KVANTNA MEHANIKA

Zadaci za vježbe 17. 3. 2025.

4 Slobodna čestica

4.1 Pretpostavimo da česticu koja je lokalizirana u intervalu $-a < x < a$ i ima valnu funkciju

$$\Psi(x,0) = \begin{cases} A\,; -a < x < a \\ 0\,; \text{drugo} \end{cases}$$

(A, a su pozitivne realne konstante) oslobodimo u $t = 0$.
(a) Odredite A tako da normalizirate $\Psi(x,0)$.
(b) Odredite Fourierov transformat funkcije $\Psi(x,0)$.
(c) Komentirajte ponašanje Fourierovog transformata $\Phi(k)$ za velike i male vrijednosti od a. U kakvoj su vezi ovakvo ponašanje i princip neodređenosti?

4.2 Slobodna čestica ima početnu valnu funkciju

$$\Psi(x,0) = A\mathrm{e}^{-ax^2}$$

gdje su A i a realne konstante ($a > 0$).
(a) Normalizirajte $\Psi(x,0)$.
(b) Nađite $\Psi(x,t)$. Po mogućnosti, upotrijebite program *Mathematica*.
(c) Nađite $|\Psi(x,t)|^2$. Izrazite rezultat pomoću veličine $w = \{a / [1 + (2\hbar at/m)^2\}^{1/2}$. Skicirajte $|\Psi|^2$ kao funkciju od x u $t = 0$ i za veliki t. Što se događa s $|\Psi|^2$ u vremenu?
(d) Nađite $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, $\langle p^2\rangle$, σ_x , σ_p .
(e) Da li relacija neodređenosti vrijedi? U kojem trenutku t sustav priđe najbliže granici neodređenosti?

4.3 Zamislite da klizač atomskih dimenzija klže bez trenja po kružnoj žici duljine a. Uočite da je ovaj problem sličan slobodnoj čestici, ali je uvjet na valnu funkciju $u(x + a) = u(x)$. Nađite stacionarna stanja i odgovarajuće energije. Primijetite da postoje dva nezavisna rješenja za svaku od nađenih energija E_n: jedno rješenje opisuje gibanje u smjeru, a drugo suprotno smjeru gibanja kazaljke na satu. Nazovite ih u_+ i u_- . Kako biste objasnili ovu degeneraciju pozivajući se na teorem kojeg ste pokazali na predavanjima? Odnosno, zašto taj teorem ne vrijedi u ovom problemu?

4.4 Pokažite da je Schrödingerova jednodimenzionalna jednadžba za *slobodnu česticu* invarijantna na Galilejeve transformacije. Nakon što primijenite Galilejeve transformacije $x' = x - vt$, $t' = t$, transformirana valna funkcija $\Psi'(x',t') = f(x,t)\,\Psi(x,t)$ zadovoljava valnu jednadžbu sa crtanim varijablama, gdje je f funkcija od x, t, $\hbar$, m, v. Nađite f i pokažite da se ravni val $\Psi(x,t) = \exp[i(kx - \omega t)]$ transformira na očekivani način.

4.5 Promotrite valnu funkciju koja je, početno, superpozicija dva dobro odvojena i uska valna paketa

$$\psi_1(x,0) + \psi_2(x,0)$$

koja su odabrana tako da je apsolutna vrijednost integrala prekrivanja

$$\gamma(0) = \int_{-\infty}^{\infty} \psi_1^*(x)\psi_2(x)dx$$

veoma mala. Kako se valni paket giba i širi, hoće li se $|\gamma(t)|$ povećavati u vremenu ako se valni paketi prekrivaju?

4.6 Neutronski interferometar visoke rezolucije sužava energijski rasap termalnih neutrona kinetičke energije 20 meV na rasap $\Delta\lambda/\lambda = 10^{-9}$ po valnim duljinama. Procijenite duljinu valnog paketa neutrona u smjeru gibanja. Za koje vrijeme će se valni paket značajno proširiti?

