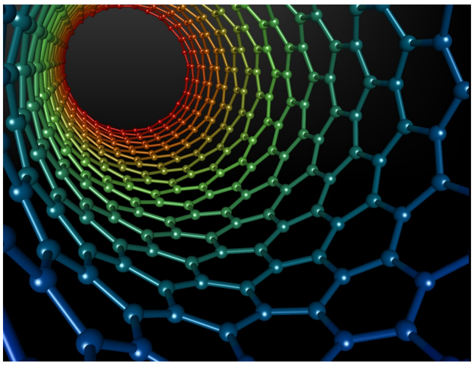
Set #3

8.
Suppose a particle is moving freely inside a carbon nanotube. If the particle if moving with a given momentum p (eigenvalue), find its quantum state (eigenfunction) by directly solving the corresponding eigenvalue equation for the momentum operator:

$$\hat{p} = -i\hbar\hat{\nabla}$$



b. Show that these particle states are orthogonal (in the Dirac sense)

c. Show that such states are also complete with respect to any square integrable function.

d. Apply part c. to a Gaussian function of width σ and centred at the origin and one centred at some position $x = a$

9.
a. For an electron moving inside a tiny nanotube (1D) give the general solution of the Schroedinger equation.

b. Discuss (briefly) whether such a solution is acceptable. In the negative what would you foresee as a way out?

10.
Work out eigenfunctions and eigenvalues of a free electron inside a box of sides {a,b,c} with impenetrable walls using the method of separation of variables for (partial) differential equations.

11.
Find under what condition the solutions of the Schroedinger eq.

$$i\hbar\,\partial_t\Psi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\Psi(x,t) + V(x,t)\Psi(x,t)$$

can be factorized as $\psi(x,t) = \psi(x)\,T(t)$. Determine the form of $T(t)$.

✦ Find under what conditions solutions of the Schroedinger eq.

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can be factorized as $\psi(x,t) = \psi(x)\,T(t)$. Determine the form of $T(t)$.

$$i\hbar\,\partial_t \psi(x,t) = \Big[-\frac{\hbar^2}{2m}\partial_x^2 + \underbrace{V(x,t)}_{\text{general (not conservative)}}\Big]\psi(x,t) \qquad (1)$$

Try: $\psi(x,t) \equiv \psi(x)\,T(t)$ (Factorization)

Insert into (1):

$$\left[i\hbar\,\partial_t T(t)\right]\psi(x) = \left[-\frac{\hbar^2}{2m}\partial_x^2\psi(x)\right]T(t) + V(x,t)\,\psi(x)\,T(t)$$

Divide by $\psi(x)T(t)$:

$$\frac{i\hbar\,\partial_t T(t)}{T(t)} = -\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\partial_x^2\psi(x) + V(x,t)$$

IF $V(x,t) = V(x)$ (conservative potential) $\Rightarrow$ left hand side is only dependent on "t" while the right hand side is only dependent on "x". Space & time dependencies can be factored out in this case and each side of the equation will be equal to the same constant, say, E

a. $i\hbar\dfrac{dT}{dt} = E\,T$ or $\dfrac{d}{dt}\ln T = \dfrac{E}{i\hbar}$ or $\ln T = -i\dfrac{E}{\hbar}t + \text{const}$

b. $-\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}\psi(x) + V(x)\,\psi(x) = E\,\psi(x)$

For conservative potentials w.f. $\psi(x,t) = \psi(x)\cdot e^{-i\frac{E}{\hbar}t}\cdot\text{const.} \Rightarrow \psi(x)\underbrace{e^{-i\frac{E}{\hbar}t}}_{\text{harmonic time-dependence.}}$

$\xrightarrow{}$ general (NOT conservative)

$$i\hbar \partial_t \psi(x,t) = \left[-\frac{\hbar^2}{2m}\partial_x^2 + V(x,t)\right]\psi(x,t)$$ ①

