

FİNAL SINAVI İLE İLGİLİ SABİT VE FORMÜLLER

Fiziksel sabitler ve genel integraller

$$\begin{aligned} h &= 6.63 \times 10^{-34} \text{ J s} & \hbar &= 1.06 \times 10^{-34} \text{ J s} & m_e &= 9.11 \times 10^{-34} \text{ kg} & c &= 3.0 \times 10^8 \text{ m/s} \\ E &= h\nu = hc/\lambda & \Delta x \Delta p &\geq \hbar/2 & \lambda &= h/p & \lambda \nu &= c \\ \int_0^\infty e^{-ax^2} dx &= \frac{1}{2} \sqrt{\frac{\pi}{a}} & \int_0^\infty x e^{-ax^2} dx &= \frac{1}{2a} & \int_0^\infty x^2 e^{-ax^2} dx &= \frac{\sqrt{\pi}}{4a^{3/2}} & \int_0^\infty x^n e^{-ax} dx &= \frac{n!}{a^{n+1}} \\ & & & & & & n > -1, a > 0 \text{ için geçerli} \end{aligned}$$

Temel Bağlantılar

Zamana Bağlı Schrödinger Denklemi

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

Zamandan Bağımsız Schrödinger Denklemi

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E \psi(x)$$

Kanonik Komütasyon Bağlantısı

$$[\hat{x}, \hat{p}] = i\hbar$$

Heisenberg Belirsizlik İlkesi

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

Fermi'nin Altın Kuralı

$$W_{fi} = \frac{2\pi}{\hbar} |V_{fi}|^2 \left[\delta(E_f - E_i - \hbar\omega) + \delta(E_f - E_i + \hbar\omega) \right]$$

$$\hat{V}(t) = \hat{V} \cos(\omega t) \quad V_{fi} = \int d^3\mathbf{r} \psi_f^*(\mathbf{r}) \hat{V} \psi_i(\mathbf{r})$$

Bir kutudaki Parçacık

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

$$V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{diğer durumlarda} \end{cases}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$\psi(0 \leq x \leq a) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

Ayrılabilen Sistemler

$$\hat{H}(x, y) = \hat{H}_x(x) + \hat{H}_y(y)$$

$$\Psi_{m,n}(x, y) = \psi_m(x)\psi_n(y)$$

$$E_{m,n} = E_m + E_n$$

Harmonik Osilatör

$$\hat{H} = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} k x^2 = \hat{a}_+ \hat{a}_+ + \frac{\hbar \omega}{2}$$

$$E_n = \hbar \omega \left(n + \frac{1}{2} \right); \quad \omega = \sqrt{\frac{k}{\mu}}$$

$$\hat{a}_\pm = \frac{1}{\sqrt{2m\hbar\omega}} (m\omega\hat{x} \mp i\hat{p})$$

$$[\hat{a}_-, \hat{a}_+] = 1$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_+ + \hat{a}_-)$$

$$\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}} (\hat{a}_+ - \hat{a}_-)$$

$$\hat{a}_+ \psi_n(x) = \sqrt{n+1} \psi_{n+1}(x)$$

$$\hat{a}_- \psi_n(x) = \sqrt{n} \psi_{n-1}(x)$$

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{\alpha}{\pi} \right)^{1/4} H_n(\alpha^{1/2} x) e^{-\frac{1}{2}\alpha x^2}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi} \right)^{1/4} e^{-\frac{1}{2}\alpha x^2}$$

$$\psi_1(x) = \frac{1}{\sqrt{2}} \left(\frac{\alpha}{\pi} \right)^{1/4} (2\alpha^{1/2} x) e^{-\frac{1}{2}\alpha x^2}$$

$$\psi_2(x) = \frac{1}{\sqrt{8}} \left(\frac{\alpha}{\pi} \right)^{1/4} (4\alpha x^2 - 2) e^{-\frac{1}{2}\alpha x^2}$$

$$\psi_3(x) = \frac{1}{\sqrt{48}} \left(\frac{\alpha}{\pi} \right)^{1/4} (8\alpha^{3/2} x^3 - 12\alpha^{1/2} x) e^{-\frac{1}{2}\alpha x^2}$$