4.1

$$\psi(x,0) = \begin{cases} A, & -a \le x \le a \\ 0, & \text{drugo} \end{cases}$$

(a) Normalizacija

$$\int_{-a}^{a} |\psi|^2 dx = |A|^2 \cdot 2a = 1 \Rightarrow A = \frac{1}{\sqrt{2a}}$$

(b) Fourierov transformat.

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \cdot \frac{1}{\sqrt{2a}} \int_{-a}^{a} e^{-ikx} dx$$

$$= \frac{\sin(ka)}{\sqrt{\pi \cdot a} \cdot k}$$

(c) Mali a; $ka \ll 1$, čestica je lokalizirana

$$\sin(ka) \simeq ka$$

$$\phi(k) \simeq \sqrt{\frac{a}{\pi}} = \text{konst.}$$

Iz definicije valnog paketa: iz gornje funkcije možemo pročitati da čestica ima širok interval k-ova.

To je u skladu s relacijom neodređenosti, $\sigma_x \sigma_p \ge \frac{\hbar}{2}$

Dobro definiran položaj, znači loše određen valni vektor, odnosno impuls ($p = \hbar k$).

Veliki a;
$$\frac{\sin(ka)}{k} \xrightarrow[a \to \infty]{} \pi \delta(k)$$

$\phi(k) \to \sqrt{\frac{\pi}{a}}\, \delta(k)$ valni vektor je oštro definiran, položaj loše.

$\boxed{4.2}$

$$\psi(x,0) = A e^{-ax^2}$$

(a)

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1$$

$$\parallel$$

$$|A|^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = |A|^2 \sqrt{\frac{\pi}{2a}} = 1$$

$$\Rightarrow \quad A = \left(\frac{2a}{\pi}\right)^{1/4}$$

[Analogija s diskretnim stanjima

$$\psi(x,t) = \sum_n c_n u_n e^{-i\omega_n(k)t}$$]

(b)

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x,0) e^{-ikx} dx$$

Računamo najprije $\phi(k)$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} A \underbrace{\int_{-\infty}^{+\infty} e^{-ax^2} e^{-ikx} dx}_{J}$$

$$J = \int_{-\infty}^{+\infty} e^{-(ax^2+ikx)} dx = \Big[ax^2 + ikx = a\left(x^2 + i\frac{k}{a}x\right)$$

$$= a(\underbrace{x + \frac{ik}{2a}}_{y})^2 + \frac{k^2}{4a}$$

$$= e^{-\frac{k^2}{4a}} \int_{-\infty}^{+\infty} e^{-a(x+\frac{ik}{2a})^2} dx$$

OPREZ: y je kompleksan broj. Vidi dodatak

$$= e^{-\frac{k^2}{4a}} \cdot \sqrt{\frac{\pi}{a}}$$

$$\phi(k) = \frac{1}{(2\pi a)^{1/4}} e^{-\frac{k^2}{4a}}$$

Natrag u izraz za $\psi(x,t)$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \cdot \frac{1}{(2\pi a)^{1/4}} \int_{-\infty}^{\infty} e^{-k^2/4a} \cdot e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} dk$$

$$-\frac{k^2}{4a} - i\frac{\hbar k^2}{2m}t + ikx = -\left(\frac{1}{4a} + i\frac{\hbar t}{2m}\right)k^2 + ikx$$

