

Note on Square Well

Ning Sun

March 25, 2016

1 ONE-DIMENSIONAL STATIC SQUARE WELL

Consider a square well potential of infinite depth

$$V_0(x) = \begin{cases} 0, & x \in [-L, L] \\ \infty, & \text{otherwise} \end{cases}$$

Hamiltonian writes $H_0(x) = \frac{p^2}{2m} + V_0(x)$.

Ground State

Eigenvalues and real space wave functions are

$$E_n = \frac{\hbar^2 \pi^2 n^2}{8mL^2}, \quad n \in \mathbb{Z}^+$$
$$\psi_n(x) = \begin{cases} \sqrt{\frac{1}{L}} \cos \left[\frac{n+1}{2} \frac{\pi x}{2L} \right], & \text{for odd } n \\ \sqrt{\frac{1}{L}} \sin \left[\frac{n}{2} \frac{\pi x}{2L} \right], & \text{for even } n \end{cases}$$

Then ground state wave function is

$$\psi_g(x) = \psi_1(x) = \begin{cases} \sqrt{\frac{1}{L}} \cos \left(\frac{\pi x}{2L} \right), & x \in [-L, L] \\ 0, & \text{otherwise} \end{cases}$$

Momentum Distribution

Take Fourier transformation,

$$\boxed{\begin{aligned} \psi(x) &= \frac{1}{2\pi} \int \phi(k) e^{ikx} dk \\ \phi(k) &= \int \psi(x) e^{-ikx} dx \end{aligned}}$$

of ground state wave function $\psi_0(x) = \sqrt{1/L} \cos(k_0 x)$ with $k_0 = \pi/2L$, we obtain

$$\begin{aligned}
\phi_0(k) &= \int \psi_0(x) e^{-ikx} dx = \sqrt{\frac{1}{L}} \int_{-L}^L \frac{e^{ik_0 x} + e^{-ik_0 x}}{2} e^{-ikx} dx \\
&= \frac{1}{2} \sqrt{\frac{1}{L}} \left[\int_{-L}^L e^{i(k_0 - k)x} dx + \int_{-L}^L e^{-i(k_0 + k)x} dx \right] \\
&= \sqrt{\frac{1}{L}} \left\{ \frac{\sin[(k - k_0)L]}{(k - k_0)} + \frac{\sin[(k + k_0)L]}{(k + k_0)} \right\} \\
&= \sqrt{\frac{1}{L}} \frac{(k + k_0) \sin[(k - k_0)L] + (k - k_0) \sin[(k + k_0)L]}{(k - k_0)(k + k_0)} \\
&= \sqrt{\frac{1}{L}} \frac{-2k_0 \cos(kL)}{k^2 - k_0^2} \\
&= \sqrt{\frac{2k_0}{\pi}} \frac{-2k_0}{k^2 - k_0^2} \cos \left[\frac{\pi}{2} \left(\frac{k}{k_0} \right) \right]
\end{aligned}$$

Thus the momentum distribution of the ground state is¹

$$\begin{aligned}
n_0(p) dp &= \left| \phi_0(p/\hbar) \right|^2 \frac{dp}{2\pi\hbar} \\
&= \frac{1}{2\pi\hbar} \frac{1}{L} \frac{4k_0^2 \cos^2(kL)}{k^2 - k_0^2} dp \\
&= \frac{8\pi\hbar^3 L}{(4p^2 L^2 - \pi^2 \hbar^2)^2} \cos^2 \left(\frac{pL}{\hbar} \right) dp
\end{aligned}$$

$$n_0(p) = \frac{8\pi\hbar^3 L}{(4p^2 L^2 - \pi^2 \hbar^2)^2} \cos^2 \left(\frac{pL}{\hbar} \right)$$

When p is large, it decays as p^{-4} power law.

¹See Landau Non-relativistic QM, Sec. 22, Problem 1.

