1. The Wave Function

1.1 The Schrödinger Equation

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

or $i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\Psi(\vec{r},t) + V(\vec{r},t)\Psi(\vec{r},t)$

where $\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^3}{\partial z^3}$

Solve for the particle's wave function $\Psi(x,t)$

$\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34}$ Js

1.2 The Statistical Interpretation

$\int_a^b |\Psi(x,t)|^2 dx = \{\text{P of finding the particle btwn } a \text{ and } b, \text{ at } t\}$

1.3 Probability

Standard deviation: $\sigma = \sqrt{\langle j^2\rangle - \langle j\rangle^2}$

Expectation value of x given Ψ: $\langle x\rangle = \int x|\Psi|^2 dx$

Probability current: $J(x,t) = \frac{i\hbar}{2m}(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x})$

1.4 Normalization

$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$

The Schrödinger equation produces unitary time evolution:

$\vec{J} = -\frac{i\hbar}{2m}(\psi((\vec{r}),t)^*\vec{\nabla}\psi(\vec{r},t) - \psi(\vec{r},t)\vec{\nabla}\psi(\vec{r},t)^*)$

The probability density satisfies the continuity equation,

$\frac{\partial}{\partial t}\mathcal{P} + \vec{\nabla}\cdot J = 0$

Because the probability for finding the particle at infinity is 0 (otherwise non-normalizable), $\vec{J} = 0$ at infinity.

Therefore, $\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\mathcal{P}d^3\vec{r} = \frac{\mathrm{d}}{\mathrm{d}t}P = 0$, where P is the total probability $\rightarrow$ the total probability is constant in time.

1.5 Momentum

For a particle in state Φ, the expectation value of x and p is

$$\langle x\rangle = \int_{-\infty}^{+\infty} x|\Psi(x,t)|^2 dx \qquad \langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int(\Psi^*\frac{\partial\Psi}{\partial x})dx$$

To calculate the expectation value of any quantity, $Q(x,p)$:

$$\langle Q(x,p)\rangle = \int\Psi^* Q(x, \frac{\hbar}{i}, \frac{\partial}{\partial x})\Psi dx$$

Position and momentum operators: $\widehat{\vec{r}} = \vec{r}$, $\widehat{\vec{p}} = -i\hbar\vec{\nabla}$

1.6: The Uncertainty Principle

The wavelength of Ψ is related to the momentum of the particle by the de Broglie formula:

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}$$

The more precisely determined a particle's position is, the less precisely is its momentum. The Heisenberg's uncertainty principle:

$$\sigma_x\sigma_p \geq \frac{\hbar}{2}$$

Commutation relation btwn position and momentum:

$$\widehat{p}_x(\widehat{x}\psi(x,t)) = -i\hbar\frac{\partial}{\partial x}[x\psi(x,t)] = -i\hbar\psi(x,t) - i\hbar x\frac{\partial}{\partial x}\psi(x,t)$$

$$\widehat{x}(\widehat{p}_x\psi(x,t)) = x(-i\hbar\frac{\partial}{\partial x}\psi(x,t))$$

$\widehat{x}\widehat{p}_x - \widehat{p}_x\widehat{x} = [\widehat{x}, \widehat{p}_x] = i\hbar$

$[\widehat{x}_i, \widehat{p}_j] = i\hbar\delta_{ij}, [\widehat{x}_i, \widehat{x}_j] = [\widehat{p}_i, \widehat{p}_j] = 0,$

where $\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq j$

Given three operators $\widehat{A}, \widehat{B}, \widehat{C}$, we have $[\widehat{A}, \widehat{B}\widehat{C}] = [\widehat{A}, \widehat{B}]\widehat{C} + \widehat{B}[\widehat{A}, \widehat{C}]$.

Other: Blackbody Spectrum

$E = hv = \hbar\omega$

The wave number k is $k = 2\pi/\lambda = \omega/c$

Only two spin states occur (quantum number m is +1 or -1).

$\rho(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3(e^{\hbar\omega/k_b T} - 1)}$

Wien displacement law: $\lambda_{\max} = \frac{2.90\times10^{-3}\text{mK}}{T}$

2. Time-Independent Schrödinger Equation

2.1 Stationary States

Suppose PE is independent of time, $V(\vec{r},t) = V(\vec{r})$.