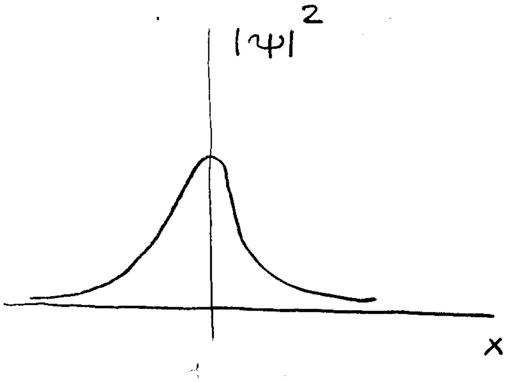
$$= -\left(\frac{1}{4a} + i\frac{\hbar t}{2m}\right)\left[k^2 + \frac{ix}{\left(\frac{1}{4a} + i\frac{\hbar t}{2m}\right)}k\right]$$

$$= -\left(\frac{1}{4a} + i\frac{\hbar t}{2m}\right)\left[k + \frac{ix}{2\left(\frac{1}{4a} + i\frac{\hbar t}{2m}\right)}\right]^2 - \frac{x^2}{4\left(\frac{1}{4a} + i\frac{\hbar t}{2m}\right)}$$

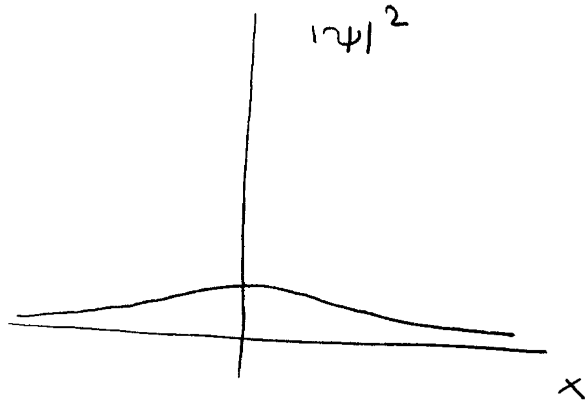
$$\psi(x,t) = \left(\frac{2a}{\pi}\right)^{1/4} \frac{e^{-ax^2/(1+2i\hbar a t/m)}}{\sqrt{1 + 2i\hbar a t/m}}$$

(c)

$$|\psi|^2 = \sqrt{\frac{2}{\pi}}\, w\, e^{-2w^2x^2}; \quad w = \left(\frac{a}{1 + \left(\frac{2\hbar a t}{m}\right)^2}\right)^{1/2}.$$



$t=0$



$t \gg 0$

$t \to 0 \quad w \to \sqrt{a}$

$t \to \infty \quad w \to 0$

Kako t raste valni paket se širi i izravnava.

(d)

$$\langle x\rangle = \int_{-\infty}^{+\infty} x\,|\psi|^2 dx \propto \int_{-\infty}^{+\infty} x\, e^{-2ax^2} = 0$$

neparna funkcija na simetričnom intervalu

$$\langle p\rangle = m\,\frac{d\langle x\rangle}{dt} = 0 \quad \text{(stacionarno stanje)}$$

$$\langle x^2\rangle = \int_{-\infty}^{+\infty} x^2|\psi|^2 dx = \sqrt{\frac{2}{\pi}}\, w \int_{-\infty}^{+\infty} x^2 e^{-2w^2x^2} dx$$

$$= \sqrt{\frac{2}{\pi}}\, w \cdot \frac{1}{4w^2}\sqrt{\frac{\pi}{2w^2}} = \frac{1}{4w^2}$$

$$\langle p^2\rangle = \hbar^2 a$$

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{1}{2w}$$

$$\sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \hbar\sqrt{a}$$

(e)

$$\sigma_x\sigma_p = \frac{1}{2w}\hbar\sqrt{a} = \frac{\hbar}{2}\sqrt{1+\left(\frac{2\hbar a t}{m}\right)^2} \geq \frac{\hbar}{2}$$

(zadovoljena je relacija neodređenosti.)

$$t = 0 \Rightarrow \sigma_x\sigma_p = \frac{\hbar}{2}$$

$\boxed{4.3}$ Potencijalna energija je $V(x)=0$, pa su rješenja oblika

$$u_+ = A e^{ikx}$$

$$u_- = A e^{-ikx}$$

$$k^2 = \frac{2mE}{\hbar^2} \; ; \quad E > 0.$$

Periodični rubni uvjet: $u_+(x+a) = u_+(x)$

$$A e^{ik(x+a)} = A e^{ikx}$$

$$e^{ik\cdot a} = 1$$

$$\Rightarrow \quad k\cdot a = 2n\pi \; ; \quad n = 0, 1, 2, \dots \; ; \quad k>0$$

