1993 ϕ507 Problems Assigned: 2/5. Due: 2/12/93.

⑩ Let the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + V$, where $\mathcal{H}_0$ is a free-particle Hamiltonian, and V accounts for all interactions. Let ξ be the space-time point (x,t). The Schrödinger Eq. is: $\underline{(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}_0')\psi(\xi') = \hbar\rho(\xi')}$, w/ $\rho(\xi') = \frac{1}{\hbar}V(\xi')\psi(\xi')$. ρ acts as a source fcn for the otherwise free propagation of ψ. Now let $G_0(\xi',\xi)$ be the free-particle Green's fcn which satisfies the point-source eqtn: $\underline{(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}_0')G_0(\xi',\xi) = \hbar\delta(\xi'-\xi)}$. Show that the general solution to the S. Eqtn is: $\underline{\underline{\psi(\xi') = \psi_0(\xi') + \int G_0(\xi',\xi)\rho(\xi)d\xi}}$, where ψ_0 is a free-particle wavefcn. This justifies the claim in class notes, p. IF7.

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⑪ Set $\hbar=1$. Consider a Schrödinger system with known eigenfcns $u_n(\mathbf{r})$ and eigenvalues ω_n [generated as usual by $\mathcal{H}u_n = \omega_n u_n$]. In class, we claimed the Green's fcn for this system was: $\underline{G(\mathbf{r},t;\mathbf{r}_0,t_0) = -i\,\theta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)u_n(\mathbf{r})e^{-i\omega_n(t-t_0)}}$, w/ θ = unit step fcn [see Eq (A5) of class notes, p. IF7]. Verify this claim by showing that G actually obeys: $\underline{\underline{[i(\partial/\partial t) - \mathcal{H}]G = \delta(\mathbf{r}-\mathbf{r}_0)\delta(t-t_0)}}$, per Eq.(15), p. IF6.

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⑫ A free particle in 1D has mean momentum k_0, and initially is localized in space to $\Delta x \sim \delta$; its wavefcn at $t=0$ is: $\underline{\psi(x,0) = Ae^{ik_0x}e^{-x^2/2\delta^2}}$. Adjust the cnst A so that $\int_{-\infty}^{\infty}|\psi(x,0)|^2dx = 1$. Now, by integrating $\psi(x,0)$ over the free-particle propagator K_0 [Eq.(19), class notes, p. IF8], show that $t>0$, ψ has evolved to:

$$\boxed{\psi(x,t) = \frac{A}{\sqrt{1+i\tau}}e^{i(k_0x-\omega_0t)}e^{-(1-i\tau)(x-v_0t)^2/2\delta^2(1+\tau^2)}},$$

w/ $\tau = \hbar t/m\delta^2$, $v_0 = \hbar k_0/m$, $\omega_0 = \hbar k_0^2/2m$.

Interpret the motion of ψ physically (e.g. draw pictures). What happens if $\delta \to 0$?

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⑬ This tidbit of complex variable arcana will be used in problem ⑮. By evaluating an appropriate contour integral in the complex ω-plane, show that the unit step fcn can be represented by: $\underline{\underline{\theta(\tau) = \lim_{\epsilon\to0+}\left(\frac{i}{2\pi}\right)\int_{-\infty}^{\infty}\frac{e^{-i\omega\tau}d\omega}{\omega+i\epsilon}}} = \begin{cases}1, & \text{for } \tau>0\\ 0, & \text{for } \tau<0\end{cases}$. If $\epsilon\to0-$, rather than $0+$, show that the integral generates $\theta(\tau)-1$, the often popular out-of-step fcn. From the form for $\theta(\tau)$, what is the integral for the Dirac delta, $\delta(\tau)$?

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⑩ Solve general Schrödinger problem by means of Green's fcn.

1. Integrate through the $(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}_0')G_0(\xi',\xi) = \hbar\,\delta(\xi'-\xi)$ eqtn by $\int d\xi\,\rho(\xi)$. Since the $\xi = (x,t)$ and $\xi' = (x',t')$ cds are independent of one another...

$$\rightarrow \left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}_0'\right)\underbrace{\int G_0(\xi',\xi)\rho(\xi)\,d\xi}_{\text{define this to be } \psi(\xi')} = \hbar\int \delta(\xi'-\xi)\rho(\xi)\,d\xi = \hbar\,\rho(\xi'). \qquad (1)$$

With the definition of $\psi(\xi')$ as indicated, we have immediately...

$$\rightarrow \left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}_0'\right)\psi(\xi') = \hbar\,\rho(\xi'), \text{ w/ } \underline{\psi(\xi') = \int G_0(\xi',\xi)\rho(\xi)\,d\xi}. \qquad (2)$$

This means $\psi(\xi')$, so defined, is a particular solution to Schrodinger's Eq.

