.

11.9 Ushbu

$$U(x) = \begin{cases} \infty, & \text{agar } x < 0, \\ 0, & \text{agar } 0 < x < a, \\ U_0, & \text{agar } x > a. \end{cases}$$

shakldagi potensial o`radan m_0 massali zarra energiyasi diskret qiymatlarini aniqlang.

12-mavzu: Markaziy maydonda harakat. Radial Shryodinger tenglamasini yechish. Holatni ifodalovchi kvant sonlariga doir masalalar

N.Bor nazariyasi yangi kvant qonuniyatlarni tushunishda katta qadam bo`ldi. Lekin boshidanoq Bor nazariyasi jiddiy kamchiliklardan holi emasligi ayon edi. U yarim klassik, yarim kvant nazariya edi. Bor nazariyasining dastlabki yutuqlarini e’tiborga olgan holda, uning bir qator muammolarni hal qila olmaganligini aytib o`tish ham zarur. Bor nazariyasi quyidagi muammolarni hal qila olmadi:

1. Nima uchun o`tishlar faqat berilgan energetik sathlar orasida bajariladi-yu, xoxlaganida emas?

2. Nima uchun statsionar orbitada harakat qilayotgan elektronlar elektromagnit nurlanish chiqarmaydi va spiralsimon harakat qilib yadroga qulab tushmaydi?

3. Murakkab atomlar, xususan geliy va litiy spektrining tabiati qanday?

Kvant mexanikasi va to`lqin funktsiya tushunchalaridan foydalangan Ervin Shryodinger atom tuzilishi tugal nazariyasini yaratish imkoniga ega bo`ldi. Shryodinger nazariyasini tushunish uchun eng oddiy strukturaga ega bo`lgan vodorod atomi misolida ko`ramiz.

Kvant mexanikasi tarixidagi eng katta yutuqlar bu oddiy atomlar spektrini detallarigacha tushuntirib berishi va kimyoviy elementlarning davriyligini ham tushuntirishi edi. Shu bilan birga kimyoviy elementlarning sirli hossalarining sifatiy tushuntirilishi kvant mexanikasining rivojlanishiga juda katta ijobiy ta'sir ko`rsatadi.

Bu masalani hal etish uchun atomda elektronning hatti-harakatini mufassal o`rganamiz: birinchi navbatda uning fazoda taqsimlanishini hisoblaymiz.

Vodorod atomini to`la tavsiflash uchun ikkala zarraning – elektron va protonning ham harakatini e'tiborga olish zarur. Biroq masalani soddalash uchun protonni elektronga nisbatan juda og`ir zarra $(1836\,m_e)$ deb uning harakatini hisobga olmaymiz va proton atomning markazida turibdi deb faraz qilamiz.

Ikkinchidan, elektronning spinini ham inobatga olmaymiz. Relyativistik mexanika qonunlari orqali tasvirlangan elektron spini umuman moddalarga kam hissa qo`shadi, deb hisoblaymiz. Boshqacha aytganda Shryodingerning norelyativistik tenglamalaridan foydalanamiz.

Yuqorida aytilgan taxminlar asosida atom fazosining u yoki bu nuqtasida elektronning qayd qilinishi (kuzatilishi) amplitudasi holat va vaqt funktsiyasi sifatida qaraladi.

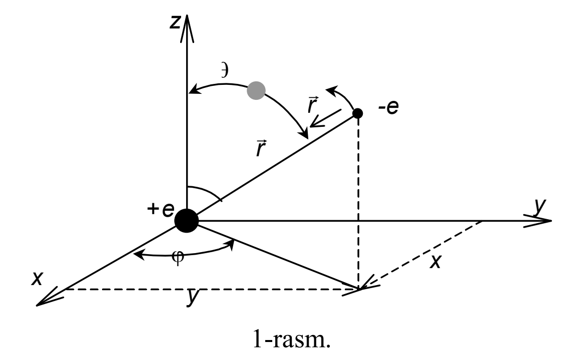
t vaqt momentida x, y, z nuqtada elektronning qayd qilinish amplitudasi $\psi(x, y, z, t)$ deb belgilaylik. Kvant mexanikasiga ko`ra, bu amplitudaning vaqt bo`yicha o`zgarish tezligi, shu funktsiyaga ta'sir etayotgan Gamilton operatorini beradi. Avvalgi bobdan bilamizki,

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\,\psi \tag{1}$$

bunda

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(r), \tag{2}$$

bu yerda m – elektron massasi, $U(\vec{r})$ – protonning elektrostatik maydonidagi elektronning potentsial energiyasi.



1-rasm.

1-rasmda vodorod atomi tasvirlangan (klassik tushuncha nuqta nazaridan). Dekart koordinatalar sistemasini boshiga proton joylashtirilgan. Kulon kuchi tajribada r radiusli orbita bo`ylab elektron harakat qilayotgan bo`lsin. 1-rasmda elektron markazida turgan protonga nisbatan aylanmoqda. Haqiqatda esa ikkala zarra ham ular uchun umumiy bo`lgan massa markazi atrofida aylanmoqda. Biz soddalashtirilgan model bilan, ya’ni protonni qo`zg`almas deb ish ko`ramiz. U holda Kulon maydonidagi elektronning potentsial energiyasi

$$U(r) = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}, \tag{3}$$

bunda e – elektron zaryadi va ε_0=8,85·10^{-12} F/m – elektr doimiysi.

Kvant mexanikasi nuqtai nazaridan elektron to`lqinlar yig`indisidan tashkil topgan sistema bo`lib, u (3) Kulon maydonining potentsial o`rasi bilan chegaralangan. Bu esa diskret energetik sathlarga va xususiy to`lqin funktsiyalar yechimi masalasiga olib keladi. Bunday qarash, o`rada ruxsat etilgan to`lqinlar sistemasining to`plami mavjudligi va ulardan har biri bo`lgan energiyaning biror mumkin bo`lgan qiymatiga mos keldai degan fikrga olib keldai. Bu holda to`lqin tenglamasini uch o`lchovli ko`rinishda yozishga to`g`ri keladi.

Bunday qarashda ψ to`lqin funktsiya

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r} \tag{4}$$

tenglikni qanoatlantirishi kerak.

Biz aniq energiyaga ega bo`lgan holatni izlaganimiz uchun yechimni

$$\psi(\vec{r},t) = \exp\left(-\frac{i}{\hbar}Et\right)\psi(\vec{r}) \tag{5}$$

ko`rinishda yozamiz. U holda $\psi(\vec{r})$ funktsiya

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \left(E + \frac{e^2}{r}\right)\psi \tag{6}$$

tenglikni yechimi bo`lishi kerak. Vodorod atomi statsionar holatda bo`lgani uchun Shryodingerning vaqtga bog`liq bo`lmagan tenglamasidan foydalanish ma’qul.

Tenglamadan ko`rinib turibdiki, Laplas operatori va psi-funktsiya $x, y, z$ ga bog`liq, ammo $U(r)$ potentsial energiya x, y, z ning emas, balki r masofaning funktsiyasidir.

Potentsial energiya faqat r ga bog`liq bo`lgani uchun (6) tenglamani qutbiy koordinatalar sistemasida yechgan ma’qul.

To`g`ri burchakli koordinatalar sistemasida Laplasian

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \tag{7}$$

Masala simmetriyaga ega bo`lgani uchun, eng qulay koordinatalar sistemasi sferik sistemadir. Bunday sistema 1-rasmda tasvirlangan. Sferik koordinatalar bo`lib, $\vec{r}$ –radius vektor, θ – qutbiy burchak va φ – azimutal burchak xizmat qiladi.

Sferik koordinatalar sistemasidan to`g`ri burchakli koordinatalarga o`tish formulasi

$$x = r\sin\theta\cos\varphi\,, \quad y = r\sin\theta\sin\varphi\,, \quad z = r\cos\varphi \tag{8}$$

Elementar hajm

$$dV = dxdydz = r^2 \sin\theta\sin\varphi d\theta d\varphi\,,$$

bunda $0 \le r \le \infty$, $0 \le \theta \le \pi$, $0 \le \varphi \le 2\pi$ va $r = \sqrt{x^2 + y^2 + z^2}$ koordinata boshidan R nuqtaga o`tkazilgan radius vektorning uzunligi. $\theta = \arccos\dfrac{z}{\sqrt{x^2 + y^2 + z^2}}$ – radius-vektor bilan $z$ o`q tashkil qilgan (qutbiy) burchak, $\varphi = \mathrm{arctg}\left(\dfrac{y}{x}\right)$ – radius-vektorning (XY) tekisligiga proektsiyasining x o`qi bilan tashkil qilgan (azimutal) burchagi.

Matematik almashtirishlar yordamida Laplas operatorini sferik koordinatalarda ifodalasak, u holda $\psi(\vec{r}) = \psi(r,\theta,\varphi)$ funktsiya uchun:

$$\nabla^2\psi(r,\theta,\varphi) = \frac{1}{r}\frac{\partial^2}{\partial x^2}(r\psi) + \frac{1}{r^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right\} \tag{9}$$

tenglikni yozish mumkin.

Bundan sferik koordinatalar sistemasida $\psi(r,\theta,\varphi)$ funktsiyani qanoatlantiruvchi statsionar Shryodinger tenglamasi

$$\begin{aligned} -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin\theta}\frac{\partial\psi}{\partial\varphi}\right] + \\ + \left(-\frac{e^2}{4\pi\varepsilon_0 r}\psi\right) = E\psi \end{aligned} \tag{10}$$

ko`rinishga ega. Shunday qilib, to`lqin funktsiya endi r, θ va φ ga bog`liq, ya'ni $\psi = \psi(r,\theta,\varphi)$.

Shryodinger tenglamasini qismlarga ajratish. Umuman olganda, to`lqin funktsiya $r$ va $\theta$, $\varphi$ burchaklarga bog`liq. To`lqin funktsiya maxsus hollarda burchakka bog`liq bo`lmasligi mumkin. Agar to`lqin funktsiya burchakka bog`liq bo`lmasa, amplituda koordinata sistemasini burilishiga bog`liq bo`lmaydi. Bu holda harakat miqdori momentining barcha komponentalari nolga teng bo`ladi. Natijada to`lqin funktsiya to`la harakat miqdori momenti nolga teng bo`lgan holatni xarakterlaydi va u s-***holat*** deyiladi.

(10) tenglamaning qulay tomoni uni uchta tenglik orqali yozish mumkinligidir. Buning uchun (10) ning yechimini uchta funktsiya ko`paytmasi tarzida ifodalaymiz:

$$\psi(r,\theta,\varphi) = R(r)\Theta(\theta)\Phi(\varphi)\,. \tag{11}$$

Bu yerda $R(r)$ – radial to`lqin funktsiya bo`lib, θ va φ burchaklarning o`zgarmas qiymatida psi-funktsiyaning radius-vektori bo`yicha o`zgarishini xarakterlaydi; $\Theta(\theta)$ – qutbiy funktsiya bo`lib, radius-vektor va φ burchakning o`zgarmas qiymatida markaziy maydon sferasi meridiani bo`ylab to`lqin funktsiya $\psi$ ning zenit (qutb) burchagi $\theta$ ga bog`liq o`zgarishini tasvirlaydi; $\Phi(\varphi)$ – azimutal to`lqin funktsiya bo`lib $r$ va $\theta$ ning o`zgarmas qiymatida ψ ning ushbu sfera paralleli bo`ylab o`zgaruvchi azimut burchagi φ ga bog`liq o`zgarishini xarakterlaydi. (11) ifodani (10) tenglamaga qo`yamiz va $2mr^2/\hbar^2$ ga ko`paytirib quyidagini olamiz.

$$\Theta\Phi\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{R\Theta}{\sin^2\theta}\frac{d^2\Phi}{d\varphi^2}+\frac{\Phi R}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+$$
$$+\frac{2mr^2}{\hbar^2}\left(E+\frac{e^2}{4\pi\varepsilon_0 r}\right)R\Theta\Phi=0. \qquad (12)$$

O`zgaruvchilarga ajratish usulidan foydalanib, (12) ni $y=R\Theta\Phi$ ga bo`lib, faqat r ga, faqat θ ga va faqat φ ga bog`liq bo`lgan uchta alohida tenglamalarga ajratish mumkin. Natijada faqat r ga bog`liq bo`lgan radial qism va faqat θ va φ ga bog`liq bo`lgan burchak qismini ajratish mumkin bo`ladi:

$$R\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\Phi}{\sin^2\theta}\frac{d^2\Phi}{d\varphi^2}+\frac{\Theta}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{2mr^2}{\hbar^2}\left(E+\frac{e^2}{4\pi\varepsilon_0 r}\right)=0. \qquad (13)$$

Har birini $l(l+1)$ ko`rinishdagi doimiylikka tenglaylik:

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left(E+\frac{e^2}{4\pi\varepsilon_0 r}\right)=l(l+1)R. \qquad (14)$$

va

$$\frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\varphi^2}+\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=l(l+1). \qquad (15)$$

ni hosil qilamiz.

Shuningdek (15) ni ikkita bir-biriga bog`liq bo`lmagan tenglama ko`rinishida yozish mumkin. Buning uchun (15) ni $\sin^2\theta$ ga ko`paytirib, guruhlab quyidagi tenglik ko`rinishiga keltiramiz.

$$\frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\varphi^2}=l(l+1)\sin^2\theta-\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)$$

hosil bo`lgan tenglikni ikki tomonini bir o`zgarmasga m_l^2 ga teng bo`lgan holdagina o`rinlidir.

$$\frac{m_l^2}{\sin^2\theta}-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=l(l+1) \qquad (16)$$

va

$$\frac{d^2\Phi}{d\varphi^2} + m_l^2\Phi = 0. \tag{17}$$

Shunday qilib, Shryodinger tenglamasini uchta oddiy differentsial tenglamalarga ajratdik.

