

Övning 9

Träpartikelsystem

$$\psi(\vec{r}_1, \vec{r}_2, t)$$

Bestäms alltid av S.E.

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

där

$$H = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 + V(\vec{r}_1, \vec{r}_2, t)$$

Bosoner och fermioner:

$$\psi_{\pm}(\vec{r}_1, \vec{r}_2) = A[\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)]$$

Normering ger $A = \frac{1}{\sqrt{2}}$.

I allmänhet:

$$\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$$

För särskiljbara partiklar $\langle x_1 x_2 \rangle = \langle x \rangle_a \langle x \rangle_b$

För identiska partiklar:

$$\langle x_1 x_2 \rangle = \langle x \rangle_a \langle x \rangle_b \pm |\langle x \rangle_{ab}|^2$$

$$\text{där } \langle x \rangle_{ab} = \int x \psi_a(x) \psi_b(x) dx$$

4.38 Tre-dimensionell harmonisk oscillator

$$V(r) = \frac{1}{2} m \omega^2 r^2$$

a) I kartesiska koordinater

$$V(r) = \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2)$$

Således

$$E^2 \psi(x, y, z) = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi + \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2) \psi$$

Potentialen oberoende i x, y, z-riktning $\Rightarrow \psi(x, y, z)$ oberoende

$$\psi(x, y, z) = X(x) Y(y) Z(z)$$

Stoppa in detta i S.E och dividera med XYZ

$$E = -\frac{\hbar^2}{2m} \frac{1}{X} \frac{\partial^2 X}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 - \frac{\hbar^2}{2m} \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} + \frac{1}{2} m \omega^2 y^2 - \frac{\hbar^2}{2m} \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} + \frac{1}{2} m \omega^2 z^2$$

Vänsterledet är konstant och vi har 3 delar enbart beroende av x, y, z respektive. Dessa måste vara konstanta. Således

$$-\frac{\hbar^2}{2m} \frac{1}{X} \frac{\partial^2 X}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 = E_x$$

$$-\frac{\hbar^2}{2m} \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} + \frac{1}{2} m \omega^2 y^2 = E_y$$

$$-\frac{\hbar^2}{2m} \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} + \frac{1}{2} m \omega^2 z^2 = E_z$$

3 harmoniska oscillatorer med

$$E_x = (n_x + \frac{1}{2}) \hbar \omega, E_y = (n_y + \frac{1}{2}) \hbar \omega, E_z = (n_z + \frac{1}{2}) \hbar \omega$$

och
$$E = E_x + E_y + E_z = (n_x + n_y + n_z + \frac{3}{2}) \hbar \omega = (n + \frac{3}{2}) \hbar \omega, n = 0, 1, 2, \dots$$

b) Degenereringen av E_n , dvs på hur många sätt man vi få energin E_n .

Om $n_x = n, n_y = n_z = 0$ ett sätt

$n_x = n-1, (n_y = 1, n_z = 0), (0, 1)$ två

$n_x = n-2, (n_y = 2, n_z = 0), (1, 1), (0, 2)$ tre osv

Antalet sätt blir summan av alla dessa fall

$$d(n) = 1 + 2 + 3 + \dots + (n+1) = \frac{(n+1)(n+2)}{2}$$

4.55

Elektron i väteatom uppstår tillståndet

$$R_{21}(\sqrt{\frac{1}{3}} Y_1^0 \chi_+ + \sqrt{\frac{2}{3}} Y_1^1 \chi_-) = 2r_{210} \sqrt{\frac{1}{3}} \chi_+ + 2r_{211} \sqrt{\frac{2}{3}} \chi_-$$

