Quantum Dynamics, NWI-SM295, exercises week 3

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Question 1: Time dependent wave packet for free particle

The time-dependent Schrödinger equation for a free particle of mass μ is in one dimension is

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\Psi(x,t) \tag{1}$$

Solutions exist that can be written as

$$\Psi(x,t) = \exp[-\frac{1}{2}\alpha_t(x-vt)^2 + ikx + c_t] \tag{2}$$

In this expression v and k are constants that satisfy the relation

$$\hbar k = \mu v \equiv p \tag{3}$$

The width of the wave packet is determined by

$$\alpha_t = \frac{\alpha_0\mu}{\mu + i\hbar(t-t_0)\alpha_0}, \tag{4}$$

where α_0 determins the width at $t = t_0$.

1a. Compute the expectation value of the position x

$$\langle x\rangle = \frac{\langle\Psi|x|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{5}$$

Answer:

$$\langle x\rangle = \frac{\int e^{-\frac{1}{2}\alpha_t^*(x-vt)^2-ikx+c_t^*}\, x\, e^{-\frac{1}{2}\alpha_t(x-vt)^2+ikx+c_t}dx}{\int e^{-\frac{1}{2}\alpha_t^*(x-vt)^2-ikx+c_t^*}\, e^{-\frac{1}{2}\alpha_t(x-vt)^2+ikx+c_t}dx} \tag{6}$$

$$= \frac{\int e^{-\frac{1}{2}\alpha_t^*(x-vt)^2}\, x\, e^{-\frac{1}{2}\alpha_t(x-vt)^2}dx}{\int e^{-\frac{1}{2}\alpha_t^*(x-vt)^2}\, e^{-\frac{1}{2}\alpha_t(x-vt)^2}dx}. \tag{7}$$

Now we use the coordinate transformation $y \equiv x - vt$, and since $dy/dx = 1$ we get

$$\langle x\rangle = \frac{\int e^{-\frac{1}{2}\alpha_t^* y^2}\,(y+vt)\, e^{-\frac{1}{2}\alpha_t y^2}dy}{\int e^{-\frac{1}{2}\alpha_t^* y^2}\, e^{-\frac{1}{2}\alpha_t y^2}dy}. \tag{8}$$

$$= \underbrace{\frac{\int e^{-\frac{1}{2}\alpha_t^* y^2}\, y\, e^{-\frac{1}{2}\alpha_t y^2}dy}{\int e^{-\frac{1}{2}\alpha_t^* y^2}\, e^{-\frac{1}{2}\alpha_t y^2}dy}}_{=0 \text{ by symmetry}} + \frac{\int e^{-\frac{1}{2}\alpha_t^* y^2}\, vt\, e^{-\frac{1}{2}\alpha_t y^2}dy}{\int e^{-\frac{1}{2}\alpha_t^* y^2}\, e^{-\frac{1}{2}\alpha_t y^2}dy} \tag{9}$$

$$= vt. \tag{10}$$

1b. Compute the expectation value of the momentm $\hat{p}$

$$\langle\hat{p}\rangle = \langle\frac{\hbar}{i}\frac{\partial}{\partial x}\rangle = \frac{\langle\Psi|\hat{p}|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{11}$$

Answer: *The derivative of $\Psi(x,t)$ is*

$$\frac{\partial}{\partial x}\Psi(x,t) = [-\alpha_t(x-vt) + ik]\Psi(x,t) \tag{12}$$

so

$$\hat{p}\Psi(x,t) = \hbar[i\alpha_t(x-vt) + k]\Psi(x,t) \tag{13}$$

$$\langle\hat{p}\rangle = \frac{\int e^{-\frac{1}{2}\alpha_t^*(x-vt)^2-ikx+c_t^*}\,\hbar[i\alpha_t(x-vt)+k], e^{-\frac{1}{2}\alpha_t(x-vt)^2+ikx+c_t}dx}{\int e^{-\frac{1}{2}\alpha_t^*(x-vt)^2-ikx+c_t^*}\, e^{-\frac{1}{2}\alpha_t(x-vt)^2+ikx+c_t}dx}. \tag{14}$$

As in the previous question, we can split the integral in two terms, and the integral involving $\hbar i\alpha_t(x - vt)$ will be zero by symmetry again, and the second term gives $\langle \hat{p} \rangle = \hbar k$.

Question 2: Flux

In one dimension, the flux j of a wave function $\Psi(x,t)$ is given by

$$j = \frac{\hbar}{\mu}\mathrm{Im}\left[\Psi^* \frac{\partial}{\partial x}\Psi\right], \tag{15}$$

where μ is the mass of the particle. This expression also applies to time-independent wave functions $\Psi(x)$.