Try: $\psi(x,t) \equiv \psi(x)\,T(t)$ (Factorization)

Insert into ①:

$$\left[i\hbar\,\partial_t T(t)\right]\psi(x) = \left[-\frac{\hbar^2}{2m}\partial_x^2\psi(x)\right]T(t) + V(x,t)\,\psi(x)\,T(t)$$

Divide by $\psi(x)\,T(t)$:

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a. $i\hbar \dfrac{dT}{dt} = E\,T$ or $\dfrac{d}{dt}\ln T = \dfrac{E}{i\hbar}$ or $\ln T = -i\dfrac{E}{\hbar}t + \text{const}$

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For conservative potentials w.f. $\psi(x,t) = \psi(x)\cdot e^{-i\frac{E}{\hbar}t}$, const, $\rightarrow \psi(x)\underbrace{e^{-i\frac{E}{\hbar}t}}_{}$

harmonic time-dependence.

Work out eigenfunctions and eigenvalues of a free electron inside a box of sides {a,b,c} with impenetrable walls using the method of separation of variables for (partial) differential equations.

S.S. Schr. Eq.

$$\left[\frac{\hbar^2}{2m}\nabla + E\right]\psi(xyz) = 0 \qquad (1)$$

Electron inside the box is subject to a vanishing potential hence its dynamics in three directions (x, y, z) is independent.

Try: $\psi(\vec{r}) \equiv \psi(xyz) \equiv X(x)Y(y)Z(z)$

$$\frac{\hbar^2}{2m}\nabla^2 X(x)Y(y)Z(z) = \frac{\hbar^2}{2m}\partial_x^2 XYZ + \cdots + \frac{\hbar^2}{2m}\partial_z^2 XYZ$$

$$\downarrow$$

$$YZ\ddot{X}\frac{\hbar^2}{2m} + \cdots + \ddot{Z}XY\frac{\hbar^2}{2m}$$

Divide both sides of (1) by XYZ:

$$\underbrace{\frac{\hbar^2}{2m}\frac{\ddot{X}}{X}} + \underbrace{\frac{\hbar^2}{2m}\frac{\ddot{Y}}{Y}} + \underbrace{\frac{\hbar^2}{2m}\frac{\ddot{Z}}{Z}} + E = 0$$

Three 1D eq.s each in an indep. variable so:

$$\frac{\hbar^2}{2m}\frac{\ddot{X}}{X} = -\alpha; \quad \ldots = -\beta; \quad \frac{\hbar^2}{2m}\frac{\ddot{Z}}{Z} = -\gamma \qquad E = \alpha + \beta + \gamma$$

$$\Downarrow$$

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}X(x) + \alpha X(x) = 0$$

1D problem  electron bound to ∞ barriers

Sol.s are $X(x) = A\sin k_x x \qquad \alpha = \frac{\hbar^2}{2m}k_x^2 \quad$ w/ $k_x = \frac{\pi}{a}\cdot n_x$

Same for Y and Z

Finally: $E = \alpha+\beta+\gamma = \frac{\hbar^2}{2m}k_x^2 + \frac{\hbar^2}{2m}k_y^2 + \frac{\hbar^2}{2m}k_z^2 = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2 n_x^2 + \dots + \left(\frac{\pi}{c}\right)^2 n_z^2\right]$

$$\psi(\bar{r}) = A \sin\frac{\pi}{a}n_x x \cdot \sin\frac{\pi}{b}n_y y \cdot \sin\frac{\pi}{c}n_z z$$