12.1. Massasi m_0 va orbital momenti 0 ga teng bo`lgan zarra radiusi $r_0$ bo`lgan cheksiz devorli potensial o`rada joylashgan bo`lsa, uning to`lqin funksiyasi va energiyasi xususiy qiymatlarini aniqlang.

Yechish: l=0 orbital momentga ega bo`lgan holda Shryodinger tenglamasi radial tenglamasi quyidagi ko`rinishga ega:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2m_0E}{\hbar^2}k = 0,$$

Bundan $R(r) = \frac{\lambda(r)}{r}$ almashtirish bajarib, $\lambda(r)$ uchun tenglama yozamiz:

$$\lambda''(r) + k^2\lambda(r) = 0, \qquad k^2 = \frac{2m_0E}{\hbar^2}.$$

Bundan

$$\lambda(r) = A\sin(kr + \alpha),$$

bu yerda A va α – integrallash doimiylari. $r \to 0$ $R(r)$ ning chekliligidan α =0 ekanini olamiz.

$$R(r_0) = 0 = \frac{A \cdot \sin kr_0}{r_0}$$

chegaraviy shartdan $kr_0 = \pi n$ (n=1, 2, 3, ...) ni olamiz. Demak, energiya xususiy qiymatlari

$$E_n = \frac{\pi^2\hbar^2}{2m_0r_0^2} \cdot n^2.$$

Unda s (l=0) holatning to`lqin funksiyasi

$$\psi_{n,0,0} = R(r)Y_{0,0}(\theta,\varphi) = C\frac{1}{2}\sin\frac{2\pi}{r_0} \cdot r.$$

Normallashtirish shartidan $C = (2\pi r_0)^{-1/2}$ ni olamiz.

Shunday qilib

$$\psi_{n,0,0} = \frac{1}{\sqrt{2\pi r_0}} \cdot \frac{1}{r} \cdot \sin\frac{\pi n}{r_0} \cdot r_0$$

ni olamiz.

12.2. Massasi m_0 bo`lgan zarra

$$U(r)=\begin{cases}0, & \text{agar } r<r_0,\\ U_0, & \text{agar } r>r_0,\end{cases}$$

potensial maydonda harakatlanadi. $R(r)=\frac{1}{r}\lambda(r)$ almashtirish bilan s (l=0) holat uchun $E<U_0$ da energiya xususiy qiymatlari uchun tenglama

$$\sin kr_0=\pm\sqrt{\frac{\hbar^2}{2m_0r_0^2U_0}}kr_0$$

ko`rinishda bo`lishini ko`rsating.

12.3. Vodorod atomida $1s$ – elektronning maydonning klassik chegarasidan tashqarisida bo`lishi ehtimolligini aniqlang.

Yechish: $1s$ – elektron uchun vodorod atomi effektiv potensiali quyidagiga teng

$$U_{ef}=-\frac{e^2}{4\pi\varepsilon_0^2}+\frac{\hbar^2 l(l+1)}{2m_0r^2}=-\frac{e^2}{4\pi\varepsilon_0 r}$$

Elektron energiyasi bu hol uchun

$$E=-\frac{m_0e^4}{32\pi^2\varepsilon_0^2\hbar^2}$$

ga teng. Klassik tasavvur bo`yicha harakat $0\le r\le r^*$ sohada $E>U_{ef}$ bo`lgan holda harakat mavjud bo`ladi,
bunda

$$r^*=2a_0=\frac{8\pi\varepsilon_0\hbar^2}{m_0e^2}$$

ga teng. Unda izlanayotgan ehtimollik quyidagicha aniqlanadi:

$$W_{r>2a_0}=\frac{U}{a_0^3}\int_{2a_0}^{\infty}r^2\exp\left(-\frac{2r}{a_0}\right)dr=13e^{-4}\approx 0{,}238.$$

12.4. $1s$ – holatdagi elektronning vodorodsimon atomning markazida hosil qilgan o`rtacha elektrostatik potensiali aniqlansin.

Yechish: Elektron bulutining ixtiyoriy $\vec{r}$ nuqtada hosil qilgan $\varphi_e(r)$ o`rtacha potensiali Puasson tenglamasining markaziy simmetrik yechimi kabi aniqlanadi.

$$\frac{1}{r}\frac{d^2}{dr^2}(r\varphi_e)=-\frac{\rho(r)}{\varepsilon_0}$$

bunda zaryad zichligi

$$\rho(r)=e|\psi_{1S}|^2$$

kabi aniqlanadi. Bu tenglamani ikki marta integrallab

$$\psi_e(r) = \frac{e_0}{4\pi\varepsilon_0}\left(\frac{1}{r} + \frac{1}{a_0}\right) \cdot e^{-\frac{2r}{a_0}} + \frac{B}{2} + A$$

yechimga kelamiz. A, B koeffitsientlarni shunday topamizki $\varphi_e(\infty) = 0$, $\varphi_e(0)$ chekli bo`lsin. Unda

$$A=0,\ B = -\frac{e_0}{4\pi\varepsilon_0}$$

ekanini topamiz. $\varphi_e(r)$ ga yadro potensiali $\varphi_e = \frac{e_0}{4\pi\varepsilon_0 r}$ ni qo`yib

$$\varphi = \frac{e_0}{4\pi\varepsilon_0}\left(\frac{1}{r} + \frac{1}{a_0}\right) \cdot e^{-\frac{2r}{a_0}}$$

ni olamiz.

12.5. Devorlari qattiq cheksiz chuqur potensial o`radagi zarraning $\frac{1}{4}a \le x \le \frac{3}{4}a$ sohada bo`lish ehtimolini aniqlang (a – chuqur kengligi).

12.6. To`gri burchakli bir o`lchovli cheksiz chuqur potensial o`radagi $n$- energetik holatidagi zarraning quyidagi kattaliklarning o`rtacha qiymatini aniqlang: $\bar{x}$, $\bar{p}_x$ va $(\Delta x)^2$.

13-mavzu: Sferik funktsiyalarga doir masalalar

Yuqorida Shryodinger tenglamasini uchta oddiy differentsial tenglamalarga ajratdik. Ikkinchi tartibli, birinchi tartibli hosilasi bo`lmagan azimutal to`lqin tenglama

$$\frac{d^2\Phi}{d\varphi^2} + m_l^2\Phi = 0$$

quyidagi yechimlarga ega:

$$\Phi = A\exp(im_l\varphi), \tag{16.19}$$

bunda Φ – xususiy azimutal to`lqin funksiya, φ – azimutal burchak, m_l – doimiy son, A – amplituda.

Azimutal to`lqin funksiya bir qiymatlilik shartini qanoatlantirishi shart. Shuning uchun

$$\Phi(\varphi) = \Phi(\varphi + 2\pi),$$

Bundan

$$e^{2i\pi m_l} = 1,$$

ya’ni

$$e^{i\frac{L_z}{\hbar}\varphi}=e^{i\frac{L_z}{\hbar}(\varphi+2\pi)}.$$

Bundan

$$e^{i\frac{L_z}{\hbar}2\pi}=1$$

kelib chiqadi. Bu shart bajarilishi uchun $\frac{L_z}{\hbar}$ – butun son bo`lishi kerak, ya’ni $\frac{L_z}{\hbar}=m_l\hbar$, bunda m_l=0, ±1, ±2,….

Normallash shartiga ko`ra

$$A=\frac{1}{\sqrt{2\pi}}$$

bo`ladi. Shunday qilib, normallangan to`lqin funksiya

$$\Phi m_l(\varphi)=\frac{1}{\sqrt{2\pi}}e^{im_l\varphi}$$

ga ega bo`lamiz (bunda m_l=0, ±1, ±2,….).

Qutbiy burchak θ uchun yozilgan tenglama

$$\frac{m_l^2}{\sin^2\theta}-\frac{1}{\theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=l(l+1)$$

differensial tenglama murakkab yechimga ega. Shu sababli uning yechimi

$$\Theta(\theta)\sim c_{l,m_l}p_{l,m_l}(\cos\theta)$$

ko`rinishda ekanligini ko`rsatamiz. $p_{l,m_l}(\cos\theta)$ – ***Lejandrning birlashtirilgan polinomi*** deyiladi va quyidagi ko`rinishga ega:

$$P_l^m(x)=\left(1-x^2\right)^{m_l/2}\frac{d^{l+m_l}}{dx^{l+m_l}}\left[\frac{(x^2-1)^l}{2^l l!}\right],$$

Bunda $x=\cos\theta$. Bu yerda

$$c_{l,m_l}=\sqrt{\frac{(2l+1)}{2}\frac{(l-m_l)!}{(l+m_l)!}},$$

va normallangan qutbiy to`lqin funksiya

$$\theta_{l,m_l}=\sqrt{\frac{(2l+1)(l-m_l)!}{2(l+m_l)!}}\cdot P_{l,m_l}(\cos\theta)$$

ko`rinishga ega bo`ladi.

$$Y(\theta,\varphi)=\Phi(\varphi)\cdot\Theta(\theta)$$

funksiya ***sferik funksiya*** deyiladi. Bu sferik funksiya L^2 – operator hususiy funksiyalaridir.

13.1. m_0 massali zarra $U(r)$ markaziy maydonda harakatlansa Shryodinger tenglamasi o`zgaruvchilarni ajratish yo`li bilan yechilishi mumkinligini ko`rsating. To`lqin funksiyasining azimutal burchakka qanday bog`liqligini aniqlang.

Yechish: $U(r)$ potensial markaziy maydonda harakatlanuvchi zarra uchun sferik koordinatalar sistemasidagi Shryodinger tenglamasi ushbu ko`rinishga ega

$$\frac{1}{2}\cdot\frac{\partial^2}{\partial r^2}\psi(\vec{r})+\frac{2m_0}{\hbar^2}\left[E-U(r)-\frac{\hat{L}^2}{2m_0r^2}\right]\cdot\psi(\vec{r})=0, \tag{1}$$

bu tenglamada o`zgaruvchilarni ajratamiz

$$\psi(\vec{r})=R_{ne}(r)\cdot Y_{em}(\theta,\varphi), \tag{2}$$

bunda $Y_{em}(\theta,\varphi)$ – sferik funksiyalar bo`lib, $\hat{L}_z^2$ va $\hat{L}_z$ operatorlarning xususiy funksiyalari hisoblanadi. Azimutal burchak $\varphi$ ga bog`liq qismini aniqlash uchun $\hat{L}_z$ operator uchun xususiy funksiyalar aniqlash tenglamasini yozamiz

$$\hat{L}_z\psi(\varphi)=L_z\psi(\varphi).$$

Sferik koordinatalar sistemasida $\hat{L}_z=-i\hbar\frac{\partial}{\partial\varphi}$ ekanligidan foydalansak,

$$-i\hbar\frac{\partial\psi(\varphi)}{\partial\varphi}=L_z\psi(\varphi),$$

bunda $0\le\varphi\le 2\pi$ sohada o`zgaradi. Bu tenglama yechimi

$$\psi(\varphi)=A\cdot\exp\left(i\frac{L_z}{\hbar}\varphi\right)$$

Endi

$$\psi(\varphi)=\psi(\varphi+2\pi)$$

shartdan

$$L_z=\hbar m\quad,\qquad m=0,\pm1,\pm2,\pm3...$$

$$\int_0^{2\pi}\psi_m^*\psi_m d\varphi=1$$

ekanidan $A=(2\pi)^{-1/2}$ ekanini aniqlab

$$\psi_m(\varphi)=(2\pi)^{-1/2}\cdot e^{im\varphi}$$

yechimni topamiz.

13.2 Ushbu operatorlarning xususiy funksiyasi va xususiy qiymatlari topilsin: a) $\hat{L}_z=-i\hbar\frac{\partial}{\partial\varphi}$; b) $\hat{L}_z^2=-\hbar^2\frac{\partial^2}{\partial\varphi^2}$ (φ – azimutal burchak).

Yechish: a) $-i\hbar\frac{\partial\psi}{\partial\varphi}=L_z\psi$

yechim

$$\psi(\varphi) = Ae^{i\frac{L_z}{\hbar}\varphi}$$
$$\psi(\varphi) = \psi(\varphi + 2a)$$

bir qiymatlili shartidan

$$L_z = m\hbar \qquad (m=0, \pm1, \pm2, \ldots)$$

ekanini aniqlaymiz. Normallashtirish shartidan

$$\int_0^{2\pi} \psi(\varphi)\psi^*(\varphi)d\varphi = 1, \qquad A = \frac{\lambda}{\sqrt{2\pi}}$$

Shuning uchun normallashgan xususiy funksiyalar quyidagi ko`rinishga ega bo`ladi.

$$\psi_m(\varphi) = (2\pi)^{-\frac{1}{2}} e^{i\varphi m}$$

b) $L_z^2 = m^2\hbar^2$, $(m=0, \pm1, \pm2, \ldots)$

$$\psi_m(\varphi) = (2\pi)^{-\frac{1}{2}} e^{i\varphi m} .$$

13.3. $U(r)$ potensial markaziy maydonda harakatlanuvchi zarra to`lqin funksiyasi $\theta$, $\varphi$ burchaklarga bog`liq qismi $Y(\theta,\varphi)$ – sferik funksiyalar ko`rinishida bo`lsa, uning impuls momenti proyeksiyalari L_x, L_y va L_z larning o`rtacha qiymatini hisoblang.

