Problems & Solutions in Quantum Mechanics

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PROBLEMS AND SOLUTIONS IN QUANTUM MECHANICS

This collection of solved problems corresponds to the standard topics covered in established undergraduate and graduate courses in quantum mechanics. Completely up-to-date problems are also included on topics of current interest that are absent from the existing literature.

Solutions are presented in considerable detail, to enable students to follow each step. The emphasis is on stressing the principles and methods used, allowing students to master new ways of thinking and problem-solving techniques. The problems themselves are longer than those usually encountered in textbooks and consist of a number of questions based around a central theme, highlighting properties and concepts of interest.

For undergraduate and graduate students, as well as those involved in teaching quantum mechanics, the book can be used as a supplementary text or as an independent self-study tool.

Kyriakos Tamvakis studied at the University of Athens and gained his Ph.D. at Brown University, Providence, Rhode Island, USA in 1978. Since then he has held several positions at CERN's Theory Division in Geneva, Switzerland. He has been Professor of Theoretical Physics at the University of Ioannina, Greece, since 1982.

Professor Tamvakis has published 90 articles on theoretical high-energy physics in various journals and has written two textbooks in Greek, on quantum mechanics and on classical electrodynamics. This book is based on more than 20 years' experience of teaching the subject.

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Preface

This collection of quantum mechanics problems has grown out of many years of teaching the subject to undergraduate and graduate students. It is addressed to both student and teacher and is intended to be used as an auxiliary tool in class or in self-study. The emphasis is on stressing the principles, physical concepts and methods rather than supplying information for immediate use. The problems have been designed primarily for their educational value but they are also used to point out certain properties and concepts worthy of interest; an additional aim is to condition the student to the atmosphere of change that will be encountered in the course of a career. They are usually long and consist of a number of related questions around a central theme. Solutions are presented in sufficient detail to enable the reader to follow every step. The degree of difficulty presented by the problems varies. This approach requires an investment of time, effort and concentration by the student and aims at making him or her fit to deal with analogous problems in different situations. Although problems and exercises are without exception useful, a collection of solved problems can be truly advantageous to the prospective student only if it is treated as a learning tool towards mastering ways of thinking and techniques to be used in addressing new problems rather than a solutions manual. The problems cover most of the subjects that are traditionally covered in undergraduate and graduate courses. In addition to this, the collection includes a number of problems corresponding to recent developments as well as topics that are normally encountered at a more advanced level.

1

Wave functions

Problem 1.1 Consider a particle and two normalized energy eigenfunctions $\psi_1(\mathbf{x})$ and $\psi_2(\mathbf{x})$ corresponding to the eigenvalues $E_1 \neq E_2$. Assume that the eigenfunctions vanish outside the two non-overlapping regions Ω_1 and Ω_2 respectively.

(a) Show that, if the particle is initially in region Ω_1 then it will stay there forever.
(b) If, initially, the particle is in the state with wave function

$$\psi(\mathbf{x}, 0) = \frac{1}{\sqrt{2}}\left[\psi_1(\mathbf{x}) + \psi_2(\mathbf{x})\right]$$

show that the probability density $|\psi(\mathbf{x}, t)|^2$ is independent of time.
(c) Now assume that the two regions Ω_1 and Ω_2 overlap partially. Starting with the initial wave function of case (b), show that the probability density is a periodic function of time.
(d) Starting with the same initial wave function and assuming that the two eigenfunctions are real and isotropic, take the two partially overlapping regions Ω_1 and Ω_2 to be two concentric spheres of radii $R_1 > R_2$. Compute the probability current that flows through Ω_1.

Solution

(a) Clearly $\psi(\mathbf{x}, t) = e^{-iEt/\hbar}\psi_1(\mathbf{x})$ implies that $|\psi(\mathbf{x}, t)|^2 = |\psi_1(\mathbf{x})|^2$, which vanishes outside Ω_1 at all times.

(b) If the two regions do not overlap, we have

$$\psi_1(\mathbf{x})\psi_2^*(\mathbf{x}) = 0$$

everywhere and, therefore,

$$|\psi(\mathbf{x}, t)|^2 = \tfrac{1}{2}\left[|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2\right]$$

which is time independent.

(c) If the two regions overlap, the probability density will be

$$|\psi(\mathbf{x},t)|^2 = \tfrac{1}{2}\left[|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2\right] + |\psi_1(\mathbf{x})|\,|\psi_2(\mathbf{x})|\cos[\phi_1(\mathbf{x}) - \phi_2(\mathbf{x}) - \omega t]$$

where we have set $\psi_{1,2} = |\psi_{1,2}|e^{i\phi_{1,2}}$ and $E_1 - E_2 = \hbar\omega$. This is clearly a periodic function of time with period $T = 2\pi/\omega$.

(d) The current density is easily computed to be

$$\mathcal{J} = \hat{\mathbf{r}}\frac{\hbar}{2m}\sin\omega t\left[\psi_2'(r)\psi_1(r) - \psi_1'(r)\psi_2(r)\right]$$

and vanishes at R_1, since one or the other eigenfunction vanishes at that point. This can be seen through the continuity equation in the following alternative way:

$$I_{\Omega_1} = -\frac{d}{dt}\mathcal{P}_{\Omega_1} = \int_{S(\Omega_1)} d\mathbf{S}\cdot\mathcal{J} = \int_{\Omega_1} d^3x\,\nabla\cdot\mathcal{J} = -\int_{\Omega_1} d^3x\,\frac{\partial}{\partial t}|\psi(\mathbf{x},t)|^2$$
$$= \omega\sin\omega t\int_{\Omega_1} d^3x\;\psi_1(r)\psi_2(r)$$

The last integral vanishes because of the orthogonality of the eigenfunctions.

Problem 1.2 Consider the one-dimensional normalized wave functions $\psi_0(x)$, $\psi_1(x)$ with the properties

$$\psi_0(-x) = \psi_0(x) = \psi_0^*(x), \qquad \psi_1(x) = N\frac{d\psi_0}{dx}$$

Consider also the linear combination

$$\psi(x) = c_1\psi_0(x) + c_2\psi_1(x)$$

with $|c_1|^2 + |c_2|^2 = 1$. The constants $N,\ c_1,\ c_2$ are considered as known.

(a) Show that ψ_0 and ψ_1 are orthogonal and that $\psi(x)$ is normalized.
(b) Compute the expectation values of x and p in the states ψ_0, ψ_1 and ψ.
(c) Compute the expectation value of the kinetic energy T in the state ψ_0 and demonstrate that

$$\langle\psi_0|T^2|\psi_0\rangle = \langle\psi_0|T|\psi_0\rangle\langle\psi_1|T|\psi_1\rangle$$

and that

$$\langle\psi_1|T|\psi_1\rangle \geq \langle\psi|T|\psi\rangle \geq \langle\psi_0|T|\psi_0\rangle$$

(d) Show that

$$\langle\psi_0|x^2|\psi_0\rangle\langle\psi_1|p^2|\psi_1\rangle \geq \frac{\hbar^2}{4}$$

(e) Calculate the matrix element of the commutator $[x^2,\ p^2]$ in the state ψ.