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2. To get the general solution for ψ (and to match boundary conditions), we can add to $\psi(\xi')$ of Eq. (2) any solution to the homogeneous eqtn, i.e.

$$\rightarrow \left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}_0'\right)\psi_0(\xi') = 0. \qquad (3)$$

Since $\mathcal{H}_0'$ is the free-particle Hamiltonian, this identifies $\psi_0(\xi')$ as a free-particle state, a fortiori. Then, as required, the general solution is

$$\psi(\xi') = \psi_0(\xi') + \int G_0(\xi',\xi)\rho(\xi)\,d\xi \leftarrow \text{ w/ } \rho(\xi) = \frac{1}{\hbar}V(\xi)\psi(\xi);$$

$$\text{or/ } \underline{\underline{\psi(\xi') = \psi_0(\xi') + \int G_0(\xi',\xi)\,\Omega(\xi)\,\psi(\xi)\,d\xi}}, \text{ w/ } \Omega(\xi) = \frac{1}{\hbar}V(\xi). \qquad (4)$$

This justifies the claim in class notes, p. IF 7, that a Green's fcn solution works for the Schrodinger Eqtn. G_0 satisfies the point-source eqtn for a free-particle $\mathcal{H}_0$: $[i\hbar(\partial/\partial t') - \mathcal{H}_0']\,G_0(\xi',\xi) = \hbar\,\delta(\xi'-\xi)$. Eq. (4) is sometimes referred to as the Lippmann-Schwinger Eqtn.

Set $\hbar = 1$

① Verify: $G(\mathbf{r},t;\mathbf{r}_0,t_0) = -i\theta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)u_n(\mathbf{r})e^{-i\omega_n(t-t_0)}$, satisfies point-source eq.

1. This is a straightforward plug-in. $\mathcal{H}$ operates only on $\mathbf{r}$-cds, w/ $\mathcal{H}u_n(\mathbf{r}) = \omega_n u_n(\mathbf{r})$, by definition of the eigenfcns u_n & eigenvalues ω_n. Then...

$$\rightarrow \mathcal{H}G = -i\,\theta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)\,u_n(\mathbf{r})\cdot\omega_n e^{-i\omega_n(t-t_0)}. \qquad (1)$$

The t-derivative of G has two terms, one from $\theta(t-t_0)$, and one from $e^{-i\omega_n(t-t_0)}$. Since $\frac{\partial}{\partial t}\theta(t-t_0) = \delta(t-t_0)$, then...

$$\rightarrow i\frac{\partial}{\partial t}G = \delta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)\,u_n(\mathbf{r})\,e^{-i\omega_n(t-t_0)} - \underbrace{-i\,\theta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)\,u_n(\mathbf{r})\cdot\omega_n e^{-i\omega_n(t-t_0)}}_{\text{this term} \equiv \mathcal{H}G \text{ of Eq.(1)}} \qquad (2)$$

Now (1) & (2) together yield...

$$\rightarrow \left(i\frac{\partial}{\partial t} - \mathcal{H}\right)G = \delta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)\,u_n(\mathbf{r})\,e^{-i\omega_n(t-t_0)}. \qquad (3)$$

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2. The RHS of Eq.(3) is nonzero only when $t=t_0$, because of the δ-fcn. We can then evaluate $e^{-i\omega_n(t-t_0)}\big|_{t=t_0} = 1$, and write (3) as...

$$\rightarrow \left(i\frac{\partial}{\partial t} - \mathcal{H}\right)G = \delta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)\,u_n(\mathbf{r}). \qquad (4)$$

But the $\{u_n(\mathbf{r})\}$ are a complete set of eigenfcns, so they satisfy the closure relation: $\sum_n u_n^*(\mathbf{r}_0)\,u_n(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}_0)$. Thus, as desired, we have that $G(\mathbf{r},t;\mathbf{r}_0,t_0) = -i\,\theta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)u_n(\mathbf{r})e^{-i\omega_n(t-t_0)}$ satisfies the point-source eqtn:

$$\boxed{\left(i\frac{\partial}{\partial t} - \mathcal{H}\right)G = \delta(\mathbf{r}-\mathbf{r}_0)\,\delta(t-t_0)}, \qquad (5)$$

and thus qualifies as a Green's fcn for the Schrödinger Eqtn.

