Computational Methods in Quantum Mechanics

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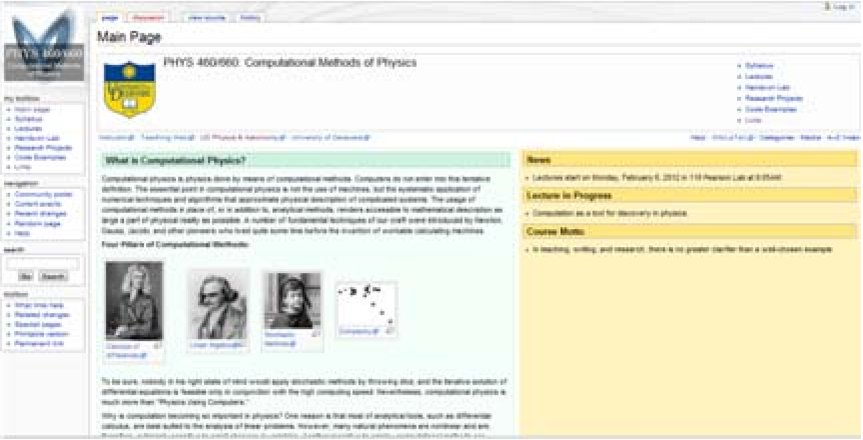
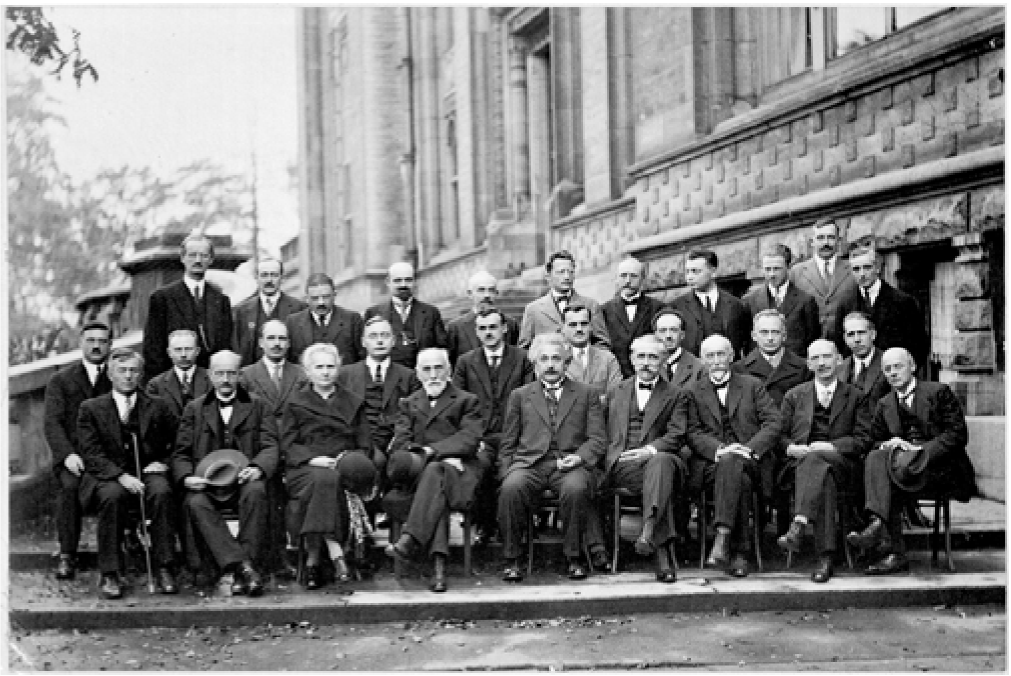
PHYS 460/660: Computational Methods of Physics

http://wiki.physics.udel.edu/phys660



Quantum Mechanics in the Words of the Founding Fathers

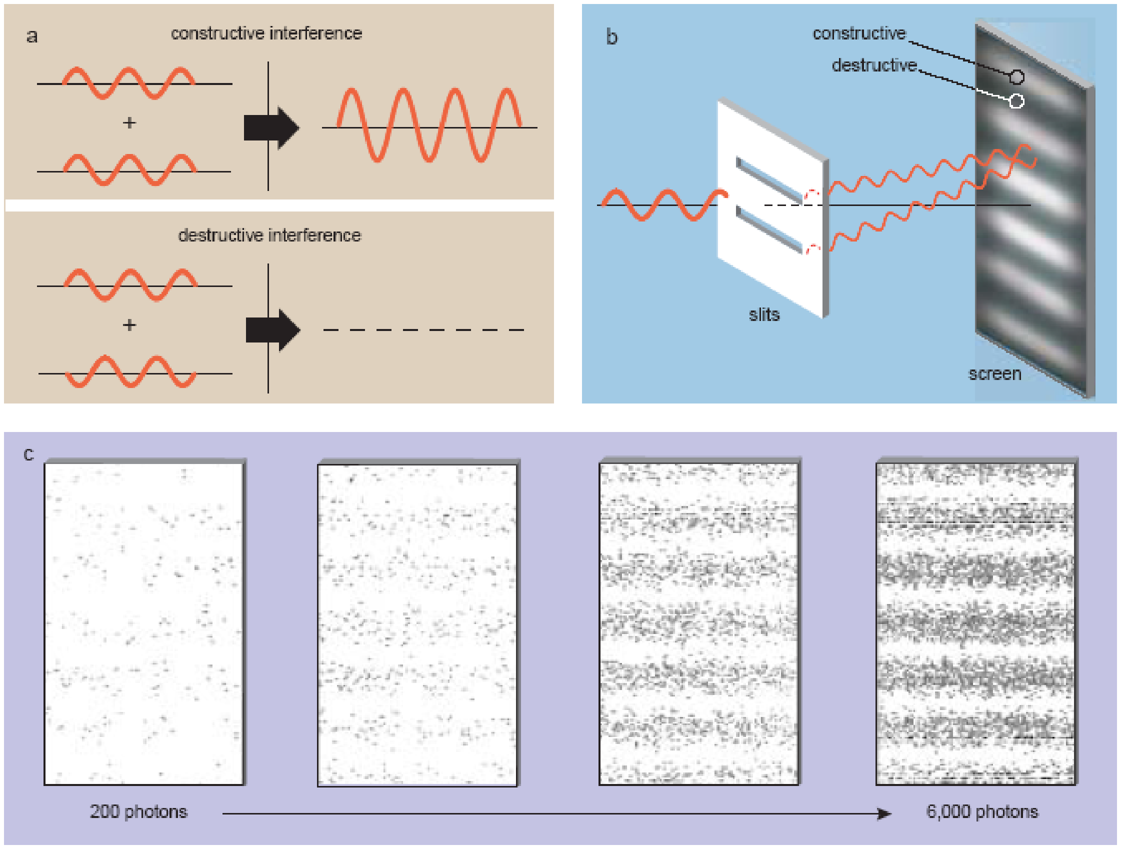
- **Albert Einstein**: "Quantum mechanics is very impressive. But an inner voice tells me that it is not yet the real thing. The theory produces a good deal but hardly brings us closer to the secret of the Old One. I am at all events convinced that He does not play dice."