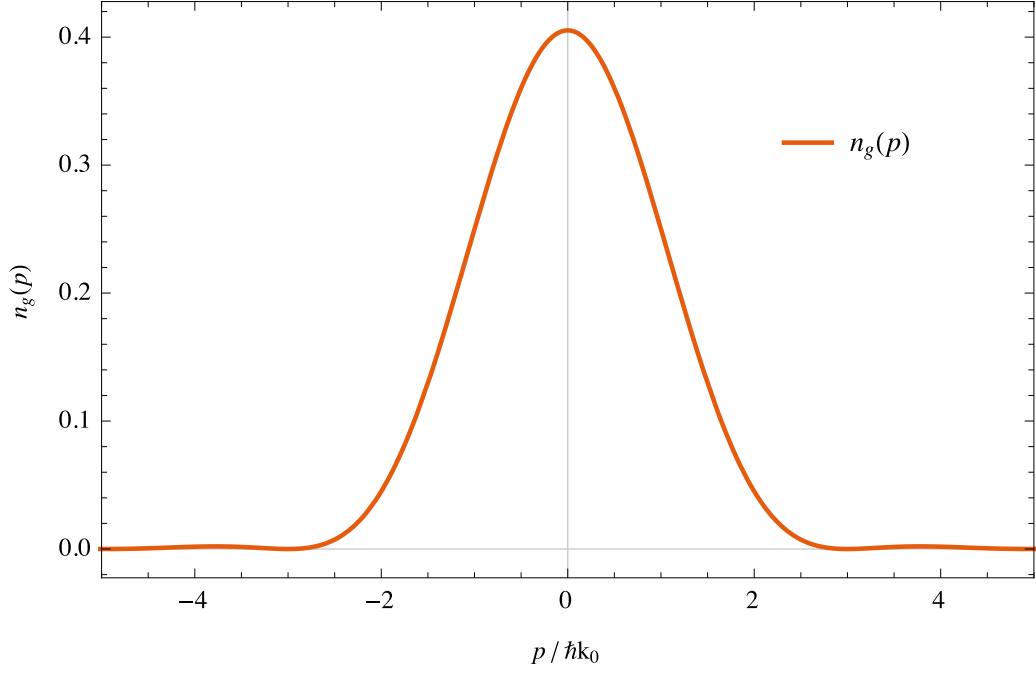


Fig. 1 (a) Momentum distribution

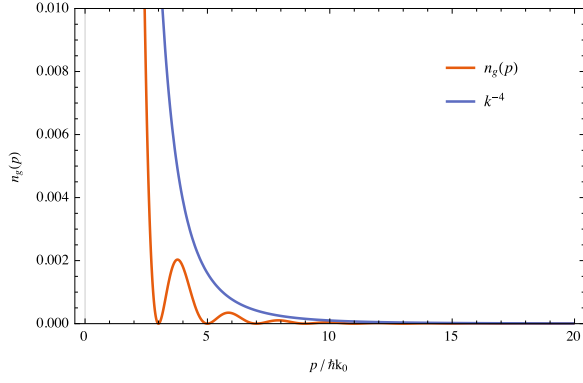


Fig. 1 (b) comparison with -4 power law curve

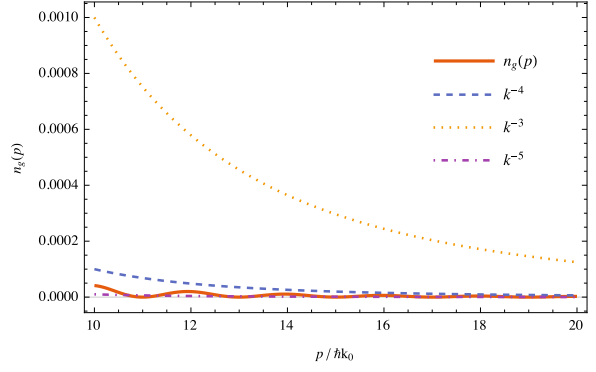


Fig. 1 (c) comparison with $-4, 3, 5$ power law curves

Fig. 1: Momentum distribution of the ground state (initial state). Tail of the curve behaves as -4 power law decay.

