Coherent and semiclassical states of a free particle

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De Broglie waves

Free particle solutions of the Schrödinger equation with a given momentum and energy:

$$\hat{p}\psi(x,t) = p\psi(x,t), \ \hat{p} = -i\hbar\frac{d}{dx},$$
$$\hat{H}\psi(x,t) = E\psi(x,t), \ \hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2},$$
$$\psi(x,t) = Ne^{\frac{i}{\hbar}(px-Et)}, \ E = \frac{p^2}{2m}.$$

According to Louis de Broglie (1924) these solutions can be treated as plane waves

$$\psi(x,t) = Ne^{i(kx-\omega t)}, \ p = \hbar k, \ E = \hbar\omega, \ \ \omega = \left(\frac{\hbar}{2m}\right)k^2.$$

that are related in a sense to a point like massive particle.

Phase and group velocities

De Broglie waves propagate with the so-called phase velocity v_{ph},

$$\varphi = kx - \omega t = \mathrm{const} \Longrightarrow$$
$$v_{\mathrm{ph}} = \frac{dx}{dt} = \left(\frac{\hbar}{2m}\right) k = \frac{p}{2m} = \frac{v}{2}, \quad v_{\mathrm{part}} = \frac{p}{m},$$

which is twice less than the particle velocity. At present, we know that De Broglie waves do not belong to the Hilbert space $L^2(\mathbb{R})$ and do not represent state vectors of any physical state. Nevertheless, one can construct some superpositions of these functions (wave packets) that are free particle solutions of the SE and belong to the Hilbert space,

$$\psi(x,t) = \int_{-\infty}^{+\infty} A(k)\, \mathrm{e}^{i(kx-\omega t)} dk.$$

We chose $A(k)$ as a nero distributed function near the point $k = k_0, \quad \Delta k \ll k_0$. Then, in fact,

$$\psi(x,t) = \int_{k_0-\Delta k}^{k_0+\Delta k} A(k)\, \mathrm{e}^{i(kx-\omega t)} dk.$$

Phase and group velocities

Calculating the latter integral, we use

$$k = k_0 + \xi, \;\; dk = d\xi, \;\;\; \omega\left(k\right) = \left(\frac{\hbar}{2m}\right) k^2 \simeq \omega_0 + \left(\frac{\partial \omega}{\partial k}\right)_{k_0} \xi,$$

$$\omega_0 = \left(\frac{\hbar}{2m}\right) k_0^2, \;\;\; \left(\frac{\partial \omega}{\partial k}\right)_{k_0} = \frac{\hbar k_0}{m} = \frac{p_0}{m} = v_{\text{part}}.$$

Then

$$\psi\left(x,t\right) = \int_{k_0-\Delta k}^{k_0+\Delta k} A\left(k\right) \mathrm{e}^{i(kx-\omega t)} dk = A\left(k_0\right) e^{i(k_0 x - \omega_0 t)} I\left(x,t\right),$$

$$I(x,t) = \int_{-\Delta k}^{+\Delta k} \mathrm{e}^{i\xi\varphi(x,t)} d\xi = \left.\frac{\mathrm{e}^{i\xi\varphi(x,t)}}{i\varphi(x,t)}\right|_{-\Delta k}^{\Delta k} = 2\frac{\sin \Delta k \varphi}{\varphi}, \;\; \varphi(x,t) = x - \frac{p_0}{m} t.$$

Group speed is defined as

$$\varphi\left(x,t\right) = \text{const} \Longrightarrow v_{\text{gr}} = \frac{\partial x}{\partial t} = \frac{p_0}{m} = v_{\text{part}}$$

and coincides with the particle velocity.

Possible questions

This is a typical content of a section devoted to free particle motion from a standart QM textbook. Everybody is happy, the De Broglie paradox $v_{\mathrm{ph}} = v_{\mathrm{part}}/2$ is solved, wave functions of free particle are normalized wave packets with some distributions $A(k)$.