a) Måttning av L^2 . För det här tillståndet $l=1$

$$\Rightarrow L^2 = l(l+1)\hbar^2 = 2\hbar^2 \quad (\text{alltid, dvs } P=1)$$

b) $L_z = 0, \hbar$

$$P_0 = \frac{1}{3}, P_1 = \frac{2}{3}$$

c) S^2 , alltid $\frac{3\hbar^2}{4}$ ← $s(s+1)\hbar^2$ för spin-1/2 partikel

d) $S_z = \pm \frac{\hbar}{2}$

$$P_+ = \frac{1}{3}, P_- = \frac{2}{3}$$

e) $\vec{J} = \vec{L} + \vec{S}$

Utveckla basen $|l, m\rangle |s, m_s\rangle$ i $|j, m_j\rangle$. Använd C-G

$$\begin{aligned} & \sqrt{\frac{1}{3}} |1, 0\rangle |1/2, 1/2\rangle + \sqrt{\frac{2}{3}} |1, 1\rangle |1/2, -1/2\rangle = \\ & = \frac{1}{\sqrt{3}} \left(\sqrt{\frac{2}{3}} |3/2, 1/2\rangle - \sqrt{\frac{1}{3}} |1/2, 1/2\rangle \right) + \sqrt{\frac{2}{3}} \left(\sqrt{\frac{1}{3}} |3/2, 1/2\rangle + \sqrt{\frac{2}{3}} |1/2, 1/2\rangle \right) \\ & = \left(\frac{\sqrt{2}}{3} + \frac{\sqrt{2}}{3} \right) |3/2, 1/2\rangle + \left(-\frac{1}{3} + \frac{2}{3} \right) |1/2, 1/2\rangle = \frac{2\sqrt{2}}{3} |3/2, 1/2\rangle + \frac{1}{3} |1/2, 1/2\rangle \end{aligned}$$

$$j = \frac{1}{2}, \frac{3}{2}, \quad m_j = \frac{1}{2}$$

$$J^2 = \frac{3}{4}\hbar^2 \quad (P = \frac{1}{9}), \quad J^2 = \frac{15}{4}\hbar^2 \quad (P = \frac{8}{9})$$

f) $m_j = \frac{1}{2} \Rightarrow J_z = \frac{\hbar}{2}, P=1$

$$\begin{aligned} g) |2, 1\rangle^2 &= |R_{21}\rangle^2 \left| \sqrt{\frac{1}{3}} Y_1^0 \chi_+ + \sqrt{\frac{2}{3}} Y_1^1 \chi_- \right|^2 = |R_{21}\rangle^2 \left[\frac{1}{3} |Y_1^0|^2 \chi_+ \chi_+ \right. \\ & \left. + \frac{2}{3} |Y_1^1|^2 \chi_- \chi_- + \frac{2}{3} Y_1^0 Y_1^1 (\chi_+ \chi_- + \chi_- \chi_+) \right] = |R_{21}\rangle^2 \left(\frac{1}{3} |Y_1^0|^2 + \frac{2}{3} |Y_1^1|^2 \right) \\ & = \frac{1}{3} \left[\frac{1}{3} \cdot \frac{1}{24} \cdot \frac{1}{a^3} \cdot \frac{r^2}{a^2} e^{-r/a} \left[\frac{3}{4\pi} \cos^2 \theta + 2 \cdot \frac{3}{8\pi} \sin^2 \theta \right] \right] = \\ & = \frac{1}{96\pi} \cdot \frac{1}{a^6} \cdot \frac{r^2}{a^2} e^{-r/a} \end{aligned}$$

$$h) \frac{1}{3} |R_{21}|^2 \underbrace{\int |Y_1^0|^2}_{\substack{\text{spin-up} \\ \text{coeff.}}} \sin^2 \theta d\theta d\phi = \frac{1}{3} |R_{21}|^2 = \frac{1}{3} \frac{1}{24a^3} r^2 e^{-r/a} = \frac{1}{72a^3} r e^{-r/a}$$

- 5.5 a) Skriv ned Hamiltonianen för två icke-interagerande identiska partiklar i den oändliga potentialbotten.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x_2^2} = E \psi \quad 0 \leq x_1, x_2 \leq a, \text{ annars } \psi = 0$$

$$\psi(x_1, x_2) = \frac{\sqrt{2}}{a} \left[\sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right) - \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right) \right]$$