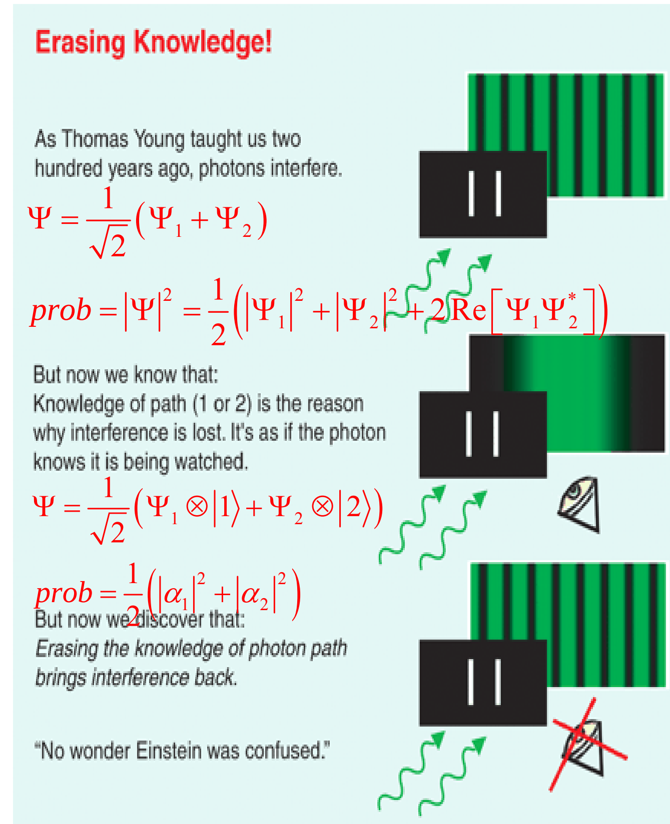


- **Niels Bohr:** "Anyone who is not shocked by quantum theory has not understood a single word."
- **Werner Heisenberg:** "I myself . . . only came to believe in the uncertainty relations after many pangs of conscience. . . "
- **Erwin Schrödinger**: "Had I known that we were not going to get rid of this damned quantum jumping, I never would have involved myself in this business!"

- Groucho Marx: "Very interesting theory - it makes no sense at all."

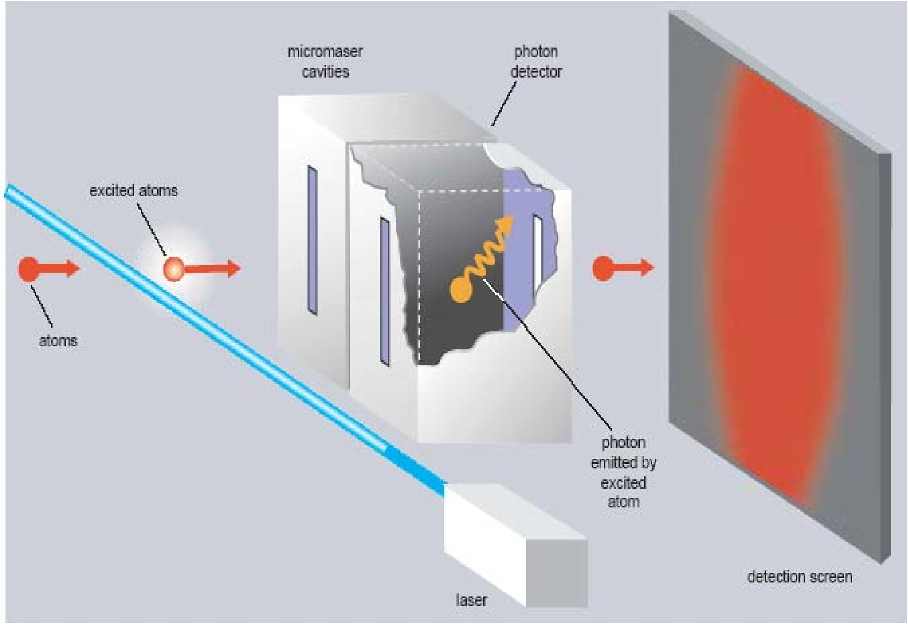
Quantum Interference in Two-Slit Experiments





❑The **self interference of individual particles** is the greatest mistery in quntum physics; in fact, Richard Feynman pronounced it "the only mystery" in quantum theory

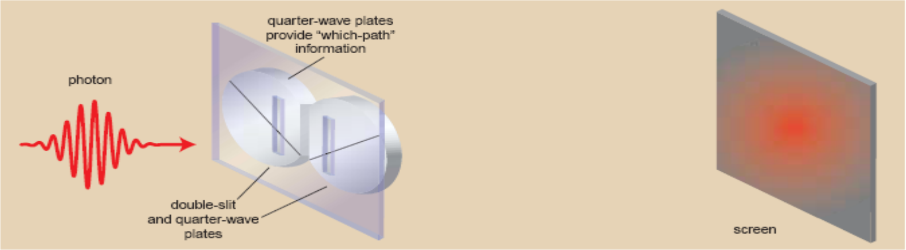
Quantum Erasure

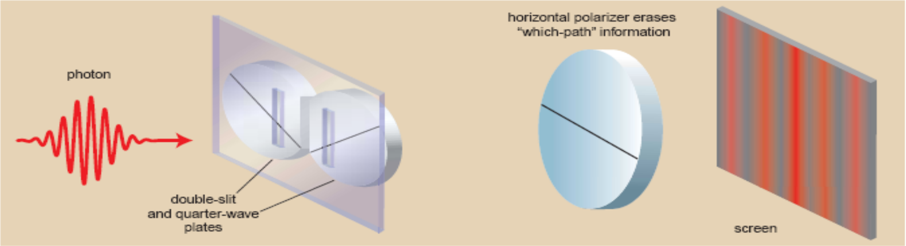


$$|\Psi_0\rangle = \frac{1}{\sqrt{2}}\left(|\text{path 1}\rangle \otimes |\nwarrow\rangle + |\text{path 2}\rangle \otimes |\nearrow\rangle\right)$$

$$|\Psi_0\rangle = \frac{1}{2}\left(|\text{path 1}\rangle + |\text{path 2}\rangle\right) \otimes |\rightarrow\rangle + \frac{1}{2}\left(|\text{path 1}\rangle - |\text{path 2}\rangle\right) \otimes |\uparrow\rangle$$

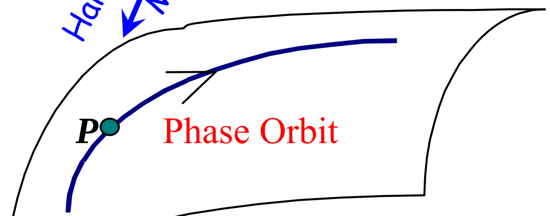
B. Green, *Fabric of Cosmos* (page 149): "These experiments are a magnificent affront to our conventional notions of space and time. Something that takes place long after and far away from something else nevertheless is vital to our description of that something else. By any classical-common sense-reckoning, that's, well, crazy. Of course, that's the point: classical reckoning is the wrong kind of reckoning to use in a quantum universe.... For a few days after I learned of these experiments, I remember feeling elated. I felt I'd been given a glimpse into a veiled side of reality. Common experience—mundane, ordinary, day-to-day activities—suddenly seemed part of a classical charade, hiding the true nature of our quantum world. The world of the everyday suddenly seemed nothing but an inverted magic act, lulling its audience into believing in the usual, familiar conceptions of space and time, while the astonishing truth of quantum reality lay carefully guarded by nature's sleights of hand."





