Boxes, operators, measurement and all that

Note Title 08-10-2009

Administrative business

Syllabus for minor - ALL material between minor 1 and minor 2

Lectures available at
http://web.iitd.ac.in/~nkurur/courses.html

Postulates

1) Wavefunction – Probabilistic interpretation

$$\Psi(\vec{r}, t)$$

N particle system

$$\Psi(\underbrace{\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots \vec{r}_N}_{3N}, t)$$

$3N, t$

2) Observable — Linear, Hermitian Operator

3) Measurement - Eigenvalues of the operator

$$\langle A \rangle = \int \Psi^* \hat{A} \Psi \, d\tau$$

4) Time development of the system

$$i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H} \Psi$$

Linear

$$\hat{A}(c_1 \psi_1 + c_2 \psi_2) = c_1 \hat{A} \psi_1 + c_2 \hat{A} \psi_2$$

$\frac{d}{dx}$ / Multiplication by x / c_q / etc

$\hat{O}_p(f) = f^2 \rightarrow$ Non linear

Hermitian

$$\int \psi^* \hat{A} \psi \, d\tau = \left(\int \psi^* \hat{A} \psi \, d\tau \right)^*$$

$$= \int (\hat{A}\psi)^* \psi \, d\tau \Big]$$

$\Downarrow$?

"real" eigenvalues

$$\boxed{\hat{A}\psi = a\psi}$$ (eigenvalue equation)

$$a\int \psi^* \hat{\psi}\, d\tau$$

$$\int \underbrace{(\hat{A}\psi)}^* \psi \, d\tau$$

$$= a^* \int \psi^* \psi \, d\tau$$

$$\Rightarrow \quad a = a^* \quad (\text{real})$$

$$\int \psi^* \hat{A} \psi \, d\tau = \int (\hat{A}\psi)^* \psi \, d\tau$$

$$\hat{A} = \frac{d}{dx}$$

$$\int_{-\infty}^{\infty} \psi^* \frac{d}{dx}\psi \, dx = \left(\Big|_{-\infty}^{\infty} - \int \right)$$

$$(= 0$$

not a Hermitian operator

ψ is an acceptable QM wf

Hamiltonian — Total energy

m_e, e

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

Kinetic energy

m_p • p

$$\hat{\mathcal{H}}_{H\ atom} = \hat{T}_p + \hat{T}_e + \hat{V}_{ne}$$

+ Potential energy

$$= -\frac{\hbar^2}{2m_p}\nabla_p^2 - \frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{Ze^2}{r}$$

He atom

$$\hat{\mathcal{H}}_{He} = \cdots \qquad \mathcal{H}\psi = E\psi$$

Nucleus is fixed

$$\mathcal{H}_H = \underbrace{-\frac{\hbar^2}{2m}\nabla^2}_{T} - \frac{e^2}{r}$$

$$\psi(r, \theta, \varphi)$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) - \frac{e^2}{\sqrt{x^2+y^2+z^2}}$$