Bestäm E

$$\frac{d^2 \psi}{dx_1^2} = -\left(\frac{\pi}{a}\right)^2 \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right) + \left(\frac{2\pi}{a}\right)^2 \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right)$$

$$\frac{d^2 \psi}{dx_2^2} = -\left(\frac{2\pi}{a}\right)^2 \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right) + \left(\frac{\pi}{a}\right)^2 \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right)$$

$$\Rightarrow E \psi = -\frac{\hbar^2}{2m} \left(-\left(\frac{\pi}{a}\right)^2 - \left(\frac{2\pi}{a}\right)^2 \right) \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right)$$

$$-\frac{\hbar^2}{2m} \left(\left(\frac{2\pi}{a}\right)^2 + \left(\frac{\pi}{a}\right)^2 \right) \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right) =$$

$$= \frac{5\pi^2 \hbar^2}{2ma^2} \psi$$

$$\Rightarrow E = \frac{5\pi^2 \hbar^2}{2ma^2}$$

- b) Hitta nästa två exiterade tillstånd om särskiljbara, identiska bosoner, identiska fermioner

Särskiljbara partiklar:

$$\psi_{22} = \left(\frac{2}{a}\right) \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right) \quad (\text{icke-degenererad})$$

$$\left\{ \begin{array}{l} \psi_{13} = \left(\frac{2}{a}\right) \sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right) \\ \psi_{31} = \left(\frac{2}{a}\right) \sin\left(\frac{3\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right) \end{array} \right. \quad \text{tvåfaldigt degenererad}$$

Identiska bosoner:

$$\psi_{22} = \left(\frac{2}{a}\right) \sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right)$$

$$\psi_{13} = \frac{\sqrt{2}}{a} \left(\sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right) + \sin\left(\frac{3\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right) \right)$$

Identiska fermioner:

$$\psi_{13} = \frac{\sqrt{2}}{a} \left[\sin\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right) - \sin\left(\frac{3\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right) \right]$$

$$\psi_{23} = \frac{\sqrt{2}}{a} \left[\sin\left(\frac{2\pi x_1}{a}\right) \sin\left(\frac{3\pi x_2}{a}\right) - \sin\left(\frac{3\pi x_1}{a}\right) \sin\left(\frac{2\pi x_2}{a}\right) \right]$$

5.6 Två icke-interagerande partiklar med massan m . En är i tillståndet

$$\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad (\text{oändlig potentialbrunn})$$

den andra i tillståndet ψ_l . Bestäm $\langle (x_1 - x_2)^2 \rangle$.

a) Antag särskiljbara partiklar

$$(5.19) \quad \langle (x_1 - x_2)^2 \rangle_d = \langle x^2 \rangle_a + \langle x^2 \rangle_b + 2\langle x \rangle_a \langle x \rangle_b$$

De här separata väntevärdena har vi bestämt förut.

$$\langle x^2 \rangle = a^2 \left(\frac{1}{3} - \frac{1}{2(n\pi)^2} \right)$$

$$\langle x \rangle = \frac{a}{2}$$

$$\begin{aligned} \Rightarrow \langle (x_1 - x_2)^2 \rangle &= a^2 \left(\frac{1}{3} - \frac{1}{2(n\pi)^2} \right) + a^2 \left(\frac{1}{3} - \frac{1}{2(m\pi)^2} \right) - 2 \cdot \frac{a}{2} \cdot \frac{a}{2} \\ &= 2 \frac{a^2}{3} - \frac{a^2}{2} - a^2 \frac{m^2 + n^2}{2m^2 n^2 \pi^2} = \frac{a^2}{6} - a^2 \frac{m^2 + n^2}{2m^2 n^2 \pi^2} = a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] \end{aligned}$$

b) Antag identiska bosoner

$$\text{Här} \quad \langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$$

$\langle x_1^2 \rangle$ och $\langle x_2^2 \rangle$ som förut $\langle x_1 x_2 \rangle$ måste bestämmas.

I fallet av identiska bosoner har vi fermioner

$$\langle x_1 x_2 \rangle = \langle x_{\frac{m}{2}} \rangle_n \pm |\langle x \rangle_{mn}|^2$$