2a. Compute the flux of

$$\Psi(x) = ae^{ikx} + be^{-ikx}. \tag{16}$$

Answer: *The flux is*

$$j = \frac{\hbar}{\mu}\mathrm{Im}\left[\left(a^* e^{-ikx} + b^* e^{ikx}\right)\frac{\partial}{\partial x}\left(ae^{ikx} + be^{-ikx}\right)\right] \tag{17}$$

$$= \frac{\hbar}{\mu}\mathrm{Im}\left[\left(a^* e^{-ikx} + b^* e^{ikx}\right)\left(ikae^{ikx} - ikbe^{-ikx}\right)\right] \tag{18}$$

$$= \frac{\hbar}{\mu}\mathrm{Im}\left[ik|a|^2 - ik|b|^2 + ik\left(b^* ae^{2ikx} - a^* be^{-2ikx}\right)\right] \tag{19}$$

The terms $b^* ae^{2ikx}$ and $a^* be^{-2ikx}$ are eachothers complex conjugate, so the difference is purely imaginary, and after multiplication with the factor (ik) it is real, so it does not contribute to the flux, and we find

$$j = \frac{\hbar k}{\mu}\left(|a|^2 - |b|^2\right). \tag{20}$$

In three dimensions, the flux is given by

$$\boldsymbol{j} = \frac{\hbar}{\mu}\mathrm{Im}[\Psi^* \boldsymbol{\nabla}\Psi] \tag{21}$$

2b. Compute the flux of

$$\Psi(\boldsymbol{r}) = Ne^{i\boldsymbol{k}\cdot\boldsymbol{r}}. \tag{22}$$

Answer: *The flux is a vector with three components, and it is parallel to the vector* $\boldsymbol{k}$,

$$\boldsymbol{j} = \frac{\hbar}{\mu}\begin{pmatrix}\mathrm{Im}(\Psi^* \frac{\partial}{\partial x}\Psi) \\ \mathrm{Im}(\Psi^* \frac{\partial}{\partial y}\Psi) \\ \mathrm{Im}(\Psi^* \frac{\partial}{\partial z}\Psi)\end{pmatrix} = |N|^2 \frac{\hbar}{\mu}\boldsymbol{k}, \tag{23}$$

where we used $\frac{\partial}{\partial x}\boldsymbol{k}\cdot\boldsymbol{r} = k_x$, $\frac{\partial}{\partial y}\boldsymbol{k}\cdot\boldsymbol{r} = k_y$, etc.

Question 3: One-dimensional scattering

The Hamiltonian for a particle with mass μ is given by

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x). \tag{24}$$

For the potential $V(x)$ we consider a step function

$$V(x) = \begin{cases} 0, & \text{for } x < 0 \\ V_1, & \text{for } x > 0. \end{cases} \tag{25}$$

The corresponding time-independent Schrödinger equation is

$$(\hat{H} - E)\Psi(x) = 0. \tag{26}$$

For $x < 0$ the solution can be written as the sum of an incoming wave and a reflected wave

$$\Psi_L(x) = e^{ik_0 x} + e^{-ik_0 x} R(E). \tag{27}$$

For $x > 0$ there is a transmitted wave

$$\Psi_R(x) = e^{ik_1 x} T(E). \tag{28}$$

3a. Find the energy dependent reflection coefficients $R(E)$ and $T(E)$.

Answer: *At $x = 0$ the wave function and its derivative should be continuous, so we have two equations*

$$\Psi_L(0) = \Psi_R(0), \tag{29}$$
$$\Psi'_L(0) = \Psi'_R(0). \tag{30}$$

That is

$$1 + R(E) = T(E), \tag{31}$$
$$ik_0 - ik_0 R(E) = ik_1 T(E) \tag{32}$$

Substituting the first of these into the second to get an equation for $R(E)$,

$$k_0 - k_0 R(E) = k_1[1 + R(E)] \tag{33}$$

so

$$k_0 - k_1 = (k_0 + k_1)R(E) \tag{34}$$

and

$$R(E) = \frac{k_0 - k_1}{k_0 + k_1} \tag{35}$$
$$T(E) = 1 + \frac{k_0 - k_1}{k_0 + k_1} = \frac{2k_0}{k_0 + k_1}. \tag{36}$$

Note that if $k_1 = k_0$, we have $R(E) = 0$ and $T(E) = 1$, i.e., nothing is reflected, as you would expect. If $k_1 \gg k_0$ we get $R(E) = -1$ and $T(E) = 0$, i.e., full reflection. When $k_1 \ll k_0$, we have $R(E) = 1$, i.e., full reflection, but still still $T(E) = 2$. This may be surprising, but note that the transmitted flux is proportional to k_1, so even though the transmission coefficient does not go to zero, the transmitted flux will go to zero.