But how these distributions look like, let say, for semiclassical motion of massive particles in acelerator, for free electrons in metals, and so on? What is a difference between a pure quantum and semiclassical motion of a free particle?.

Maybe coherent states (CS)? Let us recall Glauber CS for a harmonic oscillator.

Glauber CS for a harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}x^2, \quad \hat{H}|n\rangle = \hbar\omega\left(1/2 + n\right)|n\rangle, \; n = 0, 1, 2, \ldots ,$$

$$|z, t\rangle = \exp\left\{-\frac{i}{2}\omega t - \frac{|z|^2}{2}\right\}\sum_{n=0}^{\infty}\frac{\left(ze^{-i\omega t}\right)^n}{\sqrt{n!}}|n\rangle.$$

If $x_0 = \langle x\rangle|_{t=0}$, $p_0 = \langle p\rangle|_{t=0}$, then

$$z = \sqrt{\frac{m\omega}{2\hbar}}\left(x_0 + i\frac{p_0}{m\omega}\right) .$$

and

$$\langle x\rangle = \langle z, t|\hat{x}|z, t\rangle = x_0\cos\omega t + \frac{p_0}{m\omega}\sin\omega t,$$

$$\langle p\rangle = \langle z, t|\hat{p}|z, t\rangle = p_0\cos\omega t - m\omega x_0\sin\omega t,$$

$$\Delta x\Delta p = \frac{\hbar}{2}, \; \Delta x = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2}, \; \Delta p = \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2}.$$

Semiclassical motion $|z|^2 \gg 1$.

CS of a free massive nonrelativistic particle

CS have to form a complete set of functions in the corresponding Hilbert space, they have to minimize uncertainty relations for some physical quantities (e.g. coordinates and momenta) at a fixed time instant and mean values of some physical quantities, calculated with respect to time-dependent CS, have to move along the corresponding classical trajectories. In addition, CS have to be labelled by quantum numbers that have a direct classical analog, let say by phase-space coordinates. It is also desirable for time-dependent CS to maintain their form under the time evolution, such that this evolution affects only their parameters.

$$i\hbar\partial_t \Psi(x,t) = \hat{H}_x \Psi(x,t),\ x \in \mathbb{R},$$

$$\hat{H}_x = -\frac{\hbar^2}{2m}\partial_x^2 = \frac{\hat{p}_x^2}{2m},\ \hat{p}_x = -i\hbar\partial_x .$$

It is useful to introduce the dimensionless variables

$$q = xl^{-1},\quad \tau = \frac{\hbar}{ml^2}t,\quad \psi(q,\tau) = \sqrt{l}\Psi\left(lq, \frac{ml^2}{\hbar}\tau\right),$$

such that $|\Psi(x,t)|^2 dx = |\psi(q,\tau)|^2 dq$. Then the Schrödinger equation takes the form

Integrals of motion linear in basic canonical operators

Let us construct an integral of motion $\hat{A}(\tau)$ linear in $\hat{q}$ and $\hat{p}$,

$$\hat{A}(\tau) = f(\tau)\,\hat{q} + ig(\tau)\,\hat{p} + \varphi(\tau),$$

$\hat{A}(\tau)$ is an integral of motion, if

$$\left[\hat{S}, \hat{A}(\tau)\right] = 0.$$

If the Hamiltonian is s.a., $\hat{A}^{\dagger}(\tau)$ is also an integral of motion, $\left[\hat{S}, \hat{A}^{\dagger}(\tau)\right] = 0$,

$$\begin{aligned} &\dot{f}(\tau) = 0,\ \ \dot{g}(\tau) - if(\tau) = 0, \quad \dot{\varphi}(\tau) = 0 \Longrightarrow \\ &f(\tau) = c_1,\ \ g(\tau) = c_2 + ic_1\tau, \quad \varphi(\tau) = \text{const}. \end{aligned}$$

Without loss of the generality we can set $\varphi(\tau) = 0$.

