CHM452: Problem Set 2

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Let $\mathrm{i} = \sqrt{-1}$, $o(\cdot)$ and $O(\cdot)$ are little-o and big-O notations, respectively, and $\mathbb{N}$ is the set of natural numbers ($\mathbb{N} = \{0,\ 1,\ 2,\ 3,\ \ldots\}$) and $\mathbb{N}_+ = \mathbb{N} \setminus \{0\}$

1. (i) Since $\Psi(x,\ t)$ is a linear combination of $\Phi_n(x,\ t)$, where

$$\Phi_n(x,\ t) = \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w(t)} x\right) \exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w(t)}\right),$$

$w(t) = a + vt$, and $E_n^i = n^2\pi^2\hbar^2/2ma^2$, we only need to check that $\Phi_n(x,\ t)$ satisfies the boundary condition for all $n \in \mathbb{N}_+$

$$\Phi_n(x = 0,\ t) = 0, \qquad \Phi_n(x = w(t),\ t) = 0.$$

On the other hand,

$$\begin{aligned}
\Phi_n(x = 0,\ t) &= \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w(t)} \cdot 0\right) \exp\left(\frac{\mathrm{i}\big(-2E_n^i at\big)}{2\hbar w(t)}\right) = 0,\\
\Phi_n(x = w(t),\ t) &= \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w(t)} w(t)\right) \exp\left(\frac{\mathrm{i}\big(mvw^2 - 2E_n^i at\big)}{2\hbar w(t)}\right)\\
&= \sqrt{\frac{2}{w}} \sin(n\pi) \exp\left(\frac{\mathrm{i}\big(mvw^2 - 2E_n^i at\big)}{2\hbar w(t)}\right) = 0.
\end{aligned}$$

Therefore, $\Phi_n(x,\ t)$ satisfies the boundary conditions, and hence, $\Psi(x,\ t)$ satisfies the boundary conditions. Next, we show that the wavefunction itself also satisfies the TDSE. Since TDSE is linear, we only need to show that $\Phi_n(x,\ t)$ satisfies TDSE for all n. Note that for $0 \le x \le w$

$$\begin{aligned}
\mathrm{i}\hbar \frac{\partial}{\partial t} \Phi_n(x,\ t) &= \mathrm{i}\hbar \frac{\partial}{\partial t} \sqrt{\frac{2}{w(t)}} \sin\left(\frac{n\pi}{w(t)} x\right) \exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w(t)}\right)\\
&= \mathrm{i}\hbar \Bigg[\frac{-v}{2w} \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w} x\right) \exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\\
&\quad + \frac{-n\pi xv}{w^2} \sqrt{\frac{2}{w}} \cos\left(\frac{n\pi}{w} x\right) \exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\\
&\quad + \frac{\mathrm{i}}{2\hbar} \frac{-2E_n^i aw - v\big(mvx^2 - 2E_n^i at\big)}{w^2} \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w} x\right) \exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\Bigg]\\
&= \sqrt{\frac{2}{w}} \exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right) \left[\frac{2E_n^i a^2 + mv^2x^2 - \mathrm{i}\hbar wv}{2w^2} \sin\left(\frac{n\pi}{w} x\right) - \frac{\mathrm{i}\hbar n\pi xv}{w^2} \cos\left(\frac{n\pi}{w} x\right)\right],
\end{aligned}$$

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and for $0 \le x \le w$,

$$
\begin{aligned}
\hat{H}\Phi_n(x,\ t) = & -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Phi_n(x,\ t) \\
= & -\frac{\hbar^2}{2m}\sqrt{\frac{2}{w}}\frac{\partial}{\partial x}\exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\left[\frac{n\pi}{w}\cos\left(\frac{n\pi}{w}x\right) + \frac{\mathrm{i}mvx}{\hbar w}\sin\left(\frac{n\pi}{w}x\right)\right] \\
= & -\frac{\hbar^2}{2m}\sqrt{\frac{2}{w}}\left[\frac{\mathrm{i}mvx}{\hbar w}\exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\left[\frac{n\pi}{w}\cos\left(\frac{n\pi}{w}x\right) + \frac{\mathrm{i}mvx}{\hbar w}\sin\left(\frac{n\pi}{w}x\right)\right]\right. \\
& \left. + \exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\left[-\frac{n^2\pi^2}{w^2}\sin\left(\frac{n\pi}{w}x\right) + \frac{\mathrm{i}mv}{\hbar w}\sin\left(\frac{n\pi}{w}x\right) + \frac{\mathrm{i}n\pi mvx}{\hbar w^2}\cos\left(\frac{n\pi}{w}x\right)\right]\right] \\
= & \sqrt{\frac{2}{w}}\exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\left[\frac{\hbar^2 n^2\pi^2 + m^2v^2x^2 - \mathrm{i}\hbar mvw}{2mw^2}\sin\left(\frac{n\pi}{w}x\right) - \frac{\mathrm{i}\hbar n\pi vx}{w^2}\cos\left(\frac{n\pi}{w}x\right)\right] \\
= & \sqrt{\frac{2}{w}}\exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\left[\frac{2E_n^i a^2 + mv^2x^2 - \mathrm{i}\hbar vw}{2w^2}\sin\left(\frac{n\pi}{w}x\right) - \frac{\mathrm{i}\hbar n\pi vx}{w^2}\cos\left(\frac{n\pi}{w}x\right)\right].
\end{aligned}
$$