⑫ Analyse free propagation of a Gaussian wavepacket in 1D.

1. With: $\psi(x,0) = A\, e^{ik_0 x}\, e^{-x^2/2\delta^2}$, the normalization requires that...

$$\rightarrow \int_{-\infty}^{\infty} |\psi(x,0)|^2 dx = |A|^2 \int_{-\infty}^{\infty} e^{-x^2/\delta^2} dx = |A|^2 \delta\sqrt{\pi} = 1 \Rightarrow \underline{\underline{A = \frac{1}{\sqrt{\delta\sqrt{\pi}}}}}. \quad (1)$$

Now, since the free-particle propagator in 1D is [from class notes, p. IF8, Eq. (10)]: $K_0(x,t;\xi,0) = \left[\frac{m}{2\pi i\hbar}/t\right]^{1/2} \exp\left\{\frac{im}{2\hbar}(x-\xi)^2/t\right\}$, the desired integral for $\psi(x,t)$ is:

$$\rightarrow \psi(x,t) = \int_{-\infty}^{\infty} K_0(x,t;\xi,0)\,\psi(\xi,0)\,d\xi$$

$$= A\,[m/2i\hbar t]^{1/2} \int_{-\infty}^{\infty} e^{\frac{im}{2\hbar t}(x-\xi)^2} \left[e^{ik_0\xi - (\xi^2/2\delta^2)}\right] d\xi. \quad (2)$$

The overall exponent in the integrand of Eq. (2) may be written as

$$\frac{im}{2\hbar t}x^2 - a\xi^2 + b\xi \quad \text{w/} \quad a = (1/2\delta^2) - i(m/2\hbar t), \quad \underline{b = i\,[k_0 - (mx/\hbar t)]};$$

$$\xrightarrow{\text{So}} \psi(x,t) = A\,[m/2i\hbar t]^{1/2}\, e^{imx^2/2\hbar t} \underbrace{\int_{-\infty}^{\infty} e^{-a\xi^2 + b\xi}\, d\xi}_{=\sqrt{\pi/a}\; e^{+b^2/4a}} \quad (3)$$

G&R #(3.232.2)

After a minor amount of algebra, this is...

$$\psi(x,t) = \frac{A}{\sqrt{1+i\tau}}\, e^{-(x-v_0 t)^2/2\delta^2(1+\tau^2)}\, e^{i\frac{m}{2\hbar t}\left[x^2 - \frac{(x-v_0 t)^2}{1+\tau^2}\right]}, \quad (4)$$

where: $\underline{\underline{\tau}} = \hbar t/m\delta^2$, $\underline{\underline{v_0}} = \hbar k_0/m$ = free-particle velocity @ momentum $\hbar k_0$.

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2. To get to the desired form requires some arithmetic. Work on the exponent of the complex exponential in Eq. (4). We have...

$$\rightarrow \frac{m}{2\hbar t}[\;\;] = \frac{m}{2\hbar t}\cdot\frac{(1+\tau^2)x^2 - (x-v_0 t)^2}{1+\tau^2} = \frac{(k_0 x - \omega_0 t) + (\hbar x^2/2m\delta^4)\,t}{(1+\tau^2)}. \quad (5)$$

Here: $\omega_0 = \hbar k_0^2/2m$, is the free-particle ∡ freq. corresponding to wave # k_0.

Splitting off the free particle phase $(k_0 x - \omega_0 t)$, we can write Eq. (5) as:

$$\rightarrow \frac{m}{2\hbar t}[\;\;] = (k_0 x - \omega_0 t) + \frac{\tau}{2\delta^2}\left[x^2 - \frac{2\delta^2}{\tau}(k_0 x - \omega_0 t)\tau^2\right]/(1+\tau^2) \quad (6)$$

[next page]

φ507 Solutions

(12)... wavepacket... (Cont'd).