2 SHAKEN WELL

Unitary Transformation

The time-dependent potential writes

$$V(x, t) = \begin{cases} 0, & x \in [-L + a \sin(\omega t), L + a \sin(\omega t)] \\ \infty, & \text{otherwise} \end{cases}$$

We see the time-dependent potential goes as $V(x(t)) = V(x + a \sin(\omega t))$. By making an unitary transformation $U(t) = e^{i x m a \omega \cos(\omega t)} e^{-i a \sin(\omega t) p}$, we obtain the Hamiltonian in co-moving frame as²

$$\begin{aligned} \mathcal{H} &= U H U^\dagger + i(\partial_t U) U^\dagger \\ &= H_0 + m a \omega^2 \sin(\omega t) x \\ &= H_0 + \gamma x \sin(\omega t) \end{aligned}$$

Thus the effective potential and time-dependent Hamiltonian in co-moving frame is

$$\begin{aligned} V(x, t) &= \begin{cases} \gamma x \sin(\omega t), & x \in [-L, L] \\ \infty, & \text{otherwise} \end{cases} \\ \mathcal{H}(x, t) &= \frac{p^2}{2m} + V(x, t) \end{aligned} \tag{1}$$

In the following we solve for evolution of state dominated by this Hamiltonian.

Floquet Approach

When $t \leq 0$, system is prepared in the ground state of H_0 , i.e. $\psi_g(x) = \sqrt{\frac{1}{L}} \cos\left(\frac{\pi x}{2L}\right)$ for $x \in [-L, L]$ and vanishes otherwise. $t \geq 0$ turn on shaking. We try Floquet approach to analyse the evolution of the state when $t \geq 0$.

For time-periodic Hamiltonian $H(t + T) = H(t)$, there are solutions called Floquet states

$$\begin{aligned} \Psi^{(\alpha)}(t) &= e^{-i \varepsilon_\alpha t} \Phi^{(\alpha)}(t) \\ \Phi^{(\alpha)}(t) &= \Phi^{(\alpha)}(t + T) \end{aligned}$$

such that $H_F \Phi^{(\alpha)} = \varepsilon_\alpha \Phi^{(\alpha)}$, where $H_F = H(t) - i \partial_t$ is the Floquet Hamiltonian. We could always

²In this note, all \hbar set 1.

solve for Floquet states in real space representation. To be specific, we expand the Floquet modes as

$$\begin{aligned}\Phi^{(\alpha)}(x, t) &= \sum_n e^{in\omega t} \sum_m a_{n,m}^{(\alpha)} u_m(x) \\ &= \sum_{n,m} a_{n,m}^{(\alpha)} e^{in\omega t} u_m(x)\end{aligned}$$

Here $\{u_m(x)\}$ are eigenstates of H_0 . Also, we write down the Floquet Hamiltonian under basis of plain waves plus eigenstates of the original static square well, i.e. $\{|n, m\rangle \rightarrow e^{in\omega t} u_m(x)\}$, such that

$$\begin{aligned}H_{n,n} &= H_0 + n\omega \\ H_{n,n\pm 1} &= \frac{\gamma x}{2} \\ H_{n,n'} &= 0 \quad \text{for other } n, n'\end{aligned}$$

and, more specifically,

$$\begin{aligned}H_{n,n} &= E_m \delta_{m,m'} + n\omega \\ H_{n,n\pm 1} &= \frac{\gamma}{2} \int_{-L}^L u_m^*(x) x u_{m'}(x) dx\end{aligned}$$

where

$$\begin{aligned}E_m &= \frac{\hbar^2 \pi^2 m^2}{8\mu L} = \frac{\hbar^2 (mk_0)^2}{2\mu} \\ \text{for } m \text{ odd: } u_m(x) &= \sqrt{\frac{1}{L}} \cos \left[\frac{m+1}{2} \frac{\pi x}{2L} \right], \quad x \in [-L, L] \\ &= \sqrt{\frac{2k_0}{\pi}} \cos \left(\frac{m+1}{2} k_0 x \right) \\ \text{for } m \text{ even: } u_m(x) &= \sqrt{\frac{1}{L}} \sin \left[\frac{m}{2} \frac{\pi x}{2L} \right], \quad x \in [-L, L] \\ &= \sqrt{\frac{2k_0}{\pi}} \sin \left(\frac{m}{2} k_0 x \right)\end{aligned}$$