Energije su oblika:

$$E_n = \frac{\hbar^2}{2m}\cdot\left(\frac{2n\pi}{a}\right)^2 = \frac{2\pi^2\hbar^2}{ma^2}\, n^2 .$$

Normalizacija:

$$|A|^2 \int_0^a \left|e^{ikx}\right|^2 dx = a\cdot |A|^2 = 1$$

$$A = \frac{1}{\sqrt{a}}$$

$$u_+(x) = \frac{1}{\sqrt{a}}\, e^{i\frac{2n\pi}{a}x}$$

$$u_-(x) = \frac{1}{\sqrt{a}}\, e^{-i\frac{2n\pi}{a}x}$$

Teorem na predavanjima: u jednoj dimenziji, nema degeneracije ako postoji točka x_0 u kojoj je $u(x_0)=0$.

Kod ravnih valova takva točka ne postoji i to je razlog zašto ravni valovi u_+ i u_- imaju iste energije.

4.4 Schrödingerova jednadžba

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\psi(x,t)}{\partial t} \qquad (*)$$

Želimo pokazati da vrijedi

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi'(x',t')}{\partial x'^2} = i\hbar\frac{\partial\psi'(x',t')}{\partial t'} \qquad (**)$$

ako je

$$x' = x - vt$$
$$t' = t$$

i

$$\psi'(x',t') = f(x,t)\psi(x,t)$$
$$= f(x'+vt',t')\psi(x'+vt',t')$$

Računamo;

$$\frac{\partial^2\psi'}{\partial x'^2} = \frac{\partial^2 f}{\partial x^2}\psi + 2\frac{\partial f}{\partial x}\frac{\partial\psi}{\partial x} + f\frac{\partial^2\psi}{\partial x^2}$$

gdje smo koristili

$$\frac{\partial f}{\partial x'} = \frac{\partial f}{\partial x}\cdot\overbrace{\frac{\partial x}{\partial x'}}^{=1} = \frac{\partial f}{\partial x}$$

$$\frac{\partial\psi}{\partial x'} = \frac{\partial\psi}{\partial x}\cdot\overbrace{\frac{\partial x}{\partial x'}}^{=1} = \frac{\partial\psi}{\partial x}$$

$$\frac{\partial\psi'}{\partial t'} = \left(\frac{\partial f}{\partial x}v + \frac{\partial f}{\partial t}\right)\psi + \left(\frac{\partial\psi}{\partial x}v + \frac{\partial\psi}{\partial t}\right)f$$

gdje smo koristili

$$\frac{\partial f}{\partial t'} = \frac{\partial f}{\partial x}\cdot\frac{\partial x}{\partial t'} + \frac{\partial f}{\partial t}\cdot\frac{\partial t}{\partial t'}$$

$$\frac{\partial\psi}{\partial t'} = \frac{\partial\psi}{\partial x}\cdot\frac{\partial x}{\partial t'} + \frac{\partial\psi}{\partial t}\cdot\frac{\partial t}{\partial t'}$$

Uvrstimo u pretpostavljenu jednadžbu (* *)

$$-\frac{\hbar^2}{2m}\left\{\frac{\partial^2 f}{\partial x^2}\psi + 2\frac{\partial f}{\partial x}\frac{\partial\psi}{\partial x} + f\frac{\partial^2\psi}{\partial x^2}\right\} =$$

$$= i\hbar\left\{\left(\frac{\partial f}{\partial x}v + \frac{\partial f}{\partial t}\right)\psi + \left(\frac{\partial\psi}{\partial x}v + \frac{\partial\psi}{\partial t}\right)f\right\}$$