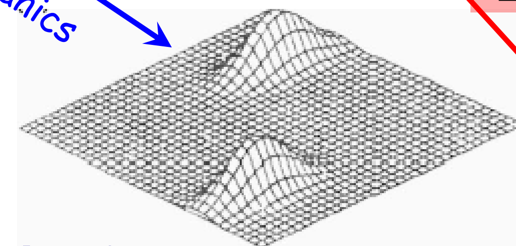
Classical vs. Three Roads to Quantum Mechanics

Hamilton-Lagrange Mechanics



$$\dot{p}_i = -\frac{\partial \boldsymbol{H}}{\partial q_i}, \quad \dot{q}_i = \frac{\partial \boldsymbol{H}}{\partial p_i}$$

Boltzmann-Gibbs Statistical Mechanics

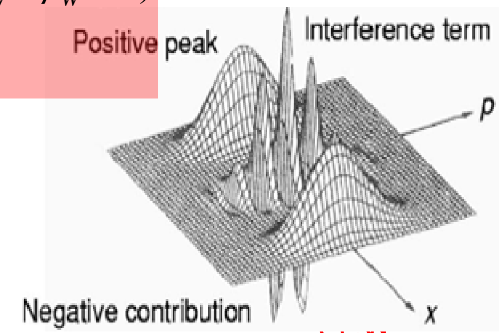


$$\frac{d\rho}{dt} \equiv \frac{\partial \rho}{\partial t} + \{\rho, \boldsymbol{H}\} = 0 \Rightarrow \rho(p,q) = \frac{e^{-\beta H(p,q)}}{Z}$$

$$\rho_W(q,p)$$

$$\frac{\partial \rho_W}{\partial t} = \frac{1}{i\hbar}(H * \rho_W - \rho_W * H)$$

$$* \equiv e^{i\hbar(\overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q)/2}$$



Moyal-Groenewala-

Deformation Quantization

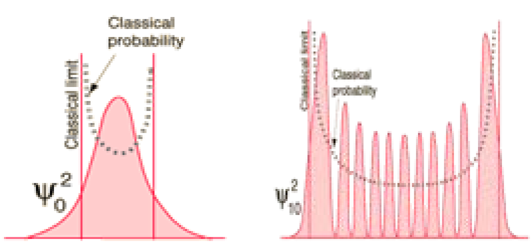
Dirac-Heisenberg-Schrödinger

Textbook Formulation in Hilbert Space

$$|\Psi\rangle, \hat{A}$$

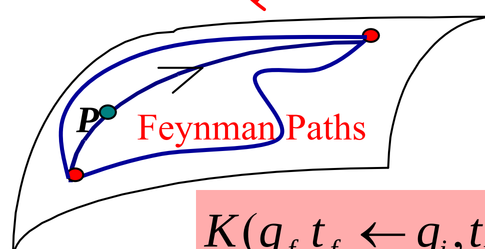
$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = \hat{H} |\Psi\rangle$$

$$i\hbar \frac{d\hat{A}}{dt} = \frac{\partial \hat{A}}{\partial t} + [\hat{A}, \hat{H}]$$



Feynman-Dirac

Path Integral



$$K(q_f, t_f \leftarrow q_i, t_i) = \int Dq(t) e^{iS[q]/\hbar}$$

Representation of Quantum Mechanics: Usual Textbook Ones Cannot Be Put on the Computer

- Coordinate Representation:

$$\left|\Psi\right\rangle = \int \left|x\right\rangle\left\langle x\middle|\Psi\right\rangle dx = \int \Psi(x)\left|x\right\rangle dx$$

- Momentum Representation:

$$\left|\Psi\right\rangle = \int \left|p\right\rangle\left\langle p\middle|\Psi\right\rangle dp = \int \left|p\right\rangle\left\langle p\middle|x\right\rangle\left\langle x\middle|\Psi\right\rangle dp\,dx$$

$$\left\langle p\middle|x\right\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \Rightarrow \Psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ipx/\hbar}\Psi(x)dx$$

- Energy representation:

$$\hat{H}\left|E_n\right\rangle = E_n\left|E_n\right\rangle$$

$$\left|\Psi\right\rangle = \sum_n \left|E_n\right\rangle\left\langle E_n\middle|\Psi\right\rangle = \sum_n \Psi_n\left|E_n\right\rangle$$

Quantum-Mechanical Probabilities in Practice

- Probability to find **coordinate** of a particle in $[x, x+dx]$

$$\langle\Psi|x\rangle\langle x|\Psi\rangle dx = \Psi^*(x)\Psi(x)dx \Rightarrow \int_{-\infty}^{+\infty}\Psi^*(x)\Psi(x)dx = 1$$

$$\hat{x}|x\rangle = x|x\rangle, \quad \Psi^*(x)\Psi(x) = |\Psi(x)|^2$$

- Probability to find **momentum** of a particle in $[p, p+dp]$

$$\langle\Psi|p\rangle\langle p|\Psi\rangle dp = \Psi^*(p)\Psi(p)dp \Rightarrow \int_{-\infty}^{+\infty}\Psi^*(p)\Psi(p)dp = 1$$

$$\hat{p}|p\rangle = p|p\rangle, \quad \Psi^*(p)\Psi(p) = |\Psi(p)|^2$$

- Probability to find **energy** of a particle to be E_n

$$\langle\Psi|E_n\rangle\langle E_n|\Psi\rangle = |\langle E_n|\Psi\rangle|^2 = \Psi^*{}_n\Psi_n \Rightarrow \sum_n \Psi^*{}_n\Psi_n = 1$$

Schrödinger Equation(s)

- time evolution of state vectors:

$$i\hbar \frac{d\left|\Psi\right\rangle}{dt} = \hat{H}\left|\Psi\right\rangle \Rightarrow \text{stationary: } \hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

- time evolution of coordinate wave functions for a single particle acted on by a conservative force with potential $V(\mathbf{x})$

$$i\hbar \frac{\partial \Psi(\mathbf{x})}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \Psi(\mathbf{x}) + V(\mathbf{x})\Psi(\mathbf{x})$$

- Momentum representation for a single particle of mass *m* acted on by a conservative force with potential $V(x) \Rightarrow V(p) = \frac{1}{2\pi\hbar}\int V(x)e^{-ipx/\hbar}dx$

$$i\hbar \frac{\partial \Psi(\mathbf{p})}{\partial t} = \frac{\mathbf{p}^2}{2m}\Psi(p) + \int_{-\infty}^{+\infty} V(\mathbf{p}-\mathbf{p}')\Psi(\mathbf{p}')d\mathbf{p}'$$

