# PHY 742 Quantum Mechanics II
# 12-12:50 PM MWF Olin 103

## Plan for Lecture 6
## Approximate solutions for stationary states
## Perturbation theory examples (Chap. 13 and 12 B) –

1. The hyperfine interaction
2. The WKB or “quasi-classical” approximation

# Course schedule for Spring 2022

(Preliminary schedule -- subject to frequent adjustment.)

| | Lecture date | Reading | Topic | HW | Due date |
|---|---|---|---|---|---|
| 1 | Mon: 01/10/2022 | Chap. 12 | Approximate solutions for stationary states -- The variational approach | #1 | 01/14/2022 |
| 2 | Wed: 01/12/2022 | Chap. 12 C | Approximate solutions for stationary states -- Perturbation theory | #2 | 01/19/2022 |
| 3 | Fri: 01/14/2022 | Chap. 12 D | Approximate solutions for stationary states -- Degenerate perturbation theory | #3 | 01/21/2022 |
| | Mon: 01/17/2022 | | MLK Holiday -- no class | | |
| 4 | Wed: 01/19/2022 | Chap. 12 C & D | Approximate solutions for stationary states -- Additional tricks | #4 | 01/24/2022 |
| 5 | Fri: 01/21/2022 | Chap. 13 | Examples of of the use of perturbation theory | #5 | 01/26/2022 |
| 6 | Mon: 01/24/2022 | Chap. 13 & 12 B | Hyperfine perturbation and also the WKB approximation | #6 | 01/28/2022 |
| 7 | Wed: 01/26/2022 | Chap. 14 | Scattering theory | | |

# PHY 742 -- Assignment #6

January 24, 2022

Complete reading Chapter 12 and 13 in **Carlson's** textbook.

1. In class, we derived the hyperfine spliting of a hydrogen atom in its ground state using a slightly different approach than found in your textbook. Check whether the two results are compatible.

**Now consider internal magnetic fields within an atom –**

**These are produced by:**

1. **The magnetic dipole moment of the electron**
2. **The magnetic field produced by the charge of the electron**
3. **The magnetic dipole moment of the nucleus**

**In PHY 712 we will derive the famous hyperfine interaction potential which arises from the interactions of the magnetic fields and moments**

Magnetic field produced by magnetic dipole moment $\boldsymbol{\mu}_e$ of the electron:

$$\mathbf{B}_{\boldsymbol{\mu}_e}(\mathbf{r}) = \frac{\mu_0}{4\pi}\left(\frac{3\hat{\mathbf{r}}\left(\boldsymbol{\mu}_e\cdot\hat{\mathbf{r}}\right)-\boldsymbol{\mu}_e}{r^3}+\frac{8\pi}{3}\boldsymbol{\mu}_e\delta(\mathbf{r})\right)$$

Magnetic field near nucleus due to orbiting electron:

$$\mathbf{B}_O(\mathbf{r}) = \frac{\mu_0}{4\pi}\frac{e}{m_e}L_z\hat{\mathbf{z}}\left\langle\frac{1}{r^3}\right\rangle$$

"Hyperfine" interaction energy due to interaction with nuclear magnetic dipole moment $\boldsymbol{\mu}_N$:

$$\mathcal{H}_{HF} = -\boldsymbol{\mu}_N\cdot\left(\mathbf{B}_{\boldsymbol{\mu}_e}(\mathbf{r})+\mathbf{B}_O(\mathbf{r})\right)$$

$$= -\frac{\mu_0}{4\pi}\left(\frac{3\left(\boldsymbol{\mu}_N\cdot\hat{\mathbf{r}}\right)\left(\boldsymbol{\mu}_e\cdot\hat{\mathbf{r}}\right)-\boldsymbol{\mu}_N\cdot\boldsymbol{\mu}_e}{r^3}+\frac{8\pi}{3}\boldsymbol{\mu}_N\cdot\boldsymbol{\mu}_e\delta(\mathbf{r})+\frac{e}{m_e}\left\langle\frac{\mathbf{L}\cdot\boldsymbol{\mu}_N}{r^3}\right\rangle\right)$$

## Notation in your textbook:

$$\mathbf{m}_p = \frac{g_p e}{2m_p}\mathbf{I}\,, \qquad \leftrightarrow \quad \mu_N$$

**Here $g_p$ denotes the g-factor for a proton $m_p$ denotes the proton mass; other nuclei can be similarly analyzed**

**Here the quantum operator I references the nuclear spin**

Magnetic dipole moment corresponding to electron spin as described in textbook --

$$\mathbf{m} = -\frac{ge}{2m}\mathbf{S} \quad \text{where } g = 2.00231930436182 \text{ and } m \text{ denotes the electron mass}$$

$\mathbf{S}$ denotes the electron spin operator

**m $\leftrightarrow$ $\mu_e$**

**Hyperfine Hamiltonian discussed in your textbook (approximating *g*=2)**

$$W_{\mathrm{HF}} = \frac{\mu_0 g_p e^2}{8\pi m m_p}\left\{\frac{1}{R^3}\mathbf{I}\cdot\mathbf{L} + \frac{1}{R^3}\left[3\left(\hat{\mathbf{R}}\cdot\mathbf{S}\right)\left(\hat{\mathbf{R}}\cdot\mathbf{I}\right) - \mathbf{I}\cdot\mathbf{S}\right] + \frac{8\pi}{3}\delta^3(\mathbf{R})\mathbf{I}\cdot\mathbf{S}\right\}.$$

**Hyperfine Hamiltonian discussed in your textbook (approximating *g*=2)**

$$W_{\mathrm{HF}} = \frac{\mu_0 g_p e^2}{8\pi m m_p}\left\{\frac{1}{R^3}\mathbf{I}\cdot\mathbf{L} + \frac{1}{R^3}\left[3\left(\hat{\mathbf{R}}\cdot\mathbf{S}\right)\left(\hat{\mathbf{R}}\cdot\mathbf{I}\right) - \mathbf{I}\cdot\mathbf{S}\right] + \frac{8\pi}{3}\delta^3(\mathbf{R})\mathbf{I}\cdot\mathbf{S}\right\}.$$

**Here, *R* denotes the distance of the electron from the nucleus.**

**Now, consider the effects of this perturbation on the ground state of a hydrogen atom where the spacial part of the electron wave function is**

$$\left|nlm\right\rangle = \left|100\right\rangle = \frac{1}{\sqrt{\pi a_0^3}} e^{-R/a_0}$$