Hence, for $0 \le x \le w$, $\mathrm{i}\hbar\frac{\partial}{\partial t}\Phi_n(x,\ t) = \hat{H}\Phi_n(x,\ t)$. Therefore, the linear combination of $\Phi_n(x,\ t)$ also satisfies TDSE.

(ii) Note that $\{\Phi_n(x,\ t)\}$ is an orthonormal basis at time t. To prove this, one only need to find that

$$
\begin{aligned}
& \int_0^w \Phi_n(x,\ t)^*\Phi_k(x,\ t)\,\mathrm{d}x \\
= & \frac{2}{w}\int_0^w \left(\sin\left(\frac{n\pi}{w}x\right)\exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_n^i at\big)}{2\hbar w}\right)\right)^*\sin\left(\frac{k\pi}{w}x\right)\exp\left(\frac{\mathrm{i}\big(mvx^2 - 2E_k^i at\big)}{2\hbar w}\right)\mathrm{d}x \\
= & \frac{2}{w}\exp\left(\frac{\mathrm{i}(E_k^i - E_n^i)at}{\hbar w}\right)\int_0^w \sin\left(\frac{n\pi}{w}x\right)\sin\left(\frac{k\pi}{w}x\right)\mathrm{d}x \\
= & -\frac{1}{w}\exp\left(\frac{\mathrm{i}(E_k^i - E_n^i)at}{\hbar w}\right)\int_0^w \left(\cos\frac{(n+k)\pi x}{w} - \cos\frac{(n-k)\pi x}{w}\right)\mathrm{d}x = \delta_{nk}.
\end{aligned}
$$

At $t = 0$,

$$
\begin{aligned}
c_n = & \int_0^a \Phi_n(x,\ 0)^*\Psi(x,\ 0)\,\mathrm{d}x = \int_0^a \left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)e^{\frac{\mathrm{i}mvx^2}{2\hbar a}}\right)^*\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\mathrm{d}x \\
= & \frac{2}{a}\int_0^a \sin\left(n\frac{\pi x}{a}\right)e^{-\mathrm{i}\frac{mva}{2\pi^2\hbar}\left(\frac{\pi x}{a}\right)^2}\sin\left(\frac{\pi x}{a}\right)\mathrm{d}x\,.
\end{aligned}
$$

Let $z = \pi x/a$, then

$$
c_n = \frac{2}{a}\int_0^\pi \sin(nz)e^{-\mathrm{i}\frac{mva}{2\pi^2\hbar}z^2}\sin(z)\frac{\mathrm{d}x}{\mathrm{d}z}\,\mathrm{d}z = \frac{2}{\pi}\int_0^\pi e^{-\mathrm{i}\alpha z^2}\sin(nz)\sin(z)\,\mathrm{d}z\,,
$$

where $\alpha = \frac{mva}{2\pi^2\hbar}$.

(iii) Without loss of generality, suppose the initial time is at $t = 0$ and the final time is at $t = \Delta t$. For the instantaneous eigenstate $\psi_n(x,\ t)$ at time t, it satisfies the TISE at some specific time

$$
-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x,\ t) = E_n(t)\psi_n(x,\ t),
$$

and it satisfies the boundary conditions at time t:

$$
\psi_n(x = 0,\ t) = 0, \qquad \psi_n(x = w(t),\ t) = 0.
$$

Solve the ODE and we have that $\psi_n(x,\ t) = N \sin\left(\frac{n\pi x}{w(t)}\right)$ and $E_n(t) = n^2\pi^2\hbar^2/2mw(t)^2$; if we require the instantaneous eigenstates are orthonormal, *i. e.*, $\int_0^{w(t)} \psi_n(x,\ t)^*\psi_m(x,\ t)\,\mathrm{d}x = \delta_{nm}$, then we have that $N = \sqrt{2/w(t)}$, and hence,

