Quantum mechanics in three dimensions

We can develop quantum mechanics in three dimensions following the analogy with classical mechanics that we used to obtain the 1D Schrödinger equation.

V. non-examinable, Aside: there is an energy-time uncertainty relation analogous to position-momentum.

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

energy, time

$\hat{H}$, $i\hbar\frac{\partial}{\partial t}$

cf. position, momentum

$\hat{x}$, $-i\hbar\frac{\partial}{\partial x}$

loosely energy and time are "conjugate" — related in the same way as position and momentum.

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We can develop quantum mechanics in three dimensions following the analogy with classical mechanics that we used to obtain the 1D Schrödinger equation. The classical state of a single particle is described by six dynamical variables: its position $\underline{x} = (x_1, x_2, x_3) = \sum_{i=1}^{3} x_i \underline{e_i}$ and momentum $\underline{p} = (p_1, p_2, p_3) = \sum_{i=1}^{3} p_i \underline{e_i}$,

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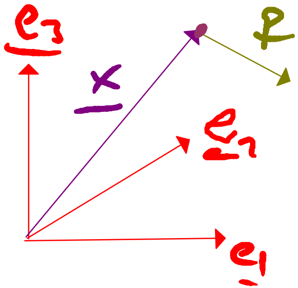

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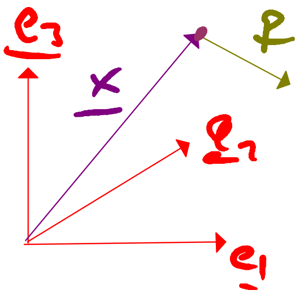

$$H = \frac{\underline{p}.\underline{p}}{2M} + V(\underline{x}) \,. \tag{7.1}$$

Quantum mechanics in three dimensions

Proceeding by analogy with the 1D case, we can introduce operators

Wavefunctions are now dependent on 3-d vector: $\psi(\underline{x})$

$$\hat{x}_i = x_i \qquad (\text{ i.e. multiplication by } x_i)\,,$$

$$\hat{x}_i \psi(\underline{x}) = x_i \psi(\underline{x})$$

Physical wavefunctions are normalisable:

$$\int_{\mathbb{R}^3} |\psi(\underline{x})|^2 \, d^3x$$

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$$\begin{aligned} \hat{x}_i &= x_i \qquad (\text{ i.e. multiplication by } x_i)\,, \\ \hat{p}_i &= -i\hbar\frac{\partial}{\partial x_i}\,, \end{aligned}$$

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$$= -\frac{\hbar^2}{2M}\nabla^2 + V(\underline{x}). \tag{7.4}$$

not a vector
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We also take the wavefunction ψ to depend on 3 space and 1 time coordinates: $\psi \equiv \psi(\underline{x}, t)$. The 3D normalisation condition is

$$\int |\psi(\underline{x}, t)|^2 d^3x = 1 \,. \tag{7.5}$$

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or more explicitly, for a time-independent potential V,

$$-\frac{\hbar^2}{2M}\nabla^2\psi(\underline{x}, t) + V(\underline{x})\psi(\underline{x}, t) = i\hbar\frac{\partial}{\partial t}\psi(\underline{x}, t)\,. \tag{7.7}$$

Using $\hat{H} = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\underline{x})\right)$

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Try ansatz: $\psi(\underline{x},t) = \psi(\underline{x})\,T(t)$.

Using the method of separation of variables, as before, we can derive the *3D time-independent Schrödinger equation*

$$-\frac{\hbar^2}{2M}\nabla^2\psi(\underline{x}) + V(\underline{x})\psi(\underline{x}) = E\psi(\underline{x})\,. \tag{7.8}$$

$$\Psi_i(\underline{x}) = \psi_i(x)\, e^{-iE_i t/\hbar}$$

stationary state

Then $|\Psi_i(\underline{x})|^2 = |\psi_i(x)|^2$ t-indep.

But $\sum_{i=1}^{\infty} c_i \Psi_i(\underline{x}) = \sum c_i \psi_i(\underline{x})\, e^{-iE_i t/\hbar}$

does not have stationary $|\Psi_i(\underline{x})|^2$.

(cf. 1D).

Recall in 1D we used an <u>ansatz</u>

$$\psi(x,t) = \psi(x) \cdot T(t)$$

and then argued the general solution is a <u>superposition</u> of these product state solutions.