Solution

(a) We have

$$\langle\psi_0|\psi_1\rangle = N\int dx\,\psi_0^*\frac{d\psi_0}{dx} = N\int dx\,\psi_0\frac{d\psi_0}{dx}$$
$$= \frac{N}{2}\int dx\,\frac{d\psi_0^2}{dx} = \frac{N}{2}\left\{\psi_0^2(x)\right\}_{-\infty}^{+\infty} = 0$$

The normalization of $\psi(x)$ follows immediately from this and from the fact that $|c_1|^2 + |c_2|^2 = 1$.

(b) On the one hand the expectation value $\langle\psi_0|x|\psi_0\rangle$ vanishes because the integrand $x\psi_0^2(x)$ is odd. On the other hand, the momentum expectation value in this state is

$$\langle\psi_0|p|\psi_0\rangle = -i\hbar\int dx\,\psi_0(x)\psi_0'(x)$$
$$= -\frac{i\hbar}{N}\int dx\,\psi_0(x)\psi_1(x) = -\frac{i\hbar}{N}\langle\psi_0|\psi_1\rangle = 0$$

as we proved in the solution to (a). Similarly, owing to the oddness of the integrand $x\psi_1^2(x)$, the expectation value $\langle\psi_1|x|\psi_1\rangle$ vanishes. The momentum expectation value is

$$\langle\psi_1|p|\psi_1\rangle = -i\hbar\int dx\,\psi_1^*\psi_1' = -i\hbar\frac{N}{N^*}\int dx\,\psi_1\psi_1'$$
$$= -i\hbar\frac{N}{2N^*}\int dx\,\frac{d\psi_1^2}{dx} = -i\hbar\frac{N}{2N^*}\left\{\psi_1^2\right\}_{-\infty}^{+\infty} = 0$$

(c) The expectation value of the kinetic energy squared in the state ψ_0 is

$$\langle\psi_0|T^2|\psi_0\rangle = \frac{\hbar^4}{4m^2}\int dx\,\psi_0\psi_0'''' = -\frac{\hbar^4}{4m^2}\int dx\,\psi_0'\psi_0'''$$
$$= \frac{\hbar^2}{2m|N|^2}\langle\psi_1|T|\psi_1\rangle$$

Note however that

$$\langle\psi_0|T|\psi_0\rangle = -\frac{\hbar^2}{2m}\int dx\,\psi_0\psi_0'' = \frac{\hbar^2}{2m}\int dx\,\psi_0'\psi_0'$$
$$= \frac{\hbar^2}{2m|N|^2}\langle\psi_1|\psi_1\rangle = \frac{\hbar^2}{2m|N|^2}$$

Therefore, we have

$$\langle\psi_0|T^2|\psi_0\rangle = \langle\psi_0|T|\psi_0\rangle\langle\psi_1|T|\psi_1\rangle$$

Consider now the *Schwartz inequality*

$$|\langle\psi_0|\psi_2\rangle|^2 \leq \langle\psi_0|\psi_0\rangle\,\langle\psi_2|\psi_2\rangle = \langle\psi_2|\psi_2\rangle$$

where, by definition,

$$\psi_2(x) \equiv -\frac{\hbar^2}{2m}\psi_0''(x)$$

The right-hand side can be written as

$$\langle\psi_2|\psi_2\rangle = \langle\psi_0|T^2|\psi_0\rangle = \langle\psi_0|T|\psi_0\rangle\,\langle\psi_1|T|\psi_1\rangle$$

Thus, the above Schwartz inequality reduces to

$$\langle\psi_0|T|\psi_0\rangle \leq \langle\psi_1|T|\psi_1\rangle$$

In order to prove the desired inequality let us consider the expectation value of the kinetic energy in the state ψ. It is

$$\langle\psi|T|\psi\rangle = |c_1|^2\langle\psi_0|T|\psi_0\rangle + |c_2|^2\langle\psi_1|T|\psi_1\rangle$$

The off-diagonal terms have vanished due to oddness. The right-hand side of this expression, owing to the inequality proved above, will obviously be smaller than

$$|c_1|^2\langle\psi_1|T|\psi_1\rangle + |c_2|^2\langle\psi_1|T|\psi_1\rangle = \langle\psi_1|T|\psi_1\rangle$$

Analogously, the same right-hand side will be larger than

$$|c_1|^2\langle\psi_0|T|\psi_0\rangle + |c_2|^2\langle\psi_0|T|\psi_0\rangle = \langle\psi_0|T|\psi_0\rangle$$

Thus, finally, we end up with the double inequality

$$\langle\psi_0|T|\psi_0\rangle \leq \langle\psi|T|\psi\rangle \leq \langle\psi_0|T|\psi_0\rangle$$

(d) Since the expectation values of position and momentum vanish in the states ψ_0 and ψ_1, the corresponding uncertainties will be just the expectation values of the squared operators, namely

$$(\Delta x)_0^2 = \langle\psi_0|x^2|\psi_0\rangle, \qquad (\Delta p)_0^2 = \langle\psi_0|p^2|\psi_0\rangle, \qquad (\Delta p)_1^2 = \langle\psi_1|p^2|\psi_1\rangle$$

We now have

$$\langle\psi_0|x^2|\psi_0\rangle\,\langle\psi_1|p^2|\psi_1\rangle \geq \langle\psi_0|x^2|\psi_0\rangle\,\langle\psi_0|p^2|\psi_0\rangle = (\Delta x)_0^2(\Delta p)_0^2 \geq \frac{\hbar^2}{4}$$

as required.

(e) Finally, it is straightforward to calculate the matrix element value of the commutator $[x^2,\ p^2]$ in the state ψ. It is

$$\langle\psi|[x^2,\ p^2]|\psi\rangle = 2i\hbar\langle\psi|(xp + px)|\psi\rangle = 2i\hbar\left(\langle\psi|xp|\psi\rangle + \langle\psi|xp|\psi\rangle^*\right)$$

which, apart from an imaginary coefficient, is just the real part of the term

$$\begin{aligned}\langle\psi|xp|\psi\rangle &= -i\hbar\int dx\ \psi^* x\psi' \\ &= |c_1|^2\int dx\ \psi_0 x\psi_0' - i\hbar|c_2|^2\int dx\ \psi_1^* x\psi_1'\end{aligned}$$

where the mixed terms have vanished because the operator has odd parity. Note however that this is a purely imaginary number. Thus, its real part will vanish and so

$$\langle\psi|[x^2,\ p^2]|\psi\rangle = 0$$

Problem 1.3 Consider a system with a *real* Hamiltonian that occupies a state having a real wave function both at time $t = 0$ and at a later time $t = t_1$. Thus, we have

$$\psi^*(x, 0) = \psi(x, 0), \qquad \psi^*(x, t_1) = \psi(x, t_1)$$

Show that the system is *periodic*, namely, that there exists a time T for which

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

In addition, show that for such a system the eigenvalues of the energy have to be integer multiples of $2\pi\hbar/T$.