Annihilation and creation operators - integrals of motion

Thus,

$$\hat{A}(\tau) = c_1 \hat{q} + ig(\tau)\hat{p}, \quad g(\tau) = c_2 + ic_1\tau,$$
$$\left[\hat{A}(\tau), \hat{A}^\dagger(\tau)\right] = 2\,\mathrm{Re}\left(g^*(\tau) f(\tau)\right) = 2\,\mathrm{Re}\left(c_1^* c_2\right) = \delta.$$

One can see that δ is real integral of motion, $\delta = \mathrm{const}$. In what follows we set $\delta = 1$, such that $\hat{A}(\tau)$ and $\hat{A}^\dagger(\tau)$ are annihilation and creation operators,

$$\left.\begin{array}{l} \delta = 2\,\mathrm{Re}\left(c_1^* c_2\right) = 1 \\ c_1 = |c_1|\, e^{i\mu_1}, \quad c_2 = |c_2|\, e^{i\mu_2} \end{array}\right\} \Longrightarrow |c_2|\,|c_1| \cos\left(\mu_2 - \mu_1\right) = 1/2$$

It follows that

$$\hat{q} = g^*(\tau)\hat{A}(\tau) + g(\tau)\hat{A}^\dagger(\tau), \quad g(\tau) = c_2 + ic_1\tau,$$
$$i\hat{p} = c_1^* \hat{A}(\tau) - c_1 \hat{A}^\dagger(\tau).$$

Time-dependent generalized CS

$$\hat{A}(\tau)|z,\tau\rangle = z|z,\tau\rangle\,, \quad \text{if } \Phi_z^{c_{1,2}}(q,\tau) \equiv \langle q|z,\tau\rangle\,,$$
$$[c_1 q + g(\tau)\partial_q]\,\Phi_z^{c_{1,2}}(q,\tau) = z\Phi_z^{c_{1,2}}(q,\tau)\ .$$

Then

$$q(\tau) \equiv \langle z,\tau|\hat{q}|z,\tau\rangle = q_0 + p\tau,\ \ q_0 = c_2^* z + c_2 z^*,$$
$$p(\tau) \equiv \langle z,\tau|\hat{p}|z,\tau\rangle = i(c_1 z^* - c_1^* z) = p,$$
$$z = c_1 q(\tau) + ig(\tau)\,p = c_1 q_0 + ic_2 p.$$

In addition, we impose on the function $\Phi_z^{c_{1,2}}(q,\tau)$ the following conditions:

$$\left(i\partial_\tau - \hat{H}\right)\Phi_z^{c_{1,2}}(q,\tau) = 0,\ \ \int_{-\infty}^{\infty}\left|\Phi_z^{c_{1,2}}(q,\tau)\right|^2 = 1.$$

Then the time-dependent generalized CS read

$$\Phi_z^{c_{1,2}}(q,\tau) = \frac{1}{\sqrt{\sqrt{2\pi} g(\tau)}} \exp\left\{ i\left(pq - \frac{1}{2}p^2\tau \right) - \frac{c_1}{g(\tau)} \frac{[q - q(\tau)]^2}{2} \right\},$$

$$\rho_z^{c_{1,2}}(q,\tau) = \left|\Phi_z^{c_{1,2}}(q,\tau)\right|^2 = \frac{1}{\sqrt{2\pi}|g(\tau)|} \exp\left\{ -\frac{[q - q(\tau)]^2}{2|g(\tau)|^2} \right\}.$$

In fact, we have different complete sets of states parametrized by c_1 and c_2 that satisfy restriction $|c_2||c_1|\cos(\mu_2 - \mu_1) = 1/2$. Each set satisfies completeness rel.:

$$\int\int \langle q|z,\tau\rangle \langle z,\tau|q'\rangle d^2z = \pi\delta(q - q'), \quad d^2z = d\,\mathrm{Re}\,z d\,\mathrm{Im}\,z, \quad \forall\tau,$$

$$\langle z',\tau|z,\tau\rangle = \exp\left(z'^* z - \frac{|z'|^2 + |z|^2}{2} \right), \quad \forall\tau;$$