**For this case, the first two terms of $W_{HF}$ do not contribute and the zero order wavefunction must include multiplicative contributions from eigenstates of electron and nuclear spin**

$$\mathbf{S}^2\left|s\ m_s\right\rangle = \hbar^2 s(s+1)\left|s\ m_s\right\rangle \quad \text{and} \quad \mathbf{S}_z\left|s\ m_s\right\rangle = \hbar m_s\left|s\ m_s\right\rangle$$

$$\mathbf{I}^2\left|I\ m_I\right\rangle = \hbar^2 I(I+1)\left|I\ m_I\right\rangle \quad \text{and} \quad \mathbf{I}_z\left|I\ m_I\right\rangle = \hbar m_I\left|I\ m_I\right\rangle$$

In our case $s=\frac{1}{2}$ and $I=\frac{1}{2}$

For our case, we will need to use degenerate perturbation theorm with the simplified hyperfine perturbation:

$$\mathrm{W}_{HF} = \frac{\mu_0 g_p e^2}{3mm_p}\delta^3(\mathbf{R})\mathbf{I}\cdot\mathbf{S}$$

and the degenerate states $\left|nlm\ sm_s\ Im_I\right\rangle = \left|100\ sm_s\ Im_I\right\rangle$

**Since *s=1/2* and *I=1/2*, then there are 4 combinations of $m_s$ and $m_I$**

$$\mathbf{S}\cdot\mathbf{I} = \tfrac{1}{2}\left(S_-I_+ + S_+I_-\right) + S_zI_z$$

$$S_\pm\left|sm_s\right\rangle = \hbar\sqrt{s^2 - m_s^2 + s \mp m_s}\left|s\left(m_s \pm 1\right)\right\rangle$$

similar expression applies to $I_\pm\left|Im_I\right\rangle$

# Matrix elements for hyperfine interaction: $\langle m_s m_I | \mathbf{I}\cdot\mathbf{S} | m_s m_I \rangle / \hbar^2$

$$
\begin{array}{cc}
 & \begin{array}{cccc} \frac{1}{2}\ \frac{1}{2} & \frac{1}{2}\,\text{-}\frac{1}{2} & \text{-}\frac{1}{2}\ \frac{1}{2} & \text{-}\frac{1}{2}\,\text{-}\frac{1}{2} \end{array} \\
\begin{array}{c} \frac{1}{2}\ \frac{1}{2} \\ \frac{1}{2}\,\text{-}\frac{1}{2} \\ \text{-}\frac{1}{2}\ \frac{1}{2} \\ \text{-}\frac{1}{2}\,\text{-}\frac{1}{2} \end{array} &
\begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}
\end{array}
$$

| Eigenvalues | Eigenvectors |
| --- | --- |
| $\frac{1}{4}$ | $\lvert m_s m_I \rangle = \lvert \frac{1}{2}\,\frac{1}{2} \rangle$ |
| $\frac{1}{4}$ | $\lvert \text{-}\frac{1}{2}\,\text{-}\frac{1}{2} \rangle$ |
| $\frac{1}{4}$ | $\frac{1}{\sqrt{2}}\left( \lvert \frac{1}{2}\,\text{-}\frac{1}{2} \rangle + \lvert \text{-}\frac{1}{2}\,\frac{1}{2} \rangle \right)$ |
| $\text{-}\frac{3}{4}$ | $\frac{1}{\sqrt{2}}\left( \lvert \frac{1}{2}\,\text{-}\frac{1}{2} \rangle - \lvert \text{-}\frac{1}{2}\,\frac{1}{2} \rangle \right)$ |

Eigenstates of the hyperfine perturbation:

$$\mathrm{W}_{HF} = \frac{\mu_0 g_p e^2}{3mm_p}\delta^3(\mathbf{R})\mathbf{I}\cdot\mathbf{S}$$ for degenerate states of the H atom:

$$\left|nlm\ sm_s\ Im_I\right\rangle = \left|100\ sm_s\ Im_I\right\rangle \qquad \left|nlm\right\rangle = \left|100\right\rangle = \frac{1}{\sqrt{\pi a_0^3}}e^{-R/a_0}$$

3 eigenvalues $$\frac{\mu_0 g_p e^2\hbar^2}{3\pi m m_p a_0^3}\frac{1}{4}$$

**Is this consistent with the results from your textbook?**

1 eigenvalue $$-\frac{\mu_0 g_p e^2\hbar^2}{3\pi m m_p a_0^3}\frac{3}{4}$$

**New topic -- WKB or "quasi-classical" approximation**

**Developed by Wentzel, Kramers, and Brillouin and several others**

**First consider exact solution to a convenient reference system --**

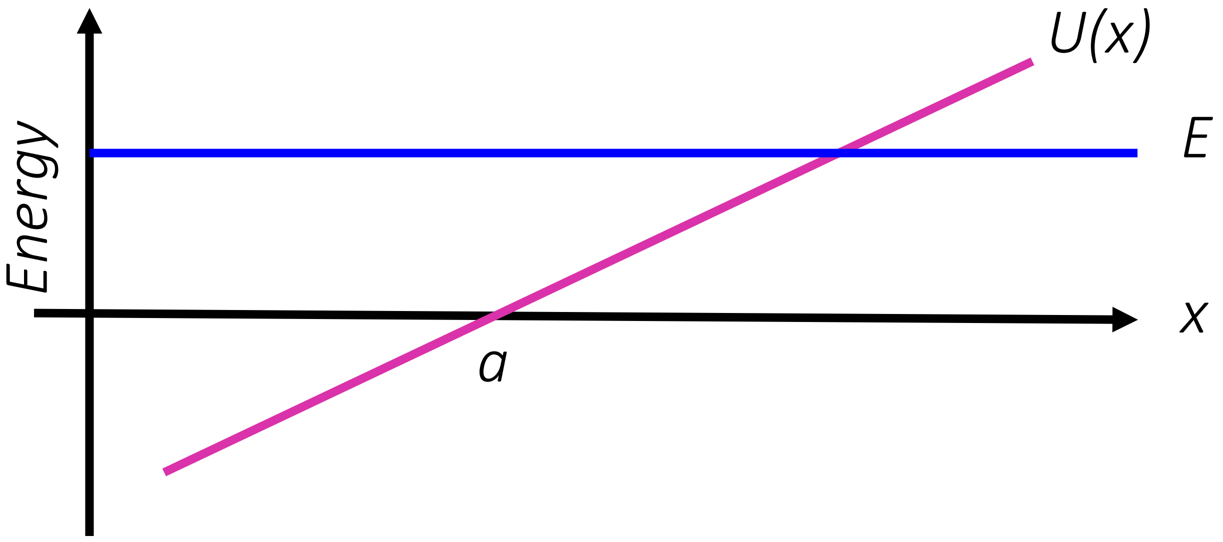
**Example of particle interacting with an electromagnetic field**