Solution

If we consider the complex conjugate of the evolution equation of the wave function for time t_1, we get

$$\psi(x, t_1) = e^{-it_1 H/\hbar}\psi(x, 0) \qquad \Longrightarrow \qquad \psi(x, t_1) = e^{it_1 H/\hbar}\psi(x, 0)$$

The inverse evolution equation reads

$$\psi(x, 0) = e^{it_1 H/\hbar}\psi(x, t_1) = e^{2it_1 H/\hbar}\psi(x, 0)$$

Also, owing to reality,

$$\psi(x, 0) = e^{-2it_1 H/\hbar}\psi(x, 0)$$

Thus, for any time t we can write

$$\psi(x, t) = e^{-itH/\hbar}\psi(x, 0) = e^{-itH/\hbar}e^{-2it_1 H/\hbar}\psi(x, 0) = \psi(x, t + 2t_1)$$

It is, therefore, clear that the system is periodic with period $T = 2t_1$.

Expanding the wave function in energy eigenstates, we obtain

$$\psi(x,t) = \sum_n C_n e^{-iE_n t/\hbar}\psi_n(x)$$

The periodicity of the system immediately implies that the exponentials $\exp(-iTE_n/\hbar)$ must be equal to unity. This is only possible if the eigenvalues E_n are integer multiples of $2\pi\hbar/T$.

Problem 1.4 Consider the following superposition of plane waves:

$$\psi_{k,\delta k}(x) \equiv \frac{1}{2\sqrt{\pi\,\delta k}}\int_{k-\delta k}^{k+\delta k} dq\, e^{iqx}$$

where the parameter δk is assumed to take values much smaller than the wave number k, i.e.

$$\delta k \ll k$$

(a) Prove that the wave functions $\psi_{k,\delta k}(x)$ are normalized and orthogonal to each other.
(b) For a free particle compute the expectation value of the momentum and the energy in such a state.

Solution

(a) The proof of normalization goes as follows:

$$\begin{aligned}
\int_{-\infty}^{+\infty} dx\, |\psi_{k,\delta k}(x)|^2 &= \frac{1}{4\pi\,\delta k}\int_{-\infty}^{+\infty} dx \int_{k-\delta k}^{k+\delta k} dq' \int_{k-\delta k}^{k+\delta k} dq''\, e^{i(q'-q'')x} \\
&= \frac{1}{2\delta k}\int_{k-\delta k}^{k+\delta k} dq' \int_{k-\delta k}^{k+\delta k} dq''\, \delta(q'-q'') \\
&= \frac{1}{2\delta k}\int_{k-\delta k}^{k+\delta k} dq'\, \Theta(k+\delta k-q')\Theta(q'-k+\delta k) \\
&= \frac{1}{2\delta k}\int_{k-\delta k}^{k+\delta k} dq' = 1
\end{aligned}$$

The proof of orthogonality proceeds similarly ($|k-k'| > \delta k + \delta k'$):

$$\begin{aligned}
\int_{-\infty}^{+\infty} dx\, \psi^*_{k,\delta k}(x)\psi_{k',\delta k'}(x) &= \frac{1}{2\sqrt{\delta k \delta k'}}\int_{k-\delta k}^{k+\delta k} dq' \int_{k'-\delta k'}^{k'+\delta k'} dq''\, \delta(q'-q'') \\
&= \frac{1}{2\sqrt{\delta k \delta k'}}\int_{k-\delta k}^{k+\delta k} dq' \Theta(k'+\delta k'-q')\Theta(q'-k'+\delta k')=0
\end{aligned}$$

since there is no overlap between the range over which the theta functions are defined and the range of integration.

(b) Proceeding in a straightforward fashion, we have

$$\begin{aligned}\langle p\rangle &= \frac{1}{4\pi\delta k}\int_{-\infty}^{+\infty} dx\int_{k-\delta k}^{k+\delta k} dq'\int_{k-\delta k}^{k+\delta k} dq''\, e^{-iq'x}\,(-i\hbar\partial_x)e^{iq''x}\\ &= \frac{1}{2\delta k}\int_{k-\delta k}^{k+\delta k} dq'\int_{k-\delta k}^{k+\delta k} dq''\,\hbar q''\delta(q'-q'')\\ &= \frac{1}{2\delta k}\int_{k-\delta k}^{k+\delta k} dq'\,\hbar q' = \frac{\hbar}{4\delta k}[(k+\delta k)^2-(k-\delta k)^2] = \hbar k + O(\delta k)\end{aligned}$$

Similarly, we obtain

$$\left\langle \frac{p^2}{2m}\right\rangle = \frac{\hbar^2 k^2}{2m} + O(\delta k)$$

Problem 1.5 Consider a state characterized by a real wave function up to a multiplicative constant. For simplicity consider motion in one dimension. Convince yourself that such a wave function should correspond to a bound state by considering the probability current density. Show that this bound state is characterized by vanishing momentum, i.e. $\langle p\rangle_\psi = 0$. Consider now the state that results from the multiplication of the above wave function by an exponential factor, i.e. $\chi(x) = e^{ip_0x/\hbar}\psi(x)$. Show that this state has momentum p_0. Study all the above in the momentum representation. Show that the corresponding momentum wave function $\tilde{\chi}(p)$ is translated in momentum, i.e. $\tilde{\chi}(p) = \tilde{\psi}(p-p_0)$.

Solution

The probability current density of such a wave function vanishes:

$$\mathcal{J} = \frac{\hbar}{2mi}[\psi^*\psi' - \psi(\psi^*)'] = 0$$

The vanishing of the probability current agrees with the interpretation of such a state as bound.

The momentum expectation value of such a state is

$$\begin{aligned}\langle\psi|p|\psi\rangle &= -i\hbar\int_{-\infty}^{+\infty} dx\,\psi(x)\psi'(x)\\ &= -\frac{i\hbar}{2}\int_{-\infty}^{+\infty} dx\,\frac{d}{dx}\psi^2(x) = -\frac{i\hbar}{2}[\psi^2(x)]_{\pm\infty} = 0\end{aligned}$$

The wave function $\chi(x) = e^{ip_0x/\hbar}\psi(x)$, however, has momentum

$$\begin{aligned}\langle\chi|p|\chi\rangle &= -i\hbar\int_{-\infty}^{+\infty} dx\, e^{-ip_0x/\hbar}\psi(x)\left[e^{ip_0x/\hbar}\psi(x)\right]'\\ &= -i\hbar\int_{-\infty}^{+\infty} dx\,\psi(x)\left[\frac{i}{\hbar}p_0\psi(x)+\psi'(x)\right] = \langle p\rangle_\psi + p_0 = p_0\end{aligned}$$

The wave function has been assumed to be normalized.

The momentum wave function is

$$\tilde{\chi}(p) = \int \frac{dx}{\sqrt{2\pi\hbar}}\, e^{-ipx/\hbar}\, \chi(x) = \int \frac{dx}{\sqrt{2\pi\hbar}}\, e^{i(p-p_0)x/\hbar}\, \psi(x) = \tilde{\psi}(p - p_0)$$

Problem 1.6 The *propagator* of a particle is defined as

$$\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) \equiv \langle \mathbf{x}| e^{-i(t-t_0)H/\hbar} |\mathbf{x}'\rangle$$

and corresponds to the probability amplitude for finding the particle at $\mathbf{x}$ at time t if initially (at time t_0) it is at $\mathbf{x}'$.