$$\psi_n(x,\ t) = \sqrt{\frac{2}{w(t)}} \sin\left(\frac{n\pi x}{w(t)}\right).$$

Now we can use the instantaneous eigenstates to represent the solution

$$\Psi(x,\ t) = \sum_{n=1}^{\infty} a_n(t)\psi_n(x,\ t)e^{\mathrm{i}\theta_n(t)},$$

where $\theta_n = -\int_0^t E_n(t')/\hbar\,\mathrm{d}t'$. From the adiabatic theorem, we have that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}a_n(t) \approx& - a_n(t)\int_0^{w(t)} \psi_n(x,\ t)\frac{\mathrm{d}}{\mathrm{d}t}\psi_n(x,\ t)\,\mathrm{d}x\\ =& - a_n(t)\frac{2}{w(t)}\frac{n\pi}{w(t)}\int_0^{w(t)} \sin\left(\frac{n\pi x}{w(t)}\right)\cos\left(\frac{n\pi x}{w(t)}\right)\mathrm{d}x = 0.\end{aligned}$$

On the other hand, at $t = 0$, we have that $a_n(0) = \delta_{1n}$. Therefore,

$$a_n(t) = \delta_{1n}.$$

Note that the well expands to twice its original time in a time Δt, which means $v = a/\Delta t$. Therefore,

$$\Psi(x,\ t) = a_1(t)\psi_1(x,\ t)e^{\mathrm{i}\theta_1(t)} = e^{\mathrm{i}\theta(t)}\sqrt{\frac{2}{w(t)}}\sin\left(\frac{\pi x}{w(t)}\right),$$

where $w(t) = a(1 + t/\Delta t)$ and

$$\theta(t) = -\frac{1}{\hbar}\int_0^t \frac{\pi^2\hbar^2}{2ma^2(1 + t'/\Delta t)^2}\,\mathrm{d}t' = -\frac{\pi^2\hbar}{2ma^2}\frac{t}{1 + t/\Delta t}.$$

On the other hand, if the velocity of expansion v is small enough, *i. e.*, $v \to 0$, from the exact solution, we will have that $\alpha = mva/2\pi^2\hbar \approx 0$ and

$$c_n(t) \approx \frac{2}{\pi}\int_0^{\pi} \sin(nz)\sin(z)\,\mathrm{d}z = \delta_{1n}.$$

Hence,

$$\begin{aligned}\Psi(x,\ t) =& \sum_{i=1}^{\infty} c_n(t)\Phi_n(x,\ t) \approx \Phi_1(x,\ t) = \sqrt{\frac{2}{w}}\sin\left(\frac{\pi}{w(t)}x\right)\exp\left(\frac{\mathrm{i}\left(mvx^2 - 2E_1^i at\right)}{2\hbar w(t)}\right)\\ =& e^{\mathrm{i}\theta'(t)}\sqrt{\frac{2}{w}}\sin\left(\frac{\pi}{w(t)}x\right),\end{aligned}$$

where $\theta'(t) = \frac{mvx^2 - 2E_1^i at}{2\hbar w(t)} \approx -\frac{\pi^2\hbar^2 at}{2ma^2\hbar a(1 + t/\Delta t)} = -\frac{\pi^2\hbar at}{2ma^2(1 + t/\Delta t)}$, which is consistent with the result from the adiabatic theorem at the limit of $v \to 0$.

(iv) If the expansion of the well can be considered as a sudden perturbation, that is, the stationary state does not change as time t goes from 0 to Δt, that is, $\Psi(x,\ \Delta t) \approx \Psi(x,\ 0) = \sqrt{2/a}\sin(\pi x/a)$;
On the other hand, since $[H(t_1), H(t_2)] = 0$ for all $t_1,\ t_2 \in [0,\ \Delta t]$,

$$\begin{aligned}\Psi(x,\ \Delta t) =& \exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t H(t_1)\,\mathrm{d}t_1\right]\sum_{n=1}^{\infty} c_n\Phi_n(x,\ 0) = e^{-\mathrm{i}\bar{H}\Delta t/\hbar}\sum_{n=1}^{\infty} c_n\Phi_n(x,\ 0)\\ =& e^{-\mathrm{i}E^i t/\hbar}\sum_{n=1}^{\infty} c_n e^{-\mathrm{i}(E_n - E^i)t/\hbar}\Phi_n(x,\ 0).\end{aligned}$$

where $\bar{H} = \int_0^t H(t_1)\,\mathrm{d}t_1$ and E^i is the energy at initial state. Notice that only terms satisfying $t > \hbar/(E_n - E^i)$ will make appreciable change, and for the sudden perturbation limit, we hence require $t \ll \hbar/(E_n - E^i)$ for all n, that is, $t \ll \hbar/\Delta\bar{H}$.