Consider a one-dimensional electrostatic field $\mathbf{E}(\mathbf{r},t) = -F\hat{\mathbf{x}}$

$$V(\mathbf{r}) = 0 \quad \mathbf{A}(\mathbf{r},t) = 0 \qquad U(\mathbf{r},t) = U(x) = qF(x-a)$$

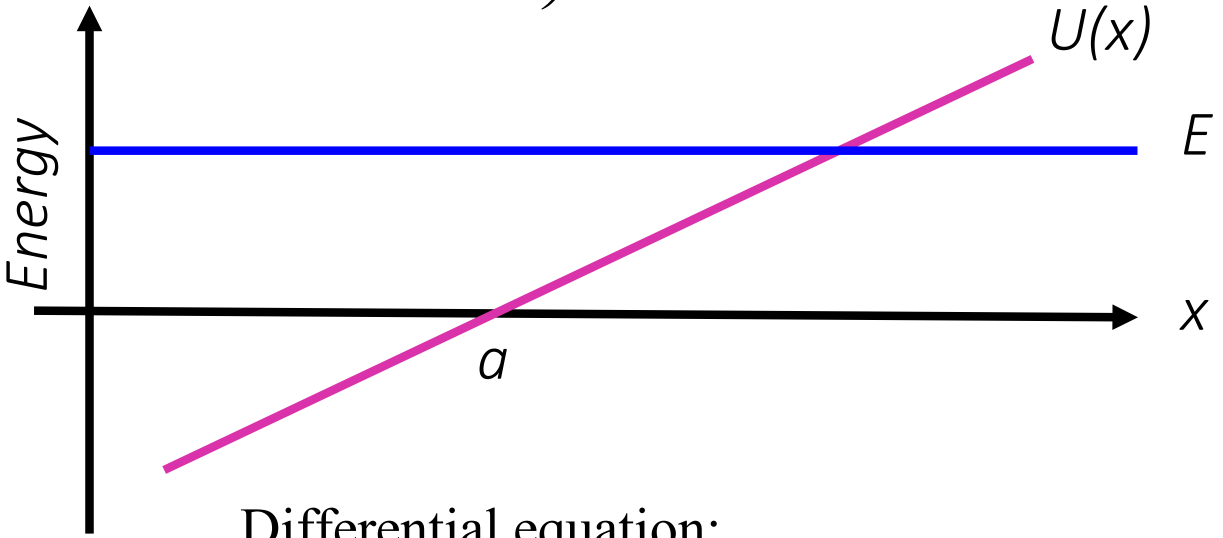
For this case, the stationary state Schrödinger equation at energy $E$ is:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + qF(x-a)\right)\psi(x) = E\psi(x)$$



# One dimensional Schrödinger equation for charged particle in an electrostatic field

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+qF(x-a)\right)\psi(x)=E\psi(x)$$