Separation of variables: $\Psi(\vec{r},t) = \psi(\vec{r})\varphi(t)$

Eq of motion for $\varphi(t)$: $\varphi(t) = e^{-iEt/\hbar}$

Eq of motion for $\psi(\vec{r})$ is the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(\vec{r})}{\mathrm{d}x^2} + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

TD of the wavefunction that corresponds to the constant E is easily written once we solve the TISE: $\Psi_E(\vec{r},t) = \psi_E(\vec{r})e^{-iEt/\hbar}$

Properties of solutions for TI potentials:

- **The constant E must be real.**
- **Stationary wavefunction.**
  $\mathcal{P}(\vec{r},t) = |\psi_E(\vec{r},t)|^2 = |\psi_E(\vec{r})|^2$ (TD cancels out).
- **Stationary wavefunction is a state of definite energy.**
  The total energy (kinetic plus potential) is the Hamiltonian:
  $H(x,p) = \frac{p^2}{2m} + V(x)$.
  Hamiltonian operator: $\widehat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
  Thus the TISE can be written as $\widehat{H}\psi = E\psi$
  $\langle\widehat{H}\rangle = E$, $\langle\widehat{H}^2\rangle = E^2$, $\Delta E = \sqrt{\langle\widehat{H}^2\rangle - \langle\widehat{H}\rangle^2} = 0$
- Spatial part of stationary wavefunction can be chosen to be real.
  $\psi^*(\vec{r})$ is a soln w/ same E
  Solns can be chosen to be real: $\psi(\vec{r}) + \psi^*(\vec{r})$ and $\frac{\psi(\vec{r}) - \psi^*(\vec{r})}{i}$.
- **Parity symmetry: even and odd wavefunctions.** Suppose $V(-\vec{r}) = V(\vec{r})$. Then, $\psi_E(-\vec{r})$ is a soln w the same energy.
  $\psi_E(\vec{r}) + \psi_E(-\vec{r})$ is even under reflection, $\psi_E(\vec{r}) - \psi_E(-\vec{r})$ is odd.
  When the potential is symmetric under reflection, we can choose the stationary states to be either even or odd under reflection.
- **Orthogonality/orthonormality.**
  $\int\psi_m(\vec{r})^*\psi_n(\vec{r})d^3\vec{r} = \delta_{mn}$ where δ_{mn} is 0 if $m \neq n$ and 1 if $m = n$.
- **Linearity.**
  The SE is linear. Given stationary states, a linear combo of these
  $$\psi(\vec{r},t) = \sum_n c_n\psi_n(\vec{r},t) = \sum_n c_n\psi_n(\vec{r})e^{-\frac{i}{\hbar}E_n t}$$
  where c_n are complex constants, is a solution to the TDSE
  $$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \widehat{H}\psi(\vec{r},t)$$
- **Time evolution.** Given
  $$\psi(\vec{r},0) = \sum_n c_n\psi_n(\vec{r},0) = \sum_n c_n\psi_n(\vec{r})$$
  at time t, the time evolution is
  $$\psi(\vec{r},t) = \sum_n c_n\psi_n(\vec{r},t) = \sum_n c_n\psi_n(\vec{r})e^{-\frac{i}{\hbar}E_n t}$$
  Once we've expanded a given initial wavefunction in terms of a linear combo of the stationary wavefunctions $\psi_n(\vec{r})$, the time evolution follows simply by putting a factor of $e^{-i/\hbar E_n t}$ to each term containing $\psi_n(\vec{r})$.
- **Normalization.**
  The constant coefficients are constrained by $\sum_n |c_n|^2 = 1$
- **Completeness.**
  The stationary states form a complete set if
  $$\sum_n\psi_n(\vec{r'},t)^*\psi_n(\vec{r},t) = \delta^3(\vec{r'} - \vec{r})$$
  where $\delta^3(\vec{r'} - \vec{r})$ is the Dirac-delta function in 3D defined by
  $$\int d^3\vec{r'}\psi(\vec{r'},t)\delta^3(\vec{r'} - \vec{r}) = \psi(\vec{r},t)$$

Euler's formula: $e^{i\theta} = \cos\theta + i\sin\theta$

sin and cos: $\cos(\theta) = \frac{1}{2}(e^{i\theta} + e^{-i\theta})$, $\sin(\theta) = \frac{1}{2}(e^{i\theta} - e^{-i\theta})$

Delta function: Given $f(x)$, $\delta(x - x')$ is defined as

$f(x') = \int f(x)\delta(x - x')dx$

$\int\delta(x - x')dx = 1$, note this is not the area

$\delta_\alpha(x) = \frac{1}{\alpha\sqrt{\pi}}e^{-\frac{x^2}{\alpha^2}}$, $\delta_\alpha(x) = \frac{1}{\pi x}\sin(\frac{x}{a})$, $\delta_\alpha(x) = \frac{\alpha}{\pi x^2}\sin^2(\frac{x}{\alpha})$

One-dimensional systems

Wavefunction for a system containing a single particle of mass m in 1D with TI potentials.