Compare Eq.(8) with EM wavepacket in a dispersive medium -- see φ520 class notes pp. Waves 25-26. Only difference is v_0 defn.

w/ $\frac{m}{2\hbar t}[\ \ ] = (k_0x - \omega_0 t) + \frac{\tau}{2\delta^2}(x-v_0t)^2/(1+\tau^2)$, w/ $\underline{\underline{\tau}} = \frac{\hbar t}{m\delta^2}$. (7)

When this result is used in Eq. (4), the desired form is obtained for $\psi(x,t)$, i.e. the wave packet @ $t>0$...

$$\boxed{\psi(x,t) = \frac{A}{\sqrt{1+i\tau}}\, e^{i(k_0x-\omega_0t)}\, e^{-(1-i\tau)(x-v_0t)^2/2\delta^2(1+\tau^2)}}, \quad (8)$$

w/ $A = 1/\sqrt{\delta\sqrt{\pi}}$, from Eq. (1). The wave intensity (probability density) is:

$$\underline{\underline{|\psi(x,t)|^2 = \left(\tfrac{1}{\sqrt{\pi}}/\delta\sqrt{1+\tau^2}\right) e^{-(x-v_0t)^2/(\delta\sqrt{1+\tau^2})^2}}}. \quad (9)$$

Note that when $t\to 0$ (& $\tau\to 0$), $\psi(x,t)$ of Eq.(8) reduces to the original $\psi(x,0)$.

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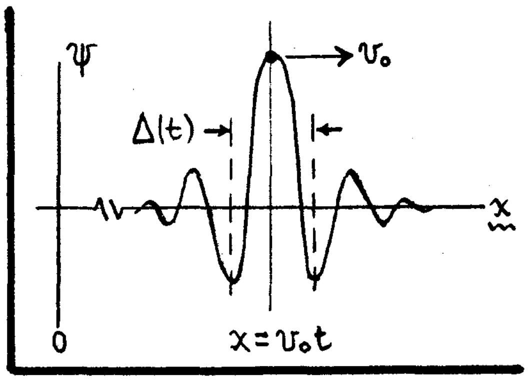
3. Interpretation of packet $\psi(x,t)$ in Eq.(8) [or $|\psi|^2$ in (9)]:



a) The center of the packet (region of max. intensity) moves according to $x = v_0 t$, w/ $v_0 = \hbar k_0/m$.

b) The packet has a plane wave phase [note factor $e^{i(k_0x-\omega_0t)}$ in (8)], but shows additional x & t dependence connected with its initial localization.

c) The packet width $\Delta(t)$ increases in time according to:

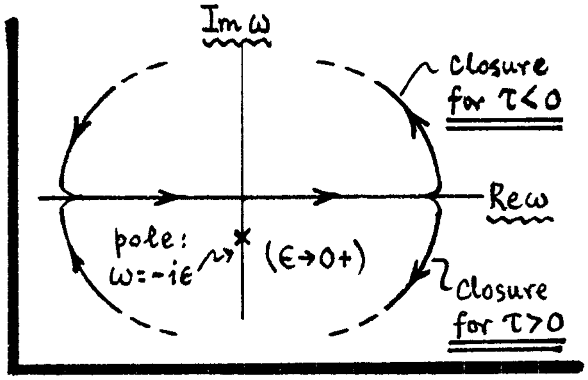
$$\to \Delta(t) = \delta\sqrt{1+\tau^2} = \left[\delta^2 + \left(\frac{\hbar}{m\delta}t\right)^2\right]^{1/2} \simeq (\hbar/m\delta)t, \text{ as } t\to\text{large}. \quad (10)$$

This broadening is in accord with the Uncertainty Principle in the following sense: the initial localization to $\Delta x\sim\delta \Rightarrow$ momentum uncertainty $\Delta p\sim\hbar/\Delta x = \hbar/\delta$, or an initial velocity uncertainty $\Delta v = \Delta p/m \sim (\hbar/m\delta)$. At time t, this Δv produces a position uncertainty $\Delta X = t\Delta v \sim (\hbar/m\delta)t$, which is Δ of Eq.(10).

d) When $\delta\to 0$, the intensity in (9) is: $|\psi(x,t)|^2 \simeq \frac{1}{\sqrt{\pi}}\left(\frac{m\delta/\hbar}{t}\right) e^{-\left(\frac{m\delta/\hbar}{t}\right)^2(x-v_0t)^2}$, at $t>0$. This packet is very broad and of low intensity, in accord w/ $\Delta v\sim\frac{\hbar}{m\delta}\to\infty$.

