III. INFINITE SQUARE WELL RESULTS IN POSITION AND MOMENTUM SPACE

Because the Wigner function can be evaluated using either position- or momentum-space wavefunctions, we review the properties of, and interconnections between, these solutions for the infinite square well (ISW). The standard problem of a particle of mass m confined by the potential

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} \end{cases} \tag{33}$$

has energy eigenvalues and position-space eigenfunctions (which are non-zero only within the well) which are given by

$$E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2} = \frac{p_n^2}{2m} \qquad (p_n \equiv n\pi\hbar/L) \qquad \text{with} \qquad u_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) . \tag{34}$$

The position-space eigenfunctions have a generalized parity property about the midpoint of the well since

$$u_n(L-x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi(L-x)}{L}\right) = -\sqrt{\frac{2}{L}}\cos(n\pi)\sin\left(\frac{n\pi x}{L}\right) = (-1)^{n+1}\, u_n(x) . \tag{35}$$

As with any such system, the eigenfunctions can be made orthonormal, which in this case can be readily checked explicitly by direct calculation of

$$\begin{aligned} \langle u_m | u_n \rangle &= \left(\frac{2}{L}\right)\int_0^L \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right) dx \\ &= \left\{ \frac{\sin[(m-n)\pi]}{(m-n)\pi} - \frac{\sin[(m+n)\pi]}{(m+n)\pi} \right\} = \delta_{m,n} . \end{aligned} \tag{36}$$

The momentum-space eigenfunctions are given by Eqn. (2) as

$$\begin{aligned} \phi_n(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_0^L u_n(x)\, e^{-ipx/\hbar}\, dx \\ &= (-i)\sqrt{\frac{L}{\pi\hbar}} e^{-ipL/2\hbar}\left[e^{+in\pi/2}\,\frac{\sin[(pL/\hbar - n\pi)/2]}{(pL/\hbar - n\pi)} - e^{-in\pi/2}\,\frac{\sin[(pL/\hbar + n\pi)/2]}{(pL/\hbar + n\pi)} \right] \end{aligned}$$

and the resulting probability density is given by

$$\begin{aligned} |\phi_n(p)|^2 &= \left(\frac{L}{\hbar\pi}\right)\left[\frac{\sin^2[(pL/\hbar - n\pi)/2]}{(pL/\hbar - n\pi)^2} + \frac{\sin^2[(pL/\hbar + n\pi)/2]}{(pL/\hbar + n\pi)^2} \right. \\ &\qquad \left. -2\cos(n\pi)\frac{\sin[(pL/\hbar - n\pi)/2]\sin[(pL/\hbar + n\pi)/2]}{(pL/\hbar - n\pi)(pL/\hbar + n\pi)} \right] \end{aligned} \tag{37}$$

which will be useful for visualization purposes.

While these forms demonstrate more explicitly the strong peaking of the probability amplitude near the expected values of $p = \pm p_n = \pm n\pi\hbar/L$, they do not make clear the finite extent (limited to the range $[0, L]$) of the position-space amplitude. In order to exemplify this dependence, we can evaluate the inverse Fourier transform, via Eqn. (1), to explicitly obtain $u_n(x)$. Because such calculations will be useful in the evaluation of the Wigner distribution using momentum-space wavefunctions, we examine this seldom-discussed analysis [11] in some detail. We require

$$\begin{aligned} u_n(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi_n(p)\, e^{ipx/\hbar}\, dp \\ &= (-i)\sqrt{\frac{L}{2\pi^2\hbar^2}} \left\{ e^{+in\pi/2} \int_{-\infty}^{+\infty} e^{ip(x-L/2)/\hbar}\, \frac{\sin[(pL/\hbar - n\pi)/2]}{(pL/\hbar - n\pi)}\, dp \right. \\ &\qquad \left. - e^{-in\pi/2} \int_{-\infty}^{+\infty} e^{ip(x-L/2)/\hbar}\, \frac{\sin[(pL/\hbar + n\pi)/2]}{(pL/\hbar + n\pi)}\, dp \right\} \\ &\equiv (-i)\sqrt{\frac{L}{2\pi^2\hbar^2}} \left\{ e^{+in\pi/2} I_A - e^{-in\pi/2} I_B \right\} . \end{aligned} \tag{38}$$