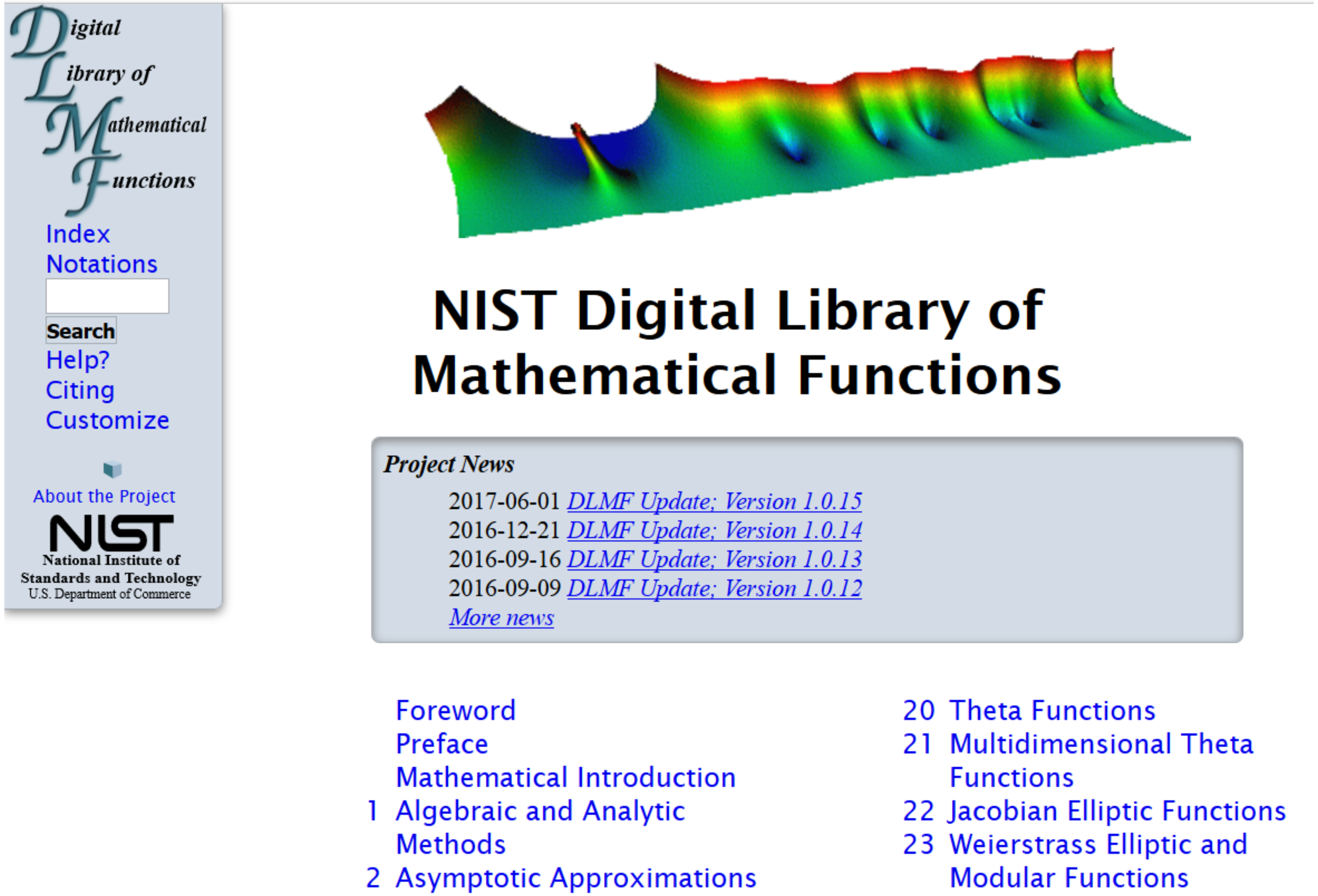


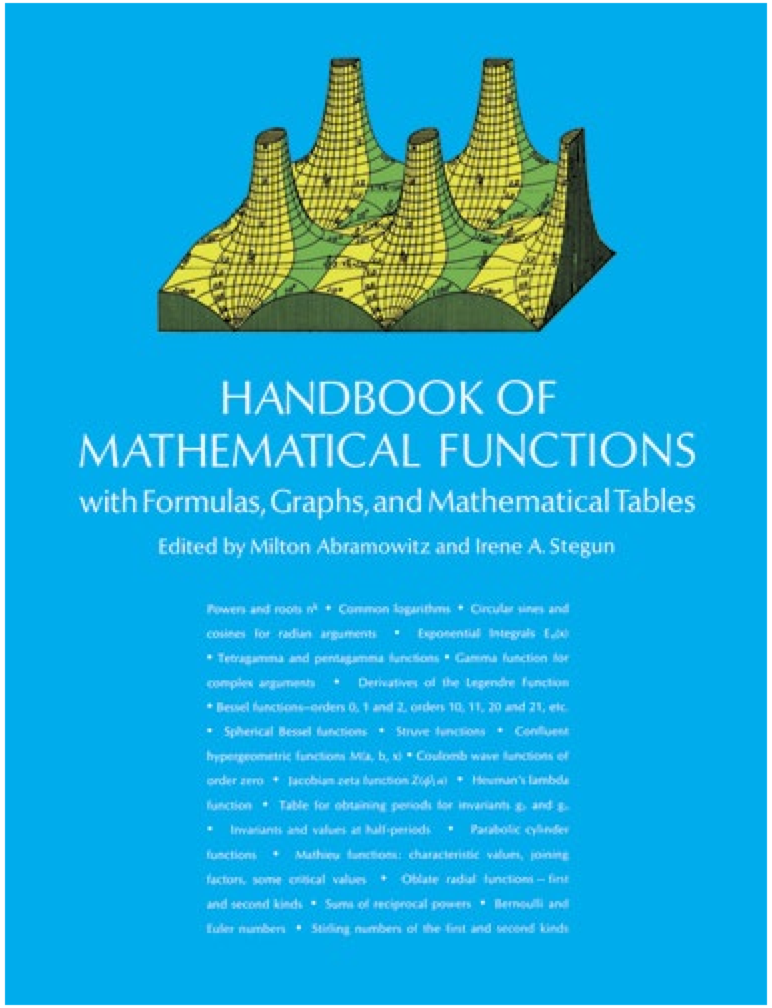

Differential equation:

$$\left(\frac{d^2}{dx^2}-\frac{2mqF}{\hbar^2}(x-b)\right)\psi(x)=0 \qquad \text{where } b\equiv a+\frac{E}{qF}$$

$$\left(\frac{d^2}{du^2}-\alpha u\right)\psi(u)=0 \qquad \text{where } u\equiv x-b \qquad \alpha\equiv\frac{2mqF}{\hbar^2}$$

## Digression – library of solutions to differential equations
http://dlmf.nist.gov/






http://store.doverpublications.com/0486612724.html

## §9.2(i) Airy's Equation

9.2.1

$$\frac{d^2 w}{dz^2} = zw.$$

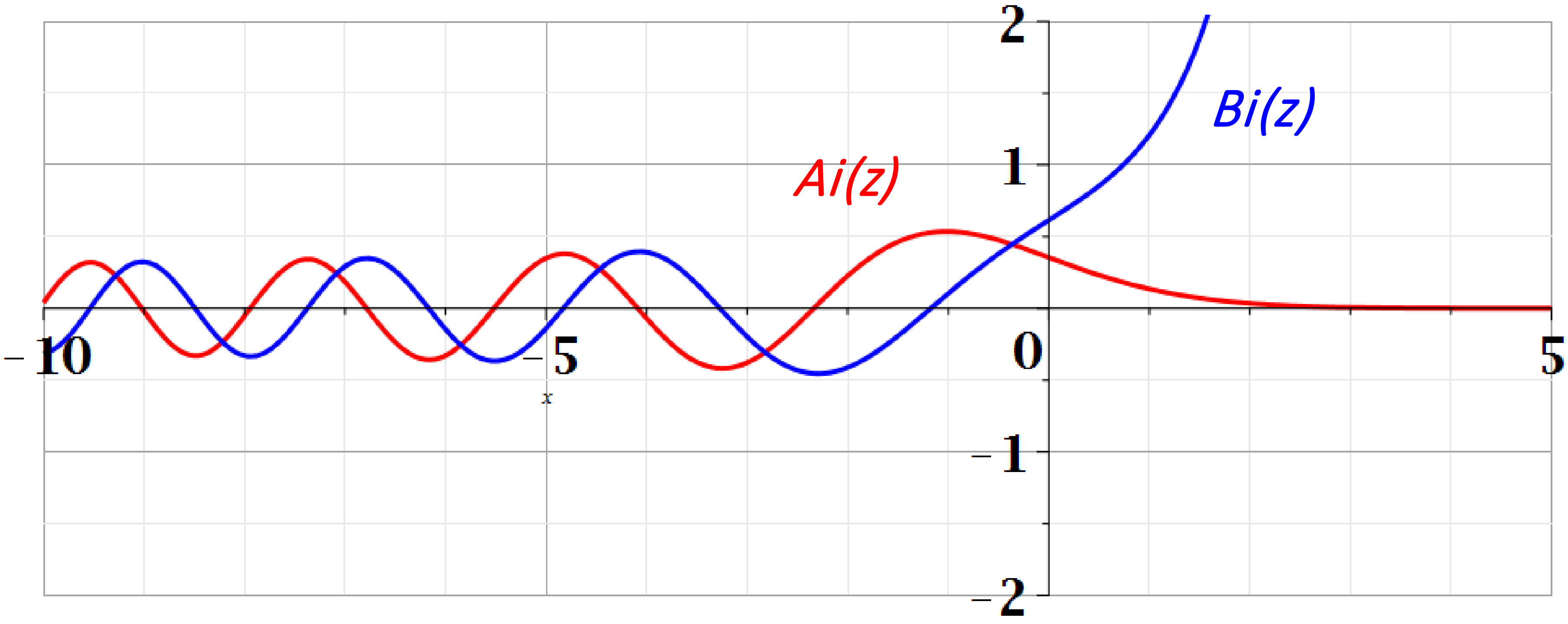
All solutions are entire functions of $z$.