$$(x, y, z)$$

$$\downarrow$$

$$(r, \theta, \varphi)$$

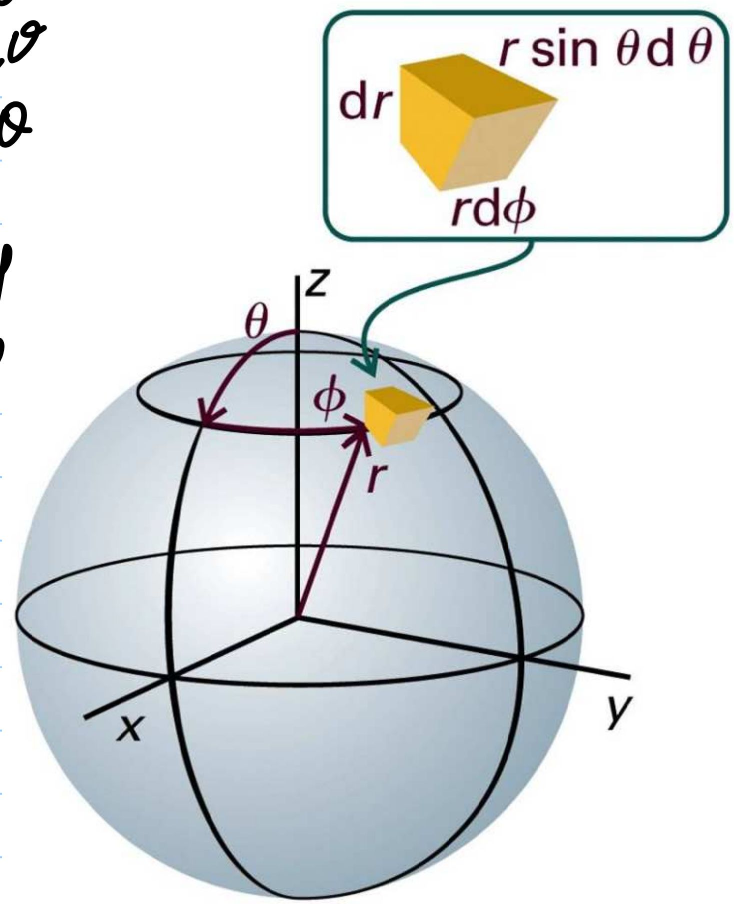
$$-\frac{\hbar^2}{2m}\left(\qquad \right) - e^2/r$$

$$\int \Psi^* \, \Psi \, \boxed{d\tau} = 1$$

$dx\,dy\,dz$ $\qquad$ $r^2 \sin\theta \, dr\, d\theta\, d\varphi$

$$\int_0^\infty f(r)\, dr \int_0^\pi g(\theta)\, r \sin\theta\, d\theta \int_0^{2\pi} h(\varphi)\, r\, d\varphi$$

$$\int f(r)\, r^2 dr \int g(\theta) \sin\theta\, d\theta \int h(\varphi)\, d\varphi$$



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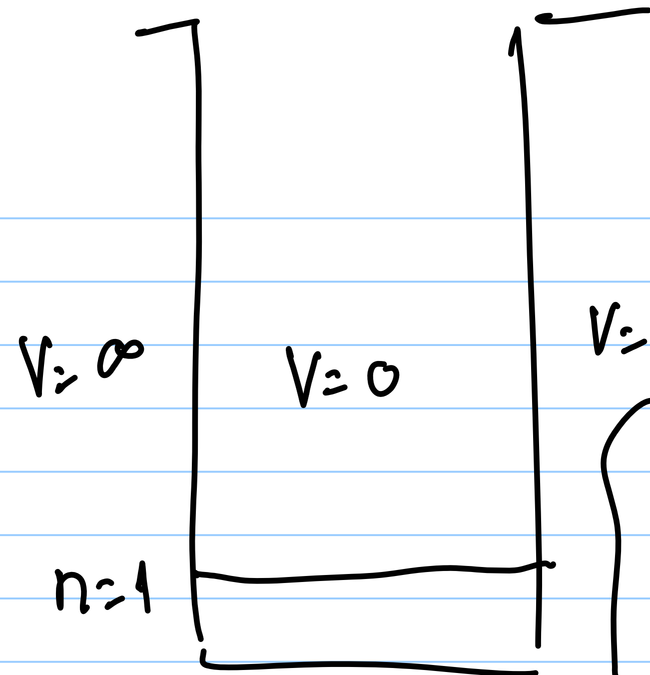


$$\boxed{\Delta p \, \Delta x \geq \hbar/2}$$

$$\begin{cases} E_1 = \dfrac{h^2}{8ma^2} \\ \psi_1 = \sqrt{\dfrac{2}{a}} \sin\left(\dfrac{\pi x}{a}\right) \end{cases}$$

$$SD = \sqrt{\overline{x^2} - \bar{x}^2}$$

by analogy

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \longrightarrow a/2$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \longrightarrow 0$$

$V = 0 \qquad \langle p^2 \rangle = 2m \langle E \rangle$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = \frac{h^2}{8ma^2}\psi_1$$