Yechish: Ma'lumki, sferik funksiyalar $Y_{em}(\theta,\varphi)$ $\hat{L}^2$ va $\hat{L}_z$ operatorlarning xususiy funksiyalari hisoblanadi

$$\hat{L}^2 Y_{em} = \hbar^2 l(l+1)Y_{em} \quad , \hat{L}_z Y_{em} = \hbar \cdot m \cdot Y_{em}$$

Shuning uchun bu holda L_z proyeksiya aniq qiymatga ega

$$L_z = m\hbar$$

$\hat{L}_x$ va $\hat{L}_y$ operatorlar $\hat{L}_z$ bilan kommutativ emas. Shu sababdan ularning o`rtacha qiymati to`g`risidagina gapirish mumkin.

$$\overline{L_x} = \int Y^*_{em} \hat{L}_x Y_{em} d\Omega \ , \quad \overline{L_y} = \int Y^*_{em} \hat{L}_y Y_{em} d\Omega$$

bunda $d\Omega = \sin\theta d\theta d\varphi$. $\overline{L_x}$ va $\overline{L_y}$ larni hisoblashdan ko`ra ushbu kattaliklar o`rtacha qiymatini hisoblash maqsadga muvofiq

$$\overline{L_x} = i\overline{L_y} = \int Y^*_{em}\left(\hat{L}_x + i\hat{L}_y\right)Y_{em} d\Omega .$$

$\hat{L}_x$ va $\hat{L}_y$ operatorlarning sferik garmonikalarga ta'sirini hisobga olib, ya'ni

$$\left(\hat{L}_x + i\hat{L}_y\right)Y_{em} = -\hbar\sqrt{(l-m)(l+m+1)}Y_{e,m+1}$$

dan ushbuni olamiz

$$\overline{L}_x + i\overline{L}_y = -\hbar\sqrt{(l-m)(l+m+1)}Y^*_{em} \cdot Y_{e,m+1}d\Omega = 0\,.$$

Shu sababdan $\overline{L}_x = 0$, $\overline{L}_y = 0$ ni olamiz.

13.4. Sferik funksiyalar jadvalidan foydalanib p - , d - , va f – holatlardagi to`lqin funksiyalar uchun normallashtirish koeffitsientlarini aniqlang.

Yechish: Biz bunda $Y_{em}(\theta,\varphi)$ larning jadvalidan foydalanamiz va normallashtirish sharti

$$\int_0^{\pi}\int_0^{2\pi} Y^*_{em}(\theta,\varphi)Y_{em}d\Omega = 1$$

dan foydalansak ushbu natijalarga ega bo`lamiz:

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta\,; \qquad Y_{1,\pm1} = \pm\sqrt{\frac{3}{8\pi}}\sin\theta\cdot e^{\pm i\varphi}\,;$$

$$Y_{2,0} = \frac{1}{2}\sqrt{\frac{5}{2\pi}}(3\cos^2\theta - 1)\,;$$

$$Y_{2,\pm1} = \pm\sqrt{\frac{15}{8\pi}}\sin\theta\cdot\cos\theta\cdot e^{\pm i\varphi}\,;$$

$$Y_{2,\pm2} = \frac{1}{2}\sqrt{\frac{15}{8\pi}}\sin^2\theta\cdot e^{\pm 2i\varphi}\,;$$

$$Y_{3,0} = \frac{1}{4}\sqrt{\frac{7}{\pi}}(5\cos^3\theta - 3\cos\theta)\,;$$

$$Y_{3,\pm1} = \pm\frac{1}{8}\sqrt{\frac{21}{\pi}}\sin\theta\left(5\cos^2\theta - 1\right)\cdot e^{\pm i\varphi}\,;$$

$$Y_{3,\pm2} = \frac{1}{4}\sqrt{\frac{105}{2\pi}}\sin^2\theta\cos\theta\cdot e^{\pm 2i\varphi}$$

$$Y_{3,\pm3} = \pm\frac{1}{8}\sqrt{\frac{35}{\pi}}\sin^3\theta\cdot e^{\pm 3i\varphi}\,.$$

13.5. L_x, L_y va L_z operatorlaring sferik koordinatalar sistemasidagi ko`rinishini oling.

13.6. L^2 operatorlaring sferik koordinatalar sistemasidagi ko`rinishini yozing.

14-mavzu: Zarrachani spin va spin operatorini xususiy funktsiyalarini aniqlash

Kvant mexanikasining postulatlaridan biri – Pauli printsipidir. To`lqin funktsiyaning simmetrik yoki antisimmetrikligi uning fazoviy va spinlari o`zgaruvchilarining amashtirilgandagi xususiyatiga bog`liq.

Agar zarralar orasidagi o`zaro ta'sir kuchlari zarralar spinlariga bog`liq bo`lmasa, sistemaning to`lqin funktsiyasini faqat koordinatalarga va faqat spinlarga bog`liq funktsiyalar ko`paytmasi ko`rinishda quyidagicha yozish mumkin:

$$\psi(x_1, x_2, ..., x_N; m_{s1}, m_{s2}, ..., m_{sN}) = \varphi(x_1, x_2, ..., x_N) U(m_{s1}, m_{s2}, ..., m_{sN}).$$

Demak, bunday zarralar, agar bozonlardan iborat bo`lsa, u holda kooordinatalar va spinlar funktsiyalari bir xil simmetriyalarga ega bo`lishlari shart, ya'ni $\varphi_c U_C$ yoki $\varphi_A U_A$ (bunda indeks "C" simmetrik "A" esa antisimmetriklikni ko`rsatadi); agar fermionlardan iborat bo`lsa, $\varphi_A U_C$ yoki $\varphi_c U_A$ dan iborat bo`lishi kerak.

Shuni ta'kidlaymizki, zarralar orasidagi o`zaro ta'sir bo`lmaganda ham, ya'ni aynan bir xil zarralardan tashkil topgan ideal gazda ham, aynanlik printsipi tufayli almashuv o`zaro ta'sir kelib chiqadi. Almashuv o`zaro ta'sir – kvant korrelyatsiya zarralar orasidagi o`rtacha masofa de Broyl to`lqin uzunligininig o`rtacha qiymati tartibida yoki undan kichik bo`lganda effektiv namoyon bo`ladi. Bunda almashuv o`zaro ta'sirini xarakteri fermionlar va bezonlar uchun har xil bo`ladi. Fermionlar uchun $\psi_A = \varphi_A U_C$ to`lqin funktsiyada spinlar parallel ekanligidan zarralarning yaqinlashuvida itarishish kuchlari namoyon bo`ladi; bu itarishish kuchlarini aks ettiruvchi Pauli printsipi ikki va undan ortiq zarralarning bir holatda bo`lishiga qarshilik (to`sqinlik) qiladi. Bozonlar uchun almashuv o`zaro ta'sir esa, spinlarning antiparallelligidan zarralarning o`zaro tortishish kuchi sodir bo`lishligidandir. Shu sababli, bozonlar bir holatda bo`la olishlari mumkin.

O`zaro ta'sirlashuvchi aynan bir xil zarralarning tashqi maydondagi energiyasiga ham kvant korrelyatsiya mavjudligi ta'sir ko`rsatadi. Ammo bu ta'sir zarralarning o`rin almashishlaridagi ta'sirga nisbatan ishorasi, odatda, teskari bo`lganligi uchun bu ta'sirlarning xissalari bir-biriga nisbatan katta yoki kichikligiga qarab, sistemaning umumiy energiyasi ortishi yoki kamayishi mumkin, ya'ni sistema holatining qulayligi spinlarning paralleligida (masalan, ferromagnetizmda) yoki antiparalleligida (masalan, N_2, O_2 molekulalarda) sodir bo`lishi mumkin.

Bir-biriga bog`liq bo`lmagan N ta zarralar sistemasi holatlari uchun

$$\psi_{n_1, n_2, ..., n_N} = \psi_{n_1} \psi_{n_2} .. \psi_{n_N} \tag{17}$$

funktsiya kiritgan edik. Ammo u simmetriklik xossasiga ega bo`lamagani uchun sistema holatini tavsiflashga yaramaydi. Sistemaning holatini tavsiflash uchun (17) ning chiziqli kombinatsiyadan simmetrik yoki antisimmetrik funktsiyalarni olish kerak.

Masalan, ikkita bir zarraviy funktsiyalar $\varphi_{n1}(x)$ va $\varphi_{n2}(x)$ berilgan bo`lsa, undan simmetriklikka ega bo`lgan holat funktsiyalarini hosil qilishimiz mumkin:

$$\varphi_c = \frac{1}{\sqrt{2}}\left[\varphi_{n1}(x_1)\varphi_{n2}(x_2) + \varphi_{n1}(x_2)\varphi_{n2}(x_1)\right],$$

$$\varphi_C = \frac{1}{\sqrt{2}}\left[\varphi_{n1}(x_1)\varphi_{n2}(x_2) - \varphi_{n1}(x_2)\varphi_{n2}(x_1)\right]. \tag{18}$$

(18) ifodadan ko`rinadiki, $n_1 = n_2$ yoki $x_1 = x_2$ bo`lganda $\varphi_A = 0$ bo`ladi, ya'ni antisimmetrik to`lqin funktsiya bilan tavsiflanuvchi ikki bir xil zarralar (fermionlar) bir holatda yoki bir joyda bo`lishi mumkin emas.

Bu (18) ifodani N ta bir-biri bilan o`zaro ta'sirlashmaydigan zarralar sistemasi uchun umumlashtiraylik:

$$\psi_C = \frac{1}{\sqrt{N!}}\sum \psi_{n1}(x_1)\psi_{n2}(x_2)...\psi_{nN}(x_N) \tag{19}$$

n_i – spin kvant sonni ham aks ettiradi. O`rin almashtirishlar soni ya'ni (19) da hadlar soni $N!$ ta. Bunda o`rin almashtirishlar ψ_C ning ishorasini o`zgartirmaydi!

Antisimmetrik funktsiya ψ_A ni quyidagi determinantdan iborat deb qaraladi:

$$\psi_A = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_{n1}(x_1)\varphi_{n1}(x_2)...\varphi_{n1}(x_N) \\ \varphi_{n2}(x_1)\varphi_{n2}(x_2)...\varphi_{n2}(x_N) \\ .... \\ \varphi_{nN}(x_1)\varphi_{nN}(x_2)...\varphi_{nN}(x_N) \end{vmatrix} \tag{20}$$

Zarralarning o`rin almashtirishga (20) determinantdagi ustunlarning o`zaro almashtirilishi mos keladi.

Agar ixtiyoriy ikki zarraning, masalan, 1 va 2 ning kvant holatlari bir xil bo`lsa, ya'ni $n_1 = n_2$ bo`lsa, u holda determinantning ikki qatori bir xil bo`ladi. Ikki qatori bir xil bo`lsa, bunday determinant har doim nolga teng bo`ladi, ya'ni $\psi_A$=0. Bunday holat amalga oshmaydi, bu esa Pauli printsipidir. Demak, bu printsipga asosan bir xil holatda 2 ta fermion bo`lishi mumkin emas.

14.1. Pauli matritsalari bilan aniqlanuvchi operatorlarning xususiy funksiya va xususiy qiymatlarini aniqlang.

Yechish: Pauli matritsalarini yozaylik

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \qquad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \qquad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Bu operatorlar xususiy qiymat va xususiy funksiyalar uchun tenglamasini yozing:

$$\hat{\sigma}_x \lambda^{(1)} = \sigma_x \lambda^{(1)}, \qquad \hat{\sigma}_y \lambda^{(2)} = \sigma_y \lambda^{(2)}, \qquad \hat{\sigma}_z \lambda^{(3)} = \sigma_z \lambda^{(3)}$$

bunda σ_x, σ_y, σ_z lar – xususiy qiymatlar, $\lambda^{(1)}$, $\lambda^{(2)}$, $\lambda^{(3)}$ lar – xususiy funksiyalar qidirilayotgan funksiyalarni $\lambda = \begin{pmatrix} a \\ b \end{pmatrix}$ shaklida qidiramiz:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \sigma_x \begin{pmatrix} a \\ b \end{pmatrix},$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \sigma_x \begin{pmatrix} a \\ b \end{pmatrix}.$$

demak

$$b = \sigma_x a, \qquad a = \sigma_x b$$

Bunda

$$\sigma_x^2 = 1, \qquad \sigma_x = \pm 1$$

ekanini olamiz. Agar σ_x=1 bo`lsa, $\lambda_{+1}^{(1)} = a\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $\sigma_x$=-1 bo`lsa $\lambda_{(-1)}^{(1)} = a\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

Normallashtirish shartidan

$$\lambda_1^{(1)^*} \lambda_1^{(1)} = |a|^2 (1 \quad 1)\begin{pmatrix} 1 \\ 1 \end{pmatrix} = 2|a|^2 = 1, \quad a = \frac{1}{\sqrt{2}}.$$

Shuning uchun

$$\lambda_{+1}^{(1)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}; \qquad \lambda_{-1}^{(1)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

ekanini aniqlaymiz.