(a) Show that, when the system (i.e. the Hamiltonian) is invariant in space translations[1] $\mathbf{x} \to \mathbf{x} + \boldsymbol{\alpha}$, as for example in the case of a free particle, the propagator has the property

$$\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) = \mathcal{K}(\mathbf{x} - \mathbf{x}'; t - t_0)$$

(b) Show that when the energy eigenfunctions are real, i.e. $\psi_E(\mathbf{x}) = \psi_E^*(\mathbf{x})$, as for example in the case of the harmonic oscillator, the propagator has the property

$$\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) = \mathcal{K}(\mathbf{x}', \mathbf{x}; t - t_0)$$

(c) Show that when the energy eigenfunctions are also parity eigenfunctions, i.e. odd or even functions of the space coordinates, the propagator has the property

$$\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) = \mathcal{K}(-\mathbf{x}, -\mathbf{x}'; t - t_0)$$

(d) Finally, show that we always have the property

$$\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) = \mathcal{K}^*(\mathbf{x}', \mathbf{x}; -t + t_0)$$

Solution

(a) Space translations are expressed through the action of an operator as follows:

$$\langle \mathbf{x}| e^{i\boldsymbol{\alpha}\cdot\mathbf{p}/\hbar} = \langle \mathbf{x} + \boldsymbol{\alpha}|$$

Space-translation invariance holds if

$$[\mathbf{p},\ H] = 0 \qquad \Longrightarrow \qquad e^{i\boldsymbol{\alpha}\cdot\mathbf{p}/\hbar} H e^{-i\boldsymbol{\alpha}\cdot\mathbf{p}/\hbar} = H$$

which also implies that

$$e^{i\boldsymbol{\alpha}\cdot\mathbf{p}/\hbar} e^{-i(t-t_0)H/\hbar} e^{-i\boldsymbol{\alpha}\cdot\mathbf{p}/\hbar} = e^{-i(t-t_0)H/\hbar}$$

Thus we have

$$\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) = \langle \mathbf{x} + \boldsymbol{\alpha}| e^{-i(t-t_0)H/\hbar} |\mathbf{x}' + \boldsymbol{\alpha}\rangle = \mathcal{K}(\mathbf{x} + \boldsymbol{\alpha}, \mathbf{x}' + \boldsymbol{\alpha}; t - t_0)$$

[1] The operator that can effect a space translation on a state is $e^{-i\mathbf{p}\cdot\boldsymbol{\alpha}/\hbar}$, since it acts on any function of $\mathbf{x}$ as the Taylor expansion operator:

$$\langle \mathbf{x}| e^{-i\mathbf{p}\cdot\boldsymbol{\alpha}/\hbar} = e^{\boldsymbol{\alpha}\cdot\nabla} \langle \mathbf{x}| = \sum_{n=0}^{\infty} \frac{1}{n!} (\boldsymbol{\alpha}\cdot\nabla)^n \langle \mathbf{x}| = \langle \mathbf{x} + \boldsymbol{\alpha}|$$

which clearly implies that the propagator can only be a function of the difference $\mathbf{x} - \mathbf{x}'$.

(b) Inserting a complete set of energy eigenstates, we obtain the propagator in the form

$$\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) = \sum_E \psi_E(\mathbf{x}) e^{-i(t-t_0)E/\hbar} \psi_E^*(\mathbf{x}')$$

Reality of the energy eigenfunctions immediately implies the desired property.

(c) Clearly

$$\begin{aligned}\mathcal{K}(-\mathbf{x}, -\mathbf{x}'; t - t_0) &= \sum_E \psi_E(-\mathbf{x}) e^{-i(t-t_0)E/\hbar} \psi_E^*(-\mathbf{x}') \\ &= \sum_E (\pm)^2 \psi_E(\mathbf{x}) e^{-i(t-t_0)E/\hbar} \psi_E^*(\mathbf{x}') = \mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0)\end{aligned}$$

(d) In the same way,

$$\begin{aligned}\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) &= \sum_E \psi_E(\mathbf{x}) e^{-i(t-t_0)E/\hbar} \psi_E^*(\mathbf{x}') \\ &= \left[\sum_E \psi_E^*(\mathbf{x}) e^{-i(t_0-t)E/\hbar} \psi_E(\mathbf{x}') \right]^* = \mathcal{K}^*(\mathbf{x}', \mathbf{x}; t_0 - t)\end{aligned}$$

Problem 1.7 Calculate the propagator of a free particle that moves in three dimensions. Show that it is proportional to the exponential of the *classical action* $\mathcal{S} \equiv \int dt\, L$, defined as the integral of the Lagrangian for a free classical particle starting from the point $\mathbf{x}$ at time t_0 and ending at the point $\mathbf{x}'$ at time t. For a free particle the Lagrangian coincides with the kinetic energy. Verify also that in the limit $t \to t_0$ we have

$$\mathcal{K}_0(\mathbf{x} - \mathbf{x}';\, 0) = \delta(\mathbf{x} - \mathbf{x}')$$

Solution

Inserting the plane-wave energy eigenfunctions of the free particle into the general expression, we get

$$\begin{aligned}\mathcal{K}_0(\mathbf{x}', \mathbf{x};\, t - t_0) &= \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} \exp\left[-i \frac{p^2}{2m\hbar}(t - t_0) \right] e^{-i\mathbf{p}\cdot\mathbf{x}'/\hbar} \\ &= \prod_{i=x,y,z} \int \frac{dp_i}{2\pi} \exp\left[-\frac{i}{\hbar}(x_i - x_i')p_i - \frac{ip_i^2}{2m\hbar}(t - t_0) \right] \\ &= \left[\frac{m\hbar}{2\pi i(t - t_0)} \right]^{3/2} \exp\left[i \frac{m(\mathbf{x} - \mathbf{x}')^2}{2\hbar(t - t_0)} \right]\end{aligned}$$

The exponent is obviously equal to $i/\hbar$ times the classical action

$$\mathcal{S} = \int_{t_0}^{t} dt\, \frac{mv^2}{2} = (t - t_0)\frac{m}{2}\left(\frac{\mathbf{x} - \mathbf{x}'}{t - t_0}\right)^2 = \frac{m(\mathbf{x} - \mathbf{x}')^2}{2(t - t_0)}$$

In order to consider the limit $t \to t_0$, it is helpful to insert a small imaginary part into the time variable, according to

$$t \to t - i\epsilon$$

Then, we can safely take $t = t_0$ and consider the limit $\epsilon \to 0$. We get

$$\mathcal{K}_0(\mathbf{x} - \mathbf{x}', 0) = \lim_{\epsilon \to 0}\left\{\left(\frac{m\hbar}{2\pi\epsilon}\right)^{3/2} \exp\left[-\frac{m(\mathbf{x} - \mathbf{x}')^2}{2\hbar\epsilon}\right]\right\} = \delta(\mathbf{x} - \mathbf{x}')$$

