time per unit area perpendicular to **j**. To regain the global conservation law, we integrate Eq. (5.3.7) over all space:

$$\frac{d}{dt}\int P(\mathbf{r}, t)\, d^3\mathbf{r} = -\int_{S_\infty} \mathbf{j}\cdot d\mathbf{S} \tag{5.3.9}$$

where S_∞ is the sphere at infinity. For (typical) wave functions which are normalizable to unity, $r^{3/2}\psi \to 0$ as $r \to \infty$ in order that $\int \psi^*\psi r^2\, dr\, d\Omega$ is bounded, and the surface integral of **j** on S_∞ vanishes. The case of momentum eigenfunctions that do not vanish on S_∞ is considered in one of the following exercises.

Exercise 5.3.1. Consider the case where $V = V_r - iV_i$, where the imaginary part V_i is a constant. Is the Hamiltonian Hermitian? Go through the derivation of the continuity equation and show that the total probability for finding the particle decreases exponentially as $e^{-2V_i t/\hbar}$. Such complex potentials are used to describe processes in which particles are absorbed by a sink.

Exercise 5.3.2. Convince yourself that if $\psi = c\tilde{\psi}$, where c is constant (real or complex) and $\tilde{\psi}$ is real, the corresponding **j** vanishes.

Exercise 5.3.3. Consider

$$\psi_{\mathbf{p}} = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar}$$

Find **j** and ϱ and compare the relation between them to the electromagnetic equation $\mathbf{j} = \varrho\mathbf{v}$, $\mathbf{v}$ being the velocity. Since ϱ and **j** are constant, note that the continuity Eq. (5.3.7) is trivially satisfied.

*Exercise 5.3.4.** Consider $\psi = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$ in one dimension. Show that $j = (|A|^2 - |B|^2)p/m$. The absence of cross terms between the right- and left-moving pieces in ψ allows us to associate the two parts of j with corresponding parts of ψ.

Ensemble Interpretation of j

Recall that $\mathbf{j}\cdot d\mathbf{S}$ is the rate at which probability flows past the area $d\mathbf{S}$. If we consider an ensemble of N particles all in some state $\psi(\mathbf{r}, t)$, then $N\mathbf{j}\cdot d\mathbf{S}$ particles will trigger a particle detector of area $d\mathbf{S}$ per second, assuming that N tends to infinity and that **j** is the current associated with $\psi(\mathbf{r}, t)$.

5.4. The Single-Step Potential: A Problem in Scattering‡

Consider the step potential (Fig. 5.2)

$$\begin{aligned} V(x) &= 0 \qquad x < 0 \quad \text{(region I)} \\ &= V_0 \qquad x > 0 \quad \text{(region II)} \end{aligned} \tag{5.4.1}$$

Such an abrupt change in potential is rather unrealistic but mathematically convenient. A more realistic transition is shown by dotted lines in the figure.

Imagine now that a classical particle of energy E is shot in from the left (region I) toward the step. One expects that if $E > V_0$, the particle would climb the barrier and travel on to region II, while if $E < V_0$, it would get reflected. We now compare this classical situation with its quantum counterpart.

First of all we must consider an initial state that is compatible with quantum principles. We replace the incident particle possessing a well-defined trajectory with a wave packet.§ Though the detailed wave function will be seen to be irrelevant in the limit we will consider, we start with a Gaussian, which is easy to handle analytically‖:

$$\psi_I(x, 0) = \psi_I(x) = (\pi\Delta^2)^{-1/4} e^{ik_0(x+a)} e^{-(x+a)^2/2\Delta^2} \tag{5.4.2}$$

This packet has a mean momentum $p_0 = \hbar k_0$, a mean position $\langle X\rangle = -a$ (which we take to be far away from the step), with uncertainties

$$\Delta X = \frac{\Delta}{2^{1/2}}, \qquad \Delta P = \frac{\hbar}{2^{1/2}\Delta}$$

We shall be interested in the case of large Δ, where the particle has essentially well-defined momentum $\hbar k_0$ and energy $E_0 \simeq \hbar^2 k_0^2/2m$. *We first consider the case* $E_0 > V_0$.