For example, a typical block $H_{n,n\pm 1}$ truncated to the first 6 bound states subspace writes

$$H_{n,n\pm 1} = \begin{pmatrix} 0 & \frac{L\gamma}{2\pi} & 0 & \frac{16L\gamma}{9\pi^2} & 0 & \frac{L\gamma}{4\pi} \\ \frac{L\gamma}{2\pi} & 0 & -\frac{20L\gamma}{9\pi^2} & 0 & -\frac{3L\gamma}{4\pi} & 0 \\ 0 & -\frac{20L\gamma}{9\pi^2} & 0 & -\frac{L\gamma}{4\pi} & 0 & \frac{52L\gamma}{25\pi^2} \\ \frac{16L\gamma}{9\pi^2} & 0 & -\frac{L\gamma}{4\pi} & 0 & -\frac{48L\gamma}{25\pi^2} & 0 \\ 0 & -\frac{3L\gamma}{4\pi} & 0 & -\frac{48L\gamma}{25\pi^2} & 0 & \frac{L\gamma}{6\pi} \\ \frac{L\gamma}{4\pi} & 0 & \frac{52L\gamma}{25\pi^2} & 0 & \frac{L\gamma}{6\pi} & 0 \end{pmatrix}$$

Now we have Floquet states exactly solutions of the time-dependent Hamiltonian,

$$i\partial_t|\Psi^{(\alpha)}(t)\rangle = H(t)|\Psi^{(\alpha)}(t)\rangle$$

Then evolution of the system is just some superposition of the evolution of Floquet state with initial condition fit. Means, we expand the initial state in the Floquet basis at $t = 0$, then the state at some moment $t > 0$ could be obtained just as superposition of those Floquet states at that time t .

$$\begin{aligned} |\psi(0)\rangle &= \sum_{\alpha} |\Psi^{(\alpha)}(0)\rangle \langle \Psi^{(\alpha)}(0) | \psi(0) \rangle \\ &= \sum_{\alpha} c_{\alpha} |\Psi^{(\alpha)}(0)\rangle \end{aligned}$$

then

$$|\psi(t)\rangle = \sum_{\alpha} c_{\alpha} |\Psi^{(\alpha)}(t)\rangle$$

because $\Psi^{(\alpha)}(t)$ is a general solution of $H(t)$.

More specifically, in real space representation the wave function of Floquet state is

$$\begin{aligned} \Psi^{(\alpha)}(x, t) &= e^{-i\varepsilon_{\alpha}t} \sum_{n,m} a_{n,m}^{(\alpha)} e^{in\omega t} u_m(x) \\ \varepsilon_{\alpha} &\in [0, \omega] \end{aligned}$$

The initial state is the ground state of infinite-depth-square-well potential

$$\psi(x, 0) = u_1(x) = \sqrt{\frac{1}{L}} \cos\left(\frac{\pi x}{2L}\right)$$

$$\Psi^{(\alpha)}(x, 0) = \sum_{n,m} a_{n,m}^{(\alpha)} u_m(x) = \sum_m \left(\sum_n a_{n,m}^{(\alpha)} \right) u_m(x)$$