Xuddi shuningdek $\hat{\sigma}_y$ va $\hat{\sigma}_z$ lar uchun ham bajarib

$$\sigma_y = \pm 1; \qquad \lambda_{+1}^{(2)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}; \qquad \lambda_{-1}^{(2)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$\sigma_z = \pm 1; \qquad \lambda_{+1}^{(3)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad \lambda_{-1}^{(3)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

ekanini topamiz, bunda $\lambda_{+1}^{(3)}$ va $\lambda_{-1}^{(3)}$ funksiyalar mos ravishda spin z o`qi bo`ylab va teskari yo`nalgan hollarga mos keladi.

14.2. Pauli matritsalar $\hat{\vec{\sigma}}$ operatorni komponentalari $\left[\hat{\vec{\sigma}} \cdot \hat{\vec{\sigma}}\right] = 2i\hat{\vec{\sigma}}$, $\left(\hat{\vec{\sigma}} \cdot \hat{\vec{\sigma}}\right) = 3\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ shaklida yozilishi mumkin bo`lgan vektor operator shaklida ifodalash mumkinligini ko`rsating hamda $\hat{\vec{\sigma}}_x \cdot \hat{\vec{\sigma}}_y \cdot \hat{\vec{\sigma}}_z$ ko`paytmani aniqlang.

Javob: $\hat{\vec{\sigma}}_x \cdot \hat{\vec{\sigma}}_y \cdot \hat{\vec{\sigma}}_z = i\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$

14.3. Elektron spini ixtiyoriy o`qdagi proyeksiyasi kvadratini hisoblang.

Yechish: Ma'lumki, $\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}}$ bunda $\hat{\vec{\sigma}}_x, \hat{\vec{\sigma}}_y, \hat{\vec{\sigma}}_z$ lar Pauli matritsalari bo`lib, ushbu shartni qanoatlantiradi:

$$\hat{\sigma}_x^2 = \hat{\sigma}_y^2 = \hat{\sigma}_z^2 = \delta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hat{\sigma}_x \cdot \hat{\sigma}_y = -\hat{\sigma}_y \cdot \hat{\sigma}_x ; \qquad \hat{\sigma}_y \cdot \hat{\sigma}_z = -\hat{\sigma}_z \cdot \hat{\sigma}_y ; \hat{\sigma}_z \cdot \hat{\sigma}_x = -\hat{\sigma}_x \cdot \hat{\sigma}_z .$$

Spinning ixtiyoriy $\vec{a}$ yo`nalishda kvadrati

$$\left(\frac{\vec{S}\cdot\vec{a}}{a}\right)^2 = \frac{\hbar^2}{4a^2}\left(\hat{\vec{\sigma}}\cdot\vec{a}\right)^2 = \frac{\hbar^2}{4a^2}\left(\hat{\sigma}_x \cdot a_x + \hat{\sigma}_y \cdot a_y + \hat{\sigma}_z \cdot a_z\right)\cdot\left(\hat{\sigma}_x \cdot a_x + \hat{\sigma}_y \cdot a_y + \hat{\sigma}_z \cdot a_z\right) =$$

$$= \frac{\hbar^2}{4a^2}\left[\hat{\sigma}_x^2 a_x^2 + \hat{\sigma}_y^2 a_y^2 + \hat{\sigma}_z^2 a_z^2 + \left(\hat{\sigma}_x \hat{\sigma}_y - \hat{\sigma}_y \hat{\sigma}_z\right) a_x a_y + \left(\hat{\sigma}_y \hat{\sigma}_z + \hat{\sigma}_z \hat{\sigma}_y\right) a_y a_z + \left(\hat{\sigma}_z \hat{\sigma}_x + \hat{\sigma}_x \hat{\sigma}_z\right) a_z a_x\right] =$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Bundan

$$S_{\vec{a}}^2 = \frac{1}{4}\hbar^2 .$$

14.4. Pauli matritsalari uchun quyidagi tengliklarni isbotlang: a) $\sin(\delta_x \varphi) = \delta_x \sin\varphi$; b) $\cos(\delta_z \varphi) = \cos\varphi$; c) $e^{i\delta_y \varphi} = \cos\varphi + i\delta_y \sin\varphi$; d) $e^{i\delta_z \varphi \cdot \delta_y} \cdot e^{-i\delta_z \varphi} = e^{2i\delta_z \varphi} = \delta_y$.

14.5. Triplet va singlet holatdagi ikkita zarra spinlarining skalyar ko`paytmasini toping. Zarralar spini $\hbar/2$ ga teng.

Yechish: Ikkita zarra operatorlari yig`indisini kvadratini qaraylik

$$\vec{S}^2 = \left(\vec{S}_1 + \vec{S}_2\right)^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2\left(\vec{S}_1 \cdot \vec{S}_2\right)$$

Triplet va singlet holatlarda S^2; S_1^2 va S_2^2 lar aniq qiymatlarga ega

$$\vec{S}^2 = \hbar^2 S(S+1),$$

(S =1 da – triplet, S =0 da – singlet holatlarda)

$$\vec{S}_1^2 = \vec{S}_2^2 = \frac{3}{4}\hbar^2 .$$

Demak,

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{\vec{S}^2 - \left(\vec{S}_1^2 + \vec{S}_2^2\right)}{2} = \frac{\hbar^2}{4}\left(2S(S+1)-3\right)$$

$\left(\vec{S}_1 \cdot \vec{S}_2\right) = \frac{1}{4}\hbar^2$ – triplet holatda, $\left(\vec{S}_1 \cdot \vec{S}_2\right) = \frac{3}{4}\hbar^2$ – singlet holatda.

14.6. B induksiyali magnit maydonida joylashgan spinga ega zarra uchun $\frac{\partial \sigma_x}{\partial t}$ operatorni hisoblang.

14.7. $\frac{\hbar}{2}$ spinli zarra spini ixtiyoriy o`qqa proeksiyasining kvadratini hisoblang.

14.8. Elektron spini kvadratining ixtiyoriy x, y, z o`qdagi proeksiyalari bir vaqtda aniq qiymatga ega bo`lishi mumkinmi?

15-mavzu: Xususiy magnit momentga doir masalalar yechish

15.1 Asosiy statsionar holatdagi vodorod atomining magnit momentini hisoblang.

15.2. P, D va F holatlarida bittadan valent elektronlari bo`lgan atom uchun Lande ko`paytuvchilarini aniqlang.

Javob: P-holatda $g_1 = \frac{2}{3}$, $g_2 = \frac{4}{3}$;

D-holatda $g_1 = \frac{4}{5}$, $g_2 = \frac{6}{5}$

F-holatda $g_1 = \frac{6}{7}$, $g_2 = \frac{8}{7}$.

15.3. Ushbu qiymatlarga ega bo`lgan spektral termlarning belgilanishini yozing: a) S= 3/2; L=2, g=0, b) S= 1/2, J=3/2 , g= /3

Javobi: a) $4D_{1/2}$; b) $2D_{3/2}$.

15.4. 3D holatdagi atomi magnit momenti qiymatining egallashi mumkin bo`lgan qiymatlarini aniqang.

16-mavzu: G`alayonlar nazariyasining holatlar energiyasi va to`lqin funktsiyasi hisoblashga tadbiqi

Shryodinger tenglanmasi juda kam hollarda aniq yechimga ega. Ko`p zarrachali sistemalarda esa faqat ikki zarrachali sistema uchun Shryodinger tenglamasi aniq yechimga ega bo`lishi mumkin. Shuning uchun ko`pincha Shryodinger tenglamasini yechish uchun taqribiy usullardan foydalanadilar. Shu usullardan biri **g`alayonlar nazaryasidir**.

G`alayonlar nazaryasining asoslarini statsionar holatlar uchun ko`rib chiqamiz. Bizga Shryodinger tenglamani yechish kerak.

$$\hat{H}\psi = E\psi, \tag{1}$$

bu yerda $\hat{H}$ – berilgan sistemaning gamiltaniani. Bu tenglamani to`g`ri integrallash bilan yechib bo`lmaydi deb hisoblaymiz. G`alayonlar nazaryasini ishlatish uchun, bizga shu sistemaga yaqin sistemaning to`lqin funksiyalari va energiya sathlari aniq bo`lishi kerak. Bu sistema uchun Shryodinger tenglamasi quyidagicha yoziladi deb hisoblaymiz:

$$\hat{H}_0\varphi_n = E_n^{(0)}\varphi_n, \tag{2}$$

bu yerda $\hat{H}$ Gamiltanian bilan beriladigan sistema ***g`alayonlanmagan sistema*** deb ataladi. Bu sistema tekshirilayotgan sistemaning taxminiy modeli bo`ladi. Chunki $\hat{H}$ va $\hat{H}_0$ bir biridan ko`p farq qilmaydi.

Agar $\hat{H}$ va $\hat{H}_0$ operatorlar orasidagi farqni hisobga olmasak

$$\psi_n = \psi_n^{(0)} = \varphi_n; E_n = E_0^{(0)}. \tag{3}$$

Bu tenglamalar g`alayonlar nazaryasining nomini darajali yondashishiga to`g`ri keladi. Operator

$$\hat{W} = \hat{H} - \hat{H}_0 \tag{4}$$

g`alayon deyiladi.

Agar $\hat{W}$ operatorni hisobga olsak, model sistemani to`lqin funksiyasini va energiya sathlarini tekshirilayotgan sistemani to`lqin funksiyasiga va energiya sathlariga yaqinlashtiradi.

Endi

$$E_n = E_n^{(0)} + \Delta E_n, \psi_n = \varphi_n + f_n \tag{5}$$

deb olamiz.

ΔE_n va f_n aniqlanishi g`alayonlanmagan sistemaga operator $\hat{W}$ bilan kiritilgan ***g`alayonlar hisoblanishi*** deb aytiladi.

Birinchi darajali yondashishida hisoblash quyidagicha bo`ladi. (1) tenglamaga $E_n, \psi_n$ qiymatlarini (5) ifodalardan foydalanib qo`yiladi:

$$\left(\hat{H}_0+\hat{W}\right)(\varphi_n+f_n)=\left(E_n^{(0)}+\Delta E_n\right)(\varphi_n+f_n) \quad (6)$$

ΔE_n, f_n va W – kichik bir darajasi deb hisoblaymiz.

(6) chi ifodada kovuslarni ochib shu kataliklar bo`yicha faqat hadlarni qoldiramiz. Olingan tenglamadan $\Delta E_n$ va $f_n$ taxminiy qiymatlarini topsa bo`ladi. Bularning $\Delta E_n^{(1)}$ va $f_n^{(1)}$ deb belgilaymiz. Gamiltanian ko`rinishi quyidagicha

$$\hat{H}_0\,\varphi_n+\hat{H}_0\,f_n^{(1)}+\hat{W}\,\varphi_n=E_n^{(0)}\varphi_n+E_n^{(0)}f_n^{(1)}+\Delta E_n^{(1)}\varphi_n.$$

(2) chi tenglikni hisobga olib yozsa bo`ladi.

$$\hat{H}_0\,f_n^{(1)}+\hat{W}\,\varphi_n=E_n^{(0)}f_n^{(1)}+\Delta E_n^{(1)}\varphi_n. \quad (7)$$

(2) chi tenglamani φ_n^* ga ko`paytirib, φ_n ning butun aniqlanish sohasida integrallaymiz

$$\int\varphi_n^*\hat{H}_0\,f_n^{(1)}dV+\int\varphi_n^*\hat{W}\,\varphi_n dV=E_n^{(0)}\int\varphi_n^*f_n^{(1)}dV+\Delta E_n^{(1)}\int\varphi_n^*\varphi_n dV \quad (8)$$

φ_n^* funksiyalarni ko`rmasa deb hisoblab,

$$\int\varphi_n^*\varphi_n dV=1.$$

$\hat{H}_0$ operatorining o`zaro qo`shmasligini hisobga olsak,

$$\int\varphi_n^*\hat{H}_0\,f_n^{(1)}dV=\int f_n^{(1)}\left(\hat{H}_0\,\varphi_n\right)^*dV=E_n^{(0)}\int\varphi_n^*f_n^{(1)}dV.$$

Endi (8)chi tenglamadan quyidagi kelib chiqadi

$$\Delta E_n^{(0)}=\int\varphi_n^*\hat{W}\varphi_n dV. \quad (9)$$

Shunday qilib, birinchi darajali yondashishda tekshirayotgan sistemaning quyidagicha bo`ladi

$$E_n^{(1)}=E_n^{(0)}+\Delta E_n^{(1)}. \quad (10)$$

To`lqin funksiyasining xatoligini keyiingi ko`rinishda izlaymiz.

$$f_n^{(1)}=\sum_k c_k\varphi_k. \quad (11)$$

(11) va (7) ga qo`ysak,

$$\hat{H}_0\,f_n^{(1)}\sum_k c_k\varphi_k+\hat{W}\,\varphi_n=E_n^{(0)}\sum_k c_k\varphi_n+\Delta E_n^{(1)}\varphi_n, \quad (12)$$

va

$$\hat{H}_0\sum_k c_k\varphi_k=\sum_k c_k E_k^{(0)}\varphi_k.$$

Hisobga olib (12) tenglamani quyidagicha yozamiz

$$\hat{W}\,\varphi_n=\Delta E_n^{(1)}\varphi_n+\sum_k\left(E_n^{(0)}-\Delta E_k^{(0)}\right)c_k\varphi_k. \quad (13)$$

(13) chi φ_m^*, $m\neq n$ ga ko`paytirib va butun sohadan integrallab

$$\int \varphi_n^* \hat{W} \varphi_n dV = E_n^{(0)} \int \varphi_m^* \varphi_n dV + \sum_k \left(E_n^{(0)} - E_k^{(0)}\right) c_k \int \varphi_m^* \varphi_k dV \cdot \qquad (14)$$

φ_k funksiyalar ermit operatorning xususiy funksiyalari, shuning uchun bular juft ortogonal. Bundan integral

$$\int \varphi_m^* \varphi_k dV$$

faqat $k = m$ bo`lganda noldan farq qiladi. Shuning uchun (14) dan

$$c_m = \frac{W_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)} . \qquad (15)$$

bu yerda $W_{mn} = \int \varphi_m^* \hat{W} \varphi_n dV$ ***g`alayon operatorining matrisaviy elementi*** deyiladi. (15) chi yordamida xolat aunksiyasini birinchi zarracha yordamida yozsa bo`ladi.

$$\psi_n^{(1)} = \varphi_n + \sum_{m \neq n} \frac{W_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)} \varphi_m \cdot \qquad (16)$$

(9) va (16) chi formulalarni faqat keying shartlar bajarilganda o`rinli bo`ladi.

$$\begin{aligned} |W_{mn}| &<< \left|E_n^{(0)}\right| \\ |W_{mn}| &<< \left|E_n^{(0)} - E_m^{(0)}\right| \end{aligned} .$$

16.1. Kengligi a ga teng potensial o`radagi zarrachaga $\overset{\wedge}{V}(x) = V_0 \cos\frac{2\pi}{a} x$ ko`rinishdagi g`alayon ta’sir qilsa, uning energiyasiga tuzatmalarni aniqlang.