After a time $t \simeq a[p_0/m]^{-1}$, the packet will hit the step and in general break into two packets: ψ_R, the reflected packet, and ψ_T, the transmitted

‡ This rather difficult section may be postponed till the reader has gone through Chapter 7 and gained more experience with the subject. It is for the reader or the instructor to decide which way to go.

§ A wave packet is any wave function with reasonably well-defined position and momentum.

‖ This is just the wave packet in Eq. (5.1.14), displaced by an amount $-a$.

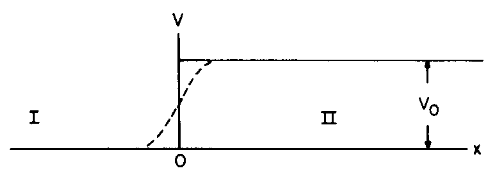

Fig. 5.2. The single-step potential. The dotted line shows a more realistic potential idealized by the step, which is mathematically convenient. The total energy E and potential energy V are measured along the y axis.

packet (Fig. 5.3). The area under $|\psi_R|^2$ at large t is the probability of finding the particle in region I in the distant future, that is to say, the probability of reflection. Likewise the area under $|\psi_T|^2$ at large t is the probability of transmission. Our problem is to calculate the *reflection coefficient*

$$R = \int |\psi_R|^2\, dx, \qquad t \to \infty \tag{5.4.3}$$

and *transmission coefficient*

$$T = \int |\psi_T|^2\, dx, \qquad t \to \infty \tag{5.4.4}$$

Generally R and T will depend on the detailed shape of the initial wave function. If, however, we go to the limit in which the initial momentum is well defined (that is, when the Gaussian in x space has infinite width), we expect the answer to depend only on the initial energy, it being the only characteristic of the state. In the following analysis we will assume that $\Delta X = \Delta/2^{1/2}$ is large and that the wave function in k space is very sharply peaked near k_0.

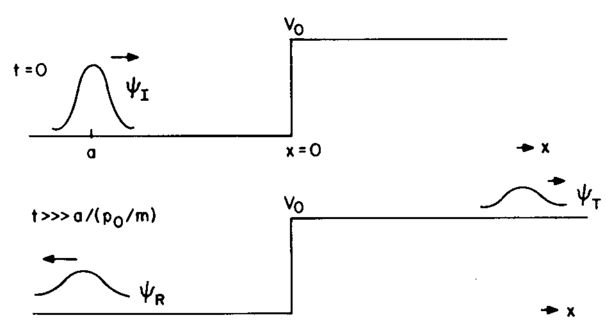

Fig. 5.3. A schematic description of the wave function long before and long after it hits the step. The area under $|\psi_I|^2$ is unity. The areas under $|\psi_R|^2$ and $|\psi_T|^2$, respectively, are the probabilities for reflection and transmission.

We follow the standard procedure for finding the fate of the incident wave packet, ψ_I:

Step 1: Solve for the *normalized* eigenfunction of the step potential Hamiltonian, $\psi_E(x)$.

Step 2: Find the projection $a(E) = \langle \psi_E | \psi_I \rangle$.

Step 3: Append to each coefficient $a(E)$ a time dependence $e^{-iEt/\hbar}$ and get $\psi(x, t)$ at any future time.

Step 4: Identify ψ_R and ψ_T in $\psi(x, t \to \infty)$ and determine R and T using Eqs. (5.4.3) and (5.4.4).

Step 1. In region I, as $V = 0$, the (*unnormalized*) solution is the familiar one:

$$\psi_E(x) = Ae^{ik_1x} + Be^{-ik_1x}, \qquad k_1 = \left(\frac{2mE}{\hbar^2}\right)^{1/2} \tag{5.4.5}$$

In region II, we simply replace E by $E - V_0$ [see Eq. (5.2.2)],

$$\psi_E(x) = Ce^{ik_2x} + De^{-ik_2x}, \qquad k_2 = \left[\frac{2m(E - V_0)}{\hbar^2}\right]^{1/2} \tag{5.4.6}$$