For the last step we needed the delta function representation

$$\delta(x) = \lim_{\epsilon \to 0}\left[(\epsilon\pi)^{-1/2} e^{-x^2/\epsilon}\right]$$

Problem 1.8 A particle starts at time t_0 with the initial wave function $\psi_{\rm i}(x) = \psi(x, t_0)$. At a later time $t \geq t_0$ its state is represented by the wave function $\psi_{\rm f}(x) = \psi(x, t)$. The two wave functions are related in terms of the propagator as follows:

$$\psi_{\rm f}(x) = \int dx'\, \mathcal{K}(x, x'; t - t_0)\psi_{\rm i}(x')$$

(a) Prove that

$$\psi_{\rm i}^*(x) = \int dx'\, \mathcal{K}(x', x; t - t_0)\psi_{\rm f}^*(x')$$

(b) Consider the case of a free particle initially in the plane-wave state

$$\psi_{\rm i}(x) = (2\pi)^{-1/2} \exp\left(ikx - i\frac{\hbar k^2}{2m}t_0\right)$$

and, using the known expression for the free propagator,[2] verify the integral expressions explicitly. Comment on the reversibility of the motion.

Solution

(a) We can always write down the inverse evolution equation

$$\psi(x, t_0) = \int dx'\, \mathcal{K}(x, x'; t_0 - t)\psi(x', t)$$

or

$$\psi_{\rm i}(x) = \int dx'\, \mathcal{K}(x, x'; t_0 - t)\psi_{\rm f}(x')$$

[2] The expresssion is

$$\mathcal{K}_0(x, x'; t - t_0) = \sqrt{\frac{m\hbar}{2\pi i(t - t_0)}}\, \exp\left[i\frac{m(x - x')^2}{2\hbar(t - t_0)}\right]$$

Taking the complex conjugate and using relation (d) of problem 1.6, we get

$$\psi_i^*(x) = \int dx' \mathcal{K}^*(x, x'; t_0 - t)\psi_f^*(x') = \int dx' \, \mathcal{K}(x', x; t - t_0)\psi_f^*(x')$$

(b) Introducing the expression for $\psi_i(x)$, an analogous expression for the evolved wave function $\psi_f(x) = (2\pi)^{-1/2} \exp(ikx - i\hbar k^2 t/2m)$ and the given expression for $\mathcal{K}_0(x - x'; t - t_0)$, we can perform a Gaussian integration of the type

$$\int_{-\infty}^{+\infty} dx' \exp[ia(x - x')^2 + ikx'] = \sqrt{\frac{\pi}{a}} \exp\left(ikx - \frac{ik^2}{4a}\right)$$

and so arrive at the required identity.

The reversibility of the motion corresponds to the fact that, in addition to the evolution of a free particle of momentum $\hbar k$ from a time t_0 to a time t, an alternative way to see the motion is as that of a free particle with momentum $-\hbar k$ that evolves from time t to time t_0.

Problem 1.9 Consider a normalized wave function $\psi(x)$. Assume that the system is in the state described by the wave function

$$\Psi(x) = C_1\psi(x) + C_2\psi^*(x)$$

where C_1 and C_2 are two known complex numbers.

(a) Write down the condition for the normalization of Ψ in terms of the complex integral $\int_{-\infty}^{+\infty} dx \; \psi^2(x) = D$, assumed to be known.
(b) Obtain an expression for the probability current density $\mathcal{J}(x)$ for the state $\Psi(x)$. Use the polar relation $\psi(x) = f(x)e^{i\theta(x)}$.
(c) Calculate the expectation value $\langle p \rangle$ of the momentum and show that

$$\langle \Psi | p | \Psi \rangle = m \int_{-\infty}^{+\infty} dx \, \mathcal{J}(x)$$

Show that both the probability current and the momentum vanish if $|C_1| = |C_2|$.

Solution

(a) The normalization condition is

$$|C_1|^2 + |C_2|^2 + C_1^* C_2 D^* + C_1 C_2^* D = 1$$

(b) From the defining expression of the probability current density we arrive at

$$\mathcal{J}(x) = \frac{\hbar}{m}(|C_1|^2 - |C_2|^2)\theta'(x) f^2(x)$$

(c) The expectation value of the momentum in the state $\Psi(x)$ is[3]

$$\langle\Psi|p|\Psi\rangle = -i\hbar\int_{-\infty}^{+\infty} dx\,\Psi^*(x)\Psi'(x)$$

$$= \hbar\left(|C_1|^2 - |C_2|^2\right)\int_{-\infty}^{+\infty} dx\,\theta'(x)f^2(x) = m\int dx\,\mathcal{J}(x)$$

Obviously, both the current and the momentum vanish if $|C_1| = |C_2|$.

Problem 1.10 Consider the complete orthonormal set of eigenfunctions $\psi_\alpha(\mathbf{x})$ of a Hamiltonian H. An arbitrary wave function $\psi(\mathbf{x})$ can always be expanded as

$$\psi(\mathbf{x}) = \sum_\alpha C_\alpha\psi_\alpha(\mathbf{x})$$

(a) Show that an alternative expansion of the wave function $\psi(\mathbf{x})$ is that in terms of the complex conjugate wave functions, namely

$$\psi(\mathbf{x}) = \sum_\alpha C'_\alpha\psi^*_\alpha(\mathbf{x})$$

Determine the coefficients C'_α.

(b) Show that the time-evolved wave function

$$\tilde{\psi}(\mathbf{x}, t) = \sum_\alpha C'_\alpha\psi^*_\alpha(\mathbf{x})e^{-iE_\alpha t/\hbar}$$

does not satisfy Schroedinger's equation in general, but only in the case where the Hamiltonian is a *real* operator ($H^* = H$).

(c) Assume that the Hamiltonian is real and show that

$$\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) = \mathcal{K}(\mathbf{x}', \mathbf{x}; t - t_0) = \mathcal{K}^*(\mathbf{x}, \mathbf{x}'; t_0 - t)$$

Solution

(a) Both the orthonormality and the completeness requirements are satisfied by the alternative set $\psi^*_\alpha(\mathbf{x})$ as well:

$$\int d^3x\,\psi^*_\alpha(\mathbf{x})\psi_\beta(\mathbf{x}) = \delta_{\alpha\beta} = \left[\int d^3x\,\psi^*_\alpha(\mathbf{x})\psi_\beta(\mathbf{x})\right]^*$$

$$= \int d^3x\,\psi_\alpha(\mathbf{x})\psi^*_\beta(\mathbf{x})$$

$$\sum_\alpha \psi_\alpha(\mathbf{x})\psi^*_\alpha(\mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}') = \sum_\alpha \psi^*_\alpha(\mathbf{x})\psi_\alpha(\mathbf{x}')$$

[3] Note the vanishing of the integrals of the type

$$\int_{-\infty}^{+\infty} dx\,ff' = \frac{1}{2}\int_{-\infty}^{+\infty} dx\frac{d}{dx}[f^2(x)] = \frac{1}{2}[f^2(x)]_{-\infty}^{+\infty} = 0$$

for a function that vanishes at infinity.