Zbog (*)

$$\left\{-\frac{\hbar^2}{2m}\frac{\partial^2 f}{\partial x^2} - i\hbar\left(\frac{\partial f}{\partial x}v + \frac{\partial f}{\partial t}\right)\right\}\psi + \left(-\frac{\hbar^2}{m}\frac{\partial f}{\partial x} - i\hbar v f\right)\frac{\partial\psi}{\partial x} = 0$$

Postavljamo

$$\frac{\partial f}{\partial x} = -i\frac{mv}{\hbar}f$$

Rješenje:

$$f = e^{-i\frac{mv}{\hbar}x}\,u(t)$$

Druge jednadžbe

$$-\frac{\hbar^2}{2m}\frac{\partial^2 f}{\partial x^2} - i\hbar v\frac{\partial f}{\partial x} - i\hbar\frac{\partial f}{\partial t} = 0$$

Uvrstimo (***) u gornju jednadžbu

$$\underbrace{\frac{mv^2}{2}u - mv^2 u}_{-\frac{mv^2}{2}u} - i\hbar\frac{du}{dt} = 0$$

$$u = e^{i\frac{mv^2}{2\hbar}t}$$

Funkcija f postaje

$$f = e^{-i\left(\frac{mv}{\hbar}x - \frac{mv^2}{2\hbar}t\right)}$$

$$\psi'(x',t') = e^{-i\left(\frac{mv}{\hbar}x - \frac{mv^2}{2\hbar}t\right)}\psi(x,t)$$

Zadani val

$$\psi'(x',t') = e^{-i\left(\frac{mv}{\hbar}x - \frac{mv^2}{2\hbar}t\right)}\cdot e^{i(kx-\omega t)}$$

$$= e^{i\left\{\left(k-\frac{mv}{\hbar}\right)(x'+vt') - \left(\omega - \frac{mv^2}{2\hbar}\right)t'\right\}}$$

$$= e^{i\left\{\left(k-\frac{mv}{\hbar}\right)x' - \left(\omega + \frac{mv^2}{2\hbar} - kv\right)t'\right\}}$$

$$k' = k - \frac{mv}{\hbar} \Rightarrow \underbrace{\hbar k'}_{p'} = \underbrace{\hbar k}_{p} - mv$$

$$\omega' = \omega + \frac{mv^2}{2\hbar} - kv \Rightarrow \underbrace{\hbar\omega'}_{E'} = \underbrace{\hbar\omega}_{E} + \frac{mv^2}{2} - \hbar k\cdot v$$

Npr.

$$E' = \frac{p'^2}{2m} = \frac{1}{2m}(p-mv)^2 = \frac{1}{2m}(\hbar k - mv)^2$$

$$= \frac{\hbar^2 k^2}{2m} - \frac{1}{\cancel{2m}}\cdot\cancel{2}\hbar k\cancel{m}v + \frac{1}{2m}m^2v^2$$

$$= \underbrace{\frac{\hbar^2k^2}{2m}}_{E=\hbar\omega} - \hbar k v + \frac{mv^2}{2}$$

$\boxed{4.5}$

Valni paketi

$$\psi_1(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi_1(k)\, e^{i(kx-\omega(k)t)} dk$$

$$\psi_2(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi_2(k)\, e^{i(kx-\omega(k)t)} dk$$

Uvrstimo u formulu za $\gamma(t)$

$$\gamma(t) = \int_{-\infty}^{\infty} \psi_1^*(x,t)\, \psi_2(x,t)\, dx$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_1 \int_{-\infty}^{\infty} dk_2\ \phi_1(k_1)\, \phi_2(k_2)\, e^{-i(\omega(k_1)-\omega(k_2))t} \underbrace{\int_{-\infty}^{\infty} dx\, e^{i(k_1-k_2)x} dx}_{2\pi\,\delta(k_1-k_2)}$$

$$= \int_{-\infty}^{\infty} dk_2\ \phi_1(k_2)\, \phi_2(k_2)$$

Posljednji integral je neovisan o vremenu pa vrijedi

$$\gamma(t) = \gamma(0)$$

Isto smo mogli zaključiti i pomoću zahtjeva za normalizacijom valnih funkcija te zahtjevom da valna funkcija u 1D može biti odabrana kao realna.