"sharp"

$$\langle E \rangle = E_1$$

$$\langle p^2 \rangle_1 = 2m\langle E \rangle = 2mE_1$$

$$\hat{O}_p \psi = a\psi$$

$$\langle p \rangle = 0$$

$$\int \psi^* \hat{O}_p \psi \, d\tau = a \int \psi^* \psi \, d\tau = a$$

$$\sin\left(\frac{\pi x}{a}\right) = \frac{1}{2i}\left(e^{ikx} - e^{-ikx}\right)$$

$$\Delta E = 0$$

$$\Delta p = \langle p^2 \rangle - \langle p \rangle^2$$

$$\int \psi^* \psi$$

$$\Delta x = \langle x^2 \rangle - \langle x \rangle^2$$

$$\int x^2 \sin^2\left(\frac{\pi x}{a}\right) dx$$

$$\Delta x \, \Delta p > \hbar/2$$

$$\langle A \rangle = \frac{\int \psi^* A \psi \, d\tau}{\int \psi^* \psi \, d\tau}$$

$$\Delta x \, \Delta p \geq \hbar/2$$

$$\Delta A \, \Delta B \geq \frac{1}{2} \left| \langle [A, B] \rangle \right|$$

$$-i\hbar\frac{\partial}{\partial x}\, x\,\psi \neq \underline{x\left(-i\hbar\frac{\partial}{\partial x}\right)\psi}$$

$$\psi'$$

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

$$\hat{A}\hat{B} - \hat{B}\hat{A} \neq 0 \qquad \Delta A\,\Delta B \quad \hat{O}_p\psi$$

$$\boxed{-i\hbar\frac{\partial}{\partial x}(x}\psi) = -i\hbar\left\{x\frac{\partial\psi}{\partial x} + \psi\right\}$$

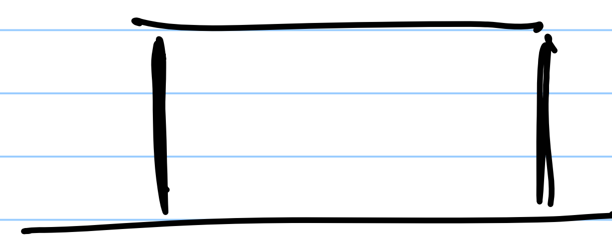
$$= \left(-i\hbar\, x\frac{\partial}{\partial x} + 1\right)\psi$$

$$\longrightarrow [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad \text{(commutator)}$$

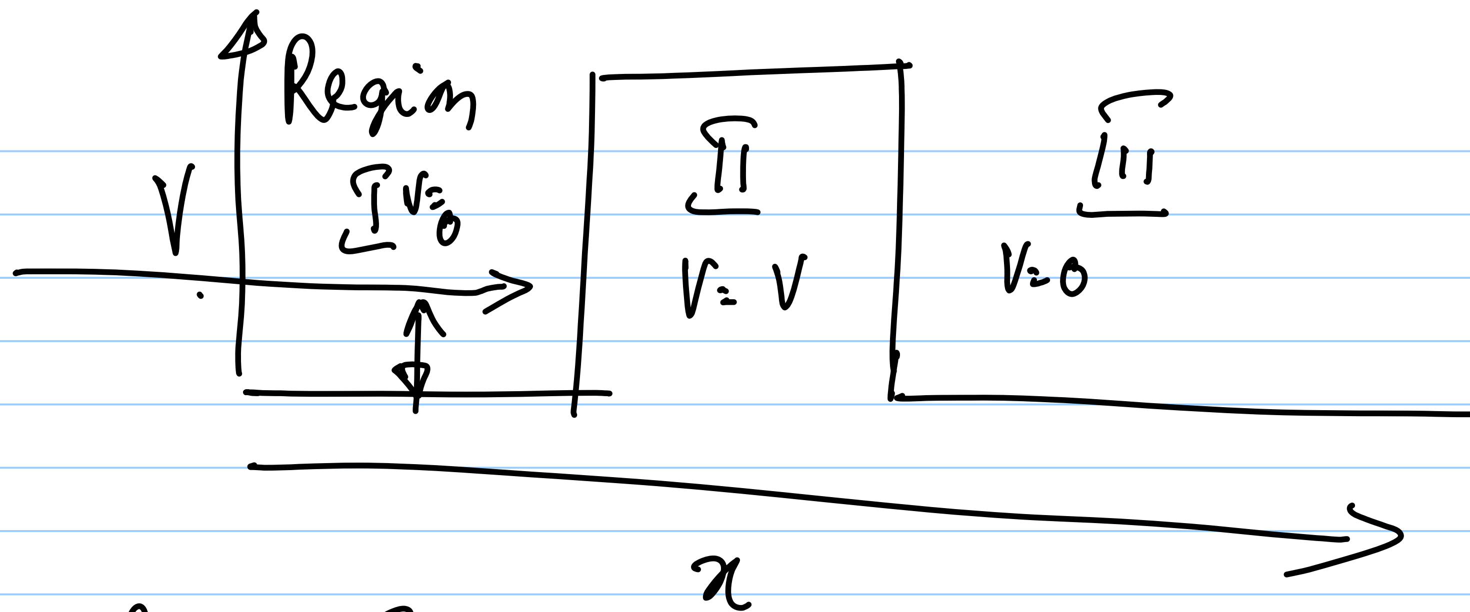
$$\boxed{\Delta E \, \Delta t \geq \hbar/2}$$