The coefficients of the standard expansion are immediately obtained as

$$C_\alpha = \int d^3x\, \psi^*_\alpha(\mathbf{x})\psi(\mathbf{x})$$

while those of the alternative (or complex-conjugate) expansion are

$$C'_\alpha = \int d^3x\, \psi_\alpha(\mathbf{x})\psi(\mathbf{x})$$

(b) As can be seen by substitution, the wave function $\tilde{\psi}$ does not satisfy the Schroedinger equation, since

$$H\psi^*_\alpha(\mathbf{x}) \neq E_\alpha\psi^*_\alpha(\mathbf{x})$$

This is true however in the case of a *real* Hamiltonian, i.e. one for which $H^* = H$.

(c) From the definition of the propagator using the reality of the Hamiltonian, we have

$$\begin{aligned}\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) &\equiv \left\langle \mathbf{x} \middle| e^{-i(t-t_0)H/\hbar} \middle| \mathbf{x}' \right\rangle = \left(\left\langle \mathbf{x} \middle| e^{i(t-t_0)H/\hbar} \middle| \mathbf{x}' \right\rangle\right)^* \\ &= \mathcal{K}^*(\mathbf{x}, \mathbf{x}'; t_0 - t)\end{aligned}$$

Also, using hermiticity,

$$\begin{aligned}\mathcal{K}(\mathbf{x}, \mathbf{x}'; t - t_0) &\equiv \left\langle \mathbf{x} \middle| e^{-i(t-t_0)H/\hbar} \middle| \mathbf{x}' \right\rangle = \left(\left\langle \mathbf{x}' \middle| e^{i(t-t_0)H/\hbar} \middle| \mathbf{x} \right\rangle\right)^* \\ &= \left\langle \mathbf{x}' \middle| e^{-i(t-t_0)H/\hbar} \middle| \mathbf{x} \right\rangle = \mathcal{K}(\mathbf{x}', \mathbf{x}; t - t_0)\end{aligned}$$

Problem 1.11 A particle has the wave function

$$\psi(r) = Ne^{-\alpha r}$$

where N is a normalization factor and α is a known real parameter.

(a) Calculate the factor N.
(b) Calculate the expectation values

$$\langle \mathbf{x} \rangle, \qquad \langle r \rangle, \qquad \langle r^2 \rangle$$

in this state.
(c) Calculate the uncertainties $(\Delta\mathbf{x})^2$ and $(\Delta r)^2$.
(d) Calculate the probability of finding the particle in the region

$$r > \Delta r$$

(e) What is the momentum-space wave function $\tilde{\psi}(\mathbf{k}, t)$ at any time $t > 0$?
(f) Calculate the uncertainty $(\Delta\mathbf{p})^2$.
(g) Show that the wave function is at all times *isotropic*, i.e.

$$\psi(\mathbf{x}, t) = \psi(r, t)$$

What is the expectation value $\langle \mathbf{x} \rangle_t$?

Solution

(a) The normalization factor is determined from the normalization condition

$$1 = \int d^3r\, |\psi(r)|^2 = 4\pi N^2 \int_0^\infty dr\, r^2 e^{-2\alpha r} = \frac{\pi N^2}{\alpha^3}$$

which gives

$$N = \sqrt{\frac{\alpha^3}{\pi}}$$

We have used the integral ($n \geq 0$)

$$\int_0^\infty dx\, x^n e^{-x} = \Gamma(n+1) = n!$$

(b) The expectation value $\langle \mathbf{x} \rangle$ vanishes owing to spherical symmetry. For example,

$$\langle x \rangle = N^2 \int d^3r\, x e^{-2\alpha r} = N^2 \int_0^\infty dr\, r^3\, e^{-2\alpha r} \int_{-1}^{1} d\cos\theta \sin\theta \int_0^{2\pi} d\phi\, \cos\phi$$
$$= 0$$

The expectation value of the radius is

$$\langle r \rangle = N^2 \int d^3r\, r e^{-2\alpha r} = 4\pi N^2 \int_0^\infty dr\, r^3 e^{-2\alpha r} = \frac{3}{2\alpha}$$

The radius-squared expectation value is

$$\langle \mathbf{x}^2 \rangle = \langle r^2 \rangle = N^2 \int d^3r\, r^2 e^{-2\alpha r} = 4\pi N^2 \int_0^\infty dr\, r^4 e^{-2\alpha r} = \frac{3}{\alpha^2}$$

(c) For the uncertainties, we have

$$(\Delta \mathbf{x})^2 \equiv \langle r^2 \rangle - \langle \mathbf{x} \rangle^2 = \langle r^2 \rangle = \frac{3}{\alpha^2}$$

and

$$(\Delta r)^2 \equiv \langle r^2 \rangle - \langle r \rangle^2 = \frac{3}{\alpha^2} - \left(\frac{3}{2\alpha}\right)^2 = \frac{3}{4\alpha^2}$$

(d) The probability of finding the particle in the region $\Delta r < r < \infty$ is

$$\int_{\Delta r}^\infty d^3r\, |\psi(r)|^2 = 4\pi N^2 \int_{\sqrt{3}/2\alpha}^\infty dr\, r^2 e^{-2\alpha r} = \frac{1}{2} \int_{\sqrt{3}}^\infty dy\, y^2 e^{-y}$$
$$= \frac{1}{2}(5 + 2\sqrt{3}) e^{-\sqrt{3}} \sim 0.7487$$

(e) From the Fourier transform

$$\tilde{\psi}(\mathbf{k}) = \int \frac{d^3r}{(2\pi)^{3/2}}\, e^{-i\mathbf{k}\cdot\mathbf{x}}\, \psi(r)$$

we obtain

$$\tilde{\psi}(k) = \frac{N}{\sqrt{2\pi}} \int_0^\infty dr\, r^2 e^{-\alpha r} \int_{-1}^{1} d\cos\theta\, e^{ikr\cos\theta}$$

$$= \frac{iN}{k\sqrt{2\pi}} \int_0^\infty dr\, r\, e^{-\alpha r}(e^{-ikr} - e^{ikr}) = \frac{4N\alpha}{\sqrt{2\pi}} \frac{1}{(\alpha^2 + k^2)^2}$$

Designating as $t = 0$ the moment at which the particle has the wave function $Ne^{-\alpha r}$, we obtain at time $t > 0$ the evolved momentum-space wave function

$$\tilde{\psi}(k, t) = \frac{4N\alpha}{\sqrt{2\pi}} \frac{e^{-i\hbar k^2 t/2m}}{(\alpha^2 + k^2)^2}$$

(f) Owing to the spherical symmetry of the momentum distribution, we have $\langle \mathbf{p} \rangle = 0$. The uncertainty squared is

$$(\Delta \mathbf{p})^2 = \langle \mathbf{p}^2 \rangle = \frac{16N^2\alpha^2}{2\pi} \int d^3k\, \frac{\hbar^2 k^2}{(k^2 + \alpha^2)^4}$$

$$= \frac{32\alpha^5}{\pi} \int_0^\infty dk \left[\frac{1}{(k^2+\alpha^2)^2} - \frac{2\alpha^2}{(k^2+\alpha^2)^3} + \frac{\alpha^4}{(k^2+\alpha^2)^4} \right]$$

$$= \frac{32\alpha^5}{\pi} \left[-\frac{\partial}{\partial\alpha^2} - \alpha^2 \left(\frac{\partial}{\partial\alpha^2}\right)^2 - \frac{\alpha^4}{6} \left(\frac{\partial}{\partial\alpha^2}\right)^3 \right] \mathcal{J}$$

where

$$\mathcal{J} = \int_0^\infty dk\, \frac{1}{k^2 + \alpha^2} = \frac{\pi}{2\alpha}$$