Determine A from orthogonality:

$$\underset{[\text{box}]}{|A|^2 \int dx \int dy \int dz} \sin^2\frac{\pi}{a}n_x x \, \sin^2\frac{\pi}{b}n_y y \, \sin^2\frac{\pi}{c}n_z z = 1$$

$$|A|^2 \underbrace{\int_0^a dx \sin^2\frac{\pi}{a}n_x x}_{\frac{a}{2}} \cdot \underbrace{\int dy \dots}_{b/2} \cdot \underbrace{\int dz}_{c/2} = 1$$

$$|A|^2 \frac{abc}{8} = 1 \Rightarrow A = \sqrt{\frac{8}{abc}} = \sqrt{\frac{2}{a}} \cdots \sqrt{\frac{2}{c}} = \sqrt{8/\text{Vol.}}$$

a. For an electron moving inside a tiny nanotube (1D) give the general solution of the Schroedinger equation.

b. Discuss (briefly) whether such a solution is acceptable. In the negative what would you foresee as a way out?

a.) General sol. is: $\underbrace{Ae^{ikx - iEt/\hbar}}_{\text{p.le moving Toward pos. } x} + \underbrace{Be^{-ikx - iEt/\hbar}}_{\text{p.le moving " neg. } x}$ (Superposition Principle)

b.) Prob. Density Function: $|\psi(x,t)|^2 \equiv P(x,t)$
$= |A|^2 + |B|^2 + 2\,\mathrm{Re}[AB^* e^{2ikx}]$

W/out loss of generality Take $A = B$ (real)

$P(x,t) = 2A^2 [1 + \cos 2kx]$ $\quad (k = \sqrt{2mE}/\hbar)$

This prob. density is not integrable or the w/function $\psi(x,t)$ is not a square integrable fcn hence gen/sol. above is not acceptable

In fact, the overall prob. of finding the p.le is infinite....

In mathematical terms:

$$\int_{-\infty}^{+\infty} dx\, P(x,t) = \int dx\, |\psi(x,t)|^2 = 2|A|^2 \int_{-\infty}^{+\infty} dx\, (1 + \cos 2kx) < \infty$$

Way out: Wave-packet (w/vector) Representation

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \times \int_{-\infty}^{+\infty} dk\, A(k)\, e^{ikx - i\frac{E(k)}{\hbar}t} \quad \Big] \text{ specific superposition}$$

represents a "free" p.le moving w/ w.vector k, energy $E_k = \frac{\hbar^2 k^2}{2m}$

and prob. density $|A(k)|^2$

Requirement is: $|A(k)|^2$ must be square integrable fcn.

$\int dk\, |A(k)|^2 \rightarrow 1$

Prob. density: $|\psi(x,t)|^2 = \frac{1}{2\pi}\int dk \int dk' \,\bar{A}(k')\, A(k)\, e^{-ik'x+ikx} \times e^{+i\frac{E(k')}{\hbar}t - i\frac{E(k)}{\hbar}t}$

One should have:

$$\int |\psi(x,t)|^2 dx = 1$$

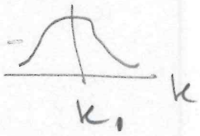
$$\hookrightarrow \quad = \frac{1}{2\pi}\int dk \int dk' \,\bar{A}A\, e^{i\frac{E(k')}{\hbar}t - i\frac{E(k)}{\hbar}t} \underbrace{\int_{-\infty}^{+\infty} dx\, e^{ix(k-k')}}_{2\pi\delta(k-k')}$$

$$= \int dk\, |A(k)|^2$$

Hence: $A(k)$ should be square integrable.

In general $A(k)$ is a sharp-peaked fcn about some k_0

$\Delta k \ll k_0$



Wave-packet: (Momentum) Representation. For a free-ple $p = \hbar k$ (DB)

change variable $k \to p/\hbar$

and $E(k) = \frac{\hbar^2}{2m}k^2 \to p^2/2m \equiv E(p)$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int \frac{dp}{\hbar}\, A(p)\, e^{i\frac{p}{\hbar}x - i\frac{E(p)}{\hbar}t}$$

In general $A(k)$ and $A(p)$ have $\neq$ dimensions, so we need to look for the proper scale-factor "C_p"