Yechish: Oldingi masalalardan ma’lumki bunday potensial o`radagi zarra xususiy funksiyasi va energiyasi quyidagicha edi:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{\pi n}{a} x; \qquad E_n^{(0)} = \frac{\pi^2 \hbar^2 n^2}{2 m_0 a^2} .$$

Energiyaga tuzatmalar $\hat{V} = \hat{V}_0 \cos\frac{2\pi}{a} x$ operatorning matritsaviy elementlari orqali ifodalanadi. Ularni hisoblaylik

$$V_{mn} = \int_0^a \psi_m^* \hat{V} \psi_n dx = \frac{2V_0}{a} \int_0^a \sin\frac{\pi m}{a} x \cos\frac{2\pi}{a} x \cdot \sin\frac{\pi n}{a} x dx .$$

Bundan

$$V_{mn} = \frac{V_0}{2} \left[\delta_{m,n+2} + \delta_{m,n-2}\right]$$

Energiyaga birinchi tartibli tuzatma ifodasidan

$$E_n^1 = V_{nn} = 0 .$$

Ikkinchi tartibli tuzatma esa

$$E_n^{(2)} = \frac{V_0^2}{2E_1^{(0)}} \cdot \frac{1}{n^2 - 4}, \quad n \neq 2$$

16.2. $V(x)=\alpha x^3+\beta x^4$ ko`rinishdagi g`alayon ta'sirida chiziqli garmonik ossilyator energiyasiga tuzatmalarni aniqlang.

Yechish: Garmonik ossilyator energiyasiga birinchi tartibli tuzatma quyidagi formula bilan aniqlanadi.

$$E^{(1)}=\beta\left(x_{nn}^4\right)$$

Chunki

$$\left(x^3\right)_{nn}=\int_{-\infty}^{+\infty}\left|\psi_n^{(0)}\right|^2 x^3dx=0$$

bo`ladi (integral ostidagi funksiya toqligi sababli).
Matritsalarni ko`paytirish qoidasi va

$$x_{n,n-1}=x_{n-1,n}=\sqrt{\frac{\hbar n}{2m_0\omega}}$$

ekanligidan foydalanib, matritsa elementlarini topamiz

$$E_n^{(1)}=\beta\left(x^4\right)_{nn}=\frac{3}{2}\beta\cdot\frac{\hbar^2}{m_0^2\omega^2}\left(n^2+n+\frac{1}{2}\right)$$

energiya ikkinchi tartibli tuzatma αx^3 ushbu formula bilan topiladi:

$$E_n^{(2)}=\frac{\alpha^2}{\hbar\omega}\sum_{k\neq n}\frac{\left|(x^3)_{nk}\right|^2}{n-k}=-\frac{15}{4}\alpha^2\frac{\hbar^2}{m_0^3\omega^4}\left(n^2+n+\frac{11}{30}\right).$$

Shuning uchun garmonik ossilyator asosiy holati (n=0) energiyasiga tuzatma

$$\Delta E=\frac{3}{4}\frac{\hbar^2}{m_0^2\omega^2}\left(\beta-\frac{11}{6}\cdot\frac{\alpha^2}{m_0\omega^2}\right)$$

ko`rinishda bo`ladi.

16.3. Inersiya momenti I va dipol momenti D bo`lgan qattiq rotator $X0Y$ tekislikda aylanmoqda. $X$ o`qi bo`ylab yo`nalgan maydon kuchlanganligi $\vec{E}$ bo'gan elektr maydonning rotator energiyasiga ta'sirini aniqlang.

Yechish: Maydon mavjud bo`lmasa rotator to`lqin funksiyasi va energiyasi

$$\psi_m^{(0)}=\frac{1}{\sqrt{2\pi}}e^{im\varphi},\qquad E_m^{(0)}=\frac{\hbar^2m^2}{2I},\qquad m=0,\pm1,\pm2,\ldots$$

edi. Elektr maydon ta'sir etsa $\vec{E}(E,0,0)$ uning potensial energiyasiga $\hat{V}=-D\cdot E\cos\varphi$ kabi had qo`shiladi va unda energiyasiga shu g`alayon ta'sir etadi deb hisoblab

$$V_{km}=-\frac{DE}{2\pi}\int_0^{2\pi}e^{i(m-k)\varphi}\cos\varphi d\varphi=-\frac{1}{2}DE\left(\delta_{k,m+1}+\delta_{k,m-1}\right).$$

Birinchi tartibli tuzatma

$$\left(\Delta E_m\right)^{(1)} = V_{mm} = 0\,.$$

Energiyaga ikkinchi tartibli tuzatma

$$\left(\Delta E_m\right)^{(2)} = \sum_{k\neq m} \frac{\left|V_{km}\right|^2}{E_m^{(0)} - E_k^{(0)}}$$

dan

$$\left(\Delta E_m\right)^{(2)} = \frac{1}{4} D^2 E^2 \cdot \frac{2I}{\hbar^2} \left[\frac{1}{m^2 - (m-1)^2} + \frac{1}{m^2 - (m+1)^2} \right]$$

Bundan

$$\left(\Delta E_m\right)^{(2)} = \left(\frac{DE}{\hbar} \right)^2 \cdot \frac{I}{4m^2 - 1}\,.$$

16.4. Massaning tezlikka relyativistik bog`liqligini hisobga olgan holda vodorod atomi energetik sathlariga tuzatmalarni aniqlang. Relyativistik massa $m(v)$ ga $v^2/c^2$ tartibidagi hadning ta'siri $\hat{V}_{rel} = -\frac{1}{8m_0^3c^2}\hat{p}^4$ g`alayon bilan aniqlanadi deb hisoblang ($\hat{p}$ – impuls operatori).

16.5. Ikki karra aynigan energiya sathi uchun energiyaga birinchi tartibli tuzatmalarni aniqlang. Bunda g`alayon operatori $\hat{V}$ vaqtga bog`liq emas deb hisoblang.

16.6. Variotsion metod yordamida $U(x) = U_0 \cdot x^4$ potensial maydondagi zarraning asosiy holati energiyasi topilsin. Ruxsat etilgan funksiyalar sifatida $\psi(x) = A \cdot e^{-\frac{x^2}{2\beta^2}}$ ni oling.

Yechish: Ma'lumki asosiy holat energiyasi ushbu funksional minimumidan topiladi

$$\overline{E} = I(\psi) = \int \psi^* \hat{H} \psi(x) dx$$

Bu holda biz ruxsat etilgan funksiya qilib

$$\psi(x) = \left(\sqrt{\pi\beta}\right)^{-1/2} \cdot e^{-\frac{x^2}{2\beta^2}}$$

ni olamiz va gamiltanian

$$\hat{H}(x) = -\frac{\hbar^2}{2m_0} \frac{d^2}{dx^2} + U_0 x^4$$

kabi olamiz va yuqoridagi funksionaldan foydalanib

$$\overline{E}=\frac{\hbar^2}{4m_0\beta^2}+\frac{3}{4}U_0\beta^4$$

ekanini aniqlaymiz. $\overline{E}$ ning minimumlaridan

$$\beta^2=\left(\frac{\hbar^2}{6m_0U_0^2}\right)^{\frac{1}{3}}$$

va shunday qilib

$$E_0=\left(\overline{E}\right)_{\min}=\frac{3}{4}\cdot\left(\frac{3}{4}\frac{U_0\hbar^4}{m_0^2}\right)^{1/3}$$

ni olamiz.

16.7. Variatsion metoddan foydalanib uch o`lchamli garmonik ossilyator energiyasining eng kichik qiymatini aniqlang. Bunda uning potensial energiyasi $U(r)=\frac{1}{2}m_0\omega^2r^2$ kabi deb olinsin. Namunaviy funksiyalar sifatida esa $\psi(r)=A(1+\alpha r)\cdot e^{-\alpha r}$ olinsin.

**Ko`rsatma:** Maydon potensialining sferik simmetriyasi hisobga olib, energiya o`rtacha qiymati ushbu integral orqali ifodalanadi

$$\overline{E}=\int_0^\infty\left(-\frac{\hbar^2}{2m_0}\left|\frac{d\psi}{dr}\right|^2+\frac{m_0\omega^2r^2}{2}|\psi|^2\right)4\pi r^2dr$$

Bunda normallashgan to`lqin funksiyalari ko`rinishi

$$\psi(r)=\left(\frac{\alpha^3}{7\pi}\right)^{1/2}\cdot(1+\alpha r)\cdot e^{-\alpha r}$$

shaklda bo`ladi:

$$E_0=\overline{E}_{\min}=\frac{9}{7}\sqrt{\frac{3}{2}}\hbar\omega\approx 1{,}575\hbar\omega.$$

17-mavzu: Kvant o`tishlar nazariyasi. Tanlash qoidalari

Dastlab m holatda bo`lgan sistemaning tashqi ta'sirdan keyin $n$ holatda topish ehtimolligi $n-m$ ***o`tish ehtimolligi*** deb yuritiladi. Bu ehtimollik g`alayonlar nazariyasida taqribiy yechiladi. Biror funksiyaning holat hususiy funksiyalari orqali yoyilmasidagi koeffitsentlarning fizik ma'nosiga ko`ra superpozitsiya prinsipiga asosan

$$W_{mn}=C_{mn}^*(\tau)C_{mn}(\tau).$$

Bu ifodadan g`alayonlar nazariyasining birinchi darajali yondashishidan $m\neq n$ o`tishlar uchun

$$W_{mn} = \frac{1}{\tau^2}\left|\int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} V_{mn}(t)e^{iw_{mn}t}dt\right|^2 .$$

Agar zarraga yoki sistema o`zgaruvchan tashqi maydonda bo`lsa, uning holatini aniqlash uchun Shryodingerning to`liq tenglamasini yechish kerak.

$$i\hbar\frac{\partial\varphi}{\partial t} = \hat{H}\psi , \qquad \hat{H} = \hat{H}(r,t), \tag{1}$$

nostatsionar holatlarda gamiltanian

$$\hat{H} = \hat{H}_0(x) + \hat{V}(x,t) \tag{2}$$

ko`rinishda yoziladi. (1) ifodani (2) ni hisobga olgan holda quyidagicha yozish mumkin:

$$i\hbar\frac{\partial\varphi}{\partial t} = \left[\hat{H}_0(x) + \hat{V}(x,t)\right]\varphi . \tag{3}$$

Agar faqat $H(x)$ qatnashadigan Shryodinger tenglamasining yechimlari ma'lum bo`lsa, (3) tenglamani nostatsionar g`alayonlar nazariyasini ishlatib yechish mumkin.