Δp :

$\longrightarrow \hbar k$



$\longleftarrow$

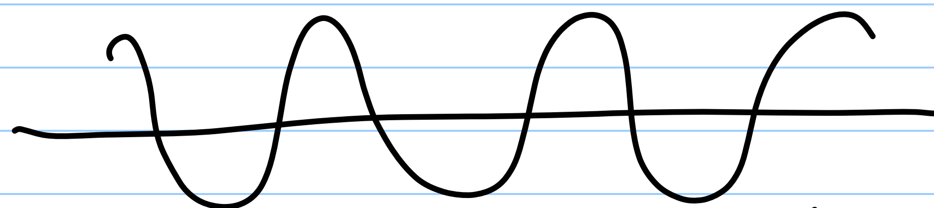


Region I :

Region II : $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)\psi_{II} = E\,\psi_{II}$

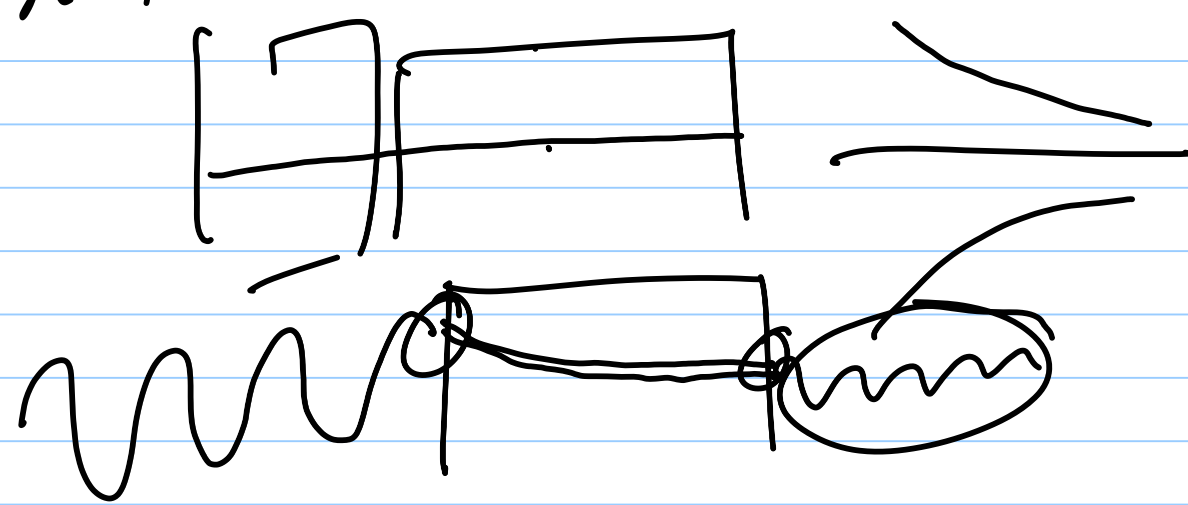
Region III :