Standard deviations, uncertainty relations

$$\sigma_q(\tau) = \sqrt{\langle q^2\rangle - \langle q\rangle^2} = |g(\tau)|,$$
$$\sigma_p(\tau) = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = |f(\tau)| = |c_1|,$$
$$\sigma_{qp}(\tau) = \frac{1}{2}\langle(\hat{q} - \langle q\rangle)(\hat{p} - \langle p\rangle) + (\hat{p} - \langle p\rangle)(\hat{q} - \langle q\rangle)\rangle$$
$$= i[1/2 - g(\tau) f^*(\tau)] \Longrightarrow \sigma_q^2(\tau)\sigma_p^2 - \sigma_{qp}^2(\tau) = 1/4.$$

The generalized CS minimize the Robertson-Schrödinger uncertainty relation. The relation $\mu_1 = \mu_2 = \mu$ provides the minimization Heisenberg uncertainty relation at the initial time instant

$$\sigma_q\sigma_p = 1/2, \quad \sigma_q(0) = \sigma_q = |c_2|, \quad \sigma_p(0) = \sigma_p = |c_1|.$$

One can see that the constant μ don't enter the gener. CS. Thus, we set $\mu = 0$ in what follows. Namely, such states we call simply CS of a free particle.

Now the restriction $2\,\mathrm{Re}\left(c_1^* c_2\right) = 1$ takes the form

$$|c_2|\,|c_1| = 1/2 \Longrightarrow c_2^* = c_1^{-1}/2.$$

Then

$$c_2 = |c_2| = \sigma_q,\ \ c_1 = |c_1| = \sigma_p = 1/(2\sigma_q),$$
$$g\left(\tau\right) = \left(\sigma_q + \frac{i\tau}{2\sigma_q}\right),\ \sigma_q\left(\tau\right) = |g\left(\tau\right)| = \sqrt{\sigma_q^2 + \frac{\tau^2}{4\sigma_q^2}}.$$

For any τ the Heisenberg uncertainty relation in the CS takes the form

$$\sigma_q\left(\tau\right)\sigma_p = \frac{1}{2}\sqrt{1 + \frac{\tau^2}{4\sigma_q^4}} \geq \frac{1}{2}$$

CS of a free particle

$$\Phi_z^{\sigma_q}(q,\tau) = \frac{\exp\left\{ i\left(pq - \frac{p^2}{2}\tau\right) - \frac{[q-q(\tau)]^2}{4\left(\sigma_q^2 + i\tau/2\right)} \right\}}{\sqrt{\left(\sigma_q + \frac{i\tau}{2\sigma_q}\right)\sqrt{2\pi}}}.$$

In fact, we have a family of complete sets CS parametrized by one real parameter σ_q. Each set of CS in the family has its specific initial standard deviations $\sigma_q > 0$. CS from a family with a given σ_q are labeled by quantum numbers z,

$$z = \frac{q_0}{2\sigma_q} + i\sigma_q p,$$

which are in one to one correspondence with trajectory initial data q_0 and p,

$$q_0 = 2\sigma_q \operatorname{Re} z \ , \quad p = \frac{\operatorname{Im} z}{\sigma_q} \ .$$

CS of a free particle

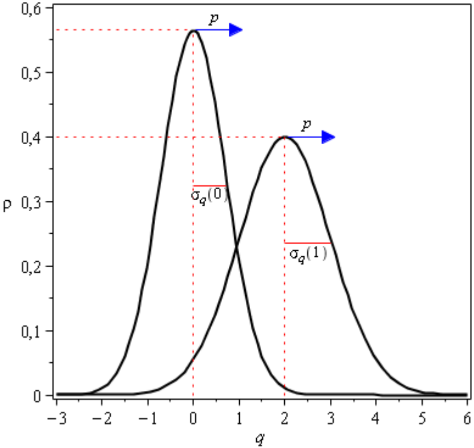
The probability densities that corresponds to the CS are

$$\rho_z^{\sigma_q}(q,\tau) = \frac{1}{\sqrt{\left(\sigma_q^2 + \frac{\tau^2}{4\sigma_q^2}\right)2\pi}} \exp\left\{ -\frac{1}{2}\frac{\left[q - q(\tau)\right]^2}{\sigma_q^2 + \frac{\tau^2}{4\sigma_q^2}} \right\}.$$