Agar zarraga o`zgaruvchan maydon ta'sir qilayotgan bo`lsa

$$\varphi_k(x,t) = \varphi_k(x)e^{-i\omega_k t}, \qquad \omega_k = \frac{E}{\hbar}, \qquad k = 1, 2, 3, \ldots .$$

$$H_0\varphi_k(x) = E_k\varphi_k(x),$$

$$\hat{V}(x,t) << \hat{H}_0(x).$$

$\varphi(x,t)$ ni statsionar holatlar to`lqin funktsiyalari superpozitsiyasi ko`rinishida yozamiz:

$$\varphi(x,t) = \sum_k C_k(t)\varphi_k(x)e^{-i\omega_k t} . \tag{4}$$

Endi bu yerda $C_k(t)$ koeffitsientlarni tanlaymiz. Bu koeffitsientlarni hisoblash uchun taqribiy usullardan foydalanamiz va ularni quyidagi ko`rinishda izlaymiz:

$$C_k(t) = C_k^{(0)}(t) + C_k^{(1)}(t) + C_k^{(2)}(t) + \ldots .$$

Nolinchi darajali yondashishda koeffitsientlar tuzatmalarga ega emas:

$$C_k(t) = C_k^{(0)}(t) .$$

Birinchi darajali yondashishda

$$C_k(t) = C_k^{(0)}(t) + C_k^{(1)}(t),$$

boshlang`ich shart

$$\varphi(x,0) = \varphi_n(x) . \tag{5}$$

Bu holda (4) ifoda quyidagi ko`rinishga ega bo`ladi:

$$\varphi(x,t) = \sum_k C_{kn}(t)\varphi_k(x)e^{-i\omega_k t} . \tag{6}$$

t=0 da

$$C_{kn} = \delta_{kn}. \tag{7}$$

G`alayonlar nazariyasining nolinchi darajali yondashishida

$$\hat{V}(x,t) = 0.$$

(7) tenglamadan

$$\frac{dC_{mn}^0(t)}{dt} = 0 \qquad \text{yoki} \quad C_{mn}^0(t) = const.$$

(7) ifodaga asosan

$$C_{mn}^0(t) = \delta_{mn}.$$

(6) ga asosan

$$\varphi^{(0)}(x,t) = \varphi_n(x)e^{-i\omega_n t}.$$

17.1. Boshlang`ich vaqtda ($t$=0) sistema $\psi_1^{(0)}$ funksiyali ikki karra ionlashgan holatda turibdi. Agar tashqi g`alayon ta'sir eta boshlasa, uning xuddi shunday energiyali $\psi_2^{(0)}$ funksiyali boshqa holatga o`tish ehtimolini toping.

Yechish: Nolinchi yaqinlashishning to`g`ri funksiyalarini yozamiz

$$\psi = C_1\psi_1 + C_2\psi_2; \qquad \psi' = C_1'\psi_1 + C_2'\psi_2. \tag{1}$$

bunda C_1, C_2, C_1', C_2' koeffitsientlar tashqi g`alayonda bog`liq holda aniqlanuvchi koeffisiyentlar. (1) formuladan foydalanib ψ_1 ni ψ va ψ' lar orqali ifodalaymiz, bu xolat energiyaga $E + E_1^{(1)}$ va $E + E_2^{(1)}$ tuzatmalar bilan aniqlanadi. $E_{1,2}^{(1)}$ energiyalar

$$E_{1,2}^{(1)} = \frac{1}{2}\left[V_{11} + V_{22} \pm \sqrt{(V_{11} + V_{22})^2 + 4(V_{12})^2}\right]$$

formuladan topiladi.

Vaqt bo`yicha ko`paytuvchi kiritib ψ_1 to`lqin funksiyalarga o`tamiz:

$$\psi_1 = \frac{e^{-\frac{i}{\hbar}Et}}{C_1C_2' - C_1'C_2}\left[C_2'\psi e^{-\frac{i}{\hbar}E_1^{(1)}t} - C_2\psi' e^{-\frac{i}{\hbar}E_2^{(1)}t}\right].$$

Boshlang`ich vaqtda (t=0)

$$\Psi_1 = \psi_1 = \frac{C_2'\varphi - C_2\varphi'}{C_1C_2' - C_1'C_2}$$

(1) ga Ψ va Ψ' larning Ψ_1 va Ψ_2 orqali ifodalarini qo`yib, Ψ_1 ning yoyilmasini topamiz

$$\Psi_1 = a_1(t)\psi_1 + a_2(t)\psi_2.$$

bunda

$$a_2(t) = \frac{\exp^{\frac{i}{\hbar}Et}}{C_1C_2' - C_2'C_2}\left(C_2'C_2e^{-\frac{i}{\hbar}E_1^{(1)}t} - C_2'C_2e^{-\frac{i}{\hbar}E_2^{(1)}t}\right).$$

Bunga koeffitsientlarning qiymatlarini qo`yib va $|a_2(t)|^2$ ni hisoblab, o`tish ehtimolini aniqlaymiz

$$W_{12} = 2\frac{|V_{12}|^2}{\left(\hbar\omega^{(1)}\right)^2}\left[1-\cos\omega^{(1)}t\right],$$

bunda

$$\omega^{(1)} = \frac{1}{\hbar}\sqrt{\left(V_{11}+V_{22}\right)^2 + 4|V_k|^2}$$

ga teng.

17.2. Asosiy kvant holatdagi zaryadlangan garmonik ostsillyatorga birdan tashqi elektr maydon qo`yildi. Bu g`alayon ta'sirida ostsillyatorning uyg`ongan holatga o`tish ehtimolini toping.

Yechish: $\vec{E}(E,0,0)$ tashqi maydonda garmonik ostsillyator energiyasi

$$U(x) = \frac{m\omega^2}{2}x^2 - e\cdot E\cdot x = \frac{m\omega^2}{2}(x-x_0)^2 + const.$$

Bunda $x_0 = \dfrac{e\cdot E}{m\omega^2}$ shu sababdan uyg`ongan garmonik ossilyator to`lqin funksiyasi

$$\psi_k = \frac{(-1)^k}{\sqrt{2^k k!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\cdot e^{\frac{(\xi-\xi_0)^2}{2}}\frac{d^k}{d\xi^k}\left[e^{-(\xi-\xi_0)^2}\right]$$

bo`ladi, bunda

$$\xi = x\left(\frac{m\omega}{\hbar}\right)^{1/2}; \qquad \xi_0 = \frac{eE}{\left(m\hbar\omega^3\right)^{1/2}}.$$

O`tish ehtimoli $\Psi_0(x-x_0)$ ning $\Psi_k(x)$ lar bo`yicha yoyilmaning a_k koeffitsientlari bilan aniqlanadi.

$$a_k = \int_{-\infty}^{+\infty}\psi_k(x)\psi_0(x-x_0)dx = \frac{(-1)^k}{\sqrt{2^k k!}}e^{-\frac{\xi_0^2}{2}}\int_{-\infty}^{+\infty}e^{\xi\xi_0}\frac{d^k}{d\xi^k}e^{-\xi^2}d\xi.$$

Bu integral k marta bo`laklab integrallash bilan Puasson integraliga keltiriladi

$$\int_{-\infty}^{+\infty}e^{\xi\xi_0}\frac{d^k}{d\xi^k}e^{-\xi^2}d\xi = (-1)^k\xi_0^k\int_{-\infty}^{+\infty}e^{\xi\xi_0}e^{-\xi^2}d\xi = (-\xi_0)^k\sqrt{\pi}e^{\frac{\xi_0^2}{4}},$$

shuning uchun

$$a_k = \frac{1}{\sqrt{2^k k!}}\xi_0^2 e^{-\frac{\xi_0^2}{4}}.$$

$0\to k$ o`tish ehtimolligi

$$W_{0k}=|a_k|^2=\frac{\xi_0^{2k}e^{-\frac{\xi_0^2}{2}}}{2^k k!}$$

ga teng.

18-mavzu: Aynan o`xshash zarrachalar sistemasi. Ko`p elektronli atomlar va molekulalar. Atomlarning to`qin funktsiyalari

G`alayonlar nazaryasining nolinchi darajasi yondashishdagi geliy atomining energiyasi va holat funksiyasi aniqlash mumkin. Ikkita elektron geliy atomi – bu murakkab sistema, shuning uchun buni o`rganish uchun taqribiy usullarni ishlatish kerak. Agar magnit ta'sirlarini hisobga olmasak, yadro bilan va o`zaro ta'sirlashayotgan ikkita elektronli sistemaning gamiltaniani quyidagi ko`rinishga ega

$$\hat{H}=-\frac{\hbar^2}{2m}\Delta_1-\frac{\hbar^2}{2m}\Delta_2-\frac{2\chi e^2}{r_1}-\frac{2\chi e^2}{r_2}+\frac{\chi e^2}{r_{1,2}}. \quad (1)$$

Bu yerda Δ_1 va Δ_2 – birinchi va ikkinchi elektronlarning koordinatalari bo`yicha Laplas operatori, $r_1$ va $r_2$ – zarrachalarning yadrogacha masofasi: $r_{1,2}$ – elektronlar orasidagi masofasi, $m$ – elektron massasi. Berilgan gamiltanian uchun Shryodinger tenglamasini aniq yechish noma'lum. Shuning uchun bu yerda g`alayonlar nazaryasini ishlatamiz. Nolinchi zarrachani yondashishini kiritish uchun yadro maydonidagi ikkita o`zaro ta'sirlashmayotgan elektronlar sistemasini ko`ramiz. Shunday qilib, g`alayonlanmagan sistema uchun Shryodinger tenglamasi quyidagicha bo`ladi.

$$\hat{H}_0 f=Ef.$$

bu yerda

$$\hat{H}=-\frac{\hbar^2}{2m}\Delta_1-\frac{\hbar^2}{2m}\Delta_2-\frac{2\chi e^2}{r_1}-\frac{2\chi e^2}{r_2}.$$

Ma'lumki, o`zaro ta'sirlashmayotgan sistemaning to`lqin uzunligini quyidagicha yosa bo`ladi

$$f_{n_1,n_2}(\vec{r}_1\vec{r}_2)=\psi_{n_1}(\vec{r}_1)\psi_{n_2}(\vec{r}_2). \quad (2)$$

Bu yerda n_1 va n_2 – zarrachaning holatini belgilaydigan kvant sonlarning to`plami.

Sistemaning energiyasi quyidagi formula bilan aniqlanadi.

$$E_{n_1n_2}=E_{n_1}+E_{n_2},$$

E_n energiya sathlari va $\psi_n(\vec{r})$ funksiyalar bitta zarracha uchun yoziladigan Shryodinger tenglamasining yechimidan topiladi.

$$\left(-\frac{\hbar^2}{2m}\Delta_1-\frac{2\chi e^2}{r}\right)\psi_n(\vec{r})=E_n\psi_n(\vec{r}). \quad (3)$$

Bu tenglamaning yechimi aniq (vodorod atomi masalasidan chiqadi)

$$E_n = -\frac{4R_y}{h^2}; \qquad \psi_n(\vec{r}) = R_{ne}(r)Y_{em}(\theta,\varphi),$$

bu yerda $R_y = \frac{m_{eff}\chi e^4 Z^2}{2\hbar^2}$, $\psi_n(\vec{r})$ – vodorodga o`xshagan sistemaning toppish formulasi.

Shunday qilib, nolinchi darajali yondashishda geliy atomi haqidagi masalani yechdik.

D.Mendeleyev tomonidan yaratilgan moddalarning davriy qonuniyati (jadval) nafaqat kimyo sohasida, balki zamonaviy atom va yadrolar fizikasida ham muhim ahamiyatga ega. Bu qonuniyat nazariyasi haligacha oxiriga yetmagan: atom yadrosining tuzilish muammosining juda ko`p tomonlari ochilmagan bo`lib, xuddi hali tug`ilmagan chaqaloq holatidadir. **Mendeleyev jadvalining** tuzilishi kvant mexanikasi yoki yadro fizikasi nuqtai nazaridan tushuntiriliishi mumkin. Ma`lumki, atom yadrosi atomning elektron qobig`ining tuzilishini ifodalaydi. Kvant yadro mexanikasi massasi va zaryadini e`tiborga olgan holda elektron sistemasini yadro elektr maydonidagi harakat qonuniyatlariga asoslanib elektron qobig`idagi davriylikni tushuntirib bera oldi. Bu masala yechimi elektronlar soni haddan tashqari ko`p bo`lganligi tufayli matematik nuqtai nazardan juda murakkabdir. Klassik mexanikada hatto shu vaqtgacha uchta jism harakati masalasining to`liq va umumiy yechimi aniqlanmagan. Atom mexanikasida ko`p masalalar yaqinlashtirish usullarini qo`llash tufayli nisbatan oson yechiladi. Yaqinlashtirishning qo`llanilishini esa atomda elektronlarning diskretlik tabiatiga ega ekanligidan kelib chiqadi. Shu usullar Pauli prinsipi hamda elektronlarning markaziy kuchlar maydonidagi harakat nazariyalariga asoslangan holda davriylikni tushunishga imkon berdi. Bunda albatta, elementlarning tartib raqami eng asosiy ahamiyatga molikdir.

Ko`rdikki, elektron energiyasi ikkita $n$ va $l$-kvant sonlariga bog`liq bo`lib, energiyaning bir qiymatiga bir necha to`lqin funksiyasi mos keladi, $E_{nl} \to \Psi_{n,l,m,m_s}$ atom tashqi ta’sir bo`lmagan holda ham aynigan. $n$ ning qiymati atom qobig`ining tartib raqamini ifodalaydi, undagi elektronlar soni Pauli prinsipiga asosan mumkin bo`lgan kvant sonlariga $l$, $m$, $m_z$ mos ravishda $n = 2n^2$ ga teng. Demak, Pauli prinsipiga asosan, berilgan to`rtta kvant soni bilan bitta qobiqda faqatgina bitta elektron turishi mumkin, ya’ni qobiqdagi elektronlar soni ham $2n^2$ ga teng bo`ladi.

$K \quad n=1 \quad 2(s \text{ sath})$

$L \quad n=2 \quad 8(s=2\overline{e},\ p=6\overline{e})$

$M \quad n=3 \quad 18(s=2\overline{e},\ p=6\overline{e},\ d=10\overline{e})$

$N \quad n=4 \quad 32(s=2\overline{e},\ p=6\overline{e},\ d=10\overline{e},\ f=14\overline{e})$

$O \quad n=5 \quad 50(s=2\overline{e},\ p=6\overline{e},\ d=10\overline{e},\ f=14\overline{e},\ e=18\overline{e})$

$P \quad n=6 \quad 72(...)$

Atomdagi E energiyasi $l \neq 0$ da ilgarilanma va aylanma harakat energiyalar yig\`indisidan tashkil topganligi tufayli, ba'zi hollarda $l$ ning katta qiymatlari uchun quyidagicha bo\`lishi mumkin: $E_{n,\,l_1} < E_{n,l_2}$, $n_1 > n_2$ lekin $l_2 > l_1$.