In 3D we try $\psi(\underline{x},t) = \psi(\underline{x}) T(t)$

$$\Rightarrow \hat{H} \psi(\underline{x}) = E \psi(\underline{x})$$

$$T(t) = e^{-iEt/\hbar}$$

(just as in 1D)

Our theorems from 1D carry over: the general solution to the 3DSE is again a superposition of stationary state solutions

ie.

$$\sum_{i=1}^{\infty} \psi_i(\underline{x}) e^{-iE_i t/\hbar}$$

(for discrete energy spectrum)

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$$\frac{\partial \rho}{\partial t} + \underline{\nabla}.\underline{J} = 0 \,. \tag{7.11}$$

$$\frac{\partial}{\partial t}\left(\int \rho(\underline{x})\, dV\right) = -\int \underline{J}.\underline{dS}$$

$\underline{J}.\underline{dS}$ = "probability flux across $\underline{dS}$"

$\rho(\underline{x}_0)\, V$ = "total probability in small volume V"

$$-\frac{\hbar^2}{2M}\nabla^2\psi(\underline{x},t)+V(\underline{x})\psi(\underline{x},t)=i\hbar\frac{\partial}{\partial t}\psi(\underline{x},t)\,. \qquad (7.7)$$

$$\underline{\nabla}\cdot\underline{J} = -\frac{i\hbar}{2m}\Big((\nabla\psi^*)(\nabla\psi)+\psi^*(\nabla^2\psi) - (\nabla^2\psi^*)\psi - (\nabla\psi^*)(\nabla\psi)\Big)$$

$$= -\frac{i\hbar}{2m}\Big(\psi^*(\nabla^2\psi) - (\nabla^2\psi^*)\psi\Big)$$

$$= -\frac{i\hbar}{2m}\psi^*\Big(-\frac{2mi\hbar}{\hbar^2}\frac{\partial\psi}{\partial t} + \frac{2M}{\hbar^2}V(x)\psi(x)\Big)$$

$$+\frac{i\hbar}{2m}\Big(\Big(\frac{2mi\hbar}{\hbar^2}\frac{\partial\psi^*}{\partial t}\Big)\psi + \frac{2m}{\hbar^2}V(x)\psi^*\psi\Big)$$

$$= -\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t} = -\frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\partial\rho}{\partial t}\,.$$

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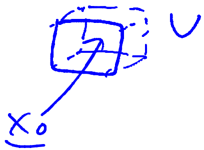

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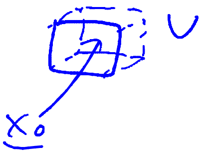

$$\int_V |\psi(\underline{x}, t)|^2 d^3x$$

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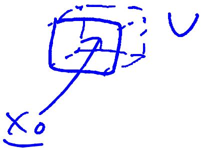
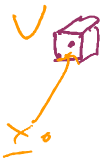


$$\int_V |\psi(x, t)|^2 d^3x \approx V\, |\psi(\underline{x_0}, t)|^2 \qquad (7.12)$$



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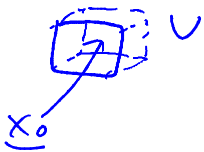

$$\begin{aligned} \int_V |\psi(\underline{x}, t)|^2 d^3x &\approx V\,|\psi(\underline{x_0}, t)|^2 \qquad (7.12) \\ &= V\,\rho(\underline{x_0}, t)\,. \end{aligned}$$

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We define the inner product of 3D wavefunctions by

$$(\psi_1, \psi_2) = \int \psi_1^*(\underset{\sim}{x})\psi_2(\underset{\sim}{x})d^3x\,.$$

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As in the 1D case, we can justify this definition directly for position and for operators with discrete eigenvalues. It can also be justified for general operators: we will take the definition (7.13) as valid for all operators.

E.g. $\langle \hat{\underline{x}} \rangle_\psi = \int_{\mathbb{R}^3} \text{Prob}(\hat{\underline{x}} = \underline{x})\, \underline{x} \; d^3x$

$$= \int |\psi(\underline{x})|^2 \, \underline{x} \; d^3x$$

$$= \int \psi^*(\underline{x})\, \underline{x}\, \psi(\underline{x})\, d^3x$$

$$= (\psi(\underline{x}), \hat{\underline{x}}\, \psi(\underline{x}))$$

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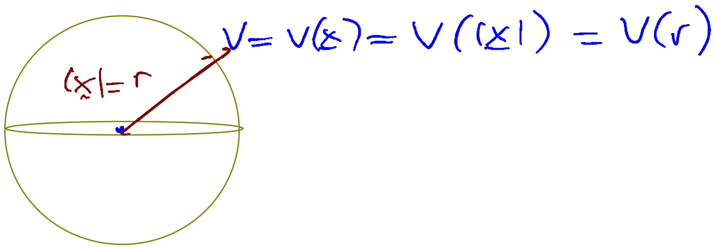
We can thus define the uncertainty $\Delta_\psi A$ as in (6.21), using the definition (7.13) for expectation values.

