Note on Square Well

Ning Sun
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I. 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 $H_0(x) = \dfrac{p^2}{2m} + V_0(x)$.

A. Ground State

Eigenvalues and real space wave functions are

$$E_n = \frac{\hbar^2 \pi^2 n^2}{8mL^2} = \frac{\hbar^2 k_0^2}{2m} \cdot n^2\,, \quad n \in \mathbb{Z}^+$$

$$\psi_n(x) = \begin{cases} \sqrt{\dfrac{1}{L}} \cos(nk_0 x)\,, & \text{for odd } n \\ \sqrt{\dfrac{1}{L}} \sin(nk_0 x)\,, & \text{for even } n \end{cases}$$

where $k_0 = \dfrac{\pi}{2L}$.
Then ground state wave function is

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

B. Momentum Distribution

Take Fourier transformation,

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

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

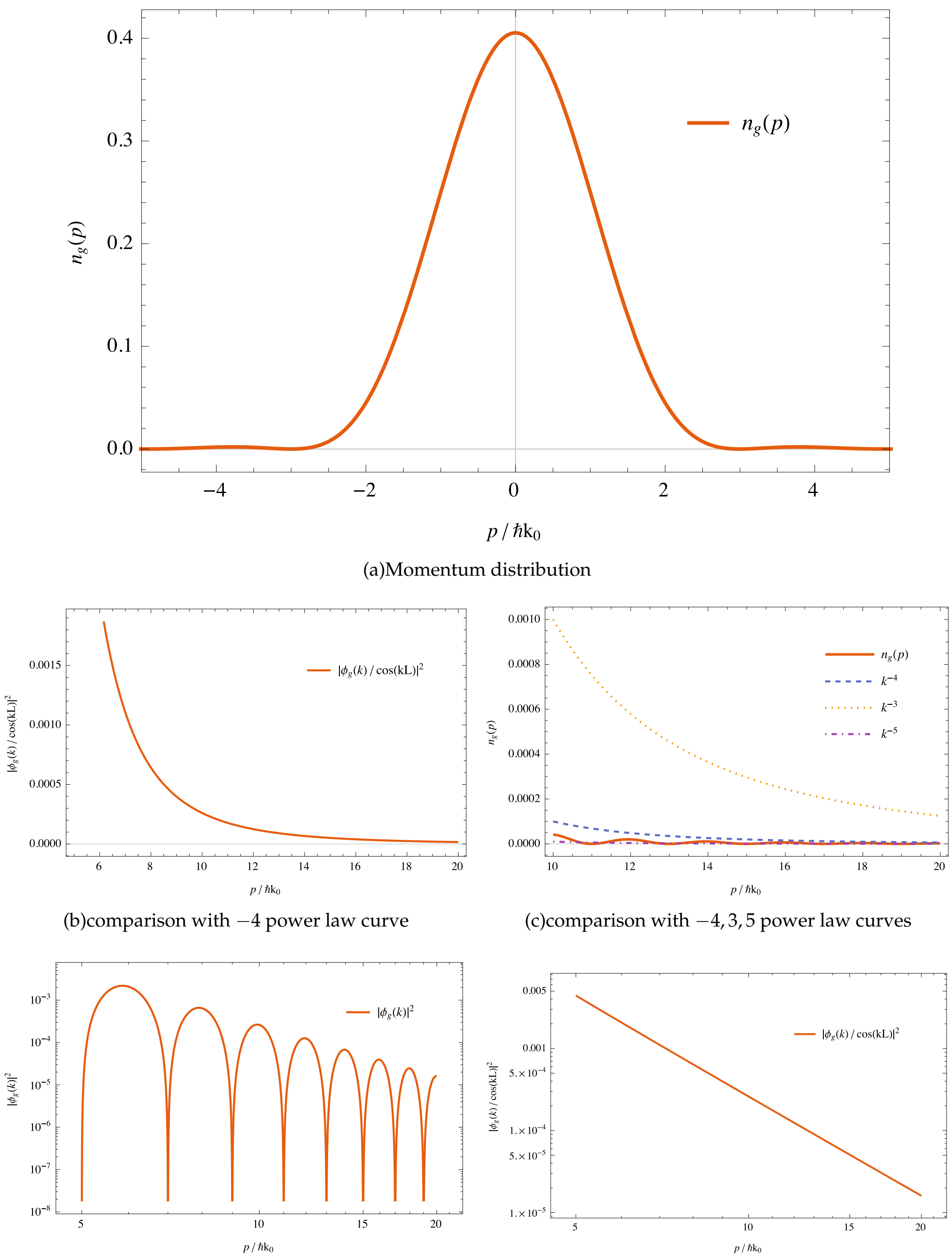
$$\begin{aligned}
\phi_0(k) &= \int \psi_0(x) e^{-\mathrm{i}kx} dx = \sqrt{\frac{1}{L}} \int_{-L}^{L} \frac{e^{\mathrm{i}k_0 x} + e^{-\mathrm{i}k_0 x}}{2} e^{-\mathrm{i}kx} dx \\
&= \frac{1}{2}\sqrt{\frac{1}{L}} \left[\int_{-L}^{L} e^{\mathrm{i}(k_0-k)x} dx + \int_{-L}^{L} e^{-\mathrm{i}(k_0+k)x} dx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