For the last step we have used the integral

$$\int dx\, \frac{1}{1 + x^2} = \arctan x$$

Thus, we end up with

$$(\Delta \mathbf{p})^2 = \hbar^2 \alpha^2$$

(g) From the Fourier transform we get

$$\psi(\mathbf{x}, t) = \int \frac{d^3k}{(2\pi)^{3/2}} \, e^{i\mathbf{k}\cdot\mathbf{x}} \, \tilde{\psi}(k, t)$$
$$= \frac{1}{\sqrt{2\pi}} \int_0^\infty dk \, k^2 \, \tilde{\psi}(k, t) \int_{-1}^{1} d\cos\theta \, e^{ikr\cos\theta} = \psi(r, t)$$

Consequently, the expectation value $\langle \mathbf{x} \rangle_t$ will vanish at all times owing to spherical symmetry.

2

The free particle

Problem 2.1 A free particle is initially (at $t = 0$) in a state described by the wave function

$$\psi(\mathbf{x}, 0) = Ne^{-\alpha r}$$

where α is a real parameter.

(a) Compute the normalization factor N.
(b) Show that the probability density of finding the particle with momentum $\hbar\mathbf{k}$ is *isotropic*, i.e. it does not depend on the direction of the momentum.
(c) Show that the spatial probability density

$$\mathcal{P}(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2$$

is also isotropic.
(d) Calculate the expectation values

$$\langle \mathbf{p} \rangle_t, \quad \langle \mathbf{x} \rangle_t$$

(e) Show that the expectation value of r^2 increases with time, i.e. it satisfies the inequality

$$\langle r^2 \rangle_t \geq \langle r^2 \rangle_0$$

(f) Modify the initial wave function, assuming that initially the particle is in a state described by

$$\psi(\mathbf{x}, 0) = Ne^{-\alpha r} e^{i\mathbf{k}_0 \cdot \mathbf{x}}$$

Calculate the expectation values $\langle \mathbf{p} \rangle_t$, $\langle \mathbf{x} \rangle_t$ for this case.

Solution

(a) $N = (\alpha^3/\pi)^{3/2}$.
(b) The momentum wave function will be

$$\tilde{\psi}(k) = N \int \frac{d^3x}{(2\pi)^{3/2}}\, e^{-\alpha r - i\mathbf{k}\cdot\mathbf{x}} \propto \frac{1}{k} \int_0^\infty dr\; re^{-\alpha r} \left(e^{ikr} - e^{-ikr}\right) = \tilde{\psi}(k)$$

where we have taken the z-axis of the integration variables to coincide with the momentum direction (so that $\mathbf{k}\cdot\mathbf{x} = kr\cos\theta$). Thus,

$$\Pi(\mathbf{k}) = |\tilde{\psi}(k)|^2 = \Pi(k)$$

Note that, since we have a free particle, its momentum wave function will also be an energy eigenfunction and will evolve in time in a trivial way:

$$\tilde{\psi}(\mathbf{k}, t) = \tilde{\psi}(k)e^{-i\hbar k^2 t/2m}$$

Its corresponding probability density $\Pi(k)$ will be time independent.

(c) The evolved wave function will be

$$\psi(\mathbf{x}, t) = \int \frac{d^3k}{(2\pi)^{3/2}}\, \tilde{\psi}(k)e^{-i\hbar k^2 t/2m}\, e^{i\mathbf{k}\cdot\mathbf{x}}$$

Taking the $\hat{\mathbf{z}}$-axis of the integration variables to coincide with the direction of $\mathbf{x}$, we obtain

$$\psi(\mathbf{x}, t) \propto \frac{1}{r}\int_0^\infty dk\, k\tilde{\psi}(k)e^{-i\hbar k^2 t/2m}\left(e^{ikr} - e^{-ikr}\right) \propto \psi(r, t)$$

Thus, the probability density

$$\mathcal{P}(\mathbf{x}, t) = |\psi(r, t)|^2 = \mathcal{P}(r, t)$$

will be isotropic at all times, i.e. it will not depend on angle.

(d) The momentum expectation value will clearly not depend on time:

$$\langle\mathbf{p}\rangle = \int d^3k\, \hbar\mathbf{k}|\tilde{\psi}(k)|^2$$

Note also that isotropy implies the vanishing of this integral. An easy way to see this is to apply the parity transformation to the integration variable by taking $\mathbf{k} \to -\mathbf{k}$, which leads to

$$\langle\mathbf{p}\rangle = -\langle\mathbf{p}\rangle = 0$$

The same argument applies to the position expectation value, which also vanishes at all times:

$$\langle\mathbf{x}\rangle_t = 0$$

(e) The expectation value of the position squared can be expressed in terms of the momentum wave function as

$$\langle r^2\rangle_t = -\int d^3k\, \tilde{\psi}(k, 0)e^{iEt/\hbar}\, \nabla_{\mathbf{k}}{}^2\left[\tilde{\psi}(k, 0)e^{-iEt/\hbar}\right]$$

Note that, in the case that we are considering, the momentum wave function is not only isotropic but also real. We have

$$\nabla_{\mathbf{k}}\left[\tilde{\psi}(k,0)e^{-iEt/\hbar}\right] = -\frac{i\hbar t}{m}\mathbf{k}\tilde{\psi}e^{-iEt/\hbar} + \hat{\mathbf{k}}\tilde{\psi}'e^{-iEt/\hbar}$$

$$\begin{aligned}\nabla^2_{\mathbf{k}}\left[\tilde{\psi}(k,0)e^{-iEt/\hbar}\right] = &-\frac{3i\hbar t}{m}\tilde{\psi}e^{-iEt/\hbar} - \frac{2i\hbar kt}{m}\tilde{\psi}'e^{-iEt/\hbar}\\ &-\frac{\hbar^2k^2t^2}{m^2}\tilde{\psi}e^{-iEt/\hbar} + \frac{2}{k}\tilde{\psi}'e^{-iEt/\hbar} + \tilde{\psi}''e^{-iEt/\hbar}\end{aligned}$$

The expectation value can be written as

$$\langle r^2\rangle_t = \langle r^2\rangle_0 + \frac{\hbar^2t^2}{m^2}\int d^3k\,k^2\tilde{\psi}^2 + \frac{2i\hbar t}{m}\int d^3k\,k\tilde{\psi}\tilde{\psi}' + \frac{3i\hbar t}{m}\int d^3k\,\tilde{\psi}^2$$

The terms linear in time vanish since

$$\int d^3k\,k\tilde{\psi}\tilde{\psi}' = 2\pi\int_0^\infty dk\,k^3(\tilde{\psi}^2)' = -2\pi\int_0^\infty dk(k^3)'\tilde{\psi}^2 = -\frac{3}{2}\int d^3k\,\tilde{\psi}^2 = -\frac{3}{2}$$

Note that we used the normalization $\int d^3k\,\tilde{\psi}^2 = 1$. Finally, we have

$$\langle r^2\rangle_t = \langle r^2\rangle_0 + \frac{\hbar^2t^2}{m^2}\int d^3k\,k^2\tilde{\psi}^2$$

which demonstrates the validity of the inequality $\langle r^2\rangle_t \geq \langle r^2\rangle_0$. Note that this inequality corresponds to the general fact that, for a free particle, the *uncertainty* $(\Delta x)^2$ always increases in time.