Each integral, I_A, I_B, can be done in turn using a change of variables, giving, for example,

$$\begin{aligned} I_A &= \int_{-\infty}^{+\infty} e^{ip(x-L/2)/\hbar}\, \frac{\sin[(pL/\hbar - n\pi)/2]}{(pL/\hbar - n\pi)}\, dp \\ &= \left(\frac{\hbar}{L}\right) e^{+in\pi x/L}\, e^{-in\pi/2} \int_{-\infty}^{+\infty} \frac{\sin(q)}{q}\, e^{imq}\, dq \\ &= \left(\frac{\hbar}{L}\right) e^{+in\pi x/L}\, e^{-in\pi/2} \int_{-\infty}^{+\infty} \frac{\sin(q)}{q}\, [\cos(mq) + i\sin(mq)]\, dq \end{aligned} \tag{39}$$

where we have used

$$q \equiv \frac{1}{2}\left(\frac{pL}{\hbar} - n\pi\right) \qquad \text{and} \qquad m \equiv \frac{(2x - L)}{L} . \tag{40}$$

The piece of I_A which includes the $\sin(mq)$ term vanishes for symmetry reasons (odd integrand over a symmetric interval), while the component with $\cos(mq)$ can be done using standard handbook [47] results, which we review in Appendix A. The result is

$$\int_{-\infty}^{+\infty} \frac{\sin(q)}{q} \cos(mq)\, dq = \begin{cases} \pi & \text{for } m^2 < 1 \\ \pi/2 & \text{for } m^2 = 1 \\ 0 & \text{for } m^2 > 1 \end{cases} \tag{41}$$

The restriction on m corresponds to

$$m^2 = \left(\frac{2x - L}{L}\right)^2 < 1 \qquad \longrightarrow \qquad -1 < \frac{2x - L}{L} < +1 \qquad \longrightarrow \qquad 0 < x < L \tag{42}$$

which explicitly demonstrates the finite extent of the position-space wavefunction which is non-vanishing only in the range $[0, L]$, as expected. Performing the second integral (I_B) in the same way, and combining factors, we find that the non-vanishing position-space wavefunction is given by

$$\begin{aligned} u_n(x) &= (-i)\sqrt{\frac{L}{2\pi^2\hbar^2}}\left(\frac{\hbar\pi}{L}\right)\left\{e^{+in\pi/2}e^{+in\pi x/L}\,e^{-in\pi/2} - e^{-in\pi/2}e^{-in\pi x/L}\,e^{+in\pi/2}\right\} \\ &= \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \qquad\qquad \text{for } 0 < x < L \end{aligned} \tag{43}$$

again, as expected. For future notational convenience, we can write this in the form

$$u_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\,\mathcal{R}(x; 0, L) \tag{44}$$

where

$$\mathcal{R}(x; a, b) = \begin{cases} 0 & \text{for } x < a, x > b \\ 1/2 & \text{for } x = a, x = b \\ 1 & \text{for } a < x < b \end{cases} . \tag{45}$$

(We note that the results from Eqns. (41), (44), and (45) can also be expressed in terms of of the Heaviside step-function, $\Theta(\xi)$, as, for example in Ref. [26].

Just as in position space, it is possible to explicitly demonstrate the orthonormality of the momentum-space eigenfunctions, by calculating $\langle\phi_m|\phi_n\rangle$. Since similar methods will also be useful in what follows, we illustrate one typical step in such an evaluation. One required integral, for example, is given by

$$\mathcal{I} = \left(\frac{L}{\pi\hbar}\right)\, e^{i(n-m)\pi/2}\int_{-\infty}^{+\infty}\frac{\sin[(pL/\hbar - m\pi)/2]\,\sin[(pL/\hbar - n\pi)/2]}{(pL/\hbar - m\pi)(pL/\hbar - n\pi)}\,dp \tag{46}$$

The denominator can be written in a form which allows use of standard integrals, namely

$$\frac{1}{(pL/\hbar - m\pi)(pL/\hbar - n\pi)} = \frac{1}{(m-n)\pi}\left[\frac{1}{(pL/\hbar - m\pi)} - \frac{1}{(pL/\hbar - n\pi)}\right] . \tag{47}$$

Appropriate changes of variables and integrals as in Eqn. (41) then give simple closed form expressions, and the complete result for $\langle\phi_m|\phi_n\rangle$ is the indeed same as in Eqn. (36).

Finally, for eventual comparison to the Wigner distributions for the ISW, we plot some standard representations of the position- and momentum-space probability densities for two low-lying states ($n = 1, 10$) in Fig. 1.