Standard solutions are:

9.2.2

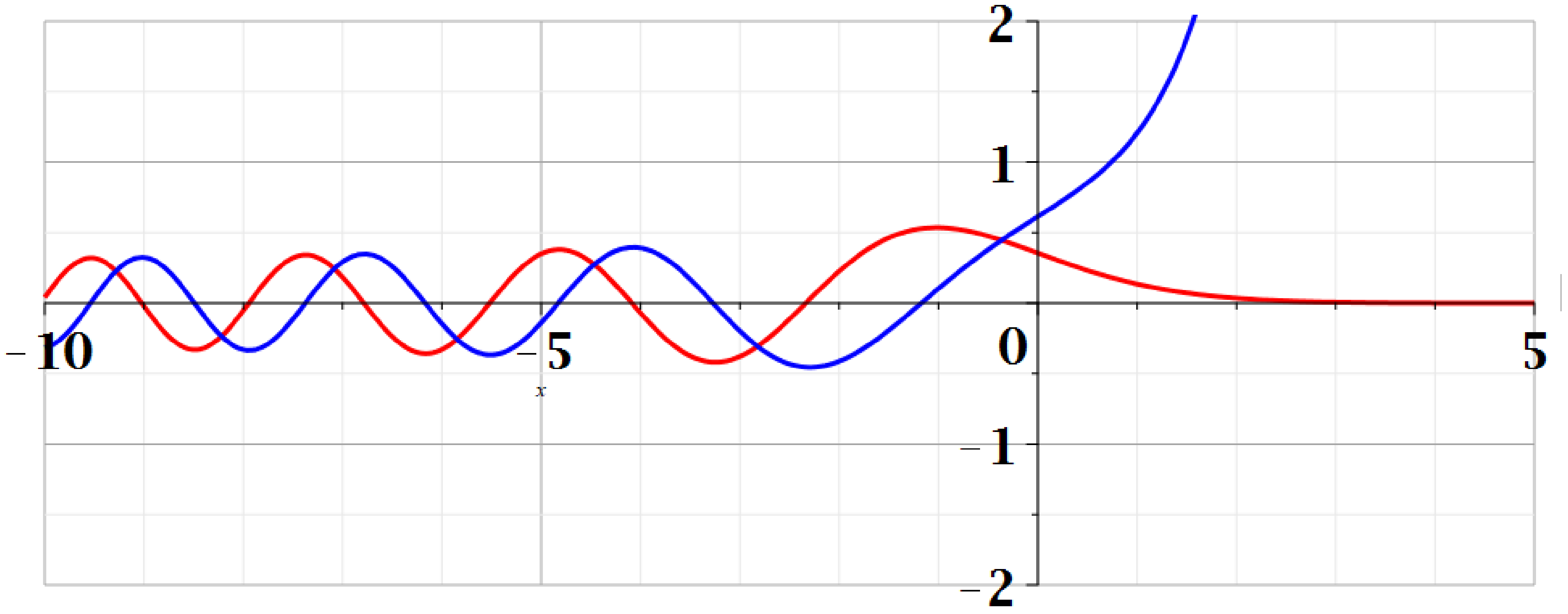
$$w = \mathrm{Ai}(z),\ \mathrm{Bi}(z),\ \mathrm{Ai}\left(z\, e^{\mp 2\pi i/3}\right).$$

$$\frac{d^2w}{dz^2} = zw$$



## Example Maple input --

```
> plot({AiryAi(x), AiryBi(x)}, x=-10..5, -2..2, font=['Times','bold', 24],
    gridlines=true, thickness=3, color=['red','blue']);
```



Differential equation:

$$\left(\frac{d^2}{dx^2}-\frac{2mqF}{\hbar^2}(x-b)\right)\psi(x)=0 \qquad \text{where } b\equiv a+\frac{E}{qF}$$

$$\left(\frac{d^2}{du^2}-\alpha u\right)\psi(u)=0 \qquad \text{where } u\equiv x-b \qquad \alpha\equiv\frac{2mqF}{\hbar^2}$$

Airy's equation

$$\left(\frac{d^2}{dz^2}-z\right)Ai(z)=0$$

Note that the Schroedinger equation can be multiplied by a constant:

$$C\left(\frac{d^2}{du^2}-\alpha u\right)\psi(u)=0$$

Changing variables: $z=C\alpha u$

$$C\frac{d^2}{du^2}=C^3\alpha^2\frac{d^2}{dz^2} \quad \Rightarrow C=\alpha^{-2/3} \qquad \Rightarrow z=\alpha^{1/3}u$$

$$\Rightarrow \psi(u)=\mathcal{N}Ai(\alpha^{1/3}u)$$

← normalization constant

**Some properties of Airy functions –**

**Integral form:**

$$\mathrm{Ai}(x) = \frac{1}{\pi}\int_0^{\infty} \cos\left(\tfrac{1}{3}t^3 + xt\right)\,\mathrm{d}t\,.$$

Behavior as $z \rightarrow \infty$

$$Ai(z) \approx \frac{1}{2\sqrt{\pi}z^{1/4}} e^{-\frac{2}{3}z^{3/2}}$$

Behavior as $-z \rightarrow \infty$

$$Ai(-z) \approx \frac{1}{\sqrt{\pi}z^{1/4}} \sin\left(\frac{2}{3}z^{3/2} + \frac{\pi}{4}\right)$$