2. Landau–Zener theory gives a formula that predicts the nonadiabatic transit probability. If the hamiltonian is

$$
\begin{aligned}
H =& H_0 + V, \\
H_0 =& E_1(t)\,|1\rangle\langle 1| + E_2(t)\,|2\rangle\langle 2|\,, \\
V =& \frac{\Delta}{2}\,|1\rangle\langle 2| + \frac{\Delta}{2}\,|1\rangle\langle 2|\,,
\end{aligned}
$$

where $E_1(t) = vt/2$, $E_2(t) = -vt/2$, and we start with $|(\psi(t = -\infty))\rangle = |1\rangle$, then for $t \to +\infty$, Laudau–Zener theory gives the nonadiabatic transit probability

$$
P_{1\to 2} = 1 - \exp\left(-\frac{\pi\Delta^2}{2\hbar v}\right).
$$

For instance, for the molecular dynamics Laudau–Zener gives the theoretical basis of surface hopping algorithms. We can plug the velocity of the classical trajectory as the group velocity and plug it in the Laudau–Zener formula, and get the probability of surface hopping for our simulation.

3. (i) The Floquet Hamiltonian is

$$
\mathcal{H} = H(t) - \mathrm{i}\hbar\frac{\partial}{\partial t}
$$

The Floquet Hamiltonian is defined on the expanded Hilbert space that spanned by basis $\{|\alpha n\rangle\} \coloneqq \{|\alpha\rangle\,|n\rangle\}$, where $|\alpha\rangle \in \{|E_1\rangle\,,\ |E_2\rangle\}$ and $\langle t|n\rangle = e^{\mathrm{i}n\omega t}$. The Floquet mode $|U_\lambda\rangle$ satisfies

$$
\mathcal{H}\,|U_\lambda\rangle = \mathcal{E}_\lambda\,|U_\lambda\rangle\,.
$$

Let

$$
\begin{aligned}
\langle \beta t|U_\lambda\rangle &= \sum_{m=-\infty}^{\infty} U_{\beta\lambda}^{(m)} e^{\mathrm{i}m\omega t}, \\
\langle \alpha|H(t)|\beta\rangle &= \sum_{n=-\infty}^{\infty} H_{\alpha\beta}^{(n)} e^{\mathrm{i}n\omega t}.
\end{aligned}
$$

Then,

$$
\langle \alpha m|\mathcal{H}|\beta n\rangle = \sum_k H_{\alpha\beta}^{(k)}\frac{1}{T}\int_0^T e^{\mathrm{i}(k-m+n)\omega t} + n\hbar\omega\delta_{\alpha\beta}\delta_{mn} = H_{\alpha\beta}^{(m-n)} + n\hbar\omega\delta_{\alpha\beta}\delta_{mn}
$$

where $T = 2\pi/\omega$. On the other hand, from the matrix representation of $H(t)$ we have that

$$
\begin{aligned}
H^{(0)} =& \begin{pmatrix} -\hbar\omega_0/2 & \\ & \hbar\omega_0/2 \end{pmatrix}, \\
H^{(-1)} =& \begin{pmatrix} & b \\ b & \end{pmatrix}, \\
H^{(1)} =& \begin{pmatrix} & b \\ b & \end{pmatrix}, \\
H^{(n)} =& 0,\ \text{otherwise}.
\end{aligned}
$$

where we have applied the fact that $\cos\omega t = \left(e^{\mathrm{i}\omega t} + e^{-\mathrm{i}\omega t}\right)/2$. Therefore, the matrix representation of $\mathcal{H}$ under basis $\{||\alpha n\rangle\rangle\}$ is

$$
\begin{pmatrix}
\ddots & \ddots & & & \\
\ddots & A - \hbar\omega & B & & \\
& B & A & B & \\
& & B & A + \hbar\omega & \ddots \\
& & & \ddots & \ddots
\end{pmatrix},
$$

where $A = \frac{\hbar\omega_0}{2}\begin{pmatrix} -1 & \\ & 1 \end{pmatrix}$ and $B = b\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$.

Truncate the basis by $\{|\alpha n\rangle\}_{n=-100}^{100}$ and diagonalize the representation matrix of $\mathcal{H}$ numerically, and note the that from the original structure of $\mathcal{H}$, if $\mathcal{E}$ is its eigenenergy then $\mathcal{E} + \hbar\omega$ is also its eigenenergy, then we only need to pick the one as quasienergy in a equivalence class that is defined by $\sim$, where $A \sim B$ if and only if there is an integer n such that $A = B + n\hbar\omega$. Here I chose the eigenvalues of the truncated matrix that most close to 0 to represent the that quasienergies of the infinite matrix. The result is in Figure 1. Note that for each given k the two curves are not crossing at around $\omega_0/\omega = 2,\ 4,\ 6,\ 8,\ etc.$