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int \frac{dp}{\hbar}\, C_p A(p)\, e^{i\frac{p}{\hbar}x - i\frac{E_p}{\hbar}t}$$

Prob. density: $|\psi(x,t)|^2 = \dots = \frac{|C_p|^2}{2\pi\hbar^2} \int dp \int dp'\, A^*(p') A(p)\, e^{-\frac{i}{\hbar}x(p'-p)} \times e^{-i\frac{t}{\hbar}(E_p - E_{p'})}$

One should have: (1)

$$\int dx\, |\psi(x,t)|^2 = 1$$

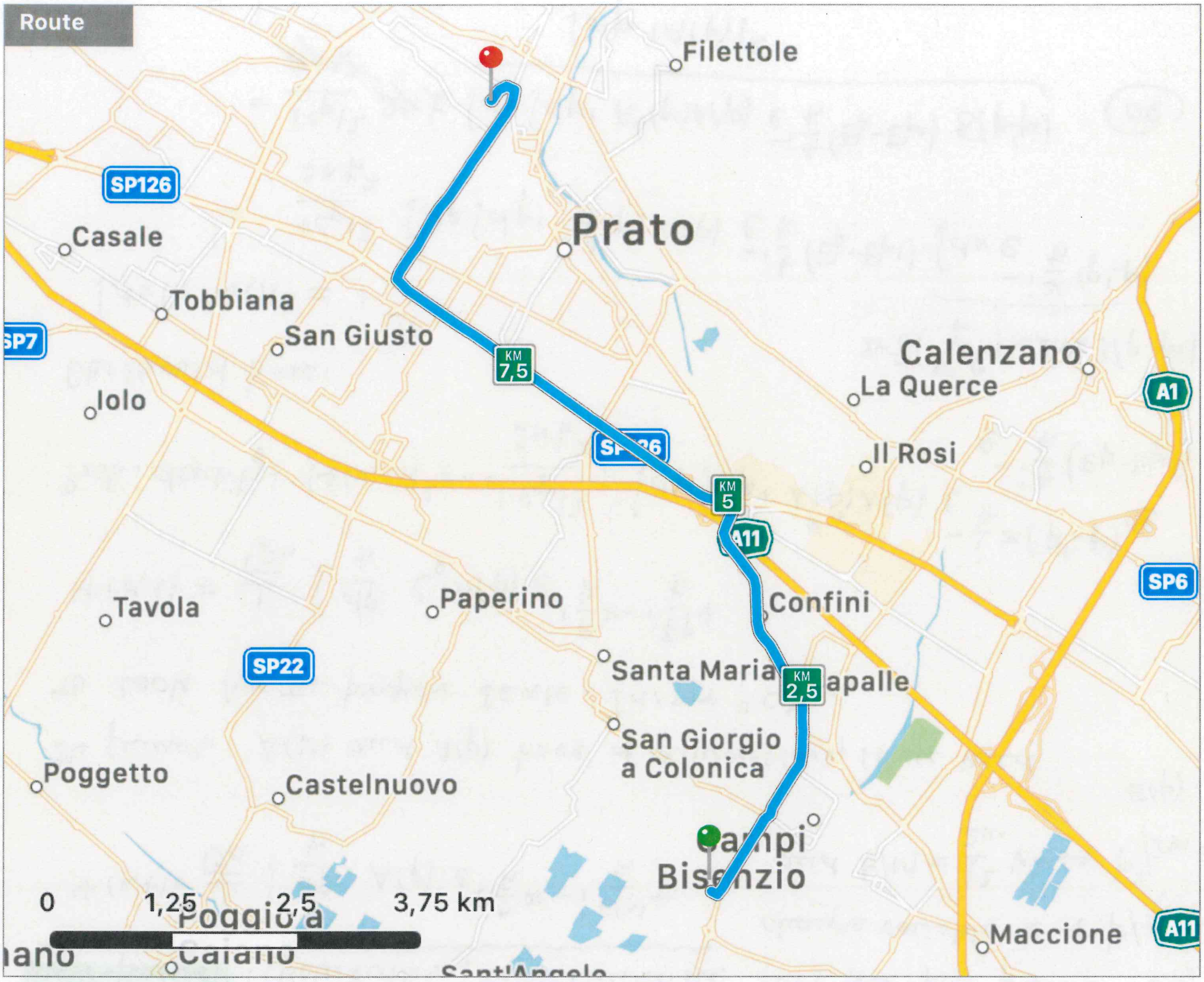
$$\hookrightarrow \quad \frac{|C_p|^2}{2\pi\hbar^2}\int dp \int dp'\, A^*(p')A(p)\, e^{-i\frac{t}{\hbar}(E_p - E_{p'})} \overbrace{\int dx\, e^{-i\frac{x}{\hbar}(p'-p)}}^{2\pi\delta\left(\frac{p'-p}{\hbar}\right) = 2\pi\hbar\,\delta(p-p')}$$