(We consider only $E > V_0$; the eigenfunction with $E < V_0$ will be orthogonal to ψ_I as will be shown on the next page.) Of interest to us are eigenfunctions with $D = 0$, since we want only a transmitted (right-going) wave in region II, and incident plus reflected waves in region I. If we now impose the continuity of ψ and its derivative at $x = 0$; we get

$$A + B = C \tag{5.4.7}$$

$$ik_1(A - B) = ik_2C \tag{5.4.8}$$

In anticipation of future use, we solve these equations to express B and C in terms of A:

$$B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)A = \left(\frac{E^{1/2} - (E - V_0)^{1/2}}{E^{1/2} + (E - V_0)^{1/2}}\right)A \tag{5.4.9}$$

$$C = \left(\frac{2k_1}{k_1 + k_2}\right)A = \left(\frac{2E^{1/2}}{E^{1/2} + (E - V_0)^{1/2}}\right)A \tag{5.4.10}$$

Note that if $V_0 = 0$, $B = 0$ and $C = A$ as expected. The solution with energy E is then

$$\psi_E(x) = A\left[\left(e^{ik_1x} + \frac{B}{A}e^{-ik_1x}\right)\theta(-x) + \frac{C}{A}e^{ik_2x}\theta(x)\right] \tag{5.4.11}$$

where

$$\theta(x) = 1 \quad \text{if } x > 0$$
$$= 0 \quad \text{if } x < 0$$

Since to each E there is a unique $k_1 = +(2mE/\hbar^2)^{1/2}$, we can label the eigenstates by k_1 instead of E. Eliminating k_2 in favor of k_1, we get

$$\psi_{k_1}(x) = A\Big[\Big(\exp(ik_1x) + \frac{B}{A}\exp(-ik_1x)\Big)\theta(-x)$$
$$+ \frac{C}{A}\exp[i(k_1{}^2 - 2mV_0/\hbar^2)^{1/2}x]\theta(x)\Big] \tag{5.4.12}$$

Although the overall scale factor A is generally arbitrary (and the physics depends only on B/A and C/A), here we must choose $A = (2\pi)^{-1/2}$ because ψ_k has to be properly normalized in the four-step procedure outlined above. We shall verify shortly that $A = (2\pi)^{-1/2}$ is the correct normalization factor.

Step 2. Consider next

$$a(k_1) = \langle\psi_{k_1}|\psi_I\rangle$$
$$= \frac{1}{(2\pi)^{1/2}}\Big\{\int_{-\infty}^{\infty}\Big[e^{-ik_1x} + \Big(\frac{B}{A}\Big)^* e^{ik_1x}\Big]\theta(-x)\psi_I(x)\,dx$$
$$+ \int_{-\infty}^{\infty}\Big(\frac{C}{A}\Big)^* e^{-ik_2x}\theta(x)\psi_I(x)\,dx\Big\} \tag{5.4.13}$$

The second integral vanishes (to an excellent approximation) since $\psi_I(x)$ is nonvanishing far to the left of $x = 0$, while $\theta(x)$ is nonvanishing only for $x > 0$. Similarly the second piece of the first integral also vanishes since ψ_I in k space is peaked around $k = +k_0$ and is orthogonal to (left-going) negative momentum states. [We can ignore the $\theta(-x)$ factor in Eq. (5.4.13) since it equals 1 where $\psi_I(x) \neq 0$.] So

$$a(k_1) = \Big(\frac{1}{2\pi}\Big)^{1/2}\int_{-\infty}^{\infty} e^{-ik_1x}\psi_I(x)\,dx$$
$$= \Big(\frac{\Delta^2}{\pi}\Big)^{1/4} e^{-(k_1-k_0)^2\Delta^2/2} e^{ik_1a} \tag{5.4.14}$$

is just the Fourier transform of ψ_I. Notice that for large Δ, $a(k_1)$ is very *sharply peaked at $k_1 = k_0$.* This justifies our neglect of eigenfunctions with $E < V_0$, for these correspond to k_1 not near k_0.

Step 3. The wave function at any future time t is

$$\psi(x, t) = \int_{-\infty}^{\infty} a(k_1)e^{-iE(k_1)t/\hbar}\psi_{k_1}(x)\,dk_1 \tag{5.4.15}$$

$$= \Big(\frac{\Delta^2}{4\pi^3}\Big)^{1/4}\int_{-\infty}^{\infty}\exp\Big(\frac{-i\hbar k_1{}^2t}{2m}\Big)\cdot\exp\Big[\frac{-(k_1-k_0)^2\Delta^2}{2}\Big]\exp(ik_1a)$$
$$\times\Big\{e^{ik_1x}\theta(-x) + \Big(\frac{B}{A}\Big)e^{-ik_1x}\theta(-x)$$
$$+ \Big(\frac{C}{A}\Big)\exp[i(k_1{}^2 - 2mV_0/\hbar^2)^{1/2}x]\theta(x)\Big\}\,dk_1 \tag{5.4.16}$$

You can convince yourself that if we set $t = 0$ above we regain $\psi_I(x)$, which corroborates our choice $A = (2\pi)^{-1/2}$.