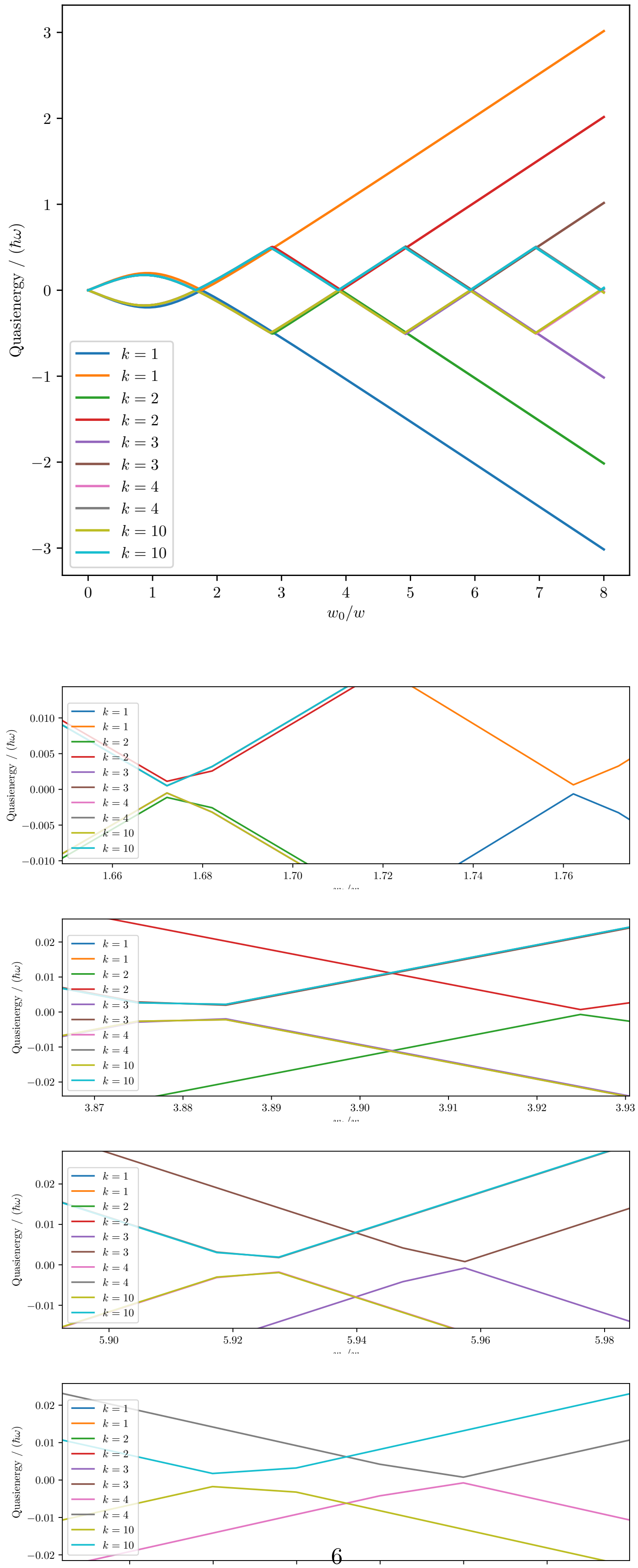


Figure 1: Quasienergies vs. ω_0

Note that the off-diagonal coupling mixes these states, and the non-zero off-diagonal terms will directly mix the the dressed states which differ in energy by $\hbar\omega$ and When $0 < \omega_0/\omega \lesssim 2$, $0 < \Delta$ to make $|E_1\rangle$ mix with $|E_2\rangle$ we need only one Floquet Brillouin zone; when $2 \lesssim \omega_0/\omega \lesssim 4$, we need 2 Floquet Brillouin zone; and so on. This can be seen by selecting specific submatrix to diagonalize for the whole matrix, *i. e.*, change the truncated basis by $\{|\alpha n\rangle\}_{n=-k}^{k}$, and the results are also plotted in Figure 1.

(ii) The time averaged transition probability in Eq. 19 in Shirley 1965 can be written in our notations as

$$\bar{P}_{\alpha\to\beta} = \sum_n \sum_\lambda |\langle \beta n|U_\lambda\rangle\langle U_\lambda|\alpha 0\rangle|^2.$$

This can be justified from the definition of $\bar{P}_{\alpha\to\beta}$

$$P_{\alpha\to\beta} = |U_{\beta\alpha}(0,\ t)|^2 = \left|\langle\beta|e^{-\mathrm{i}Ht/\hbar}|\alpha\rangle\right|^2.$$