One can see that at any time instant τ the probability densities are given by Gaussian distributions with standard deviations $\sigma_q(\tau)$. The mean values $\langle q\rangle = q(\tau) = q_0 + p\tau$ are moving along the classical trajectory with the particle velocity p. With the same velocity are moving the maxima of the probability densities.

The figure below shows plots of function $\rho_z^{\sigma_q}(q,\tau)$ with $\sigma = 2^{-1/2}$, $p = 2$, $q_0 = 0$, for two time instants, $\tau = 0$ and $\tau = 1$.

CS of a free particle



Evolution of the probability density

Semiclassical CS of free particle

$$\Psi(x,t)=\frac{1}{\sqrt{\sqrt{2\pi}\left(\sigma_x+\frac{i\hbar t}{2m\sigma_x}\right)}}\exp\left\{\frac{i}{\hbar}\left(p_x x-\frac{p_x^2}{2m}t\right)-\frac{\left[x-x(t)\right]^2}{4\left(\sigma_x^2+\frac{i\hbar t}{2m}\right)}\right\},$$

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

$$x(t)=x_0+\frac{p_x}{m}t,\quad \sigma_x^2(t)=\sigma_x^2+\frac{\hbar^2t^2}{4m^2\sigma_x^2}$$

Semiclassical motion implies that $\rho(x,t)$ is changing with time slowly. It changes due to the change of $\frac{\hbar^2}{4m^2\sigma_x^2}t^2$. We suppose that in case of semiclassical motion this quantity is much less than the distance square that the particle passes for the same time.

$$\frac{\hbar^2}{4m^2\sigma_x^2}t^2\ll\left(\frac{p_x}{m}t\right)^2\Longrightarrow p_x\gg\frac{\hbar}{2\sigma_x}\sim v\gg\frac{\hbar}{2m\sigma_x}. \tag{1}$$

which can be rewritten in another form

$$\lambda \ll 4\pi\sigma_x, \quad \lambda = \frac{2\pi\hbar}{p_x},$$

where λ is the Compton wavelength of the particle. Thus, CS of a free particle can be considered as semiclassical states if the Compton wavelength of the particle is much less than the coordinate standard deviation σ_x at the initial time moment. It is known that in a cyclotron nonrelativistic electrons are moving with velocities $v \simeq 10^3\,\frac{\mathrm{m}}{\mathrm{s}}$. Then, according to eq. (1), CS of such electrons with $2\sigma_x \simeq 10^{-7}\mathrm{m}$ can be treated as semiclassical states.

Concluding remarks

CS families are parametrized by one real-valued parameter, being the coordinate standard deviation σ_q at the initial time instant.

CS from a family with a given σ_q form a complete system of functions and are labeled by a complex-valued quantum number z, which is in one-to-one correspondence with initial data of the corresponding trajectory.

CS minimize the Robertson–Schrödinger uncertainty relation at all time instants and the Heisenberg uncertainty relations at the initial time instant.

The coordinate standard deviation $\sigma_q(\tau)$ at an arbitrary time instant grows with time the faster the smaller it was at the initial time instant.

At any time instant, the probability density is given by Gaussian distributions with the standard deviations $\sigma_q(\tau)$.

The coordinate mean value propagates along the classical trajectory with the particle mean velocity. The maximum of probability density propagates with the same velocity.

The constructed CS are wave packets being the solutions of the Schrödinger equation for a free particle. They belong to the Hilbert space $L^2(\mathbb{R})$.

CS allow one to provide a natural relation between the classical and quantum descriptions of a free particles.

The end