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x)\psi(x) = E\psi(x)$$

Once we find the wavefunction $\psi_E(x)$ of energy E, its time dependence follows easily:

$$\psi_E(x,t) = \psi_E(x)e^{-\frac{i}{\hbar}Et}$$

Boundary conditions

1. When the potential $V(x)$ has a finite jump at $x = a$, both $\psi(x)$ and $\psi'(x)$ are continuous across $x = a$.
2. When the potential $V(x)$ has an infinite jump at $x = a$, $\psi(x)$ is continuous but $\psi'(x)$ is discontinuous across $x = a$.

Futhermore, the wavefunction must vanish at $x = \pm\infty$ for a normalizable wavefunction.

2.2 The Infinite Square Well

$$V(x) = \begin{cases} 0, \text{if } 0 \leq x \leq a \\ \infty, \text{otherwise} \end{cases}$$

$$\psi(x) = 0 \text{ for } x < 0 \text{ and } x > a$$

For $0 \leq x \leq a$, $V(x) = 0$ and the Schrödinger equation reduces to

$$\psi''(x) + k^2\psi(x) = 0, \text{ where } k = \sqrt{\frac{2mE}{\hbar^2}} \text{ and } E > 0$$

Classic **simple harmonic oscillator**: $\psi(x) = A\sin(kx) + B\cos(kx)$

Boundary conditions:

Continuity of $\psi(x)$ at $x = 0$ sets $\psi(0) = B = 0 \rightarrow \psi(x) = A\sin(kx)$ at $x = a$ sets $\psi(a) = A\sin(ka) = 0$

$$k_n = \frac{n\pi}{a}, n = 1, 2, ...$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \qquad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

ψ_1 is the ground state, others are excited states.

Properties of $\psi_n(x)$:

1. Alternatively even and odd.
2. As you go up in energy, each successive state has one more node.
3. They are mutually orthogonal, in the sense that
$\int\psi_m(x) * \psi_n(x)dx = 0$ whenever $m \neq n$.
$\int\psi_m(x) * \psi_n(x)dx = \delta_{mn}$ where δ_{mn} (Kronecker delta) is 0 if $m \neq n$ and 1 if $m = n$. We say that the ϕ's are orthonormal.
4. They are complete, in the sense that any other function, $f(x)$, can be expressed as a linear combination of them (Fourier series), Dirichlet's theorem:

$$f(x) = \sum_{n=1}^{\infty} c_n\psi_n(x) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} c_n\sin\left(\frac{n\pi}{a}x\right)$$

Fourier's trick: $c_n = \int\psi_n(x)^* f(x)dx$

$$c_m = \frac{2}{a}\int_0^a f(x)\sin\left(\frac{m\pi x}{a}\right)dx$$

$|c_n|^2$ tells you the probability that a measurement of the energy would yield the value E_n.

Sum of these probabilities should be 1:

$$\sum_{n=1}^{\infty} |c_n|^2 = 1$$

The expectation value of the energy is

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

Conservation of energy in QM

2.3 The Harmonic Oscillator

Hooke's law (mass m w/ spring constant k): $F = -kx = m\frac{d^2x}{dt^2}$

Solution is $x(t) = A\sin(\omega t) + B\cos(\omega t)$, where $\omega = \sqrt{\frac{k}{m}}$

Potential energy: $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$

Expanding $V(x)$ in a **Taylor series** about the min:

$V(x) = V(x_0) + V'(x_0)(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \cdots$

Simple harmonic oscillaton, $V(x) \cong \frac{1}{2}V''(x_0)(x-x_0)^2, k = V''(x_0)$

The Schrödiner Equation for the harmonic oscillator:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi$$

Boundary conditions: $\psi(-\infty) = 0, \qquad \psi(+\infty) = 0$

1. Simplify notation with change of variables

Introduce $\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x$.