$$\begin{aligned} (\Delta_\psi A)^2 &= \langle (A - \langle A \rangle_\psi)^2 \rangle_\psi \\ &= \langle A^2 \rangle_\psi - (\langle A \rangle_\psi)^2 \,. \end{aligned} \tag{6.21}$$

Spherically symmetric potentials

The 3D time-independent Schrödinger equation simplifies considerably when the potential $V(\underline{x})$ is *central*, i.e. spherically symmetric about the origin.



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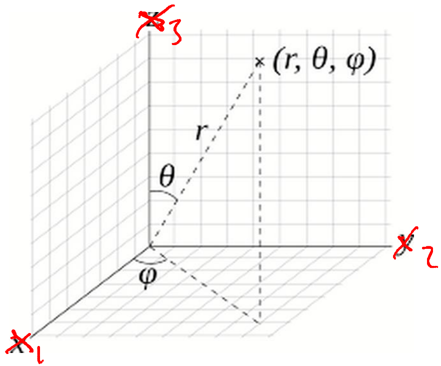

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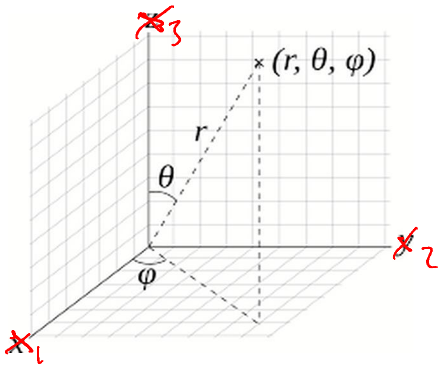
which have ranges $0 \leq r < \infty$, $0 \leq \phi < 2\pi$, $0 \leq \theta \leq \pi$.



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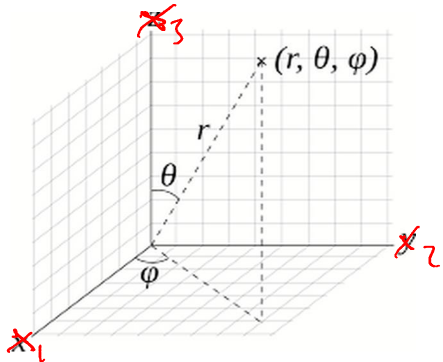
In spherical polars, a central potential $V(\underline{x}) \equiv V(r,\theta,\phi)$ depends only on $r = |\underline{x}|$.



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$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \quad (7.15)$$

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$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\phi^2} \quad (7.15)$$

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time-indep SE.

Hence

$$-\frac{\hbar^2}{2M}\frac{1}{r}\frac{d^2}{dr^2}(r\psi(r)) + V(r)\psi(r) = E\psi(r)\,, \tag{7.17}$$

Spherically symmetric potentials

For spherically symmetric stationary states $\psi(r)$, the time-independent SE simplifies.We have $\frac{\partial\psi}{\partial\theta} = \frac{\partial\psi}{\partial\phi} = 0$ and so

$$\begin{aligned} \nabla^2\psi &= \frac{1}{r^2}\frac{d}{dr}(r^2\frac{d}{dr})\psi \\ &= \frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr} \\ &= \frac{1}{r}\frac{d^2}{dr^2}(r\psi)\,. \end{aligned} \tag{7.16}$$

Hence

$$-\frac{\hbar^2}{2M}\frac{1}{r}\frac{d^2}{dr^2}(r\psi(r)) + V(r)\psi(r) = E\psi(r)\,, \tag{7.17}$$

which we can rewrite as

solve for $\phi = r\psi$ $\Longrightarrow$ solve for $\psi = r^{-1}\phi$.

$$-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}(r\psi(r)) + V(r)(r\psi(r)) = E(r\psi(r))\,. \tag{7.18}$$

Spherically symmetric potentials

Notice that (7.18) is the 1D time-independent SE for $\phi(r) = r\psi(r)$, on the interval $0 \leq r < \infty$.