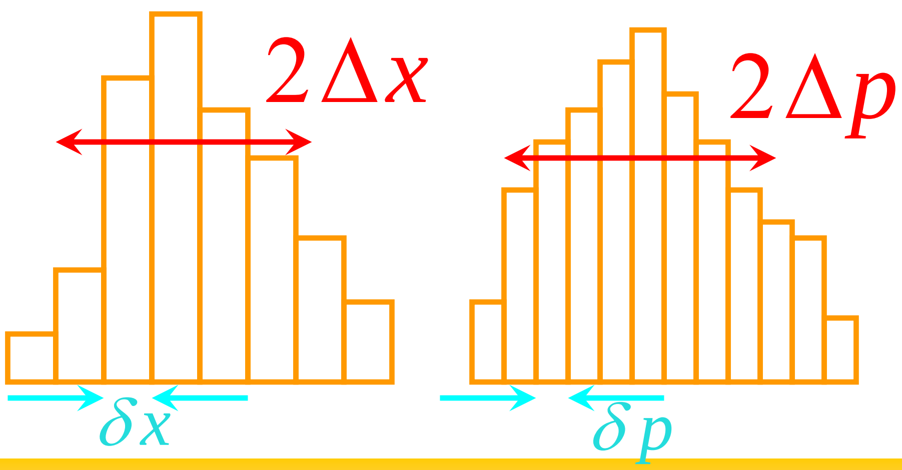
Heisenberg Uncertainty Relations

- Operators (of course, Hermitian) which represent physical quantities in QM in general do not commute:

$$\left[\hat{A},\hat{B}\right]=\hat{A}\cdot\hat{B}-\hat{B}\cdot\hat{A}\neq 0 \Rightarrow \Delta\hat{A}\Delta\hat{B}\geq\frac{1}{2}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|$$

$$\left(\Delta\hat{A}\right)^2=\left\langle\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)^2\right\rangle=\left\langle\hat{A}^2\right\rangle-\left\langle\hat{A}\right\rangle^2 \Rightarrow \Delta\hat{A}=0 \text{ iff } \hat{A}\left|\Psi\right\rangle=a\left|\Psi\right\rangle$$

- Coordinate and momentum are c-numbers $xp-px=0$ in classical physics, but in QM: $\left[\hat{x},\hat{p}_x\right]=i\hbar \Rightarrow \Delta\hat{x}\Delta\hat{p}_x\geq\frac{\hbar}{2}$



- The experimental test of the Heisenberg inequality **does not involve** simultaneous measurements of **x** and **p**, but rather it involves the measurement of one or the other of these dynamical variables on each independently prepared representative of the particular state $\left|\Psi\right\rangle$ being studied.

Quantum Tunneling Through Single Barrier in Solid State Systems

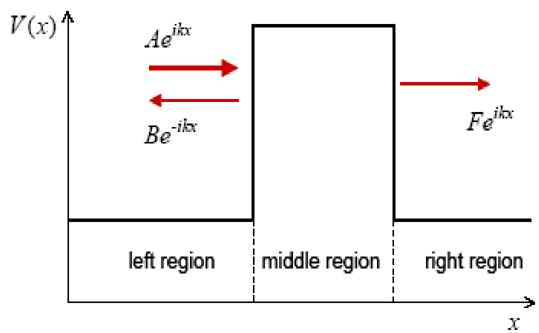


Figure 1.3: Simple approximation of the potential along the transport direction of a tunnel junction, see Fig. 1.2. In the metal (left and right regions) the potential is constant, $V(x) = V_1$. In the insulator the potential is also constant, $V(x) = V_0$, where $V_0 > V_1$. The incoming, reflected and transmitted waves are given by Ae^{ikx}, Be^{-ikx} and Fe^{ikx}.

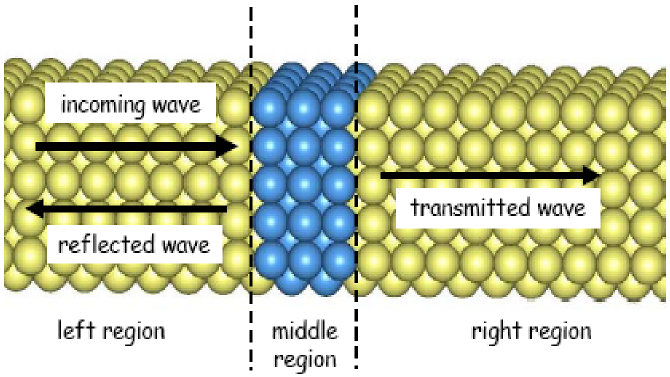
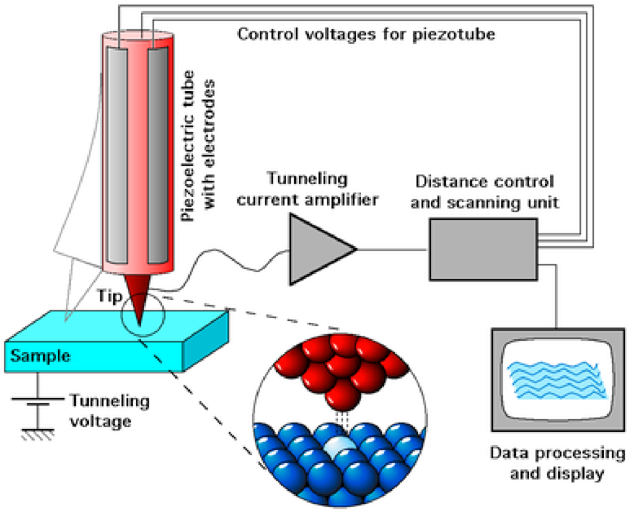
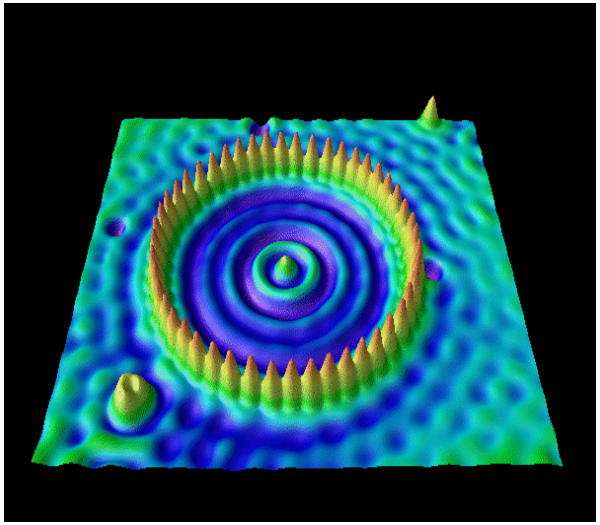
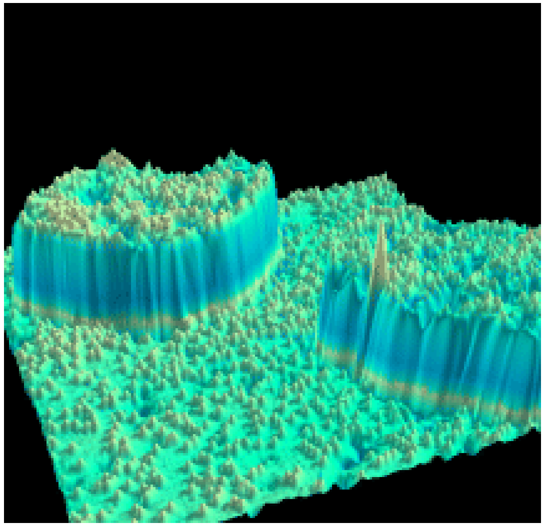