$\boxed{4.6}$

Rasap po impulsima je iz

$$p = \frac{h}{\lambda}$$

$$dp = -\frac{h}{\lambda^2}\, d\lambda = -p\,\frac{d\lambda}{\lambda}$$

jednak (po apsolutnoj vrijednosti)

$$\frac{\Delta p}{p} = \frac{\Delta \lambda}{\lambda}$$

Prosječnu vrijednost impulsa neutrona možemo dobiti iz kinetičke energije $T \ll mc^2$

$$T = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mT}$$

Duljinu valnog paketa procijenit ćemo iz neodređenosti koordinate

$$\Delta x \Delta p \sim \hbar$$

$$\Delta x \sim \frac{\hbar}{\Delta p} = \frac{1}{p}\,\frac{\hbar}{\Delta p/p} = \frac{1}{\sqrt{2mT}} \cdot \frac{\hbar}{\Delta\lambda/\lambda}$$

$T = 20\ \text{meV} = 20 \cdot 10^{-3} \cdot 1{,}6 \cdot 10^{-19}\ \text{J} = 3{,}2 \cdot 10^{-21}\ \text{J}$

$m = 1{,}67 \cdot 10^{-27}\ \text{kg}$ (neutron)

$\hbar = 1{,}054 \cdot 10^{-34}\ \text{Js}$

$\frac{\Delta\lambda}{\lambda} = 10^{-9}$

$$\Delta x = \frac{1}{\sqrt{2 \cdot 1{,}67 \cdot 10^{-27} \cdot 3{,}2 \cdot 10^{-21}}} \cdot \frac{1{,}054 \cdot 10^{-34}}{10^{-9}} = 3{,}2 \cdot 10^{-2}\ \text{m}$$

~ 1 cm

Vrijeme širenja valnog paketa dano je izrazom

$$t_s = \frac{m\hbar}{(\Delta p)^2} = \frac{\hbar m}{p^2}\cdot\frac{1}{(\Delta\lambda/\lambda)^2} = \frac{\hbar m}{2mT}\cdot\frac{1}{(\Delta\lambda/\lambda)^2}$$

$$= \frac{\hbar}{2T}\cdot\frac{1}{(\Delta\lambda/\lambda)^2}$$

$$t_s = \frac{1{,}054\cdot 10^{-34}}{2\cdot 3{,}2\cdot 10^{-21}}\cdot\frac{1}{(10^{-9})^2} = 1{,}647\cdot 10^{4}\,s = 4{,}57\,h$$

To je veoma veliko vrijeme i možemo zaključiti da se valni paket tijekom mjerenja ne proširi značajno.

DODATAK

Gaussian Integral with Complex Offset

Theorem:

$$\int_{-\infty}^{\infty} e^{-p(t+c)^2} dt = \sqrt{\frac{\pi}{p}}, \quad p, c \in \mathbf{C}, \ \text{re}\{p\} > 0 \tag{D.12}$$

Proof: When $c = 0$, we have the previously proved case. For arbitrary $c = a + jb \in \mathbf{C}$ and real number $T > |a|$, let $\Gamma_c(T)$ denote the closed rectangular contour $z = (-T) \to T \to (T + jb) \to (-T + jb) \to (-T)$, depicted in Fig.D.1.