ϕ507 Solutions

⑬ Verify step-fcn representation: $\theta(\tau) = \lim_{\epsilon\to 0+} \frac{i}{2\pi}\int_{-\infty}^{\infty} \frac{e^{-i\omega\tau}\,d\omega}{\omega+i\epsilon} = \begin{cases} 1, & \tau>0; \\ 0, & \tau<0. \end{cases}$



1. For $\epsilon>0$ (i.e. $\epsilon\to 0+$), the integrand has a simple pole at $\omega=-i\epsilon$; this lies on the (−)ve Im ω axis as shown. Whatever the sign of ϵ, the contour must be closed such that the factor $e^{-i\omega\tau}$ vanishes on the large semi-circles. With $\omega = (\mathrm{Re}\,\omega)+i(\mathrm{Im}\,\omega)$ on those semi-circles, note

$$\rightarrow e^{-i\omega\tau} = \left(e^{\tau\,\mathrm{Im}\,\omega}\right) e^{-i\tau\,\mathrm{Re}\,\omega} \begin{cases} \text{for } \tau>0, \text{ vanishes as } \mathrm{Im}\,\omega\to-\infty; \\ \text{for } \tau<0, \text{ vanishes as } \mathrm{Im}\,\omega\to+\infty. \end{cases} \tag{1}$$

So the closure is in the <u>upper</u> half-plane for $\tau<0$, <u>lower</u> half-plane for $\tau>0$.

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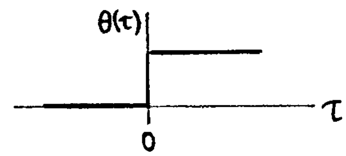
2. With $\epsilon\to 0+$, the contour integral for $\theta(\tau)$ will be zero when $\tau<0$, since closure in the <u>upper</u> half-plane contains no poles. When $\tau>0$, closure in the <u>lower</u> half-plane contains the pole at $\omega=-i\epsilon$, and so...

$$\rightarrow \theta(\tau>0) = \frac{i}{2\pi}\underbrace{(-2\pi i)}_{(-)\text{ sign because of CW contour}} \lim_{\epsilon\to 0+} \mathrm{Res}\left\{\frac{e^{-i\omega\tau}}{\omega+i\epsilon}, \omega=-i\epsilon\right\} = \lim_{\epsilon\to 0+} e^{-i(-i\epsilon)\tau}$$



or/ $\underline{\theta(\tau>0) = \lim_{\epsilon\to 0+} e^{-\epsilon\tau} = 1}$, and : $\underline{\theta(\tau<0)=0}$. (2)

So, indeed : $\theta(\tau) = \frac{i}{2\pi}\lim_{\epsilon\to 0+}\int_{-\infty}^{\infty}\frac{e^{-i\omega\tau}\,d\omega}{\omega+i\epsilon} = \begin{cases} 1, & \text{for } \tau>0, \\ 0, & \text{for } \tau<0; \end{cases}$ is the step fcn.

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3. If $\epsilon\to 0-$, i.e. $\epsilon<0$, the pole in the above diagram moves up the Im ω axis to a position <u>above</u> the Re ω axis. Closure in the lower half-plane gives $\tilde{\theta}(\tau>0)=0$, while $\tilde{\theta}(\tau<0)=-1$, by a calculation similar to Eq. (2) [get an extra (−) from the CCW contour]. This $\epsilon\to 0-$ result can be written: $\underline{\tilde{\theta}(\tau)=\theta(\tau)-1}$. (3)

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4. $\rightarrow \delta(\tau) = \frac{d}{d\tau}\theta(\tau) = \frac{i}{2\pi}\lim_{\epsilon\to 0+}\frac{d}{d\tau}\int_{-\infty}^{\infty}\frac{e^{-i\omega\tau}\,d\omega}{\omega+i\epsilon} = \frac{1}{2\pi}\lim_{\epsilon\to 0+}\int_{-\infty}^{\infty}\left(\frac{\omega}{\omega+i\epsilon}\right)e^{-i\omega\tau}\,d\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega\tau}\,d\omega.$

This is a standard repn of the Dirac delta fcn, $\delta(\tau)$. It is independent of sgn ϵ. (4)