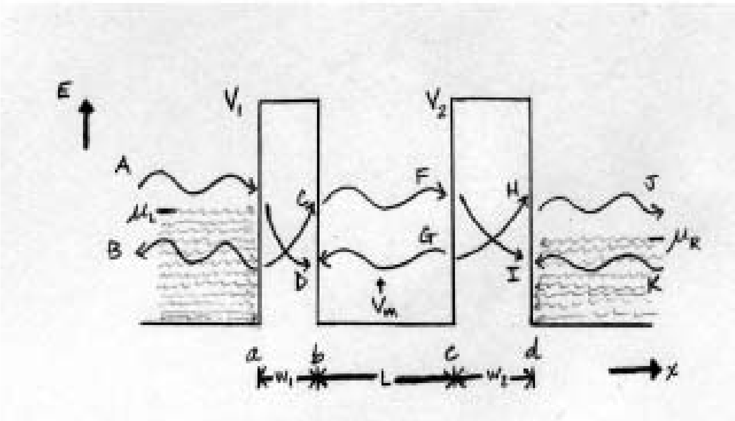
Figure 1.2: Schematic representation of a tunnel junction. The yellow balls represent atoms of a metal, the blue balls represent atoms of an insulator. The left and right regions stretch macroscopically far into the left and right, respectively. The electron waves in the metal are reflected or transmitted by the insulator in the middle region







Quantum Tunneling Through Double Barrier in Textbooks



$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = (E-V)\Psi(x)$$

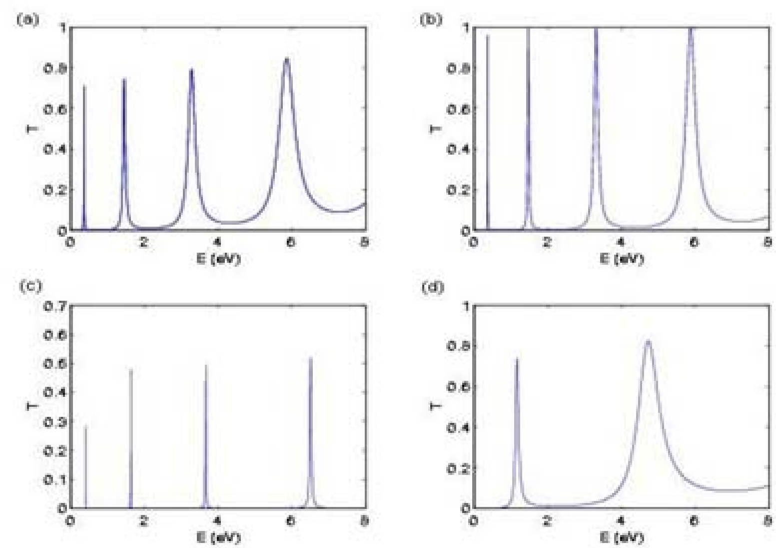
$$\boxed{\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, x < a \\ Ce^{qx} + De^{-qx}, a < x < b \\ Fe^{ik_m x} + Ge^{-ik_m x}, b < x < c \\ He^{px} + Ie^{-px}, c < x < d \\ Je^{ikx} + Ke^{-ikx}, x > d \end{cases}}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad q = \sqrt{\frac{2m(V_1 - E)}{\hbar^2}}$$

$$k_m = \sqrt{\frac{2m(E - V_m)}{\hbar^2}}, \quad p = \sqrt{\frac{2m(V_2 - E)}{\hbar^2}}$$

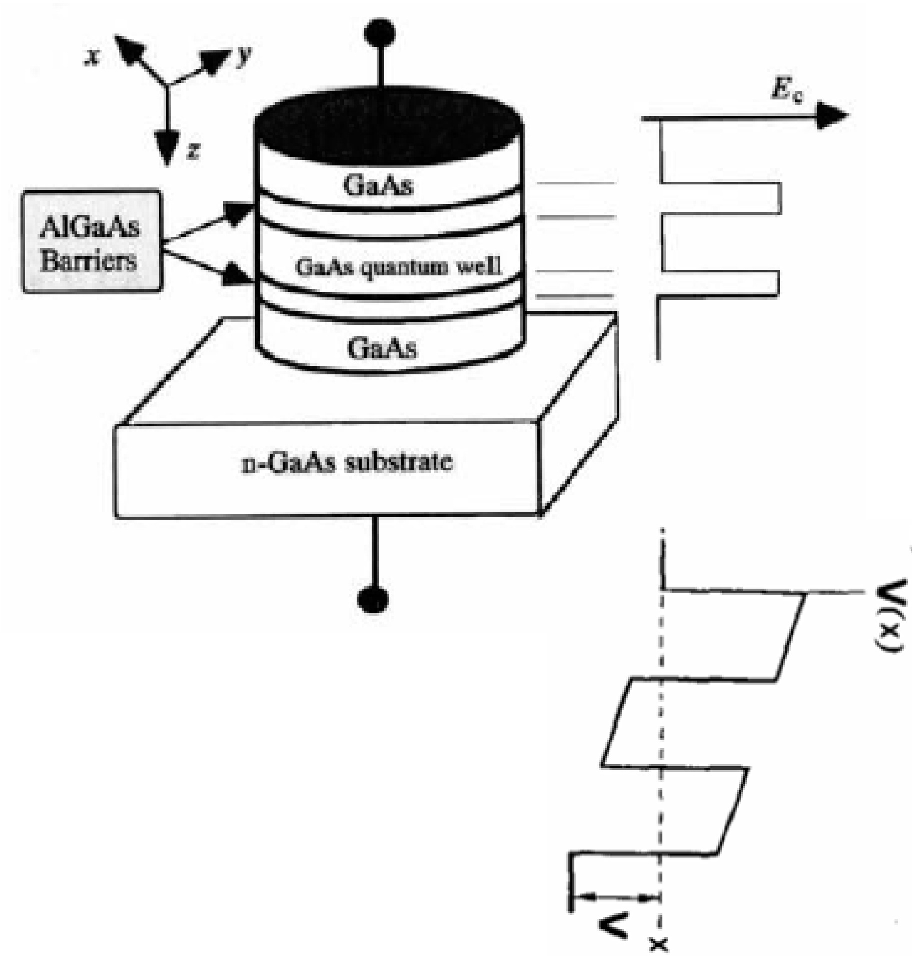
$$j_x = \frac{\hbar}{2mi}\left(\Psi^*(x)\frac{\partial\Psi(x)}{\partial x} - \Psi(x)\frac{\partial\Psi^*(x)}{\partial x}\right)$$

$$\boxed{T = \frac{j_{transmitted,x>d}}{j_{incident,x<a}} = \begin{cases} \dfrac{|H|^2}{|A|^2}, \text{ for electrons incident from the left } (+k \text{ states}) \\ \dfrac{|B|^2}{|K|^2}, \text{ for electrons incident from the right } (-k \text{ states}) \end{cases}}$$



Transmission probability versus incident energy for: **(a)** asymmetric barriers; **(b)** symmetric barriers; **(c)** tall barriers; and **(d)** narrow well.