## Summary of results

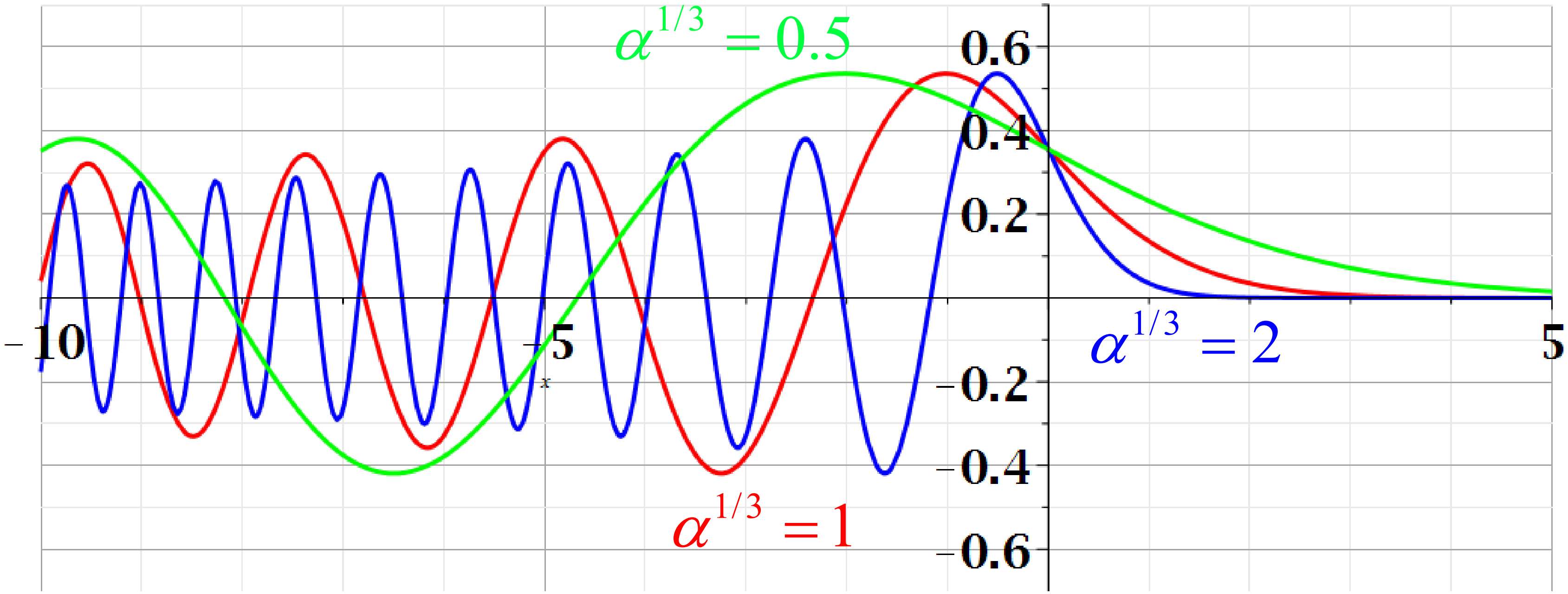
Differential equation:

$$\left(\frac{d^2}{dx^2} - \frac{2mqF}{\hbar^2}(x-b)\right)\psi(x) = 0 \qquad \text{where } b \equiv a + \frac{E}{qF}$$

$$\left(\frac{d^2}{du^2} - \alpha u\right)\psi(u) = 0 \qquad \text{where } u \equiv x - b \qquad \alpha \equiv \frac{2mqF}{\hbar^2}$$

$$\psi(u) = \mathcal{N} Ai(\alpha^{1/3} u)$$

**Note that in this case, physical solutions exist for all energies *E*; the wavefunction oscillates for *x<a+E/qF* and decays for *x>a+E/qF*.**



## Summary of results

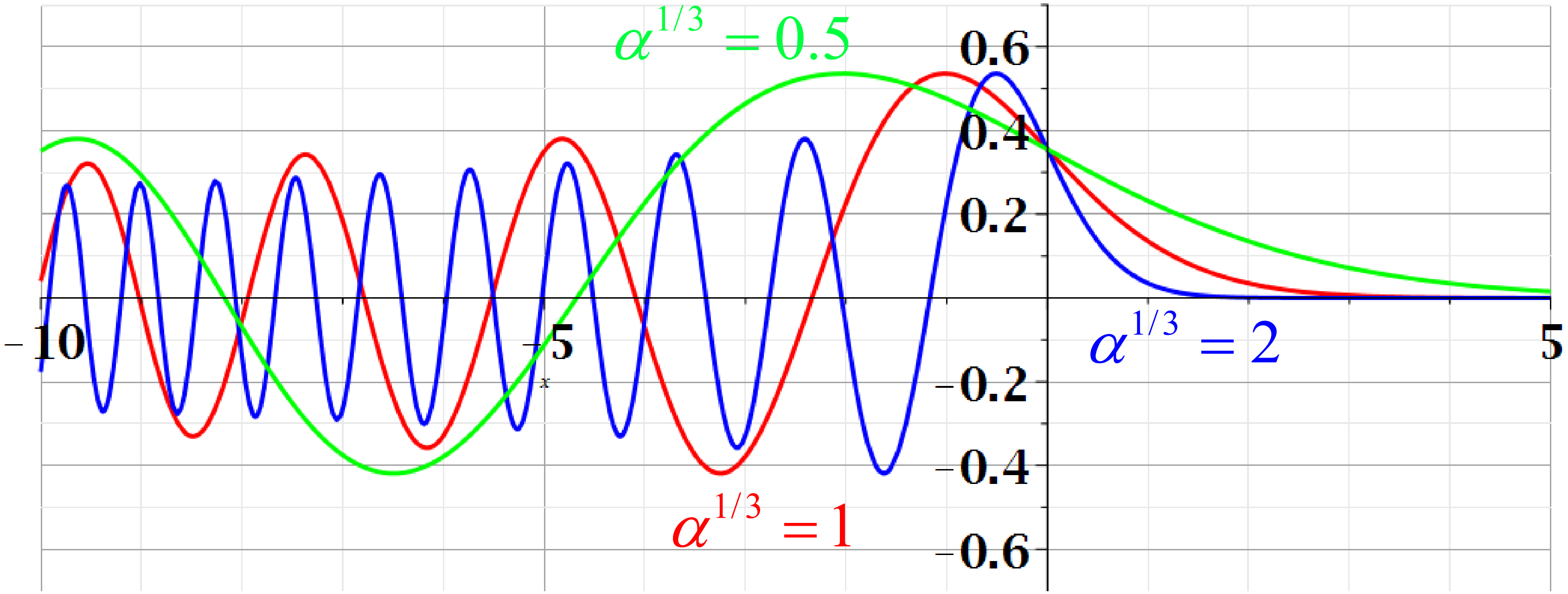
Differential equation:

$$\left(\frac{d^2}{dx^2} - \frac{2mqF}{\hbar^2}(x-b)\right)\psi(x) = 0 \qquad \text{where } b \equiv a + \frac{E}{qF}$$

$$\left(\frac{d^2}{du^2} - \alpha u\right)\psi(u) = 0 \qquad \text{where } u \equiv x - b \qquad \alpha \equiv \frac{2mqF}{\hbar^2}$$