(f) It is not difficult to see that in this case

$$\tilde{\psi}(\mathbf{k},0) = \tilde{\psi}(|\mathbf{k}-\mathbf{k}_0|,0)$$

and that

$$\psi(\mathbf{x},t) = e^{i\mathbf{k}_0\cdot\mathbf{x}}f(|\mathbf{x}-\hbar t\mathbf{k}_0/m|)$$

Thus we have

$$\langle\mathbf{p}\rangle_t = \hbar\int d^3k\,\mathbf{k}\,\tilde{\psi}^2(|\mathbf{k}-\mathbf{k}_0|,0) = \hbar\int d^3q\,\mathbf{q}\,\tilde{\psi}(q,0) + \hbar\mathbf{k}_0\int d^3k\,\tilde{\psi}^2 = \hbar\mathbf{k}_0$$

and

$$\begin{aligned}\langle\mathbf{x}\rangle_t &= \int d^3r\,\mathbf{x}\left|\psi\left(\left|\mathbf{x}-\frac{\hbar t}{m}\mathbf{k}_0\right|,t\right)\right|^2\\ &= \int d^3\rho\,\boldsymbol{\rho}|\psi(\rho,t)|^2 + \frac{\hbar t}{m}\mathbf{k}_0\int d^3r\,|\psi|^2 = \frac{\hbar t}{m}\mathbf{k}_0\end{aligned}$$

Problem 2.2 Show that the 'spherical waves'

$$\psi_{\pm}(r,t) = \frac{N}{r} e^{\pm ikr - i\hbar k^2 t/2m}$$

satisfy the Schroedinger equation for a free particle of mass m except at the origin $r = 0$. Show also that, in contrast with a plane wave, which satisfies the continuity equation everywhere, the above spherical waves do not satisfy the continuity equation at the origin. Give a physical interpretation of this non-conservation of probability. Does the probability interpretation of $\psi_{\pm}$ break down at the origin? Find a linear combination of the above spherical waves $\psi_{\pm}$ that is finite at the origin and reexamine the validity of the continuity equation everywhere.

Solution

The current density corresponding to $\psi_{\pm}$ is

$$\mathcal{J}_{\pm} = \pm\frac{\hbar k}{m}|N|^2\frac{\hat{\mathbf{r}}}{r} = \mp\frac{\hbar k}{m}|N|^2\nabla\left(\frac{1}{r}\right)$$

The probability density is $\mathcal{P}_{\pm} = |N|^2/r^2$ and it is independent of time. Thus, we have

$$\nabla\cdot\mathcal{J} + \dot{\mathcal{P}} = \mp\frac{\hbar k}{m}|N|^2\nabla^2\left(\frac{1}{r}\right) = \pm 4\pi|N|^2\left(\frac{\hbar k}{m}\right)\delta(\mathbf{x})$$

The physical interpretation of this non-zero probability density rate, in the framework of a statistical ensemble of identical systems, is *the number of particles created or destroyed per unit volume per unit time*. The non-conservation of probability arises here from the fact that the $\psi_{\pm}$ are not acceptable wave functions since they diverge at the origin.

In contrast, the spherical wave

$$\psi_0(r) = \frac{1}{2i}\left[\psi_+(r) - \psi_-(r)\right] = N\frac{\sin kr}{r}\,e^{-i\hbar k^2 t/2m}$$

is finite at the origin and satisfies everywhere the free Schroedinger equation and the continuity equation. In fact, we get $\mathcal{J} = 0$ and $\dot{\mathcal{P}} = 0$.

Problem 2.3 A free particle is initially (at $t = 0$) in a state corresponding to the wave function

$$\psi(r) = \left(\frac{\gamma}{\pi}\right)^{3/4} e^{-\gamma r^2/2}$$

(a) Calculate the probability density of finding the particle with momentum $\hbar\mathbf{k}$ at any time t. Is it isotropic?

(b) What is the probability of finding the particle with energy E?

(c) Examine whether the particle is in an eigenstate of the square of the angular momentum $\mathbf{L}^2$, and of its z-component L_z, for any time t.

Solution

(a) The momentum wave function derived from $\psi(r)$ is[1]

$$\tilde{\psi}(k) = \int \frac{d^3x}{(2\pi)^{3/2}}\, \psi(r)\, e^{-i\mathbf{k}\cdot\mathbf{x}} = (\gamma\pi)^{-3/4}\, e^{-k^2/2\gamma}$$

Since the particle is free, the momentum wave function will also be an eigenfunction of energy and will evolve trivially with a time phase:

$$\tilde{\psi}(k,t) = (\gamma\pi)^{-3/4}\, e^{-k^2/2\gamma}\, e^{-i\hbar k^2 t/2m}$$

The corresponding momentum probability density is obviously constant and isotropic.

(b) If we denote by $\mathcal{P}(E)$ the probability density for the particle to have energy $E = \hbar^2 k^2/2m$, we shall have

$$1 = \int_0^\infty dE\, \mathcal{P}(E) = \frac{\hbar^2}{m} \int_0^\infty dk\, k\mathcal{P}(E)$$

Comparing this formula with

$$1 = \int d^3k\, |\tilde{\psi}(k)|^2 = 4\pi \int_0^\infty dk\, k^2\, (\gamma\pi)^{-3/2}\, e^{-k^2/\gamma}$$

we can conclude that

$$\mathcal{P}(E) = \frac{m}{\hbar^2}\, 4\pi k(\gamma\pi)^{-3/2}\, e^{-k^2/\gamma}$$

(c) Since the initial wave function is spherically symmetric, it will be an eigenfunction of angular momentum with vanishing eigenvalues. Moreover, since the Hamiltonian of the free particle is spherically symmetric or, equivalently, it commutes with the angular momentum operators, the time-evolved wave function will continue to be an angular momentum eigenfunction with the same eigenvalue.

Problem 2.4 Consider a free particle that moves in one dimension. Its initial ($t = 0$) wave function is

$$\psi(x,0) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{ik_0 x - \alpha x^2/2}$$

where α and k_0 are real parameters.

[1] We can use the Gaussian integral

$$\int d^3x\, e^{-ar^2}\, e^{-i\mathbf{q}\cdot\mathbf{x}} = \left(\frac{\pi}{a}\right)^{3/2} e^{-q^2/4a}$$

with $\mathrm{Re}(a) > 0$.