Quantum Tunneling Through Double Barrier in Solid State Systems



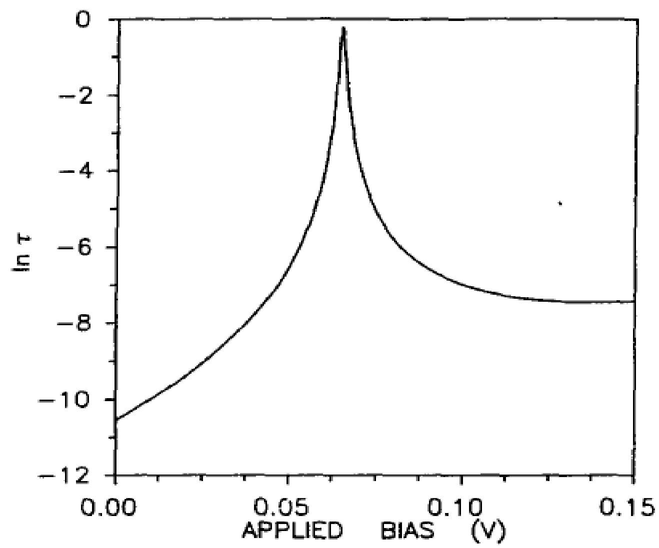


Fig. 3. Transmission coefficient obtained numerically as a function of the applied voltage in a double barrier heterostructure. The potential barrier is 0.25 eV height, $L = 3d = 150$ Å and the energy of the incident electron is 50 meV.

Plane Wave Solutions of the Free Particle Schrödinger Equation

- Plane waves are solution of the **free particle** Schrödinger equation in coordinate representation:

$$i\hbar \frac{\partial}{\partial t}\Psi_p(t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_p(x,t)$$

$$\Psi_p(x) = \frac{1}{(2\pi\hbar)^{1/2}}\exp\left[-\frac{i}{\hbar}\left(Et - px\right)\right], E = \frac{p^2}{2m}$$

- Plane waves are eigenstates of the **free particle** Hamiltonian:

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\hat{H}}\underbrace{\frac{1}{(2\pi\hbar)^{1/2}}e^{\frac{i}{\hbar}px}}_{|E\rangle} = \underbrace{\frac{p^2}{2m}}_{E}\underbrace{\frac{1}{(2\pi\hbar)^{1/2}}e^{\frac{i}{\hbar}px}}_{|E\rangle}$$

Construction of Gaussian Wave Packet From Plane Waves

$$\Psi_p(x) = \frac{1}{(2\pi\hbar)^{1/2}} \exp\left[-\frac{i}{\hbar}(Et - px)\right], E = \frac{p^2}{2m}$$

❑**Linear superpositions** of plane waves are also solutions!

$$\Psi(x,t) = \sum_n w_n \Psi_p(x,t) \rightarrow \Psi(x,t) = \int_{-\infty}^{+\infty} f(p)\Psi_p(x - x_0, t)dp$$

❑For Gaussian wave packet use Gaussian spectral function:

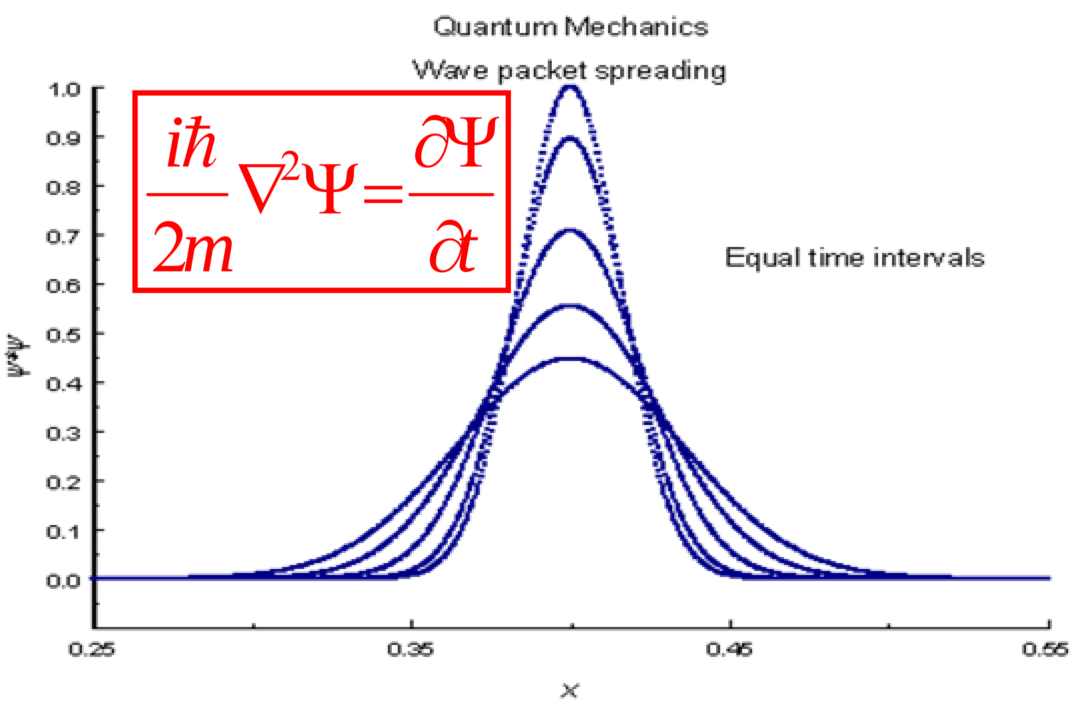
$$f(p) = \frac{1}{(2\pi)^{1/4}\sqrt{\sigma_p}} \exp\left[-\frac{(p - p_0)^2}{4\sigma_p^2}\right]$$

Spreading of Gaussian Wave Packet for Particle at Rest

❑The probability density that the particle is located at some location in space is determined from the wave function (in coordinate representation):

$$\rho(\mathbf{x}) = \Psi^*(\mathbf{x})\Psi(\mathbf{x}) = \langle \Psi | \mathbf{x} \rangle \langle \mathbf{x} | \Psi \rangle$$

❑For a free particle $V(\mathbf{x})=0$ the Schrödinger equation has the form of a diffusion equation with diffusion coefficient $i\hbar/2m$.



$$\frac{i\hbar}{2m}\nabla^2\Psi = \frac{\partial\Psi}{\partial t}$$

As time progresses the width of the distribution increases $\propto (\hbar t/m)^{1/2}$. This width is proportional to the standard deviation of the position x. In quantum mechanics the standard deviation of the probability distribution of a variable is often called the uncertainty in the variable. If we have an object of mass 1 kg then the time scale for the uncertainty in the position of this object to increase by about $10^{-6}\,m$ is estimated to be $3\cdot10^{6}$ years. Hence classical physics is amply adequate to describe the dynamics of macroscopic objects.