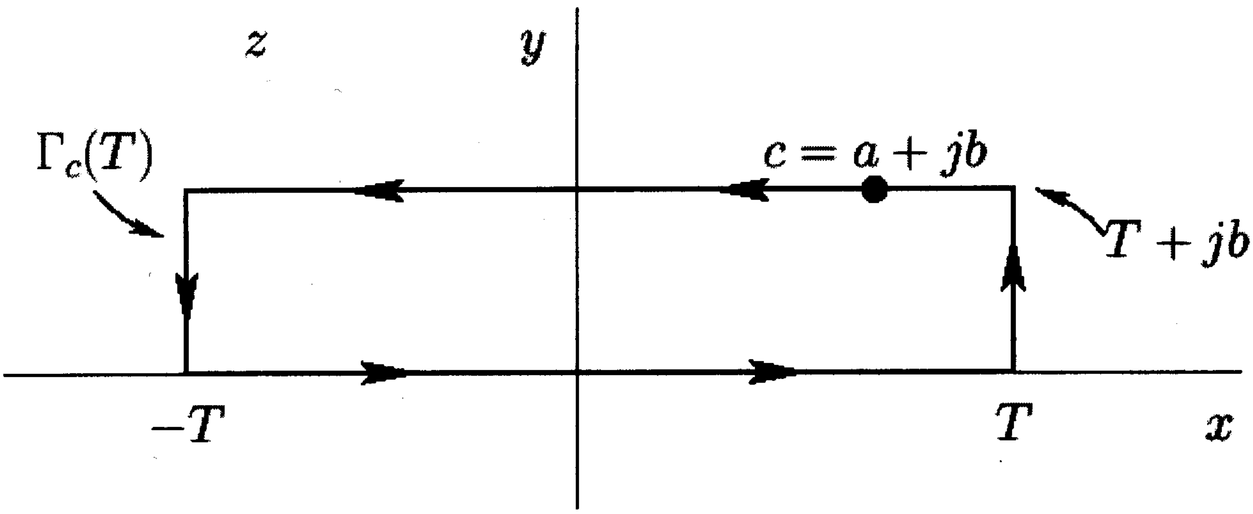


Figure D.1: Contour of integration in the complex plane.

Clearly, $f(z) \triangleq e^{-pz^2}$ is analytic inside the region bounded by $\Gamma_c(T)$. By Cauchy's theorem [41], the line integral of $f(z)$ along $\Gamma_c(T)$ is zero, *i.e.*,

$$\oint_{\Gamma_c(T)} f(z)dz = 0 \tag{D.13}$$

This line integral breaks into the following four pieces:

$$\oint_{\Gamma_c(T)} f(z)dz = \underbrace{\int_{-T}^{T} f(x)dx}_{1} + \underbrace{\int_{0}^{b} f(T+jy)jdy}_{2} + \underbrace{\int_{T}^{-T} f(x+jb)dx}_{3} + \underbrace{\int_{b}^{0} f(-T+jy)jdy}_{4}$$

where x and y are real variables. In the limit as $T \to \infty$, the first piece approaches $\sqrt{\pi/p}$, as previously proved. Pieces 2 and 4 contribute zero in the limit, since $e^{-p(t+c)^2} \to 0$ as $|t| \to \infty$. Since the total contour integral is zero by Cauchy's theorem, we conclude that piece 3 is the negative of piece 1, *i.e.*, in the limit as $T \to \infty$,

$$\int_{-\infty}^{\infty} f(x+jb)dx = \sqrt{\frac{\pi}{p}}. \qquad \text{(D.14)}$$

Making the change of variable $x = t + a = t + c - jb$, we obtain

$$\int_{-\infty}^{\infty} f(t+c)dt = \sqrt{\frac{\pi}{p}} \qquad \text{(D.15)}$$

as desired.

Next | **Prev** | **Up** | **Top** | **Index** | **JOS Index** | **JOS Pubs** | **JOS Home** | **Search**

[How to cite this work] [Order a printed hardcopy] [Comment on this page via email]

``Spectral Audio Signal Processing'', by Julius O. Smith III, W3K Publishing, 2011, ISBN 978-0-9745607-3-1.

Center for Computer Research in Music and Acoustics (CCRMA), Stanford University