Thus the momentum distribution of the ground state is[1]

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

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

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



(a)Momentum distribution

(b)comparison with -4 power law curve

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

(d)Log-Log plot of $n_g(k)$

(e)double log plot of $|\phi_g(k) / \cos(kL)|^2$

FIG. 1: Momentum distribution of the ground state (initial state). Tail of the curve shows algebraic decay. Specifically, the distribution at large momentum decays as -4 power law.

II. SHAKEN WELL GENERAL

A. 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 $U(t) = e^{\mathrm{i}ma\omega\cos(\omega t)x/\hbar} e^{-\mathrm{i}a\sin(\omega t)p/\hbar}$, we obtain the Hamiltonian in co-moving frame as

$$\begin{aligned} \mathcal{H} &= UHU^\dagger + \mathrm{i}(\partial_t U)U^\dagger \\ &= H_0 + (ma\omega^2/\hbar)x\sin(\omega t) \\ &= H_0 + \gamma x\sin(\omega t) \end{aligned}$$

Here we have defined $\gamma = ma\omega^2/\hbar$.
Thus the effective potential and time-dependent Hamiltonian in co-moving frame is

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

$$\mathcal{H}(x,t) = \frac{p^2}{2m} + V(x,t) \tag{1}$$

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

B. Floquet Approach

When $t \le 0$, 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. $t \ge 0$ turn on shaking. We try Floquet approach to analyse the evolution of the state when $t \ge 0$.
For time-periodic Hamiltonian $H(t+T) = H(t)$, there are solutions called Floquet states

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

such that $H_F\Phi^{(\alpha)} = \varepsilon_\alpha\Phi^{(\alpha)}$, where $H_F = H(t) - \mathrm{i}\partial_t$ is the Floquet Hamiltonian. We could always solve for Floquet states in real space representation. To be specific, we expand the Floquet modes as

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

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. $\{|n,m\rangle \to e^{\mathrm{i}n\omega t}u_m(x)\}$, such that

$$\begin{aligned}H_{n,n} &= H_0 + n\omega\\ H_{n,n\pm1} &= \frac{\gamma x}{2}\\ H_{n,n'} &= 0 \quad \text{for other } n,n'\end{aligned}$$

and, more specificly,

$$\begin{aligned}H_{\substack{n,n\\ m,m'}} &= E_m\delta_{m,m'} + n\omega\\ H_{\substack{n,n\pm1\\ m,m'}} &= \frac{\gamma}{2}\int_{-L}^{L} u^*_m(x)xu_{m'}(x)dx\end{aligned}$$

where

$$\begin{aligned} E_m &= \frac{\hbar^2\pi^2m^2}{8\mu L} = \frac{\hbar^2(mk_0)^2}{2\mu}\\ \text{for } m \text{ odd:} \qquad u_m(x) &= \sqrt{\frac{1}{L}}\cos\left[\frac{m+1}{2}\frac{\pi x}{2L}\right], \quad x\in[-L,L]\\ &= \sqrt{\frac{2k_0}{\pi}}\cos\left(\frac{m+1}{2}k_0x\right)\\ \text{for } m \text{ even:} \qquad u_m(x) &= \sqrt{\frac{1}{L}}\sin\left[\frac{m}{2}\frac{\pi x}{2L}\right], \quad x\in[-L,L]\\ &= \sqrt{\frac{2k_0}{\pi}}\sin\left(\frac{m}{2}k_0x\right)\end{aligned}$$

For example, a typical block $H_{n,n\pm1}$ truncated to the first 6 bound states subspace writes

$$H_{n,n\pm1} = \begin{pmatrix} 0 & \frac{L\gamma}{2\pi} & 0 & \frac{16L\gamma}{9\pi^2} & 0 & \frac{L\gamma}{4\pi}\\ \frac{L\gamma}{2\pi} & 0 & -\frac{20L\gamma}{9\pi^2} & 0 & -\frac{3L\gamma}{4\pi} & 0\\ 0 & -\frac{20L\gamma}{9\pi^2} & 0 & -\frac{L\gamma}{4\pi} & 0 & \frac{52L\gamma}{25\pi^2}\\ \frac{16L\gamma}{9\pi^2} & 0 & -\frac{L\gamma}{4\pi} & 0 & -\frac{48L\gamma}{25\pi^2} & 0\\ 0 & -\frac{3L\gamma}{4\pi} & 0 & -\frac{48L\gamma}{25\pi^2} & 0 & \frac{L\gamma}{6\pi}\\ \frac{L\gamma}{4\pi} & 0 & \frac{52L\gamma}{25\pi^2} & 0 & \frac{L\gamma}{6\pi} & 0 \end{pmatrix}$$

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

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

Then evolution of the system is just some superposition of the evoluton 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.