18.1. Ushbu holatlardagi atomlarda elektronlar soni aniqlansin: 1). $K-$, $L-$qobiqlar va $3S$ va $3P$ qobiqchalari to\`lgan; 2) $K-$, $L-$, $M-$ qobiqlar va $4S$, $4P$, $4D$, $5S$ qobiqchalari to\`lgan.

Javob: 1) N_c=18 – argon atomi; 2) N_c=48 – kadmiy atomi.

18.2. Ushbu atomlarning elektron konfiguratsiyalarini yozing: argon (Z=18), kripton (Z=36), palladiy (Z=46), seziy (Z=55).

Javob: ${}_{18}Ar - 1s^2 2s^2 2p^6 3s^2 3p^6$;

${}_{36}Kr - 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$;

${}_{46}Pd - 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10}$;

${}_{55}Cs - 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6 6s^1$.

19-mavzu: Sochilish nazariyasi. Born formulasining tadbiqi

Sochilish deb klassik zarrachaning boshqa zarrachalar ta'sirida dastlabki yo\`nalishdan og\`ishiga aytiladi. Kvant fizikada sochilish kengroq ma'noda tushuniladi. Bunda zarrachalarning o\`zaro ta'sirida harakat yo\`nalishining o\`zgarishidan tashqari, zarrachalarning holati ham o\`zgarishi mumkin, ya'ni boshqa zarracha hosil bo\`lishi mumkin. Sochilishning ikki turi farqlanadi: 1) elastik sochilishda – faqat harakat yo\`nalishi o\`zgarib zarrachalar soni ularning energiyasi, massasi, zaryadi va boshqalari o\`zgarmaydi, 2) noelastik sochilishda – zarracha turi yoki energiyasi o\`zgaradi.

Elastik sochilish. Bu yerda biz faqat elastik sochilishni ko\`ramiz. Lekin ikkita sochilish uchun ham, ya'ni elastik va noelastik sochilish uchun ham umumiy harakteristikalari mavjud. Bu diferensial va to\`liq sochilish kesimidir. ***Sochilishning differensial kesim*** deb birlik vaqtda $d\Omega$ fazoviy burchak elementiga sochilgan zarrachalar sonining tushayotgan zarrachalar oqimining zichligiga nisbatiga aytiladi.

$$d\delta = \frac{dN}{j_{tush}}. \qquad (1)$$

Bu ifodadagi dN ni quyidagicha yozish mumkin.

$$dN = j_{soch}(Q,\varphi)dS,$$

bunda $j_{soch}(Q,\varphi)$ – sferik koordinatalar burchak yo`nalishida sochilgan zarrachalar oqimi, dS – sochilgan zarrachalar tushadigan yuza. Demak (1) va keyingi ifodalardan

$$d\delta = \frac{j_{soch}dS}{j_{tush}} \qquad (2)$$

kelib chiqadi. Bu ifodadan ko`rinib turibdiki, diferensial kesim birligi – yuza birligi bilan bir hil. (2) ifodada $j_{soch}$ va $j_{tush}$ o`rinlariga ularga mos ehtimoliy oqimlar zichliklariga o`tib, keyin bu formulani bitta zarracha sochilishi uchun ham ishlatsa bo`ladi. ***To`liq*** yoki ***integral sochilish kesimi*** deb hamma yo`nalish bo`yicha birlik vaqtda sochilgan zarralar sochishining tushayotgan zarralar oqimiga nisbatiga aytiladi:

$$\Sigma = \frac{N_{soch}}{j_{tush}}.$$

Integral kesim bilan diferensial kesim quyidagicha bog`langan:

$$\Sigma = \int d\delta$$

Sharni sochma bilan bombardimon qilsa, bu sharning ko`ndalang kesimi integrall sochilishi tenglamasini bildiradi. Mikrodunyoda ham, agar o`zaro ta’sir qisqa masofasi bo`lsa integrall kesim deb nishonning ko`ndalang kesimini olish mumkin.

Kuch maydonida sochilish amplitudasi. Sochiluvchi va sochuvchi zarrachalar o`zaro ta’sir potensial energiya operatori $\hat{U}(\vec{r})$ bo`lsa, sochilish masalasi μ keltirilgan massa zarrachaning ikkinchi zarrachaga nisbatan harakati masalasi keladi. Bu hol uchun Shryodinger tenglamasi

$$\left[-\frac{\hbar^2}{2\mu}\Delta + u(r)\right]\psi(r,Q,\varphi) = E\psi(r,Q,\psi). \qquad (3)$$

Harakat bu holda albatta infinit, demak energiyalar spektri uzluksiz.

Zarralar OZ o`q bo`ylab harakatlanadi va nishon zarra koordinata boshida joylashgan deb olamiz. Sochilishdan oldin nishondan uzoqda zarrachalar yassi to`lqin bilan ifodalanadi.

$$\psi_{tush} = e^{ikz}; \qquad k = \frac{p}{\hbar}. \qquad (4)$$

Zarrachalar har xil tomonga sochilishi mumkin va ularning birlik hajmda topilishi nishondan masofa kvadratiga teskari proporsional bo`lganligi uchun sochilgan zarrachaning to`lqin funksiyasini quyidagicha yozish mumkin:

$$\psi_{soch} = \frac{f(Q,\varphi)}{r}e^{ikz}, \qquad (5)$$

bundagi $f(Q,\varphi)$ funksiyalar zarrachaning har xil yo`nalishlari sochilish ehtimolini bildirib, ***sochilish amplitudasi*** deb yuritiladi. Tushayotgan va sochilayotgan to`lqinlarda ehtimoliy oqim zichligini hisoblaymiz. Ehtimoliy oqim zichligi ta'rifidan foydalanib yozish mumkin.

$$j_{tush} = (j_z)_{tush} = \frac{p}{\mu}; \qquad j_{soch} = (j_r)_{soch} = \frac{p}{\mu r^2}|f(Q,\varphi)|^2.$$

(2) formulaga asosan differensial sochilish kesimi uchun quyidagini yozish mumkin:

$$d\sigma = |f(Q,\varphi)|^2 d\Omega. \tag{6}$$

Bunda ko`rinib turibdiki $|f(Q,\varphi)|^2$ kattalik zarrachaning Q,φ burchaklarda sochilish ehtimoli zichligini bildiradi.

Sochish markazining kuch maydonida koordinata boshidan uzoqlikda (4) va (5) ifodalarga asosan zarrachaning to`lqin funksiyasining $\psi_{tush}$ va $\psi_{soch}$ to`lqin funksiyalar superpozitsiyasi ko`rinishida yozish mumkin.

$$\psi = e^{ikz} + \frac{f(Q,\varphi)}{r}e^{ikz}. \tag{7}$$

Sochilish amplitudasi $f(Q,\varphi)$ Shryodinger tenglamasini (6) dagi ψ ga nisbatan yechib topiladi. Bu masalani yechish uchun $U(r)$ potensialning aniq ko`rinishini bilish kerak. Umumiy holda yechim quyidagi ko`rinishda toppish mumkin:

$$\psi(\vec{r}) = e^{ikz} - \frac{\mu}{2\pi\hbar^2}\frac{e^{ikz}}{r}\int U(r')\psi(r')e^{ik\frac{r'\bar{r}'}{r}}dV\,\frac{f(Q,\varphi)}{r}, \quad (r>>1,\ |z|>>1) \tag{8}$$

Bu ifodadan (7) ni hisobga olib, sochilish amplitudasini toppish mumkin:

$$f(Q,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int U(\vec{r}')\psi(\vec{r}')e^{ik\frac{r'\bar{r}'}{r}}dV'. \tag{9}$$

(9) formula yordamida sochilish amplitudasini taqribiy hisoblasa bo`ladi. Buning uchun g`alayonlar nazaryasini ishlatamiz. Nolinchi darajali yondashishda g`alayonlanmagan sistemaga erkin zarracha to`g`ri keladi va uning to`lqin funksiyasi

$$\psi_0(\vec{r}) = e^{ikz}`, \tag{10}$$

bo`ladi. Bu yondashishda sochilish bo`lmaydi:

$$f_0(Q,\varphi) = 0.$$

Agar endi (10) ga to`lqin funksiyasi $\psi(\vec{r})$ ning o`rniga (9) formulani ishlatsak, g`alayonlar nazaryasining birinchi darajasi yordamida sochilish amplitudasini topamiz:

$$f(Q,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int U(\bar{r}^1)e^{ikr'}e^{-ik\frac{r'\bar{r}'}{r}}dV'. \tag{11}$$

Zarrachalarning markaziy maydonda sochilishi. Ko`p hollarda zarrachalar orasida o`zaro ta'sir markaziy bo`ladi. Bu holda sochilish markazining maydoni markaziy simmetrik bo`ladi. Bunda $U = U(r)$ deb yozish mumkin. (11) ifodani qulayloq ko`rinishda yozish uchun $\vec{k}_0$ va $\vec{k}$ vektorlar kiritamiz. $\vec{k}_0$ vektorni $OZ$ o`qi bo`ylab zarracha harakai yo`nalishi bo`yicha yo`nalgan deb olamiz. Sochilish elastik bo`lsa, $\vec{k}_0$ va $\vec{k}$ bo`ladi. Bu belgilarni kiritib, (11) ni quyidagicha yozish mumkin.

$$f(Q,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int U(\vec{r}\,')e^{-i\vec{k}\vec{r}\,'}e^{-i\vec{k}_0\vec{r}\,'}dV'. \qquad (12)$$

Bu ifodada yana yangi belgi kiritamiz $\vec{q} = \vec{k}_0 - \vec{k}$. Natijada (12) quyidagicha yoziladi

$$f(Q,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int U(\vec{r}\,')e^{-i\vec{q}\vec{r}}dV'. \qquad (13)$$

Bu formulani ***Born formulasi*** deb va uning asosida amplitudaning hisoblanishi ***Born yaqinlashishi*** deyiladi.

(13) dagi integralni hisoblash uchun OZ oqini $\vec{q}$ vektor bo`yicha yo`naltiramiz:

$$f(Q,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi}U(r')e^{i\vec{q}\vec{r}\cos\theta}r'^2\sin\theta' dr' d\theta d\varphi'.$$

φ' bo`yicha integrallab olamiz

$$f(Q,\varphi) = -\frac{\mu}{\hbar^2}\int_0^{\infty}U(r')r'^2\,dr'\int_0^{\pi}e^{iqr'\cos\theta'}\sin\theta' d\theta'.$$

Bunda $x = \sin\theta'$ o`zgartirish kiritamiz:

$$\int_0^{\pi}e^{iqr'\cos\theta'}\sin\theta' d\theta' = \int_{-1}^{-1}e^{iqr'x}dx = \frac{e^{iqr'x}}{iqr'}\Big|_{-1}^{1} = \frac{r\sin qr'}{qr'}.$$

r' da shtrix belgisini tashlab sochilish amplitudasini topamiz:

$$f(Q,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int_0^{\infty}U(r)r\sin qr dr. \qquad (14)$$

Topilgan formulani (6) ga qo`yib va quyidagini

$$q = rk\sin\frac{\theta}{2}$$

hisobga olib, sochilish kesimini topamiz:

$$d\sigma = \frac{\mu^2}{k^2\hbar^4\sin^2\dfrac{\theta}{2}}\left[\int_0^{\infty}U(r)r\sin\left(2kr\sin\frac{\theta}{2}\right)dr\right]^2 d\Omega. \qquad (15)$$

Bu formula yordamida birinchi darajali yondashish sochilish kesimi topiladi.

Agar $\theta \to 0$ (sochilish burchagi kichik bo`lsa),

$$\sin\left(2kr\sin\frac{\theta}{2}\right)\approx rkr\sin\frac{\theta}{2}$$

va

$$d\sigma=\frac{4\mu^2}{\hbar^2}\left[\int_0^\infty U(r)r^3drr\right]^2 d\Omega$$

bo`ladi va sochilish izotrop, ya’ni fazadagi yo`nalishga bog`liq bo`lmaydi.

Rezerford formulasi. Sochilish kesimini topish misoli sifatida α-zarrachalarning atom yadrolarida sochilishni ko`rib chiqamiz. Maydon potensiallarini quyidagicha yozamiz:

$$U=\frac{\beta}{r}e^{-\lambda r}, \qquad \beta=\chi 2Ze^2,$$

bu ifodaning $\frac{\beta}{r}$ ko`paytuvchisi $\alpha$-zarrachaning yadrodan Kulon itarishishini ifodalaydi, ikkinchi ko`paytuvchi esa – atomdan tashqarida elektron ekranlashi elektr maydon tez susayishini ifodalaydi.

Endi sochilish kesimini toppish uchun (15) chi ifodadagi integralni hisoblaymiz. Uni hisoblash uchun quyidagini

$$\sin qr=\frac{1}{2i}\left(e^{iqr}-e^{iqr}\right)$$

e’tiborga olamiz.