Step 4. Consider the first of the three terms. If $\theta(-x)$ were absent, we would be propagating the original Gaussian. After replacing x by $x + a$ in Eq. (5.1.15), and inserting the $\theta(-x)$ factor, the first term of $\psi(x, t)$ is

$$\theta(-x)\pi^{-1/4}\Big(\Delta + \frac{i\hbar t}{m}\Big)^{-1/2}\exp\Big[\frac{-(x + a - \hbar k_0t/m)^2}{2\Delta^2(1 + i\hbar t/m\Delta^2)}\Big]$$
$$\times\exp\Big[ik_0\Big(x + a - \frac{\hbar k_0t}{2m}\Big)\Big] \equiv \theta(-x)G(-a, k_0, t) \tag{5.4.17}$$

Since the Gaussian $G(-a, k_0, t)$ is centered at $x = -a + \hbar k_0t/m \simeq \hbar k_0t/m$ as $t \to \infty$, and $\theta(-x)$ vanishes for $x > 0$, the product θG vanishes. Thus the initial packet has disappeared and in its place are the reflected and transmitted packets given by the next two terms. In the middle term if we replace B/A, which is a function of k_1, by its value $(B/A)_0$ at $k_1 = k_0$ (because $a(k_1)$ is very sharply peaked at $k_1 = k_0$) and pull it out of the integral, changing the dummy variable from k_1 to $-k_1$, it is easy to see that apart from the factor $(B/A)_0\theta(-x)$ up front, the middle term represents the free propagation of a normalized gaussian packet that was originally peaked at $x = +a$ and began drifting to the *left* with mean momentum $-\hbar k_0$. Thus

$$\psi_R = \theta(-x)G(a, -k_0, t)(B/A)_0 \tag{5.4.18}$$

As $t \to \infty$, we can set $\theta(-x)$ equal to 1, since G is centered at $x = a - \hbar k_0t/m \simeq -\hbar k_0t/m$. Since the gaussian G has unit norm, we get from Eqs. (5.4.3) and (5.4.9),

$$R = \int |\psi_R|^2\,dx = \left|\frac{B}{A}\right|_0^2 = \left|\frac{E_0^{1/2} - (E_0 - V_0)^{1/2}}{E_0^{1/2} + (E_0 - V_0)^{1/2}}\right|^2$$

where

$$E_0 = \frac{\hbar^2 k_0^2}{2m} \tag{5.4.19}$$

This formula is exact only when the incident packet has a well-defined energy E_0, that is to say, when the width of the incident Gaussian tends to infinity. But it is an excellent approximation for *any* wave packet that is narrowly peaked in momentum space.

To find T, we can try to evaluate the third piece. But there is no need to do so, since we know that

$$R + T = 1 \tag{5.4.20}$$

which follows from the global conservation of probability. It then follows that

$$T = 1 - R = \frac{4E_0^{1/2}(E_0 - V_0)^{1/2}}{[E_0^{1/2} + (E_0 - V_0)^{1/2}]^2} = \left|\frac{C}{A}\right|_0^2 \frac{(E_0 - V_0)^{1/2}}{E_0^{1/2}} \tag{5.4.21}$$

By inspecting Eqs. (5.4.19) and (5.4.21) we see that both R and T are readily expressed in terms of the ratios $(B/A)_0$ and $(C/A)_0$ and a kinematical factor, $(E_0 - V_0)^{1/2}/E_0^{1/2}$. Is there some way by which we can directly get to Eqs. (5.4.19) and (5.4.21), which describe the dynamic phenomenon of scattering, from Eqs. (5.4.9) and (5.4.10), which describe the static solution to Schrödinger's equation? Yes.