Vi känner $\langle x_{\frac{m}{2}} \rangle_m = \frac{a}{2}$. Kvar att bestämma är nu

$$\begin{aligned} \langle x \rangle_{mn} &= \frac{2}{a} \int_0^a x \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx = \frac{1}{a} \int_0^a x \left[\cos\left(\frac{(m-n)\pi x}{a}\right) - \cos\left(\frac{(m+n)\pi x}{a}\right) \right] dx \\ &= \frac{1}{a} \left[x \frac{a}{(m-n)\pi} \sin\left(\frac{(m-n)\pi x}{a}\right) - x \frac{a}{(m+n)\pi} \sin\left(\frac{(m+n)\pi x}{a}\right) \right]_0^a - \int_0^a \frac{1}{(m-n)\pi} \sin\left(\frac{(m-n)\pi x}{a}\right) - \frac{1}{(m+n)\pi} \sin\left(\frac{(m+n)\pi x}{a}\right) dx \\ &= + \left[\frac{a}{(m-n)^2 \pi^2} \cos\left(\frac{(m-n)\pi x}{a}\right) + \frac{a}{(m+n)^2 \pi^2} \cos\left(\frac{(m+n)\pi x}{a}\right) \right]_0^a = \\ &= \frac{a}{\pi^2} \left[\frac{1}{(m-n)^2} \left((-1)^{(m-n)} - 1 \right) - \frac{1}{(m+n)^2} \left((-1)^{m+n} - 1 \right) \right] = \\ &= \frac{a}{\pi^2} \left((-1)^{m+n} - 1 \right) \cdot \left(\frac{1}{(m-n)^2} - \frac{1}{(m+n)^2} \right) = \begin{cases} -\frac{a \cdot 8mn}{\pi^2 (m^2 - n^2)^2} & m, n \text{ udda} \\ 0 & \text{annars} \end{cases} \end{aligned}$$

Säledes:

$$\langle (x_1 - x_2)^2 \rangle = a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] - \frac{128a^2 m^2 n^2}{\pi^4 (m^2 - n^2)^4}$$

c) Identiska fermioner \Rightarrow andra tecknet

$$\langle (x_1 - x_2)^2 \rangle = a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] + \frac{128a^2 m^2 n^2}{\pi^4 (m^2 - n^2)^4}$$

5.7

Tre partiklar. En i tillstånd $\psi_a(x)$, en i $\psi_b(x)$ och en i $\psi_c(x)$.

Antag ψ_a, ψ_b, ψ_c ortonormala. Konstruera tre-partikeltillstånd för särskiljbara partiklar, identiska bosoner, identiska fermioner

a) Särskiljbara partiklar

$$\psi(x_1, x_2, x_3) = \psi_a(x_1) \psi_b(x_2) \psi_c(x_3)$$

b) Identiska bosoner. Tillståndet måste vara helt symmetriskt mot byte av vilka två partiklar som helst.

$$\psi(x_1, x_2, x_3) = \frac{1}{\sqrt{6}} \left[\psi_a(x_1) \psi_b(x_2) \psi_c(x_3) + \psi_a(x_1) \psi_c(x_2) \psi_b(x_3) + \psi_c(x_1) \psi_b(x_2) \psi_a(x_3) \right. \\ \left. + \psi_b(x_1) \psi_a(x_2) \psi_c(x_3) + \psi_c(x_1) \psi_a(x_2) \psi_b(x_3) + \psi_b(x_1) \psi_c(x_2) \psi_a(x_3) \right]$$

c) Identiska fermioner. Tillståndet måste vara helt anti-symmetriskt

$$\psi(x_1, x_2, x_3) = \frac{1}{\sqrt{6}} \left[\psi_a(x_1) \psi_b(x_2) \psi_c(x_3) - \psi_a(x_1) \psi_c(x_2) \psi_b(x_3) \right. \\ \left. - \psi_c(x_1) \psi_b(x_2) \psi_a(x_3) - \psi_b(x_1) \psi_a(x_2) \psi_c(x_3) + \psi_c(x_1) \psi_a(x_2) \psi_b(x_3) \right. \\ \left. + \psi_b(x_1) \psi_c(x_2) \psi_a(x_3) \right]$$

5.11 a) Bestäm $\langle 1/|\vec{r}_1 - \vec{r}_2| \rangle$ för tillståndet

$$\psi_0(\vec{r}_1, \vec{r}_2) = \frac{8}{\pi a^3} e^{-2(r_1+r_2)/a}$$

$$\left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle = \iint \frac{1}{|\vec{r}_1 - \vec{r}_2|} |\psi_0(\vec{r}_1, \vec{r}_2)|^2 d\vec{r}_1 d\vec{r}_2 = \left(\frac{8}{\pi a^3} \right)^2 \iint \frac{e^{-4(r_1+r_2)/a}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta}} d\vec{r}_2 d\vec{r}_1$$