$$\begin{aligned} c_{\alpha} &= \langle \Psi^{(\alpha)}(0) | \psi(0) \rangle = \int_{-L}^L \left[\sum_m \left(\sum_n a_{n,m}^{(\alpha)} \right) u_m(x) \right] u_1(x) dx \\ &= \left[\sum_m \left(\sum_n a_{n,m}^{(\alpha)} \right) \int_{-L}^L u_m(x) u_1(x) dx \right] \\ &= \sum_m \left(\sum_n a_{n,m}^{(\alpha)} \right) \delta_{m,1} = \sum_n a_{n,1}^{(\alpha)} \end{aligned}$$

and

$$\begin{aligned}
\psi(x, t) &= \sum_{\alpha} c_{\alpha} \Psi^{(\alpha)}(x, t) \\
&= \sum_{\alpha} \left[\left(\sum_{n'} a_{n',1}^{(\alpha)} \right) e^{-i\epsilon_{\alpha} t} \sum_{n,m} a_{n,m}^{(\alpha)} e^{in\omega t} u_m(x) \right] \\
&= \sum_m \left[\sum_{\alpha} \left(\sum_{n'} a_{n',1}^{(\alpha)} \right) e^{-i\epsilon_{\alpha} t} \sum_n a_{n,m}^{(\alpha)} e^{in\omega t} \right] u_m(x) \\
&= \sum_m \left\{ \sum_n \left[\sum_{\alpha} \left(\sum_{n'} a_{n',1}^{(\alpha)} \right) e^{-i\epsilon_{\alpha} t} a_{n,m}^{(\alpha)} \right] e^{in\omega t} \right\} u_m(x) \\
&= \sum_{\alpha, n, m} c_{\alpha} a_{n,m}^{(\alpha)} e^{-i\epsilon_{\alpha} t} e^{in\omega t} u_m(x)
\end{aligned}$$

Fourier Transformation

We obtain wave function in momentum space by doing Fourier transformation on both sides³

$$\begin{aligned}
\phi(k, t) &= \sum_m \left[\sum_{\alpha} \left(\sum_{n'} a_{n',1}^{(\alpha)} \right) e^{-i\epsilon_{\alpha} t} \sum_n a_{n,m}^{(\alpha)} e^{in\omega t} \right] f_m(k) \\
&= \sum_m \left[\sum_{\alpha} c_{\alpha} e^{-i\epsilon_{\alpha} t} \sum_n a_{n,m}^{(\alpha)} e^{in\omega t} \right] f_m(k) \\
&= \sum_m \sum_n \sum_{\alpha} c_{\alpha} a_{n,m}^{(\alpha)} e^{-i\epsilon_{\alpha} t} e^{in\omega t} f_m(k)
\end{aligned}$$

where

$$\begin{aligned}
\phi(k, t) &= \int \psi(x, t) e^{-ikx} dx \\
f_m(k) &= \int u_m(x) e^{-ikx} dx
\end{aligned}$$

Then momentum distribution at time $t(> 0)$ is thus

$$n(p, t) dp = \left| \phi(k, t) \right|^2 \frac{dp}{2\pi\hbar}$$

where

$$\begin{aligned}
\left| \phi(k, t) \right|^2 &= \left(\sum_{m'} \sum_{n'} \sum_{\alpha'} c_{\alpha'} a_{n',m'}^{(\alpha')} e^{i\epsilon_{\alpha'} t} e^{-in'\omega t} f_{m'}^*(k) \right) \left(\sum_m \sum_n \sum_{\alpha} c_{\alpha} a_{n,m}^{(\alpha)} e^{-i\epsilon_{\alpha} t} e^{in\omega t} f_m(k) \right) \\
&= \sum_{m,m'} \sum_{n,n'} \sum_{\alpha,\alpha'} c_{\alpha'} c_{\alpha} a_{n',m'}^{(\alpha')} a_{n,m}^{(\alpha)} e^{-i(\epsilon_{\alpha} - \epsilon_{\alpha'}) t} e^{i(n-n')\omega t} f_{m'}^*(k) f_m(k)
\end{aligned}$$

³This works because Fourier transformation is linear.