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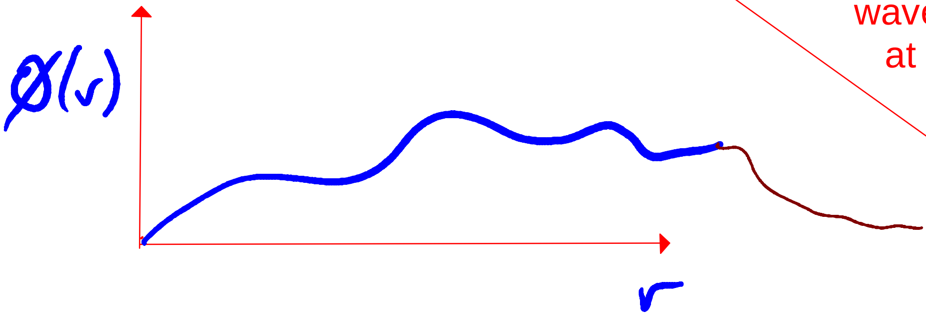
We require $\phi(r) \to 0$ as $r \to 0$, otherwise $\psi(r) \approx O(1/r)$ as $r \to 0$ and so is singular at $r = 0$.

Remember we are solving for a 3D wavefunction. If V is not singular at the origin then psi should be finite and continuous there.



$$-\frac{\hbar^2}{2M}\nabla^2\psi(\underline{x}) + V(\underline{x})\psi(\underline{x}) = E\psi(\underline{x})\,. \qquad (7.8)$$

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Any solution to (7.18) with $\phi(r) \to 0$ as $r \to 0$ can be extended to an odd parity solution $\tilde{\phi}(r)$ of the 1D SE in $-\infty < r < \infty$ of the same energy,

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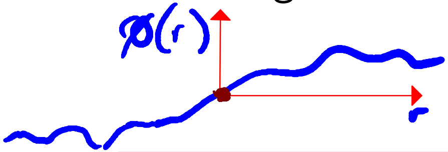


$$\tilde{\phi}(r) = \begin{cases} \phi(r) & r \geq 0\,, \\ -\phi(-r) & r < 0\,. \end{cases} \tag{7.19}$$

mathematical trick: we don't have a 3D physical interpretation of $\tilde{\phi}$.

$$-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}(r\psi(r)) + V(r)(r\psi(r)) = E(r\psi(r))\,. \tag{7.18}$$

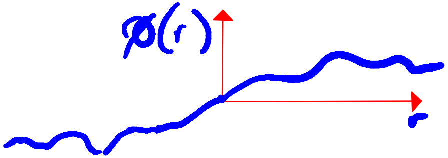
Spherically symmetric potentials

Conversely, any odd parity solution of the 1D SE for $-\infty < r < \infty$ defines a solution to (7.18) with $\phi(r) \to 0$ as $r \to 0$ and $\frac{d\phi}{dr}$ finite at $r = 0$.

Spherically symmetric potentials

Conversely, any odd parity solution of the 1D SE for $-\infty < r < \infty$ defines a solution to (7.18) with $\phi(r) \to 0$ as $r \to 0$ and $\frac{d\phi}{dr}$ finite at $r = 0$. Provided that $V(r)$ is finite and continuous at $r = 0$, these continuity conditions imply that ψ and ψ' are continuous at the origin.

$$-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}(r\psi(r)) + V(r)(r\psi(r)) = E(r\psi(r))\,. \qquad (7.18)$$



$$\phi(r) = r\psi(r) = \phi(0) + r\phi'(0) + \dots$$

$$\Rightarrow \lim_{r\to 0} \psi(r) = \phi'(0).$$

$$-\frac{\hbar^2}{2m}\phi''(r) + V(r)\phi(r) = E\phi(r)$$

$$\Rightarrow \lim_{r\to 0^+}\left(\phi''(r)\right) = 0 \quad \text{(if } V \text{ non-singular)}$$

$$\phi''(r) = 2\psi'(r) + r\psi''(r)$$

$$\Rightarrow \lim_{r\to 0^+}\left(\psi'(r)\right) = \lim_{r\to 0^+}\frac{1}{2}\left(\phi''(r) - r\psi''(r)\right)$$

$$= 0.$$

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Solving (7.18) thus becomes equivalent to finding odd parity solutions to the 1D SE for $-\infty < r < \infty$.

Spherically symmetric potentials

We will show later (see Thm. 15) that the ground state (the lowest energy bound state, if there is one) of a 3D quantum system with spherically symmetric potential is itself spherically symmetric.

i.e. if ground state then our ansatz always gives at least one physical solution.