$$= \frac{|C_p|^2}{\cancel{2\pi\hbar^2}}\cancel{2\pi\hbar}\underbrace{\int dp \int dp'\, A^*(p')A(p)\, e^{-i\frac{t}{\hbar}(E_p - E_{p'})}\,\delta(p'-p)}_{\int dp\, |A(p)|^2} \quad \text{OR}$$

$\frac{|C_p|^2}{\hbar}\int dp\, |A_p|^2 = 1$ Thus $\psi(x,t)$ is square integrable (1) iF

Via Vincenzo da Filicaia 81

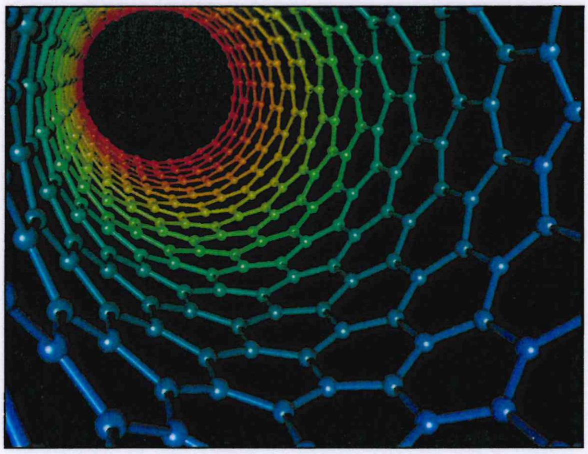
12 km, 25 min



• $C_p = \sqrt{\hbar}$ and • $\int dp\, |A(p)|^2 = 1$

Finally: $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, A(p)\, e^{i\frac{p}{\hbar}x - i\frac{E_p}{\hbar}t}$

is the correct momentum representation of the w/packet provided the momentum prob. density $|A(p)|^2$ be square integrable.



a. Suppose a particle is moving freely inside a very long (carbon) nanotube. If the particle if moving with a given momentum p (eigenvalue), find its quantum state (eigenfunction) by directly solving the corresponding eigenvalue equation for the momentum operator:

$$\hat{p} = -\, i\hbar\, \hat{\nabla}$$

b. Show that these particle states are *orthogonal* (in the Dirac sense)

c. Show that such states are also *complete* with respect to any square integrable function.

d. Apply part c. to a *Gaussian* function of width σ and centred at the origin and one centred at some position $x = a$

a.) $\hat{\vec{p}} = -i\hbar \vec{\nabla} \xrightarrow{1D}$ $\hat{p} = -i\hbar \frac{d}{dx}$