Consider the unnormalized eigenstate

$$\begin{aligned}\psi_{k_0}(x) &= [A_0 \exp(ik_0 x) + B_0 \exp(-ik_0 x)]\theta(-x) \\ &\quad + C_0 \exp\left[i\left(k_0^2 - \frac{2mV_0}{\hbar^2}\right)^{1/2} x\right]\theta(x)\end{aligned} \tag{5.4.22}$$

The incoming plane wave $Ae^{ik_0 x}$ has a probability current associated with it equal to

$$j_I = |A_0|^2 \frac{\hbar k_0}{m} \tag{5.4.23}$$

while the currents associated with the reflected and transmitted pieces are

$$j_R = |B_0|^2 \frac{\hbar k_0}{m} \tag{5.4.24}$$

and

$$j_T = |C_0|^2 \frac{\hbar(k_0^2 - 2mV_0/\hbar^2)^{1/2}}{m} \tag{5.4.25}$$

(Recall Exercise 5.3.4, which provides the justification for viewing the two parts of the j in region I as being due to the incident and reflected wave functions.) In terms of these currents,

$$R = \frac{j_R}{j_I} = \left|\frac{B_0}{A_0}\right|^2 \tag{5.4.26}$$

and

$$T = \frac{j_T}{j_I} = \left|\frac{C_0}{A_0}\right|^2 \frac{(k_0^2 - 2mV_0/\hbar)^{1/2}}{k_0} = \left|\frac{C_0}{A_0}\right|^2 \frac{(E_0 - V_0)^{1/2}}{E_0^{1/2}} \tag{5.4.27}$$

Let us now enquire as to why it is that R and T are calculable in these two ways. Recall that R and T were exact only for the incident packet whose momentum was well defined and equal to $\hbar k_0$. From Eq. (5.4.2) we see that this involves taking the width of the Gaussian to infinity. As the incident Gaussian gets wider and wider (we ignore now the $\Delta^{-1/2}$ factor up front and the normalization) the following things happen:

(i) It becomes impossible to say when it hits the step, for it has spread out to be a right-going plane wave in region I.

(ii) The reflected packet also gets infinitely wide and coexists with the incident one, as a left-going plane wave.

(iii) The transmitted packet becomes a plane wave with wave number $(k_0^2 - 2mV_0/\hbar^2)^{1/2}$ in region II.

In other words, the dynamic picture of an incident packet hitting the step and disintegrating into two becomes the steady state process described by the eigenfunction Eq. (5.4.22). We cannot, however, find R and T by calculating areas under $|\psi_T|^2$ and $|\psi_R|^2$ since all the areas are infinite, the wave packets having been transformed into plane waves. We find instead that the ratios of the probability currents associated with the incident, reflected, and transmitted waves give us R and T. The equivalence between the wave packet and static descriptions that we were able to demonstrate in this simple case happens to be valid for any potential. When we come to scattering in three dimensions, we will assume that the equivalence of the two approaches holds.

Exercise 5.4.1 (Quite Hard). Evaluate the third piece in Eq. (5.4.16) and compare the resulting T with Eq. (5.4.21). [*Hint*: Expand the factor $(k_1^2 - 2mV_0/\hbar^2)^{1/2}$ near $k_1 = k_0$, keeping just the first derivative in the Taylor series.]

Before we go on to examine some of the novel features of the reflection and transmission coefficients, let us ask how they are used in practice. Consider a general problem with some $V(x)$, which tends to constants V_+ and V_- as $x \to \pm\infty$. For simplicity we take $V_\pm = 0$. Imagine an accelerator located to the far left $(x \to -\infty)$ which shoots out a beam of nearly monoenergetic particles with $\langle P \rangle = \hbar k_0$ towards the potential. The question one asks in practice is what fraction of the particles will get transmitted and what fraction will get reflected to $x = \pm\infty$, respectively. In general, the question cannot be answered because we know only the mean momenta of the particles and not their individual wave functions. But the preceding analysis shows that *as long as the wave packets are localized sharply in momentum space, the reflection and transmission probabilities* (R *and* T) *depend only on the mean momentum and not the detailed shape of the wave functions.* So the answer to the question raised above is that a fraction $R(k_0)$ will get reflected and a fraction $T(k_0) = 1 - R(k_0)$ will get transmitted. To find R and T we solve for the time-independent eigenfunctions of $H = T + V$ with energy eigenvalue $E_0 = \hbar^2 k_0^2/2m$, and asymptotic behavior