On the other hand, note that $\langle t|\alpha 0\rangle = |\alpha\rangle$ for all t. Insert the spectrum decomposition of identity operator in the space spanned by $\{|n\rangle\}$ and we have

$$\langle\beta|U(0,\ t)|\alpha\rangle = \langle\beta|\sum_n |n\rangle\langle n|\,U\,\langle t|\alpha 0\rangle = \sum_n \langle t|n\rangle\,\langle\beta n|\,U\,|\alpha 0\rangle = \sum_n e^{\mathrm{i}n\omega t}\,\langle\beta n|\sum_\lambda |U_\lambda\rangle\,e^{-\mathrm{i}\mathcal{E}_\lambda t/\hbar}\,\langle U_\lambda|\alpha 0\rangle\,.$$

Therefore,

$$P_{\alpha\to\beta} = \left|\sum_n\sum_\lambda e^{\mathrm{i}(n\omega-\mathcal{E}_\lambda/\hbar)t}\,\langle\beta n|U_\lambda\rangle\,\langle U_\lambda|\alpha 0\rangle\right|^2$$

If we take the time average, then contributions of the crossing phases are zeros, and the diagonal phases are ones. Hence

$$\bar{P}_{\alpha\to\beta} = \sum_n \sum_\lambda |\langle \beta n|U_\lambda\rangle\langle U_\lambda|\alpha 0\rangle|^2.$$

(iii) See Figure 2. Here the size of the truncated basis k is 10 and has been verified consistency with the case that $k = 100$.

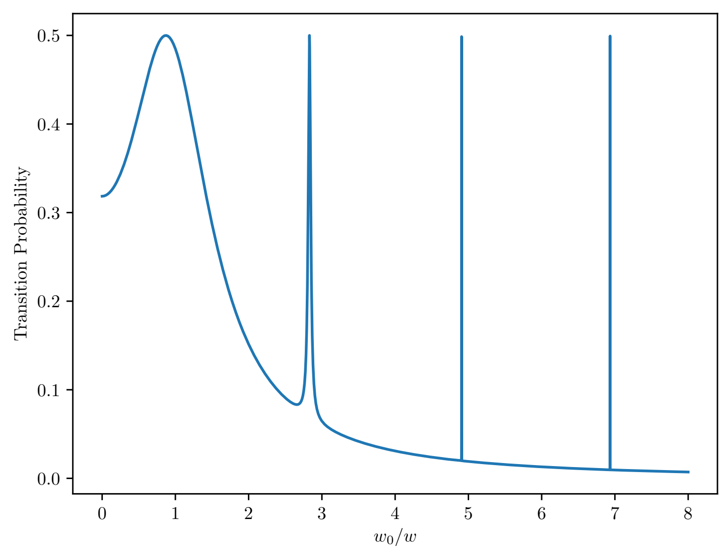


Figure 2: Transition probability vs. ω_0

(iv) It is clear that there are peaks in Figure 2 at $\omega_0/\omega \approx 1,\ 3,\ 5,\ 7,$ *etc.* These results coincide with the ones from perturbation theory, where only odd order of perturbations gives nonzero terms between the two states.

4. (i) Let $\{|n\rangle\}_{n=1}^{\infty}$ be an orthonormal and complete basis. Then

$$\begin{aligned}\operatorname{tr}\left(\hat{A}\hat{B}\right) &= \sum_n \langle n|\hat{A}\hat{B}|n\rangle = \sum_n \langle n|\,\hat{A}\sum_m |m\rangle\,\langle m|\,\hat{B}\,|n\rangle = \sum_n\sum_m \langle n|\hat{A}|m\rangle\,\langle m|\hat{B}|n\rangle\\ &= \sum_m\sum_n \langle m|\hat{B}|n\rangle\,\langle n|\hat{A}|m\rangle = \sum_m \langle m|\hat{B}\hat{A}|m\rangle = \operatorname{tr}\left(\hat{B}\hat{A}\right);\end{aligned}$$

and if the system is a mixed state with $\hat{\rho} = \sum_k p_k\,|\Psi_k\rangle$, then

$$\begin{aligned}\left\langle\hat{A}\right\rangle &= \sum_k p_k\,\langle\Psi_k|\hat{A}|\Psi_k\rangle = \sum_k p_k\,\langle\Psi_k|\,\hat{A}\sum_n |n\rangle\,\langle n|\Psi_k\rangle\\ &= \sum_{nk} p_k\,\langle\Psi_k|\,\hat{A}\,|n\rangle\,\langle n|\Psi_k\rangle = \sum_n \langle n|\sum_k p_k\,|\Psi_k\rangle\,\langle\Psi_k|\,\hat{A}\,|n\rangle = \sum_n \langle n|\,\hat{\rho}\hat{A}\,|n\rangle = \operatorname{tr}\left(\hat{\rho}\hat{A}\right).\end{aligned}$$