SE becomes $\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} = (\xi^2 - K)\psi$, where $K \equiv \frac{2E}{\hbar\omega}$.

2. Asymptotic behavior

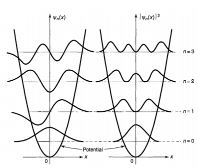
Working in the large $\xi^2 >> K$ region,

Hermite eqn: $H''(\xi) - 2\xi H'(\xi) + (K-1)H(\xi) = 0$

Hermite polynomials: $H_0 = 1$, $H_1 = 2\xi$, $H_2 = 4\xi^2 - 2$,

$H_3 = 8\xi^3 - 12\xi$, $H_4 = 16\xi^4 - 48\xi^2 + 12$, $H_5 = 32\xi^5 - 160\xi^3 + 120\xi$

3. Method of power series



The recursion formula: $a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j$

Recursion formula for allowed K:

$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)}a_j$

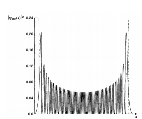
$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j\xi^j$

$h(\xi) = h_{\text{even}}(\xi) + h_{\text{odd}}(\xi)$

4. Infinite series produces a diverging function

For large n, we have $a_{n+2} \approx \frac{2}{n}a_n$

5. Truncate series



$K = 2n+1$, so $E_n = (n+\frac{1}{2})\hbar\omega$

The normalized stationary states:

$\psi_n(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\frac{1}{\sqrt{2^n n!}}H_n(\xi)e^{-\xi^2/2}$

Rodrigues formula: $H_n(\xi) = (-1)^n e^{\xi^2}(\frac{\mathrm{d}}{\mathrm{d}\xi})^n e^{-\xi^2}$

2.4 The Free Particle

$$\frac{\partial^2\xi}{\partial x^2} = -k^2\xi, k = \frac{\sqrt{2mE}}{\hbar}$$

General solution to the TISE: wave packet,

$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}\infty\psi(k)e^{i(kx - \frac{\hbar k^2}{2m}t)}dk$

$$\phi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)e^{-ikx}dx$$

Plancherel's theorem:

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}F(k)e^{ikx}dk \leftrightarrow F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)e^{-kx}dx$$

$F(k)$ is the Fourier transform of $f(x)$; $f(x)$ is the inverse Fourier transform of $F(k)$

Phase velocity: speed of individual ripples; group velocity: speed of the envelope

Dispersion relation: the formula for ω as a function of k

2.5 The Delta-Function Potential

Dirac delta function is an infinitely high, infinitesimally narrow spike at the origin, whose area is 1:

$$\delta(x) = \begin{cases} 0, \text{if } x \neq 0 \\ \infty, \text{if } x = 0 \end{cases}$$

$f(x)\delta(x-a) = f(a)\delta(x-a)$ bc the product is 0 anyway except at a. In particular, $\int_{-\infty}^{\infty} f(x)\delta(x-a)dx = f(a)$. $a-\epsilon$ to $a+\epsilon$ would do, for any $\epsilon > 0$.

Consider $V(x) = -\alpha\delta(x)$, where α is some positive constant.

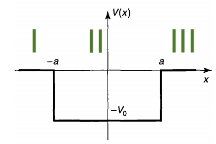
$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - \alpha\delta(x)\psi = E\psi$$

Bound states (E ¡ 0):

Scattering states (E ¿ 0):

2.6 The Finite Square Well

$$V(x) = \begin{cases} -V_0, \text{for } -a < x < a \\ 0, \text{for } |x| > a \end{cases},$$



where V_0 is a positive constant.

Both bound states ($E < 0$) and scattering states ($E > 0$).

Bound states:

Potential is piecewise and discontinuous, can split into regions.

REGION I

$$-\frac{\hbar}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi, \text{ or } \psi_I''(x) - \kappa^2\psi_I(x) = 0, \qquad \kappa \equiv \sqrt{-\frac{2mE}{\hbar}}$$

where $E < 0$ for a bound state.

General sol: $\psi_I(x) = Ae^{-\kappa x} + Be^{\kappa x}$.