Moving Gaussian Wave Packet

$$\Psi(x,t) = \int_{-\infty}^{+\infty} f(p)\Psi_p(x-x_0,t)dp = M(x,t)e^{i\phi(x,t)}$$

$$\text{amplitude function}: M(x,t) = \frac{1}{(2\pi)^{1/4}\sqrt{\sigma_p}}\exp\left[-\frac{(x-x_0-v_0t)^2}{4\sigma_x^2}\right]$$

$$\text{phase}: \phi(x,t) = \frac{1}{\hbar}\left[p_0 + \frac{\sigma_p^2}{\sigma_x^2}\frac{t}{2m}(x-x_0-v_0t)\right](x-x_0-v_0t) + \frac{p_0}{2\hbar}v_0t - \frac{\arctan\frac{2\sigma_p^2 t}{\hbar m}}{2}$$

$$\text{group velocity}: v_0 = \frac{p}{m} \qquad \text{localization in space}: \sigma_x^2 = \frac{\hbar^2}{4\sigma_p^2}\left(1+\frac{4\sigma_p^2}{\hbar^2}\frac{t^2}{m^2}\right)$$

- Physical **(i.e., measurable)** properties are contained in:

$$\rho(x,t) = \Psi(x,t)\Psi^*(x,t) = \frac{1}{\sqrt{2\pi}\sigma_x(t)}\exp\left[-\frac{(x-\langle x(t)\rangle)^2}{2\sigma_x^2}\right]$$

$$\langle \hat{x} \rangle = \int_{-\infty}^{+\infty} \Psi(x,t)x\Psi^*(x,t) = x_0 + v_0 t$$

Gaussian Wave Packet: Uncertainty Relations

$$\mathrm{var}(\hat{x}) = \left\langle \left(\hat{x} - \langle \hat{x} \rangle \right)^2 \right\rangle = \int_{-\infty}^{+\infty} \Psi(x,t) \left(\hat{x} - \langle \hat{x} \rangle \right)^2 \Psi^*(x,t) dx = \sigma_x^2$$

$$\mathrm{var}(\hat{p}) = \left\langle \left(\hat{p} - \langle \hat{p} \rangle \right)^2 \right\rangle = \int_{-\infty}^{+\infty} \Psi(x,t) \left(\frac{\hbar}{i} \frac{\partial}{\partial x} - p_0 \right)^2 \Psi^*(x,t) dx = \sigma_p^2$$

$$\Delta\hat{x}\Delta\hat{p} = \sqrt{\mathrm{var}(\hat{x})}\sqrt{\mathrm{var}(\hat{p})} = \sigma_x(t)\sigma_p \geq \frac{\hbar}{2}$$

$$t = 0 \Rightarrow \begin{cases} \Psi(x,0) = M(x,0) e^{i\phi(x,0)} = \dfrac{1}{(2\pi)^{1/4}\sqrt{\sigma_x}} \exp\left[-\dfrac{(x-x_0)^2}{4\sigma_x^2} \right] \exp\left[\dfrac{i}{\hbar} p_0 (x - x_0) \right] \\ \Delta\hat{x}\Delta\hat{p} = \sigma_x(t=0)\sigma_p = \dfrac{\hbar}{2\sigma_p}\sigma_p = \dfrac{\hbar}{2} \leftarrow \text{minimum uncertainty state} \end{cases}$$

Time-Dependent Schrödinger Equation: Direct Solution

- The time dependent Schrödinger equation can be compactly written a

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi, \quad \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$$

where we assume Hamiltonian for a single particle in a potential $V(\mathbf{r})$.

- Lets try to use **naïve Euler method** to convert this into a difference equation:

$$\Psi^{n+1} = \Psi^n - \frac{i\Delta t}{\hbar}\hat{H}\Psi^n$$

Where the superscript represent time and Δt is the time increment.

- The **second derivative** in the Hamiltonian is approximated by:

$$\left.\frac{\partial^2 \Psi^n}{\partial x^2}\right|_k \simeq \frac{\Psi^n_{k+1} - 2\Psi^n_k + \Psi^n_{k-1}}{\Delta x^2}$$

where Δx is the interval in *x*, with similar expressions for the contributions from the *y* and *z* coordinates.

Stability Problem of Direct Euler Approach

- This finite difference equation is unstable:

$$\Psi_k^{n+1} = \Psi_k^n + iQ\left(\Psi_{k+1}^n - 2\Psi_k^n + \Psi_{k-1}^n\right), Q = \frac{\hbar\Delta t}{2m\Delta x^2}$$

- This is a **linear second order difference equation** in two variables. We can solve it by Fourier analysis in the x direction. What this means is that x-dependence can be taken to be a superposition of solutions of form e^{ikx}:

$$\left.\begin{aligned} &\Psi_k^n = \zeta^n \exp\left(i\kappa k\Delta x\right) \\ &x = k\Delta x + \text{a constant} \end{aligned}\right\} \Rightarrow \zeta^{n+1} = \zeta^n + iQ\left[\exp\left(i\kappa\Delta x\right) - 2 + \exp\left(-i\kappa\Delta x\right)\right]\zeta^n$$

$$\zeta^{n+1} = \zeta^n\left[1 - 2iQ\left(1 - \cos(\kappa\Delta x)\right)\right]$$

- Thus, at each time step ζ is multiplied by the amplification factor:

$$\alpha = 1 - 2iQ\left[1 - \cos\left(\kappa\Delta x\right)\right] \Leftrightarrow \left|\alpha\right| = \sqrt{1 + 4Q^2\left[1 - \cos\left(\kappa\Delta x\right)\right]^2}$$

$$\exists\kappa \Rightarrow \left|\alpha\right| > 1 \text{ for } Q > 0$$

Implicit Method Cure?

- The instability of the Euler method is cured by **time-reversal**, i.e., we can use the implicit method. For the free particle:

$$\Psi_k^{n+1} = \Psi_k^n + iQ\left(\Psi_{k+1}^{n+1} - 2\Psi_k^{n+1} + \Psi_{k-1}^{n+1}\right), Q = \frac{\hbar\Delta t}{2m\Delta x^2}$$

so that "amplification" factor is now:

$$\alpha = \frac{1}{1+2iQ\left[1-\cos\left(\kappa\Delta x\right)\right]} \Rightarrow |\alpha| = \frac{1}{\sqrt{1+4Q^2\left[1-\cos\left(\kappa\Delta x\right)\right]^2}} \leq 1$$

- However, we now have new problem with unitarity: The implicit method does not preserve **unitarity**, i.e., it does not keep the normalization integral constant

$$\int \Psi(x)^* \Psi(x) dx = 1$$

- This is related to the fact that the amplification factor has magnitude less than or equal to one.

A Cure for both Stability and Unitarity

- The unitarity problem is cured by using a more accurate method — evaluate the time derivative at the midpoint of the time interval by taking the average of the implicit and explicit Euler methods approximations for the Hamiltonian.