(ii) For $|E_1\rangle$:

$$\rho_1 = \begin{pmatrix}1 & 0\end{pmatrix}^\dagger\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix};$$

for $|E_2\rangle$:

$$\rho_2 = \begin{pmatrix}0 & 1\end{pmatrix}^\dagger\begin{pmatrix}0 & 1\end{pmatrix} = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix};$$

for $(|E_1\rangle + \mathrm{i}\,|E_2\rangle)/\sqrt{2}$:

$$\rho_3 = \frac{1}{2}\begin{pmatrix}1\\ \mathrm{i}\end{pmatrix}\begin{pmatrix}1 & -\mathrm{i}\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & -\mathrm{i}\\ \mathrm{i} & 1\end{pmatrix};$$

for a mixture with P_1 to be in $|E_1\rangle$ and P_2 to be in $(|E_1\rangle + \mathrm{i}\,|E_2\rangle)/\sqrt{2}$:

$$\rho_4 = P_1\rho_1 + P_2\rho_3 = \begin{pmatrix}P_1 + P_2/2 & -\mathrm{i}P_2/2\\ \mathrm{i}P_2/2 & P_2/2\end{pmatrix};$$

(iii) Consider a two-level system $\rho = \sum_n P_n\,|\phi_n\rangle\langle\phi_n|$, where $|\phi_n\rangle = c_{n1}\,|E_1\rangle + c_{n2}\,|E_2\rangle$ is normalized, and $|E_1\rangle$ and $|E_2\rangle$ construct an orthonormal basis of the Hilbert space, P_n is the (positive) possibility of finding the system in $|\phi_n\rangle$. It is clear that ρ is hermite since $\rho^\dagger = \sum_n P_n^*\,|\phi_n\rangle\langle\phi_n| = \sum_n P_n\,|\phi_n\rangle\langle\phi_n| = \rho$. And hence, we can diagonalize ρ such that

$$\rho = w_1\,|\psi_1\rangle\langle\psi_1| + w_2\,|\psi_2\rangle\langle\psi_2|\,,$$

where w_1 and w_2 are nonnegative, and$\{|\psi_1\rangle\,,\ |\psi_2\rangle\}$ spans the same Hilbert space as $\{|E_1\rangle\,,\ |E_2\rangle\}$, and is orthonormal. Note that

$$\operatorname{tr}\rho = w_1 + w_2 = 1,$$

and therefore, $\rho^2 = w_1^2\,|\psi_1\rangle\langle\psi_1| + w_2^2\,|\psi_2\rangle\langle\psi_2|$

$$\operatorname{tr}\rho^2 = w_1^2 + w_2^2 = w_1^2 + (1-w_1)^2 = 2w_1^2 - 2w_1 + 1.$$

Since $0 \le w_1 \le 1$, therefore, $1/2 \le \operatorname{tr}\rho^2 \le 1$. Note that when $w_1 = w_2 = 1/2$, $\operatorname{tr}\rho^2$ gets its minimal $1/2$ and when $w_1 = 0$ or $w_1 = 1$, $\operatorname{tr}\rho^2$ gets its maximal 1.

The entropy of such a two-level system is

$$\begin{aligned}S &= -\operatorname{tr}(\rho\ln\rho) = -\operatorname{tr}((w_1\,|\psi_1\rangle\langle\psi_1| + w_2\,|\psi_2\rangle\langle\psi_2|)(\ln w_1\,|\psi_1\rangle\langle\psi_1| + \ln w_2\,|\psi_2\rangle\langle\psi_2|))\\ &= -\operatorname{tr}(w_1\ln w_1\,|\psi_1\rangle\langle\psi_1| + w_2\ln w_2\,|\psi_2\rangle\langle\psi_2|) = -w_1\ln w_1 - w_2\ln w_2 = -w_1\ln w_1 - (1-w_1)\ln(1-w_1),\end{aligned}$$

where $0 \le w_1 \le 1$. Note that when $w_1 = w_2 = 1/2$, S gets its maximal $\ln 2$ and when $w_1 = 0$ or $w_1 = 1$, $\operatorname{tr}\rho^2$ gets its minimal 0.

We can relate the two quantities by defining the Rényi entropy

$$R_\alpha = \frac{1}{1-\alpha} \ln \operatorname{tr} \rho^\alpha,$$

and notice that

$$R_2 = \frac{1}{1-2} \ln \operatorname{tr} \rho^2 = -\ln \operatorname{tr} \rho^2,$$

and

$$R_1 = \lim_{\alpha\to 1} \frac{1}{1-\alpha} \ln \operatorname{tr} \rho^\alpha = -\lim_{\alpha\to 1} \frac{\operatorname{tr} \rho^\alpha \ln \rho}{\operatorname{tr} \rho^\alpha} = -\frac{\operatorname{tr} \rho \ln \rho}{\operatorname{tr} \rho} = -\operatorname{tr} \rho \ln \rho = S.$$

(iv) The entropy is not time independent: consider a spin–boson model (SBM) stating with the initial state $(|E_1\rangle + |E_2\rangle)/\sqrt{2} \otimes |0\rangle$, where $|0\rangle$ is at the ground state of the harmonic oscillator. The numerical simulation gives Figure 3.