Spherically symmetric potentials

We will show later (see Thm. 15) that the ground state (the lowest energy bound state, if there is one) of a 3D quantum system with spherically symmetric potential is itself spherically symmetric. Hence we can always use the method above to obtain the ground state.

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One might wonder whether there might not exist even parity solutions $\phi_+(r)$ of the 1D SE with the property that $\phi_+(0) = \frac{d\phi_+}{dr}(0) = 0$,

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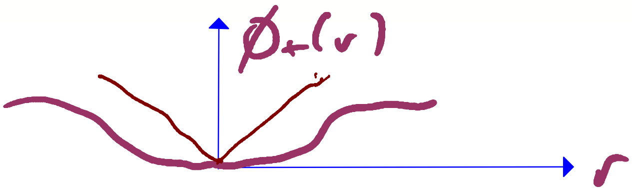

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One might wonder whether there might not exist even parity solutions $\phi_+(r)$ of the 1D SE with the property that $\phi_+(0) = \frac{d\phi_+}{dr}(0) = 0$,which would also define solutions to (7.18) for $0 \leq r < \infty$ with the appropriate properties.

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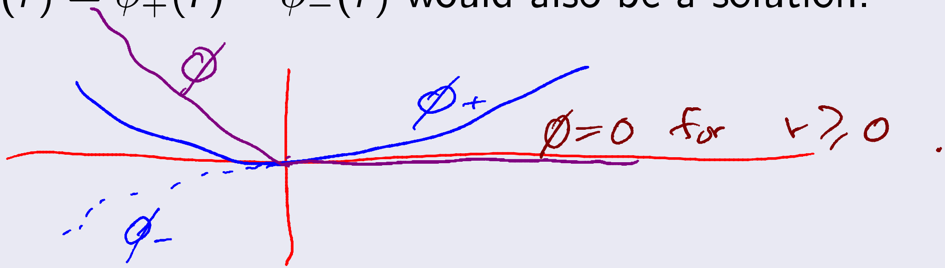
Then $\phi(r) = \phi_+(r) - \phi_-(r)$ would also be a solution.



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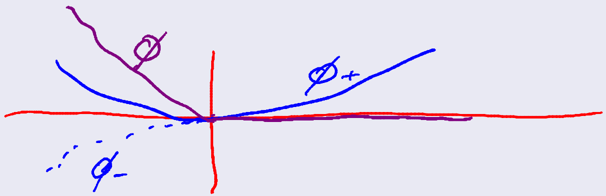

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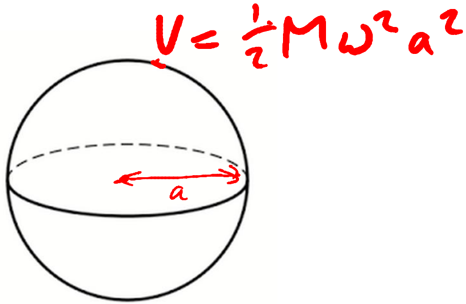
Examples of spherically symmetric potentials

The spherical harmonic oscillator has potential $V(r) = \frac{1}{2}M\omega^2 r^2$.



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$$-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}(r\psi(r)) + V(r)(r\psi(r)) = E(r\psi(r)) \,. \qquad (7.18)$$

NEED SOLUTIONS FOR ODD PARITY ϕ.

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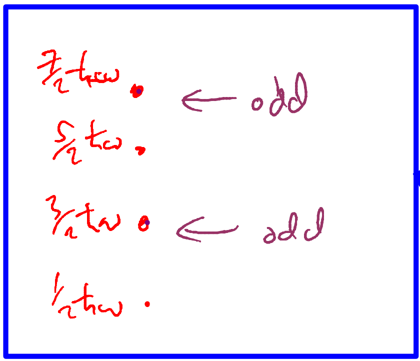