Region I : ψ_I e^{-ikx}

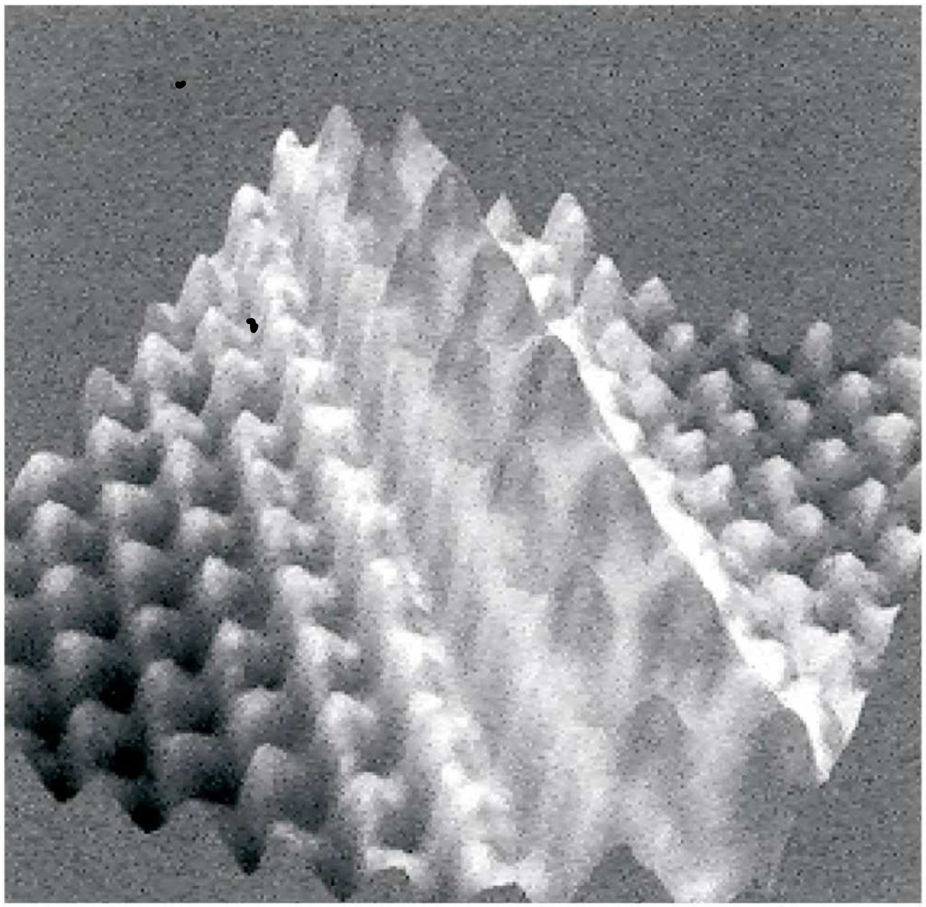


$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

Region II:



Tunneling



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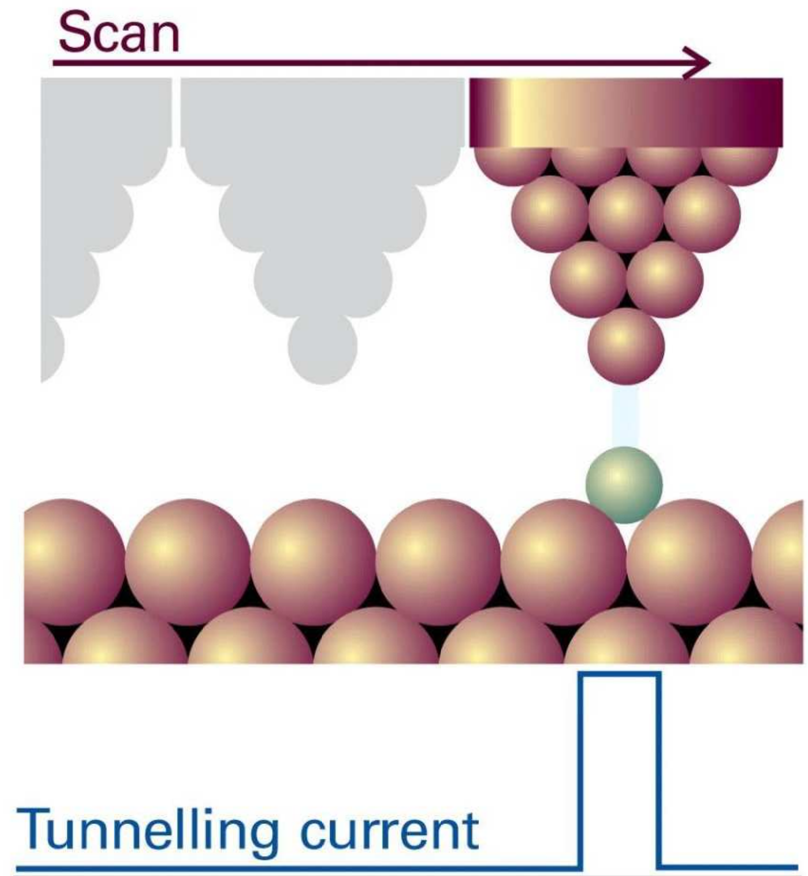