$$\psi(u) = \mathcal{N} Ai(\alpha^{1/3} u)$$

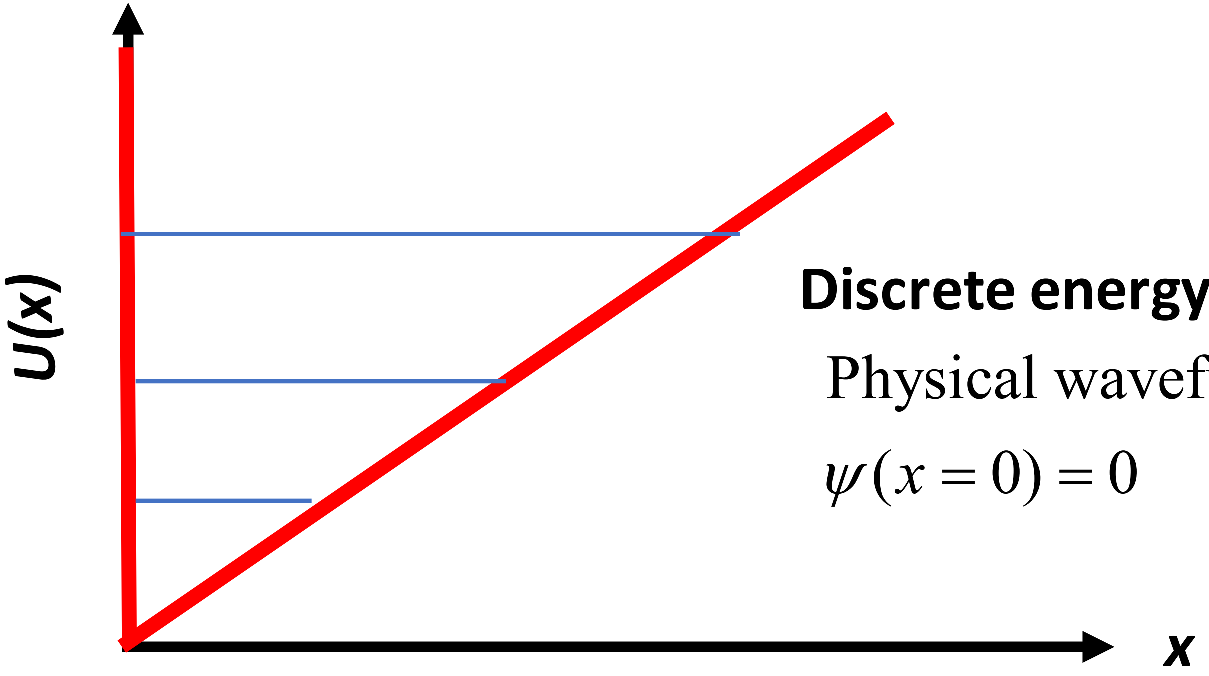
**Note that in this case, physical solutions exist for a continuous range of energies *E*; the wavefunction oscillates for *x<a+E/qF* and decays for *x>a+E/qF*.**



**Related example with bound stationary state solutions --**

Consider a spatially confined one-dimensional electrostatic field :

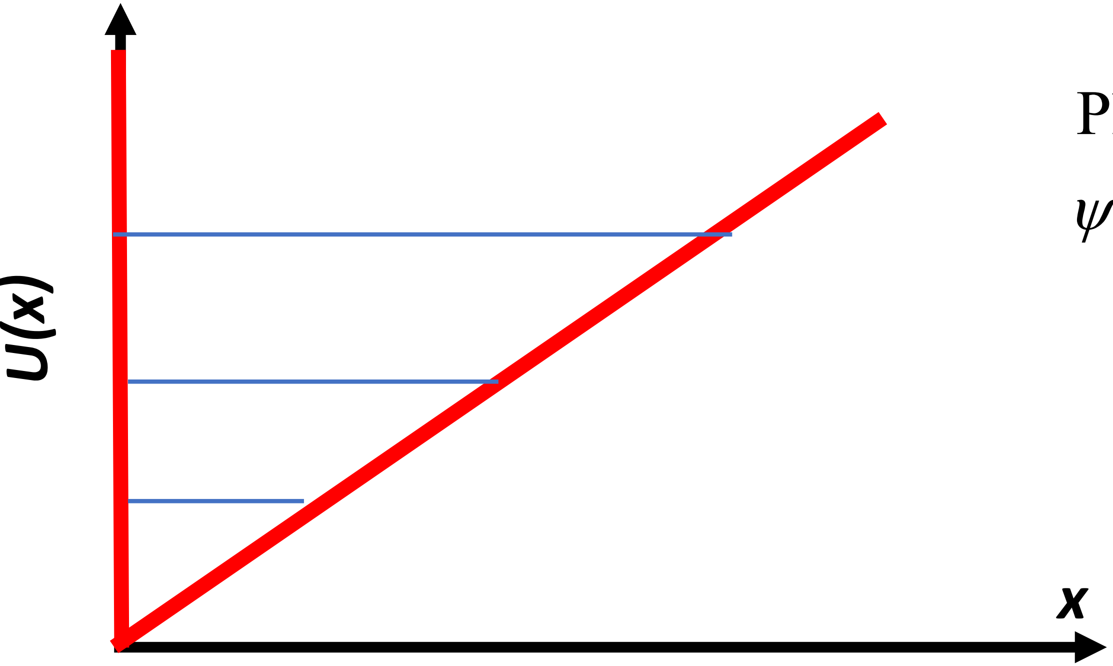
$$V(\mathbf{r}) = 0 \quad \mathbf{A}(\mathbf{r},t) = 0 \qquad U(\mathbf{r},t) = U(x) = \begin{cases} \infty & \text{for } x < 0 \\ Fx & \text{for } x > 0 \end{cases}$$




**Discrete energy levels**

Physical wavefunctions must satisfy

$$\psi(x=0) = 0 \qquad \psi(x \to \infty) = 0$$




Physical wavefunctions must satisfy

$$\psi(x=0)=0 \qquad \psi(x\to\infty)=0$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+qFx\right)\psi(x)=E\psi(x)$$

$$\left(\frac{d^2}{dx^2}-\frac{2mqF}{\hbar^2}(x-b)\right)\psi(x)=0 \qquad \text{where } b\equiv\frac{E}{qF}$$

$$\left(\frac{d^2}{du^2}-\alpha u\right)\psi(u)=0 \quad \text{where } u\equiv x-b \qquad \alpha\equiv\frac{2mqF}{\hbar^2}$$