- For free particle such finite difference method yields the equation:

$$\Psi_k^{n+1} = \Psi_k^n + i\frac{Q}{2}\left(\Psi_{k+1}^{n+1} - 2\Psi_k^{n+1} + \Psi_{k-1}^{n+1}\right) + i\frac{Q}{2}\left(\Psi_{k+1}^{n} - 2\Psi_k^{n} + \Psi_{k-1}^{n}\right)$$

$$\alpha = \frac{1 - iQ\left[1-\cos\left(\kappa\Delta x\right)\right]}{1 + iQ\left[1-\cos\left(\kappa\Delta x\right)\right]} \Rightarrow |\alpha| = 1$$

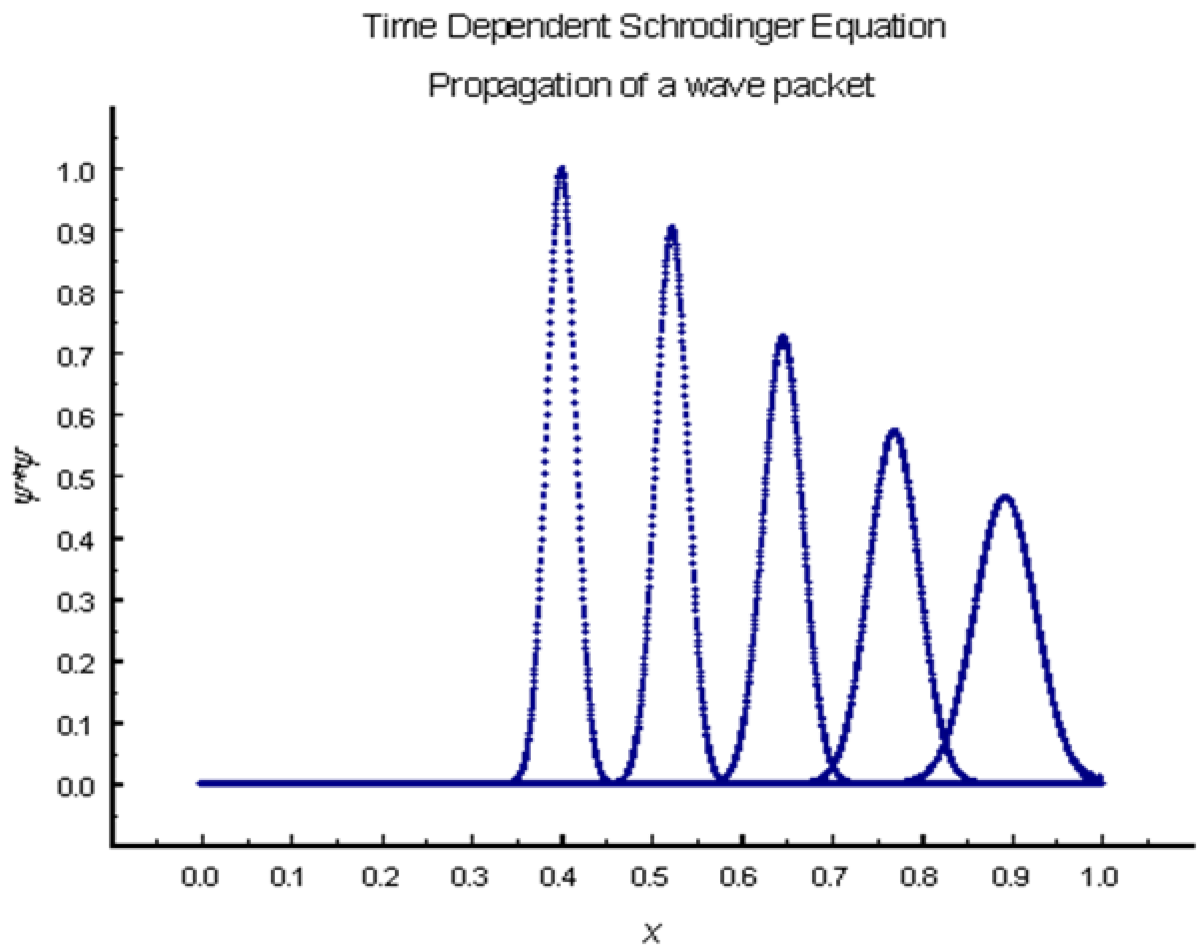
- This is now finally a stable method that preserves unitarity; for a particle in 1 dimension with potential $V(x)$, the finite difference TDSE is:

$$\Psi_k^{n+1} - iq\left(\Psi_{k+1}^{n+1} - 2\Psi_k^{n+1} + \Psi_{k-1}^{n+1}\right) + irV_k\Psi_k^{n+1} = \Psi_k^n + iq\left(\Psi_{k+1}^{n} - 2\Psi_k^{n} + \Psi_{k-1}^{n}\right) - irV_k\Psi_k^n$$

$$V_k = V(x_k),\ q = \frac{Q}{2} = \frac{\hbar\Delta t}{4m(\Delta x)^2},\ r = \frac{\Delta t}{2\hbar}$$

- If considered as a set of linear equations for the unknowns $\Psi_1^{n+1}, \Psi_2^{n+1}, \ldots, \Psi_K^{n+1}$, we have a **tri-diagonal system** of **linear equations** that can be solved much easier than standard LU decomposition + forward-backward substitution. Note, however, that you need to use **complex arithmetic**.

Test Example for Computational Algorithm Ensuring Unitary Evolution of Wave Packet



- The figure shows the probability distribution at equal time intervals for a Gaussian wave packet propagating to the right.

Solving Time-Independent Schrödinger Equation via Exact Diagonalization

- Separation of variables to solve the partial differential equation:

$$\Psi(\mathbf{r},t) = R(\mathbf{r})T(t) \Rightarrow \frac{1}{R}\left[-\frac{\hbar^2}{2m}\nabla^2 R + V(\mathbf{r})R\right] = i\hbar\frac{1}{T}\frac{dT}{dt} = E$$

$$T(t) = \exp\left(-\frac{iEt}{\hbar}\right), \quad -\frac{\hbar^2}{2m}\nabla^2 R + V(\mathbf{r})R = ER$$

- The spatial part has boundary conditions that often lead to an **eigenvalue problem**, i.e., there is a solution for R only for a discrete set of values of E This is formally similar to oscillations in a linear chain from Project 3.

- If we label the eigenvalues $E_1, E_2, E_3, \ldots$ and the corresponding eigenfunctions $R_1, R_2, R_3, \ldots$ then the complete solution is:

$$\Psi(\mathbf{r},t) = \sum_{l=1}^{\infty} \alpha_l R_l(\mathbf{r}) \exp\left(-\frac{iE_l t}{\hbar}\right)$$

$$|\Psi(t)\rangle = \exp\left(-\frac{i\hat{H}t}{\hbar}\right)|\Psi(0)\rangle = \sum_l \exp\left(-\frac{iE_l t}{\hbar}\right)|l\rangle\langle l|\Psi(0)\rangle$$

- The constants α_l are determined from the initial conditions at $t = 0$