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

then

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

because $\Psi^{(\alpha)}(t)$ is a general solution of $H(t)$.
More specificly, in real space representation the wave function of Floquet state is

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

at initial time $t_0 = 0$

$$\Psi^{(\alpha)}(x,0) = \sum_{n,m} a^{(\alpha)}_{n,m} u_m(x) = \sum_{m}\left(\sum_{n} a^{(\alpha)}_{n,m}\right) u_m(x)$$

Thus for some initial states, expansion as superposition of Floquet states could be derived through

$$\begin{aligned}c_{\alpha} &= \left\langle\Psi^{(\alpha)}(0)\right|\psi(0)\right\rangle = \int dx \left\langle\Psi^{(\alpha)}(0)\right|x\right\rangle\left\langle x\right|\psi(0)\right\rangle \\ &= \int \Psi^{(\alpha)}(x,0)\psi(x,0)dx \\ &= \int \Big[\sum_{m,n} a^{(\alpha)}_{n,m} u_m(x)\Big]\psi(x,0)dx \\ &= \sum_{m}\left[\Big(\sum_{n} a^{(\alpha)}_{n,m}\Big)\int u_m(x)\psi(x,0)\right]\end{aligned}$$

When we start with the ground state of the square well of infinite depth $\psi(x,0) = u_1(x)$, then

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

and if we start from some other eigenstate $u_{m'}$ of the static potential H_0 then $c_\alpha = \sum_n a_{n,m'}^{(\alpha)}$. Then the evolution of the given state is

$$\begin{aligned} \psi(x,t) &= \sum_\alpha c_\alpha \Psi^{(\alpha)}(x,t) \\ &= \sum_{\alpha,n,m} c_\alpha a_{n,m}^{(\alpha)} e^{-\mathrm{i}\varepsilon_\alpha t} e^{\mathrm{i}n\omega t} u_m(x) \end{aligned}$$

C. Fourier Transformation

We obtain wave function in momentum space by doing Fourier transformation on both sides[2]

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

where

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

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

$$\left|\phi(k,t)\right|^2 = \left(\sum_{m'}\sum_{n'}\sum_{\alpha'} c_{\alpha'} a_{n',m'}^{(\alpha')} e^{\mathrm{i}\varepsilon_{\alpha'} t} e^{-\mathrm{i}n'\omega t} f_{m'}^*(k)\right)\left(\sum_{m}\sum_{n}\sum_{\alpha} c_{\alpha} a_{n,m}^{(\alpha)} e^{-\mathrm{i}\varepsilon_{\alpha} t} e^{\mathrm{i}n\omega t} f_{m}(k)\right)$$
$$= \sum_{m,m'}\sum_{n,n'}\sum_{\alpha,\alpha'} c_{\alpha'} c_{\alpha} a_{n',m'}^{(\alpha')} a_{n,m}^{(\alpha)} e^{-\mathrm{i}(\varepsilon_\alpha-\varepsilon_{\alpha'})t} e^{\mathrm{i}(n-n')\omega t} f_{m'}^*(k) f_m(k)$$

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

$u_1(x) = \sqrt{\frac{2k_0}{\pi}}\cos(k_0 x)$	$f_1(k) = -2\sqrt{\frac{2}{\pi k_0}}\frac{\cos(kL)}{(k/k_0)^2-1}$
$u_2(x) = \sqrt{\frac{2k_0}{\pi}}\sin(2k_0 x)$	$f_2(k) = 4\mathrm{i}\sqrt{\frac{2}{\pi k_0}}\frac{\sin(kL)}{(k/k_0)^2-2^2}$
$u_3(x) = \sqrt{\frac{2k_0}{\pi}}\cos(3k_0 x)$	$f_3(k) = 6\sqrt{\frac{2}{\pi k_0}}\frac{\cos(kL)}{(k/k_0)^2-3^2}$
$u_4(x) = \sqrt{\frac{2k_0}{\pi}}\sin(4k_0 x)$	$f_4(k) = -8\mathrm{i}\sqrt{\frac{2}{\pi k_0}}\frac{\sin(kL)}{(k/k_0)^2-4^2}$
$u_5(x) = \sqrt{\frac{2k_0}{\pi}}\cos(5k_0 x)$	$f_5(k) = -10\sqrt{\frac{2}{\pi k_0}}\frac{\cos(kL)}{(k/k_0)^2-5^2}$
$u_6(x) = \sqrt{\frac{2k_0}{\pi}}\sin(6k_0 x)$	$f_6(k) = 12\mathrm{i}\sqrt{\frac{2}{\pi k_0}}\frac{\sin(kL)}{(k/k_0)^2-6^2}$
$\ldots$	$\ldots$

[1] See Landau Non-relativistic QM, Sec. 22, Problem 1.
[2] This works because Fourier transformation is linear.