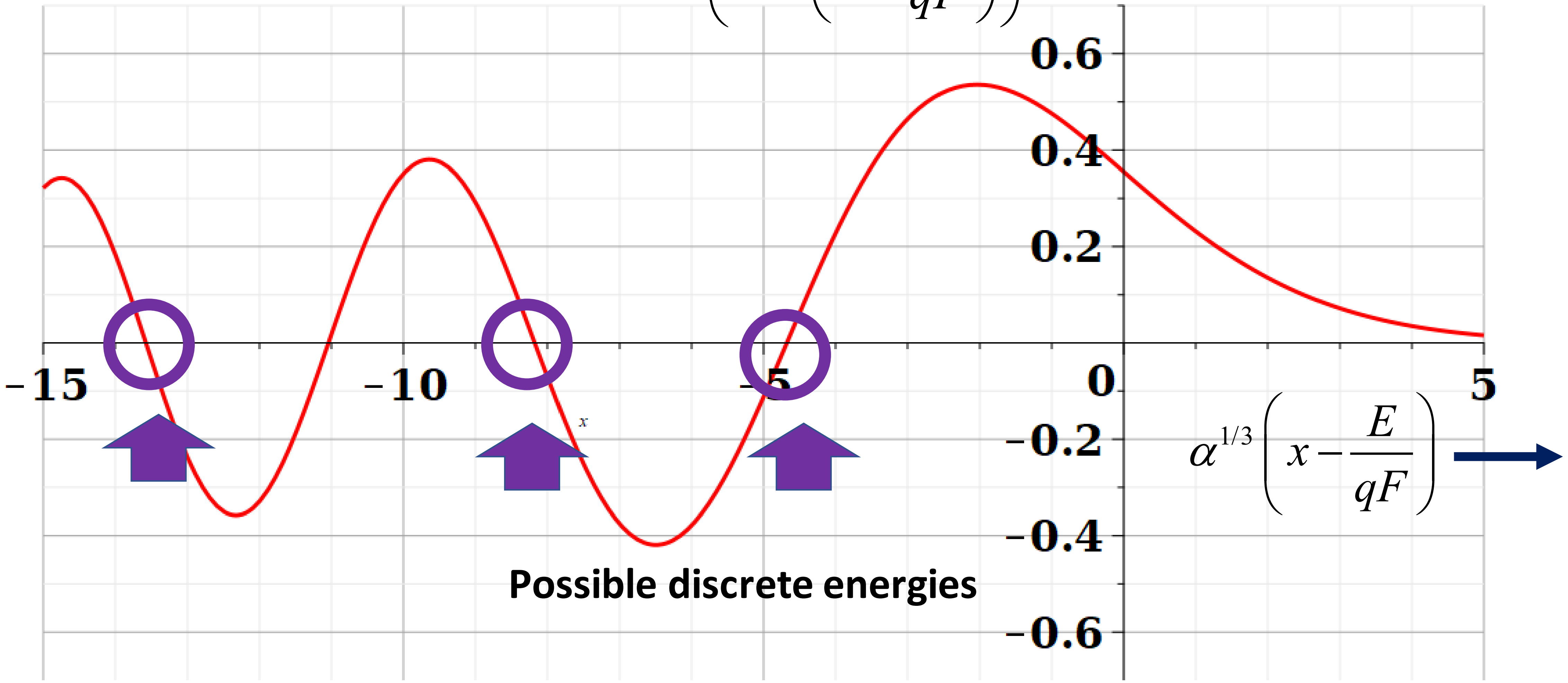
$$\psi(x)=\mathcal{N}Ai\left(\alpha^{1/3}\left(x-\frac{E}{qF}\right)\right)$$

Airy's equation

$$\left(\frac{d^2}{dz^2}-z\right)Ai(z)=0$$

$$\text{where} \quad \psi(x=0)=\mathcal{N}Ai\left(\alpha^{1/3}\left(-\frac{E}{qF}\right)\right)=0$$

$$\psi(x) = \mathcal{N} Ai\left(\alpha^{1/3}\left(x - \frac{E}{qF}\right)\right)$$




**Possible discrete energies**

## Back to the WKB or quasi classical approximation

Consider the stationary state Schrödinger equation at energy $E$ in 1-d:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)-E\right)\psi(x)=0$$

$$\frac{d^2}{dx^2}\psi(x)=-\frac{2m}{\hbar^2}\left(E-V(x)\right)\psi(x)\equiv -k^2(x)\psi(x) \qquad \#1$$

or

$$\frac{d^2}{dx^2}\psi(x)=\frac{2m}{\hbar^2}\left(V(x)-E\right)\psi(x)\equiv \kappa^2(x)\psi(x) \qquad \#2$$

Note that when $E>>V(x)$, $\psi(x) \simeq Ce^{\pm i\int^x k(x')dx'}$ #1

Note that when $V(x)>>E$, $\psi(x) \simeq Ce^{\pm\int^x \kappa(x')dx'}$ #2

These forms of the wave function are reasonably accurate except when $E \approx V(x)$

In order to estimate the forms of the wavefunction as it passes between $E >> V(x)$ and $V(x) >> E$, we use the example of the linear potential and use the properties of the Airy function solutions. More details are given in your textbook. A famous general formula for estimating the bound state energies is given by

$$\int_a^b k(x)dx = (n+1)\pi , \qquad (12.22)$$

**Your textbook shows that when *V(x)* is a harmonic oscillator potential, this formula gives the exact energy eigenvalues.**

**Classical turning points**

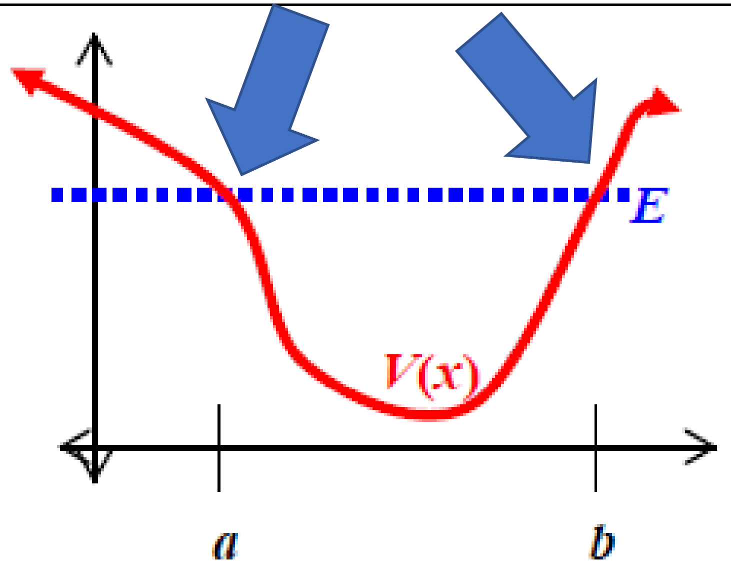



**Figure 12-3:** A potential well that smoothly crosses the energy line at the two classical turning points $a$ and $b$.