

with  $E_a < V_0$  and  $E_b > V_0$ .

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## APPENDIX A: TRIGONOMETRIC INTEGRALS

For many of the calculations included here, we require versions of the integral

$$\int_{-\infty}^{+\infty} \frac{\sin(z) \cos(mz)}{z} dz = \begin{cases} 0 & \text{for } m < -1 \text{ and } m > +1 \\ \pi/2 & \text{for } m = \pm 1 \\ \pi & \text{for } m^2 < 1 \end{cases} \quad (\text{A1})$$

which is a handbook [47] result. We can briefly justify these results, starting with the single integral

$$\int_{-\infty}^{+\infty} \frac{\sin(z)}{z} dz = \pi \quad (\text{A2})$$

which itself can be derived using contour integration. This can be generalized to

$$\int_{-\infty}^{+\infty} \frac{\sin(mz)}{z} dz = \begin{cases} +\pi & \text{for } m > 0 \\ 0 & \text{for } m = 0 \\ -\pi & \text{for } m < 0 \end{cases} \quad (\text{A3})$$

by a change of variables, and considering the special  $m = 0$  case separately. The general integral in Eqn. (A1) can then be obtained by writing

$$\sin(z) \cos(mz) = \frac{1}{2} \{ \sin[(1+m)z] + \sin[(1-m)z] \} \quad (\text{A4})$$

and using Eqn. (A3) twice. The special case of  $m = 1$  is done by noting that

$$\int_{-\infty}^{+\infty} \frac{\sin(z) \cos(z)}{z} dz = \int_{-\infty}^{+\infty} \frac{\sin(2z)}{2z} dx = \frac{1}{2} \int_{-\infty}^{+\infty} \frac{\sin(w)}{w} dw = \frac{\pi}{2} \quad (\text{A5})$$

where  $w = 2z$  and a simple trig identity is used. Another integral that is useful for normalization calculations is

$$\int_{-\infty}^{+\infty} \frac{\sin^2(z)}{z^2} dz = \pi \quad (\text{A6})$$

which is another handbook result derivable using contour integration techniques.

## APPENDIX B: WIGNER DISTRIBUTION FROM MOMENTUM-SPACE WAVEFUNCTIONS

The evaluation of the Wigner function, using momentum-space wavefunctions as in Eqn. (5), requires the integral

$$P_W^{(n)}(x, p) = \left( \frac{L}{(\pi\hbar)^2} \right) \int_{-\infty}^{+\infty} dq e^{-2iqx/\hbar} e^{+i(p+q)L/2\hbar} e^{-i(p-q)L/2\hbar} \quad (\text{B1})$$

$$\times \left\{ e^{-in\pi/2} \frac{\sin[((p+q)L/\hbar - n\pi)/2]}{[(p+q)L/\hbar - n\pi]} - e^{+in\pi/2} \frac{\sin[((p+q)L/\hbar + n\pi)/2]}{[(p+q)L/\hbar + n\pi]} \right\}$$

$$\times \left\{ e^{+in\pi/2} \frac{\sin[((p-q)L/\hbar - n\pi)/2]}{[(p-q)L/\hbar - n\pi]} - e^{-in\pi/2} \frac{\sin[((p-q)L/\hbar + n\pi)/2]}{[(p-q)L/\hbar + n\pi]} \right\}$$

and we briefly sketch out some of the necessary steps in the evaluation of  $P_W^{(n)}(x, p)$  in this approach.

Combining the various complex exponentials and using the fact that the Wigner function must be real, we are left with integrals such as

$$\mathcal{I}_1 = \int_{-\infty}^{+\infty} \cos \left[ \frac{qL}{\hbar} \left( \frac{L-2x}{L} \right) \right] \frac{\sin[((p+q)L/\hbar - n\pi)/2]}{[(p+q)L/\hbar - n\pi]} \frac{\sin[((p-q)L/\hbar - n\pi)/2]}{[(p-q)L/\hbar - n\pi]} dq. \quad (\text{B2})$$

In this case, the appropriate partial fraction identity to rewrite the denominators is

$$\frac{1}{((p+q)L/\hbar - n\pi)((p-q)L/\hbar - n\pi)} = \frac{1}{2(pL/\hbar - n\pi)} \left\{ \frac{1}{((p+q)L/\hbar - n\pi)} + \frac{1}{((p-q)L/\hbar - n\pi)} \right\} \quad (\text{B3})$$

and the remaining integrals can be done using variations on Eqn. (41). Upon combining various factors, one obtains integrals of that form not only with  $m = (L-2x)/L$ , as in Eqn. (40), but similar ones with  $m = (L-4x)/L$  and  $m = (3L-4x)/L$ . These terms give rise to limits on the  $x$  dependence of the form  $\mathcal{R}(x; 0, L/2)$  and  $\mathcal{R}(x; L/2, L)$  where  $\mathcal{R}(x; a, b)$  is defined in Eqn. (45). For example, one intermediate result can be written in the form

$$\mathcal{T} = \cos \left[ \left( \frac{pL}{\hbar} - n\pi \right) \left( \frac{L-2x}{L} \right) \right] \sin \left[ \left( \frac{pL}{\hbar} - n\pi \right) \right] \mathcal{R}(x; 0, L) \quad (\text{B4})$$