↳ nanotube

eigenvalue

Eigenvalue Eq: $A(\ ) = \lambda (\ ) \xrightarrow[\text{operator}]{}$ $\hat{p} f_p(x) = p\, f_p(x)$

eigenfunction

Solution of $-i\hbar \frac{d}{dx} f_p(x) = p\, f_p(x)$ .... $\frac{df}{f} = i p \hbar^{-1} dx$ or $f_p(x) = A e^{i\frac{p}{\hbar}\cdot x}$

continuous variable

b.) orthogonality: $\int_{-\infty}^{+\infty} dx\, f_p^*(x) f_{p'}(x) = |A|^2 \int_{-}^{+} dx\, e^{i(p'-p)x/\hbar}$ $\quad x/\hbar \equiv x'$

$$= |A|^2 \hbar \underbrace{\int_{-}^{+} dx'\, e^{i(p'-p)x'}}_{2\pi\,\delta(p'-p)} = |A|^2 h\, \delta(p'-p)$$

When we compare this w/ orthogonality condition for cont/ variables (Dirac)

it follows: $h|A|^2 = 1$ or $|A| = 1/\sqrt{h}$ $\quad f_p(x) = \frac{1}{\sqrt{h}} e^{i\frac{p}{\hbar}\cdot x}$

c.) Suppose we can use $\{f_p..\}$ as a basis.

Then $\bar{f}(x) = \int_-^+ dp\, c(p)\, f_p(x)$

- where $c(p)$ are the Fourier (inverse) coeff.

$$e^{-ip'x/\hbar}\,\bar{f}(x) = \int dp\; c(p)\, \frac{1}{\sqrt{h}}\, e^{ipx/\hbar}\, e^{-ip'x/\hbar}$$

$$\int_-^+ dx \quad \downarrow \quad = \frac{1}{\sqrt{\ }} \int dp\, c(p) \underbrace{\int_-^+ dx\, e^{i\frac{x}{\hbar}(p-p')}}_{2\pi\,\delta[(p-p')/\hbar]} = \frac{1}{\sqrt{h}} \cdot 2\pi\hbar \underbrace{\int_-^+ dp\, c(p)\, \delta(p-p')}_{c(p')}$$

or:

$$c(p') = \frac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} dx\, \bar{f}(x)\, e^{-ip'x/\hbar}$$

- where $c(p)$ should satisfy:

$$\int dx\, |\bar{f}(x)|^2 =$$

$$= \int \left[\int dp\, c^*(p)\, f_p^*(x) \int dp'\, c(p')\, f_{p'}(x)\right] dx$$

$$= \int dp \int dp'\, c^*(p)\, c(p') \underbrace{\int dx\, f_p^*(x)\, f_{p'}(x)}_{\delta(p-p')}$$

$$= \int dp\, |c(p)|^2 < \infty$$

If $\bar{f}(x)$ is square-integrable $\Rightarrow$ $c(p)$ should (also) be square-integrable.

d.) $\bar{f}(x) = N\, e^{-(x-a)^2/2\sigma^2}$ (gaussian) (N = norm / a = center / σ = width)

$$c(p) = \frac{1}{\sqrt{h}} \int_-^+ dx\, N\, e^{-(x)^2/2\sigma^2}\, e^{-ipx/\hbar} = \frac{N}{\sqrt{h}} \underbrace{\int_-^+ dx\, e^{-x^2/2\sigma^2}\, e^{-ipx/\hbar}}_{\sigma\sqrt{2\pi}\, e^{-p^2\sigma^2/2}}$$

$$= \frac{N\sigma}{\sqrt{\hbar}}\, e^{-p^2\sigma^2/2} \quad (\text{real}) \quad (a \equiv 0)$$

$$c(p) = \cdots = \frac{N}{\sqrt{h}} \int dx\, e^{-(x-a)^2/2\sigma^2}\, e^{-ipx/\hbar} = \cdots$$

$$= \frac{N\sigma}{\sqrt{\hbar}}\, e^{-p^2\sigma^2/2}\, e^{-ipa} \quad (\text{complex}) \quad (a \neq 0)$$