$x = -\infty \rightarrow \psi(x) = 0$, so $A = 0$, and we have $\psi_I(x) = Be^{\kappa x}$

REGION II

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - V_0\psi = E\psi, \text{ or } \psi'' = -l^2\psi, \qquad l \equiv \sqrt{\frac{2m(E+V_0)}{\hbar}}$$

General sol: $\psi(x) = C\sin(lx) + D\cos(lx)$, for $-a < x < a$

REGION III

SE and general sol same as region I, but $x = \infty \rightarrow \psi(x) = 0$, so $G = 0$ and $\psi_{III}(x) = Fe^{-\kappa x}$

Even bound states

$\psi(-x) = \psi(x)$, $\psi_{II}(x) = D\cos(lx)$

Bc the potential has only a finite discontinuity at $x = \pm a$, both ψ and ψ' must be continuous at $x = \pm a$.

$x = a$, $\psi_{II}(a) = \psi_{III}(a)$ imposes $D\cos(la) = Fe^{-\kappa a}$

$x = a$, $\psi_{II}'(a) = \psi_{III}'(a)'$ imposes $-lD\sin(la) = -\kappa Fe^{-\kappa a}$

Continuity of $\psi(x)$ and $\psi'(x)$ at $x = -a$ does not add anything new.

Dividing the above two, we get $\kappa = l\tan(la)$

This is a formula for the allowed energies, since κ and l are both functions of E. Let $z \equiv la$, and $z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$. $\kappa^2 + l^2 = 2mV_0/\hbar^2$, so $\kappa a = \sqrt{z_0{}^2 - z^2}$.

Transcendental eq for z (and hence E) as a function of z_0 (which is a measure of size of well): $\tan z = \sqrt{(\frac{z_0}{z})^2 - 1}$

Odd bound states

$\psi_{II}(x) = C\sin(lx)$

$x = -a, \psi_{II}(-a) = \psi_I(-a)$ imposes $C\sin(la) = Be^{-\kappa a}$

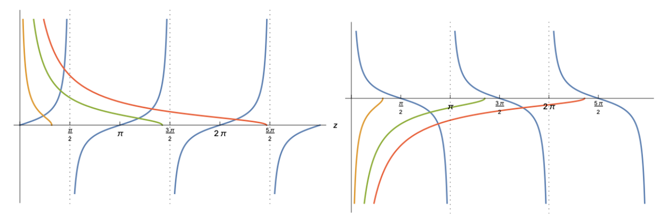
$x = -a, \psi_{II}'(-a) = \psi_I'(-a)$ imposes $lC\cos(la) = -\kappa Be^{-\kappa a}$

Dividing the above two, $l\cot(la) = -\kappa$.

Rewriting this in terms of z and z_0,

$$\cot(z) = -\sqrt{(\frac{z_0}{z})^2 - 1}$$

V_1 does not support an odd bound state, since there is no intersection pt, V_2 produces only one bound state, and V_3 produces two bound states. Finite well potential supports at least one even state, the ground state, and it may not support any of the excited states.



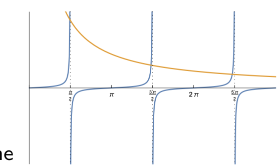
Wide and deep well

$z_n \approx \frac{n\pi}{2}, n = 1, 2, 3, \ldots.$

Using the def of z and solving for E,

$E_n = -V_0 + \frac{\hbar^2\pi^2n^2}{2m(2a)^2}, n = 1, 2, \ldots$

Thus, the energy levels of the infinite square well of width $2a$ are reproduced for $E_n - (-V_0) = E_n + V_0$, which is the energy above the bottom of the well. As $V_0 \rightarrow \infty$, finite sq well goes to infinite sq well.



Shallow and narrow well

Any shallow or narrow well supports at least one bound state. But we need at least $z_0 = \sqrt{\frac{2mV_0a^2}{\hbar^2}} \geq \frac{\pi}{2}$ to support any odd state.

Gaussian integrals

$$\int_{-\infty}^{\infty} e^{-ax^2}dx = \sqrt{\frac{\pi}{a}} \text{ and } \int_0^{\infty} e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{\infty} x^{2n+1}e^{-ax^2}dx = 0 \text{ for } n = 0, 1, 2, \ldots$$

$$\int_{-\infty}^{\infty} x^{2n}e^{-ax^2}dx = (-1)^n\frac{\mathrm{d}^n}{\mathrm{d}a^n}\sqrt{\frac{\pi}{a}} \text{ for } n = 0, 1, 2, \ldots$$

$$\int_{-\infty}^{\infty} e^{-ax^2+bx}dx = \sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}} \qquad \int_{-\infty}^{\infty} x^n e^{-ax^2+bx}dx = \frac{\mathrm{d}^n}{\mathrm{d}b^n}\sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}}$$