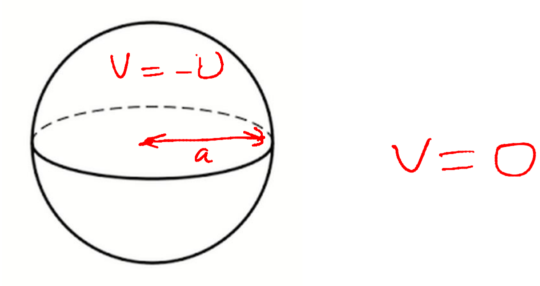
spherically symmetric

1D harmonic oscillator
bound states

Examples of spherically symmetric potentials

The spherical "square" well has potential

$$V(r) = \begin{cases} -U & r < a\,, \\ 0 & r > a\,. \end{cases} \tag{7.21}$$



Examples of spherically symmetric potentials

The spherical square well has potential

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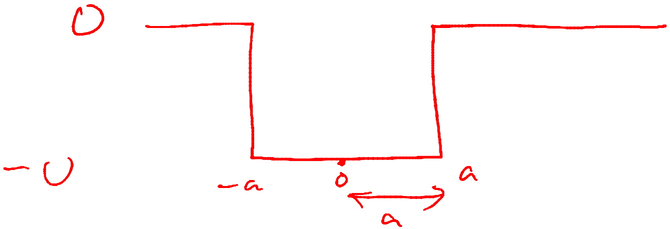
By the above argument, spherically symmetric stationary states correspond to odd parity bound states of the 1D square well potential

$$V(x) = \begin{cases} -U & |x| < a\,, \\ 0 & |x| > a\,. \end{cases} \tag{7.22}$$



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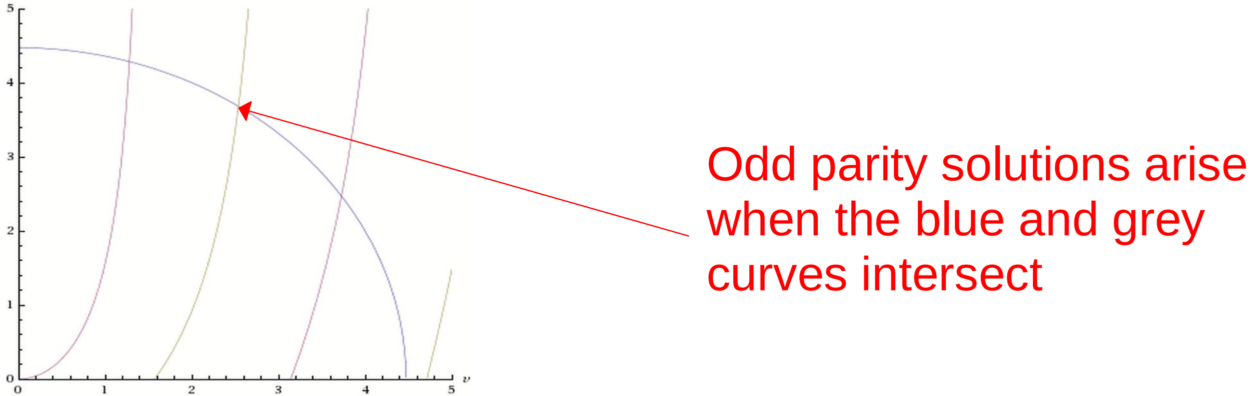
$$\sqrt{\frac{2MU}{\hbar^2}} \geq \frac{\pi}{2a} \,. \tag{7.23}$$



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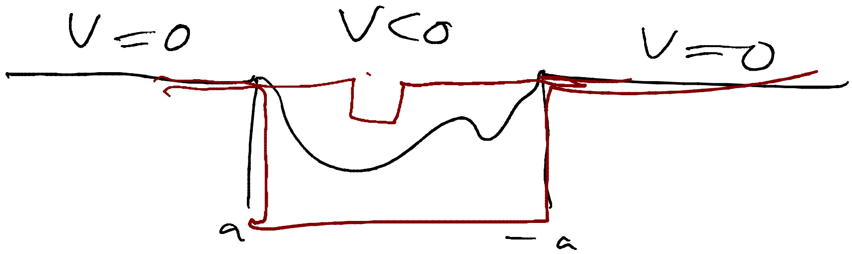
Remember: we stated (and will prove later) that the ground state of a particle in a spherically symmetric potential is always spherically symmetric

Examples of spherically symmetric potentials

As this illustrates, 3D potential wells (continuous potentials with $V(x) \leq 0$ for all x, $V(x) < 0$ for some x, and $V(x) = 0$ for $|x| > a$, for some finite a) do not necessarily have bound states.

Examples of spherically symmetric potentials

As this illustrates, 3D potential wells (continuous potentials with $V(x) \leq 0$ for all x, $V(x) < 0$ for some x, and $V(x) = 0$ for $|x| > a$, for some finite a) do not necessarily have bound states. In contrast, we can show that all 1D potential wells have at least one bound state.



Hint: consider a square pot'l V' s.t. $V'(x) \geq V(x)$ $\forall x \in \mathbb{R}$.