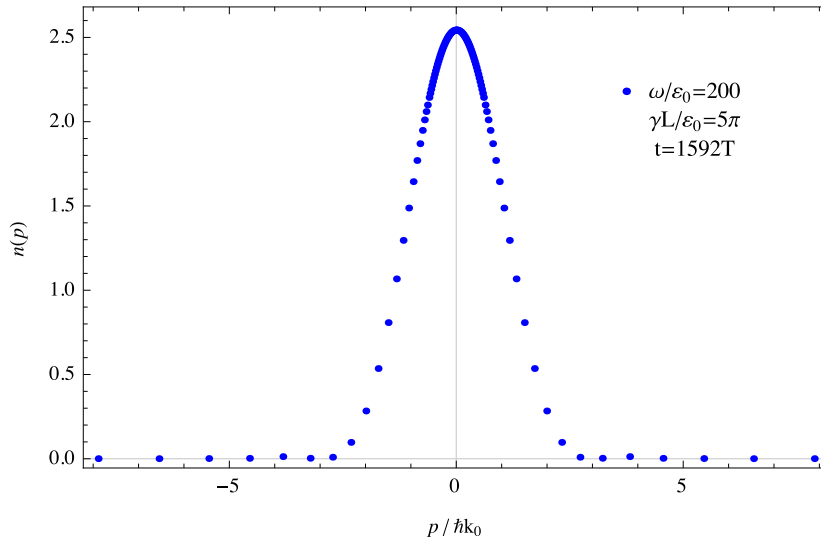
Some $u_m(x)$ and $f_m(k)$ are listed here. PS: $k_0 \cdot 2L = \pi$

$u_1(x) = \sqrt{\frac{2k_0}{\pi}} \cos(k_0 x)$	$f_1(k) = -2\sqrt{\frac{2}{\pi k_0}} \frac{1}{(k/k_0)^2 - 1} \cos\left[\frac{\pi}{2} \left(\frac{k}{k_0}\right)\right]$
$u_2(x) = \sqrt{\frac{2k_0}{\pi}} \sin(k_0 x)$	$f_2(k) = 2i\sqrt{\frac{2}{\pi k_0}} \frac{k/k_0}{(k/k_0)^2 - 1} \cos\left[\frac{\pi}{2} \left(\frac{k}{k_0}\right)\right]$
$u_3(x) = \sqrt{\frac{2k_0}{\pi}} \cos(2k_0 x)$	$f_3(k) = -2\sqrt{\frac{2}{\pi k_0}} \frac{k/k_0}{(k/k_0)^2 - 2^2} \sin\left[\frac{\pi}{2} \left(\frac{k}{k_0}\right)\right]$
$u_4(x) = \sqrt{\frac{2k_0}{\pi}} \sin(2k_0 x)$	$f_4(k) = 4i\sqrt{\frac{2}{\pi k_0}} \frac{1}{(k/k_0)^2 - 2^2} \sin\left[\frac{\pi}{2} \left(\frac{k}{k_0}\right)\right]$
$u_5(x) = \sqrt{\frac{2k_0}{\pi}} \cos(3k_0 x)$	$f_5(k) = 6\sqrt{\frac{2}{\pi k_0}} \frac{1}{(k/k_0)^2 - 3^2} \cos\left[\frac{\pi}{2} \left(\frac{k}{k_0}\right)\right]$
$u_6(x) = \sqrt{\frac{2k_0}{\pi}} \sin(3k_0 x)$	$f_6(k) = -2i\sqrt{\frac{2}{\pi k_0}} \frac{k/k_0}{(k/k_0)^2 - 3^2} \cos\left[\frac{\pi}{2} \left(\frac{k}{k_0}\right)\right]$
...	...

Result

We numerically calculate momentum distribution after a period of evolution using above approach.

For some parameters, we carry out the following result.



Power law fitting shows its decay at large p is also of power law of index around 4, which is astounding to me. Numerical result gives $n(p) \propto 3.57 \times p^{-3.90}$ at large p .