Demak,

$$\int_0^\infty U(r)r\sin qrdr=\beta\int_0^\infty e^{-\lambda r}\sin qrdr=-\frac{\beta}{q\left(1+\frac{\lambda^2}{q^2}\right)},$$

buni (15) ga qo`yib, quyidagini topamiz:

$$d\sigma=\left(\frac{\chi\mu Ze^2}{\hbar^2k^2\sin^2\frac{\theta}{2}}\right)^2\frac{d\Omega}{\left(1+\frac{\lambda^2}{4k^2\sin^2\frac{\theta}{2}}\right)^2} \qquad (16)$$

Bunda λ juda kichik, shuning uchun $\frac{\lambda^2}{4k^2\sin^2\frac{\theta}{2}}$ ham juda kichik bo`lib, uni hisobga olmasa bo`ladi. U holda (16) ifoda quyidagi ko`rinishga keladi:

$$d\sigma=\left(\frac{\chi\mu Ze^2}{o^2}\right)^2\frac{d\Omega}{\sin^4\frac{\theta}{2}}.$$

19.1 Lagranj polinomlari $P_l(\cos\theta)$ ning ortogonalligidan foydalanib, sochilishning umumiy kesimi partsial kesimlar yig`indisi ko`rinishida $\sigma = \sum_{l=0}^{\infty} \sigma_l$ ifodalanishi mumkinligini ko`rsating, bunda $\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l$.

Yechish: Sochilish amplitudasi

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left(e^{2i\delta_l} - 1\right)P_l(\cos\theta)$$

dan umumiy kesim uchun

$$\sigma = \int |f(\theta)|^2 d\Omega = \frac{1}{4k^2}\int d\Omega \left|\sum_{l=0}^{\infty}(2l+1)\left(e^{2i\delta_l} - 1\right)P_l(\cos\theta)\right|^2$$

integrallash va yig`ishning o`rnini almashtirib va φ bo`yicha integrallab

$$\sigma = \frac{2\pi}{4k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)\left(e^{2i\delta_l} - 1\right)\left(e^{2i\delta_{l'}} - 1\right)\cdot\int_0^{\pi} P_l P_{l'} \cdot \sin\theta d\theta.$$

Endi Lagranj polinomlarining ortogonalligidan, ya'ni

$$\int_0^{\pi} P_l(\cos\theta)P_{l'}(\cos\theta)\sin\theta d\theta = \frac{2}{2l+1}\delta_{ll'}$$

va l' bo`yicha yig`ib yuborib

$$\sigma = \sum_{l=0}^{\infty}\sigma_l$$

ni olamiz, bunda

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l.$$

19.2. m massali zarralarning zarra o`tkazmaydigan $a$ radiusli sferada sochilishi effektiv kesimini aniqlang. Bunda $a << 1$ bo`lganda, S – sochilish xossasini eng yuqori deb hisoblang.

Yechish: $r > a$ sohada $U(r) = 0$, shuning uchun to`lqin tenglamasi

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) + k^2\psi = 0$$

ko`rinishga keladi, bunda

$$k^2 = \frac{2m_0E}{\hbar^2}.$$

Sferaning o`tkazmasligi xususiyatidan $\psi(r)|_{r=a} = 0$ shartni olamiz va tenglamaning bu shartni qanoatlantiruvchi yechim

$$\psi(r) = A\frac{\sin(kr - ka)}{r}$$

bo`ladi. Bundan δ_i ni aniqlaymiz:

$$\delta_0 = -ka, \quad \delta_l = 0, \text{ agar } \ l \neq 0.$$

Shu sababdan

$$\sigma = \sigma_0 = \frac{4\pi}{k^2}\sin^2 ka.$$

Sekin zarralar uchun ($ka << 1$), $\sin ka \approx ka$, shu sababdan

$$\sigma = 4\pi a^2.$$

Kvant mexanikasiga asosan o`tkazmaydigan sfera kesimi klassik holatidan 4 marta katta bo`lar ekan.

19.3. Partsial to`lqinlar metodidan foydalanib, sekin harakatlanuvchi zarralarning kengligi $a$ ga va chuqurligi $U_0$ ga teng potensial sochilish to`la kesimini toping ($ka << 1$).

Yechish: Radial Shryodinger tenglamasini

$$\psi(r) = \frac{1}{2}\lambda(r)$$

almashtirish bilan o`zgartiramiz.

($ka << 1$) holda faqat S – sochilish ahamiyatli bo`lganidan

$$\lambda'' + k^2\lambda(r) = 0; \qquad k^2 = \frac{2m_0E}{\hbar^2} \qquad \text{agar} \quad r > a$$

$$\lambda'' + k_1^2\lambda(r) = 0; \qquad k_1^2 = \frac{2m_0}{\hbar^2}(E + U_0) \qquad \text{agar} \quad r < a$$

λ(r) uchun chegaraviy shart $\begin{cases} \lambda(0) = 0 \\ \lambda(\infty) = M \end{cases}$ bo`lishi kerak.

Yuqoridagi tenglamalarning bu chegaraviy shartlarini qanoatlantiruvchi yechimlari

$$\lambda(r) = \sin(kr + \delta_0); \qquad r > a$$

$$\lambda(r) = A\sin k_1 r; \qquad r < a$$

r=0 da $\frac{\lambda'}{\lambda}$ nisbatning uzluksizligidan

$$\mathrm{tg}(ka + \delta_0) = \frac{k}{k_1}\mathrm{tg}k_1 a,$$

bundan

$$\delta_0 = arctg\left(\frac{k}{k_1}tgk_1 a\right) - ka.$$

Kichik tezliklarda ($k \to 0$) S sochilish fazosi k ga proporsional

$$\delta_0 = ka\left(\frac{tgk_0 a}{k_0 a} - 1\right); \qquad k_1 \to k_0 = \frac{\sqrt{2m_0U_0}}{\hbar}$$

va

$$\sigma = 4\pi a^2 \left(\frac{tgk_0 a}{k_0 a} - 1 \right)^2 .$$

19.4. Sekin harakatdagi zarralarning sferik potensial o`radagi sochilish effektiv kesimi ifodasini tahlil qilib

$$\sigma = 4\pi a^2 \left(\frac{tgk_0 a}{k_0 a} - 1 \right)^2, \qquad k_0 = \sqrt{\frac{2m_0 U_0}{\hbar^2}}$$

bu kesimning potensial chuqurligi U_0 ga bog`lanish tabiatini aniqlang.

Yechish: Unchalik chuqur bo`lmagan o`rada $\vec{k}_0 a << 1$ va

$$\sigma = 4\pi a^2 \left(\frac{tgk_0 a}{k_0 a} - 1 \right)^2$$

ifodadan

$$\sigma = 4\pi a^2 \frac{k_0^4 a^4}{9} = \frac{16\pi}{9} \cdot \frac{U_0^2 m_0^2 a^6}{\hbar^4}$$

ni olamiz.

Ko`rinadiki $U_0$ oshishi bilan sochilish kesimi keskin oshadi va $k_0 a \to \frac{\pi}{2}$ cheksiz bo`lib qoladi.

$k_0 a \to \frac{\pi}{2}$ shart o`rada birinchi energetik holat paydo bo`lish sharti bilan mos keladi. U_0 ning keyingi oshishida, σ kamayadi va $\mathrm{tg} k_0 a = k_0 a$ da nolga teng bo`ladi, keyin σ yana osha boshlaydi. Shunday qilib U_0 ning monoton oshishida σ kesim 0 va ∞ orasida tebranib turadi.

19.5. Ixtiyoriy tashqi maydondagi $f(k)$ sochilish amplitdasi ψ - funksiya bilan $f(k) = -\frac{\mu}{2\pi\hbar^2} \int e^{-ikr} U\psi dV$ kabi ifodalanishini ko`rsating.

Yechish: Bu masala holida Shryodinger tenglamasi quyidagicha bo`ladi:

$$-\frac{\hbar^2}{2\mu} \Delta\psi + U\psi = E\psi .$$

Odatdagidek $k^2 = \frac{2\mu E}{\hbar^2}$ belgilash kiritib, yuqoridagi ifodani

$$\Delta\psi + k^2 \psi = \frac{2\mu}{\hbar^2} U\psi$$

kabi yozamiz. Biz shunday boshlangich shart kiritamiz:

$$\psi_{r\to\infty} \approx e^{ik_0 r} + f \frac{e^{ikr}}{r} .$$

Endi yuqoridagi boshlangich shartni ushbu Grin funksiyasini

$$G(r-r')=-\frac{1}{4\pi}\frac{e^{ik|r-r'|}}{|r-r'|}$$

kiritib, quidagicha yozamiz:

$$\psi=e^{ik_0r}-\frac{\mu}{2\pi\hbar^2}\int U(r')\psi(r')\frac{e^{ik|r-r'|}}{|r-r'|}dV'.$$

Katta r lar uchun

$$\frac{e^{ik|r-r'|}}{|r-r'|}\approx\frac{e^{ikr}}{r}\cdot e^{-ikr'},\qquad (r\to\infty),$$

bunda $\vec{k}=k\frac{\vec{r}}{r}$. Yuqoridagilardan foydalanib

$$\psi\approx e^{i\vec{k}_0\vec{r}}-\frac{\mu}{2\pi\hbar^2}\frac{e^{i\vec{k}\vec{r}}}{\vec{r}}\int dV'e^{-i\vec{k}\vec{r}'}U(\vec{r}')\psi(\vec{r}')$$

ni olamiz, bundan

$$f(\vec{k})=-\frac{\mu}{2\pi\hbar^2}\int dVe^{-i\vec{k}\vec{r}}U(\vec{r})\psi(\vec{r})$$

ekanini topamiz.

20-mavzu: Relyativistik kvant mexanikasi. Dirak tengnlamasining sodda hollarda yechish

Relyativistik fizika – bu yuqori tezliklar va yuqori energiyalar fizikasidir. Relyativistik zarralar o`zaro ta'sirida tinchlikdagi massa saqlanmaydi va bunda zarralar hosil bo`lishi hamda yo`qotilishi va bir-biriga aylanishi kuzatilishi mumkin. Bu hollarda relyativistik kvant fizikasi qonunlari ishlatiladi. Relyativistik kvant mexanikasi qonunlarining ishlatish chegarasi erkin zarrachaning energiyasi va impulsi orasidagi munosabatdan kelib chiqadi. Umumiy holda erkin zarrachaning energiyasi

$$E=c^2p^2+m^2c^2 \tag{1}$$

bo`ladi, bunda $mc^2$ – tinchlikdagi energiya. Agar implus $p\geq mc$ bo`lsa, bu holda zarracha uchun reletivistik kvant mexanikasi qonunlari ishlatiladi.

Kleyn-Gordon-Fok tenglamasi. Relyativistik tenglamani olish uchun E va p orasidagi relyativistik bog`lanishdan ya'ni (1) formuladan foydalanamiz.

$$\hbar^2\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\Delta\right)\Psi=m^2c^2\psi\,.$$

Bu tenglamaga to`rt o`lchamli shakl beramiz:

$$\sum_{\alpha=0}^{3}\left(\widehat{P}_\alpha\right)^2\psi=-m^2c^2\psi$$

yoki

$$\hbar \Pi \psi = -m^2 c^2 \psi$$

bu yerda Π – Lorens invariantli Dalamber operatori. Agar bu ifodada ψ Lorens almashtirishlar bo`lsa, bu tenglama ***Kleyn-Gordon-Fok*** (Shryodingerning relyativistik tenglamasi) ***tenglamasi*** deyiladi. Umumiy holda $\psi$ tenzor ham bo`lishi mumkin – $\psi_{\alpha,\beta,\ldots}$. Bu tenglama spini 0 ga teng bo`lgan $\pi$ mezon kabi zarralar uchun o`rinli.

Spini $1/2$ ga teng bo`lgan zarralar uchun esa Dirak tenglamasi o`rinli bo`ladi. Formal ravishda bu tenglama umumiy Shryodinger relyativistik tenglamasidan kelib chiqadi:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \hat{H}\, \Psi(\vec{r}, t).$$

Bunda faqat Gamilton operatori shaklini tanlashdadir. Dirak ushbu operatorni quyidagicha tanladi:

$$\hat{H} = -c\vec{\alpha} \cdot \hat{\vec{p}} - \beta m_0 c^2,$$

bunda α, β lar koeffisiyentlar. Sunday qilib

$$\left(i\hbar \frac{\partial}{\partial t} - i\hbar c \vec{\alpha} \cdot \vec{\nabla} + \beta m_0 c^2 \right) \Psi(\vec{r}, t) = 0$$

ni olamiz. Bu **Dirak tenglamasi** deyiladi.

20.1. To`rt qatorli funksiya uchun Dirak tenglamasida

$$i\hbar \frac{\partial \psi}{\partial t} = (C \sum_{i=1}^{3} \alpha_i (\hat{P}_i - eA_i) + m_0 C^2 \alpha_4 + e\varphi)\psi$$

norelyativistik yondashishga o`ting va ikki qatorli funksiya uchun Pauli tenglamasini oling. Bu yerda $\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$, i=1, 2, 3 $\alpha_4 = \begin{pmatrix} I \ldots 0 \\ 0 - I \end{pmatrix}$.

20.2. $V(r)$ maydon tomonidan erkin elektronning sochilish ehtimollik ifodasi uchun relyativistik o`zgarishini toping. Elektronning spini dastlabki va oxirigi holatlarda bir xil.

Foydalaniladigan darsliklar va o`quv qo`llanmalar ro`yxati

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Mundarija

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Kvant mexanikasidan masalalar yechish
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