$$\psi_{k_0}(x) \begin{cases} \xrightarrow[x \to -\infty]{} A e^{ik_0 x} + B e^{-ik_0 x} \\ \xrightarrow[x \to \infty]{} C e^{ik_0 x} \end{cases}$$

and obtain from it $R = |B/A|^2$ and $T = |C/A|^2$. Solutions with this asymptotic behavior (namely, free-particle behavior) will always exist provided V vanishes rapidly enough as $|x| \to \infty$. [Later we will see that this means $|xV(x)| \to 0$ as $|x| \to \infty$.] The general solution will also contain a piece $D \exp(-ik_0 x)$ as $x \to \infty$, but we set $D = 0$ here, for if $A \exp(ik_0 x)$ is to be identified with the incident wave, it must only produce a right-moving transmitted wave $Ce^{ik_0 x}$ as $x \to \infty$.

Let us turn to Eqs. (5.4.19) and (5.4.21) for R and T. These contain many nonclassical features. First of all we find that an incident particle with $E_0 > V_0$ gets reflected some of the time. It can also be shown that a particle with $E_0 > V_0$ *incident from the right* will also get reflected some of the time, contrary to classical expectations.

Consider next the case $E_0 < V_0$. Classically one expects the particle to be reflected at $x = 0$, and never to get to region II. This is not so quantum mechanically. In region II, the solution to

$$\frac{d^2\psi_{\mathrm{II}}}{dx^2} + \frac{2m}{\hbar^2}(E_0 - V_0)\psi_{\mathrm{II}} = 0$$

with $E_0 < V_0$ is

$$\psi_{\mathrm{II}}(x) = Ce^{-\varkappa x}, \qquad \varkappa = \left(\frac{2m\,|(E_0 - V_0)|}{\hbar^2}\right)^{1/2} \tag{5.4.28}$$

(The growing exponential $e^{\varkappa x}$ does not belong to the physical Hilbert space.) Thus there is a finite probability for finding the particle in the region where its kinetic energy $E_0 - V_0$ is negative. There is, however, no steady flow of probability current into region II, since $\psi_{\mathrm{II}}(x) = C\tilde{\psi}$, where $\tilde{\psi}$ is real. This is also corroborated by the fact the reflection coefficient in this case is

$$R = \left|\frac{(E_0)^{1/2} - (E_0 - V_0)^{1/2}}{(E_0)^{1/2} + (E_0 - V_0)^{1/2}}\right|^2 = \left|\frac{k_0 - i\varkappa}{k_0 + i\varkappa}\right|^2 = 1 \tag{5.4.29}$$

The fact that the particle can penetrate into the classically forbidden region leads to an interesting quantum phenomenon called *tunneling*. Consider a modification of Fig. 5.2, in which $V = V_0$ only between $x = 0$ and L (region II) and is once again zero beyond $x = L$ (region III). If now a plane wave is incident on this barrier from the left with $E < V_0$, there is an exponentially small probability for the particle to get to region III. Once a particle gets to region III, it is free once more and described by a plane wave. An example of tunneling is that of α particles trapped in the nuclei by a barrier. Every once in a while an α particle manages to penetrate the barrier and come out. The rate for this process can be calculated given V_0 and L.

Exercise 5.4.2. (a)* Calculate R and T for scattering off a potential $V(x) = V_0 a\delta(x)$. (b) Do the same for the case $V = 0$ for $|x| > a$ and $V = V_0$ for $|x| < a$. Assume that the energy is positive but less than V_0.

Exercise 5.4.3. Consider a particle subject to a constant force f in one dimension. Solve for the propagator in momentum space and get

$$U(p, t; p', 0) = \delta(p - p' - ft)e^{i(p'^3 - p^3)/6m\hbar f} \tag{5.4.30}$$

Transform back to coordinate space and obtain

$$U(x, t; x', 0) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \exp\left\{\frac{i}{\hbar}\left[\frac{m(x - x')^2}{2t} + \frac{1}{2}ft(x + x') - \frac{f^2 t^3}{24m}\right]\right\} \tag{5.4.31}$$

[*Hint*: Normalize $\psi_E(p)$ such that $\langle E | E' \rangle = \delta(E - E')$. Note that E is not restricted to be positive.]