Börja med integralen över $d\vec{r}_2$

$$\int \frac{e^{-4(r_1+r_2)/a}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}} r_2^2 \sin\theta_2 d\theta_2 d\phi_2 = 2\pi \int_0^\pi \frac{e^{-4(r_1+r_2)/a}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}} r_2^2 \sin\theta_2 d\theta_2$$

$$= 2\pi \int_0^\pi \frac{e^{-4(r_1+r_2)/a}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}} r_2^2 \sin\theta_2 d\theta_2 = 2\pi \int_0^\pi \frac{e^{-4(r_1+r_2)/a}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}} r_2^2 \sin\theta_2 d\theta_2$$

$$= 2\pi \int_0^{r_1} \frac{2r_2^2 e^{-4(r_1+r_2)/a}}{r_1} dr_2 + 2\pi \int_{r_1}^\infty 2r_2 e^{-4(r_1+r_2)/a} dr_2 =$$

$$= \underbrace{\frac{4\pi}{r_1} \int_0^{r_1} r_2^2 e^{-4r_2/a} dr_2}_{I_1} + \underbrace{4\pi e^{-4r_1/a} \int_{r_1}^\infty r_2 e^{-4r_2/a} dr_2}_{I_2} =$$

$$I_1: \int_0^{r_1} r_2^2 e^{-4r_2/a} dr_2 = \left[-\frac{a}{4} r_2^2 e^{-4r_2/a} + \frac{a^2}{2} \left(\frac{a}{4} \right) e^{-4r_2/a} \left(-\frac{4r_2}{a} - 1 \right) \right]_0^{r_1} =$$

$$= -\frac{a}{4} \left[r_1^2 e^{-4r_1/a} + \frac{ar_1}{2} e^{-4r_1/a} + \frac{a^2}{8} e^{-4r_1/a} - \frac{a^2}{8} \right]$$

$$\int_{r_1}^\infty r_2 e^{-4r_2/a} dr_2 = \left[\left(\frac{a}{4} \right)^2 e^{-4r_2/a} \left(-\frac{4r_2}{a} - 1 \right) \right]_{r_1}^\infty = \left(\frac{a}{4} \right)^2 e^{-4r_1/a} \left(\frac{4r_1}{a} + 1 \right)$$

Således

$$\frac{4\pi}{r_1} e^{-4r_1/a} (I_1 + I_2) = \frac{\pi a^2}{8} \left\{ \frac{a}{r_1} e^{-4r_1/a} - \left(2 + \frac{a}{r_1} \right) e^{-8r_1/a} \right\}$$

$$\Rightarrow \left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle = \frac{8}{\pi a^4} \cdot 4\pi \int_0^\infty \left[\frac{a}{r_1} e^{-4r_1/a} - \left(2 + \frac{a}{r_1} \right) e^{-8r_1/a} \right] r_1^2 dr_1 =$$

$$= \frac{32}{a^4} \left\{ a \int_0^\infty r_1 e^{-4r_1/a} dr_1 - 2 \int_0^\infty r_1^2 e^{-8r_1/a} dr_1 - a \int_0^\infty r_1 e^{-8r_1/a} dr_1 \right\}$$

$$= \frac{32}{a^4} \left\{ a \cdot \left(\frac{a}{4} \right)^2 - 2 \cdot 2 \cdot \left(\frac{a}{8} \right)^3 - a \cdot \left(\frac{a}{8} \right)^2 \right\} = \frac{32}{a} \left(\frac{1}{16} - \frac{1}{128} - \frac{1}{64} \right) = \frac{5}{4a}$$

b) Uppskatta elektronens interaktionsenergi

$$V_{ee} \approx \frac{e^2}{4\pi\epsilon_0} \left\langle \frac{1}{|r_1 - r_2|} \right\rangle = \frac{5}{4} \frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{a} = \frac{5}{4} \frac{m}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 = \frac{5}{2} (-E_1) = \frac{5}{2} (13.6 \text{ eV}) = 34$$