$$- \sin \left[ \left( \frac{pL}{\hbar} - n\pi \right) \left( \frac{L-2x}{L} \right) \right] \cos \left[ \left( \frac{pL}{\hbar} - n\pi \right) \right] \{ \mathcal{R}(x; 0, L/2) - \mathcal{R}(x; L/2, L) \}$$

which, in turn, gives

$$\mathcal{T} = \begin{cases} 0 & \text{for } x < 0, x > L \\ \sin[(2(p/\hbar - n\pi/L)x)] & \text{for } 0 < x < L \\ \sin[(2(p/\hbar - n\pi/L)(L-x))] & \text{for } L/2 < x < L \end{cases} \quad (\text{B5})$$

so that the ‘split’ definition of  $P_W^{(n)}(x, p)$  in the two half intervals arises very naturally and the complete result in Eqn. (60) is reproduced using momentum-space methods, including the non-trivial  $x$  dependence.

### APPENDIX C: PROBLEMS

**P1:** Complete the proof that the  $\phi_n(p)$  for the ISW are orthonormal by explicit calculation of  $\langle \phi_m | \phi_n \rangle$ , completing the steps in Sec. III, and making use of identities such as Eqn. (47).

**P2:** Using results from any quantum mechanics textbook, evaluate the Wigner distribution for the ground state and first excited state of the simple harmonic oscillator. **Answer:** The harmonic oscillator eigenstates can be written in the form

$$u_n(z) = A_n H_n(z) e^{-z^2/2} \quad \text{where} \quad A_n \equiv \frac{1}{\sqrt{2^n n!} \sqrt{\pi}} \quad \text{and} \quad z \equiv \frac{x}{b} = \frac{x}{\sqrt{\hbar/m\omega}} \quad (\text{C1})$$

and the  $H_n(z)$  are the Hermite polynomials of order  $n$ . The Wigner functions for  $n = 0, 1$  are then given by

$$P_W^{(0)}(x, p) = \frac{1}{\pi \hbar} e^{-\rho^2} \quad (\text{C2})$$

$$P_W^{(1)}(x, p) = \frac{1}{\pi \hbar} e^{-\rho^2} (2\rho^2 - 1) \quad (\text{C3})$$

where

$$\rho^2 \equiv \frac{x^2}{b^2} + \frac{b^2 p^2}{\hbar^2}. \quad (\text{C4})$$

This is one of the simpler results which shows explicitly that the Wigner function need not be positive-definite. Note that the first of these results is consistent with the expression for the free-particle Gaussian in Eqn. (18) for vanishing  $x_0$ ,  $p_0$ , and  $t$ . The Wigner function for arbitrary  $n$  has been evaluated (see, *e.g.*, Ref. [7]) with the result that

$$P_W^{(n)} = \frac{(-1)^n}{\pi \hbar} e^{-\rho^2} L_n(2\rho^2) \quad (\text{C5})$$

where  $L_n(z)$  are the Laguerre polynomials.

**P3:** Show how the phase-space plot for the 1-D harmonic oscillator can be used to generate the classical probability densities for position- and momentum-variables, namely, show how

one obtains

$$P_{CL}(x) = \frac{1}{\pi \sqrt{x_A^2 - x^2}} \quad \text{and} \quad P_{CL}(p) = \frac{1}{\pi \sqrt{p_A^2 - p^2}}. \quad (\text{C6})$$

**Partial answer:** The classical probability distribution from Eqn. (50) can be written in the form

$$P_{CL}(x, p) \propto \delta(p(x)^2 - p^2) = \frac{1}{2p(x)} [\delta(p(x) - p) + \delta(p(x) + p)] \quad (\text{C7})$$

where

$$p(x) = \sqrt{2mE - m^2\omega^2x^2} = m\omega \sqrt{x_A^2 - x^2}. \quad (\text{C8})$$

Integration of Eqn. (C7) over  $dp$  then gives

$$P_{CL}(x) \propto \frac{1}{p(x)} \propto \frac{1}{\sqrt{x_A^2 - x^2}} \quad (\text{C9})$$

which when properly normalized (integrated over the classically allowed interval  $(-x_A, +x_A)$ ) gives the first term in Eqn. (C6).

**P4:** Using either the momentum- or position-space wavefunctions in Eqns. (14) or (15) for the free-particle Gaussian wave packet, show that the Wigner function is of the form in Eqn. (18).

**P5:** Complete the proof that the result for the Wigner function for eigenstates of the ISW in Eqn. (60) can be obtained using momentum-space wavefunctions, using the techniques in Appendix B.

**P6:** Use the results in Eqn. (30) and (63) to write down the time-dependent Wigner function for the simple two-state system in the infinite well

$$\psi(x, 0) = \frac{1}{\sqrt{2}} [u_1(x) + u_2(x)] \quad (\text{C10})$$

and generate plots of  $P_W^{(\psi)}(x, p; t)$  for various times. Compare the results to standard images of the position-space and momentum-space probability densities for this problem [48], [49]. What is the only time scale associated with this system? and does it have anything to do with a classical periodicity?