Figure 9-16
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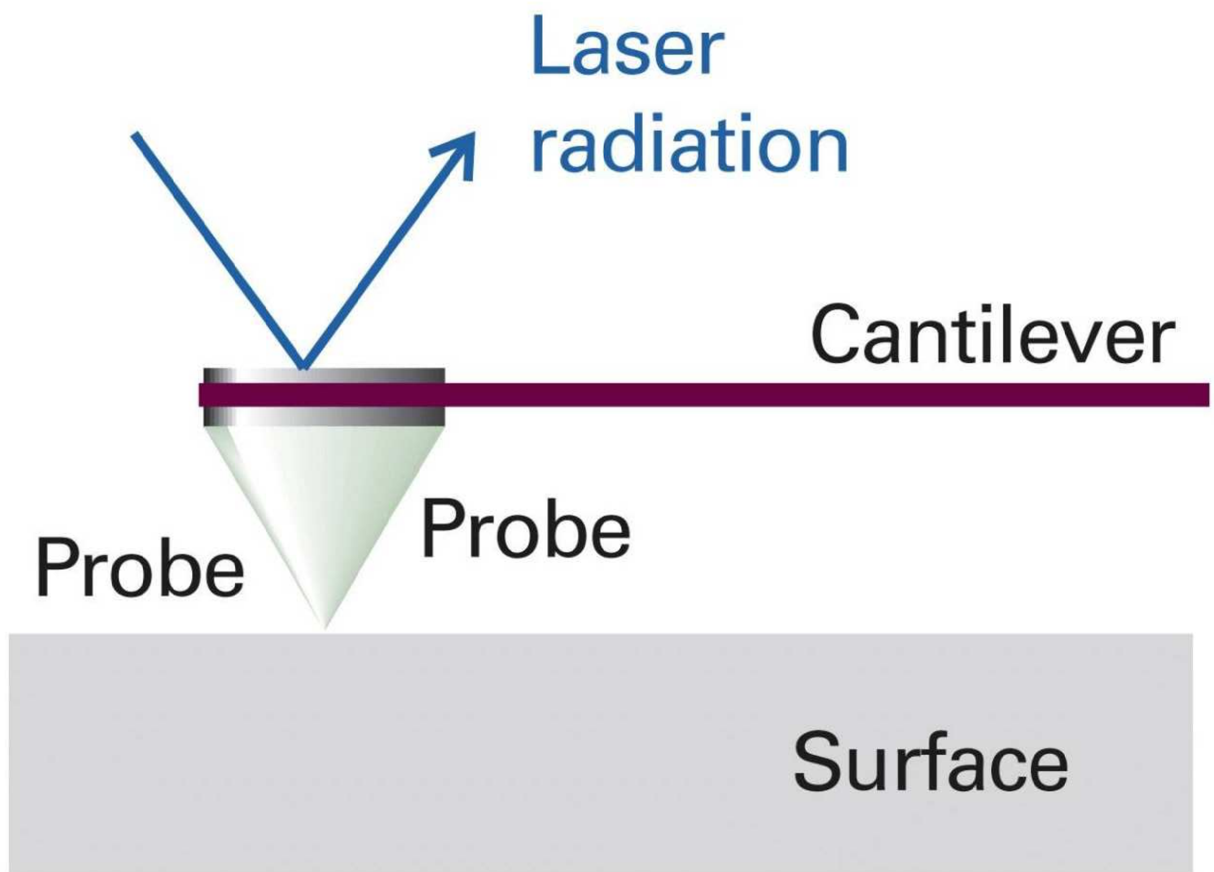

Figure 9-18
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