Açısal Momentum Operatörleri ve Küresel Harmonikler

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

$$\hat{L}_z = i\hbar \frac{\partial}{\partial\phi}$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$[\hat{L}^2, \hat{L}_i] = 0$$

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$$

$$\hat{L}^2 Y_l^m = \hbar^2 l(l+1) Y_l^m$$

$$\hat{L}_z Y_l^m = \hbar m Y_l^m$$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_1^{\pm 1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}$$

Rijit Rotor

$$\hat{H} = \frac{\hat{J}^2}{2I}; \quad I = \mu R^2 \text{ (diatomik)}$$

$$\begin{aligned} \hat{H} Y_j^{j_z} &= E_j Y_j^{j_z}; & E_j &= \hbar^2 j(j+1) \\ j &= 0, 1, 2, 3, \dots & j_z &= -j, -j+1, \dots, j-1, j \end{aligned}$$

Hidrojenik Atom

$$\hat{H} = -\frac{\hbar^2}{2m_e} \nabla^2 - \frac{Ze^2}{r};$$

atomik birimde, $\hbar = m_e = e = 4\pi\epsilon_0 = a_0 = 1$.

$$E_n = -\frac{Z^2 e^2}{8\pi\epsilon_0 a_0 n^2} = \frac{Z^2}{2n^2} \text{ (a.b.)}$$

Hidrojenik Atom Dalga Fonksiyonları

$$n=1 \quad l=0 \quad m=0$$

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$$

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma} = \psi_{1s}$$

$$n=2 \quad l=0 \quad m=0$$

$$\psi_{200}(r, \theta, \phi) = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (2-\sigma) e^{-\frac{\sigma}{2}} = \psi_{2s}$$

$$l=1 \quad m=0$$

$$\psi_{210}(r, \theta, \phi) = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\frac{\sigma}{2}} \cos \theta = \psi_{2p_z}$$

$$l=1 \quad m=\pm 1$$

$$\psi_{21\pm 1}(r, \theta, \phi) = \frac{1}{\sqrt{64\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\frac{\sigma}{2}} \sin \theta e^{i\phi}$$

$$\frac{1}{\sqrt{2}} (\psi_{21+1} + \psi_{21-1}) = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\frac{\sigma}{2}} \sin \theta \cos \phi = \psi_{2p_x}$$

$$\sigma = \frac{Zr}{a_0}$$

$$\frac{1}{\sqrt{2}i} (\psi_{21+1} - \psi_{21-1}) = \frac{1}{\sqrt{32\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\frac{\sigma}{2}} \sin \theta \sin \phi = \psi_{2p_y}$$

Spin ½ Matrisleri

$$\mathbf{S}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \mathbf{S}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \mathbf{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Bağımsız Parçacık Modeli

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \begin{vmatrix} \psi_1(\mathbf{x}_1) & \psi_1(\mathbf{x}_2) & \psi_1(\mathbf{x}_3) \\ \psi_2(\mathbf{x}_1) & \psi_2(\mathbf{x}_2) & \psi_2(\mathbf{x}_3) \\ \psi_3(\mathbf{x}_1) & \psi_3(\mathbf{x}_2) & \psi_3(\mathbf{x}_3) \end{vmatrix}$$

$$E_{\text{ort}} = \sum_i \varepsilon_i + \sum_i \sum_{j < i} \tilde{J}_{ij} - \tilde{K}_{ij} \quad \text{burada } \tilde{J}_{ij} = J_{ij} \quad \text{ve } \tilde{K}_{ij} = \begin{cases} K_{ij} & \sigma_i = \sigma_j \text{ ise} \\ 0 & \sigma_i \neq \sigma_j \text{ ise} \end{cases}$$

Varyasyon Metodu ve Moleküler Orbital Teori

$$\mathbf{Hc} = E_{\text{avg}} \mathbf{Sc} \quad \mathbf{H} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}$$
$$\psi(\mathbf{r}) = \sum_i \phi_i(\mathbf{r}) \quad H_{ij} = \int d^3r \phi_i^*(\vec{r}) \hat{H} \phi_j(\vec{r}) \quad S_{ij} = \int d^3r \phi_i^*(\vec{r}) \phi_j(\vec{r})$$