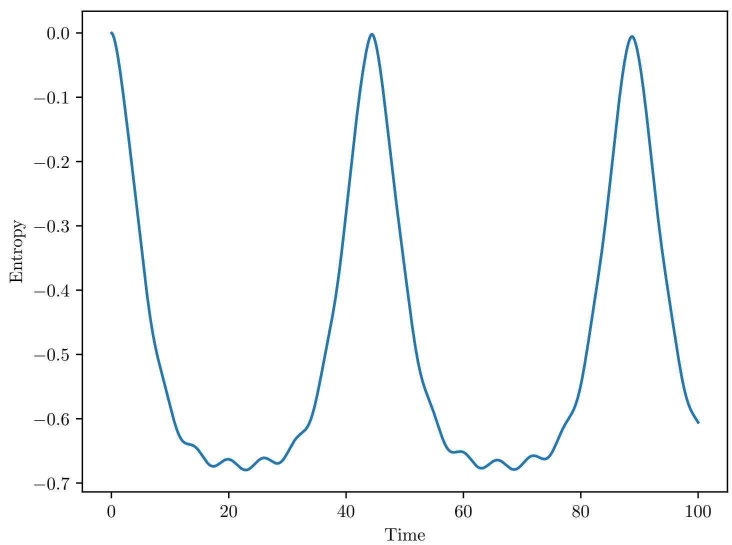


Figure 3: Time-dependency of entropy for spin–boson model.

Now consider a closed system, that is, its density operator satisfies the Liouville equation $\frac{\partial \rho}{\partial t} = -\frac{\mathrm{i}}{\hbar}[H, \rho]$, then

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\frac{\mathrm{d}}{\mathrm{d}t} \operatorname{tr}(\rho \ln \rho) = \operatorname{tr}\left(\frac{\mathrm{d}}{\mathrm{d}t} \rho \ln \rho\right) = -\operatorname{tr}\left(\frac{\partial \rho}{\partial t} \ln \rho + \frac{\partial \rho}{\partial t}\right) = \frac{\mathrm{i}}{\hbar}(\operatorname{tr}(H\rho \ln \rho) - \operatorname{tr}(\rho H \ln \rho) + \operatorname{tr}(H\rho) - \operatorname{tr}(H\rho)).$$

From 4i we know that $\operatorname{tr}(\rho H) = \operatorname{tr}(H\rho)$ and $\operatorname{tr}(\rho H \ln \rho) = \operatorname{tr}(H(\ln \rho)\rho)$. On the other hand, since $\ln \rho$ is a function of ρ, it commutes with ρ, and hence $\operatorname{tr}(H(\ln \rho)\rho) = \operatorname{tr}(H\rho \ln \rho)$. Therefore,

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}(\operatorname{tr}(H\rho \ln \rho) - \operatorname{tr}(H\rho \ln \rho) + \operatorname{tr}(H\rho) - \operatorname{tr}(H\rho)) = 0.$$

5. (i) Recall the definition of $A_{\mathrm{W}}(q,\ p) = \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{A}(\hat{q},\ \hat{p})|q + y/2\rangle\, e^{\mathrm{i}py/\hbar}$. Therefore,

$$\begin{aligned} q_{\mathrm{W}} &= \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{q}|q + y/2\rangle\, e^{\mathrm{i}py/\hbar} \\ &= \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x - q + y/2)(q + y/2)\delta(x - q - y/2) e^{\mathrm{i}py/\hbar} \\ &= \int_{-\infty}^{\infty} \mathrm{d}y\, (q + y/2)\delta(y) e^{\mathrm{i}py/\hbar} = q e^{\mathrm{i}p\cdot 0/\hbar} = q, \end{aligned}$$

and similarly,

$$\begin{aligned}
p_{\mathrm{W}} =& \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{p}|q + y/2\rangle\, e^{\mathrm{i}py/\hbar} \\
=& \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x - q + y/2)\mathrm{i}\hbar\frac{\partial}{\partial x}\delta(x - q - y/2)e^{\mathrm{i}py/\hbar} \\
=& \mathrm{i}\hbar \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x - q + y/2)\delta'(x - q - y/2)e^{\mathrm{i}py/\hbar} \\
=& \mathrm{i}\hbar \int_{-\infty}^{\infty} \mathrm{d}y\, \delta'(-y)e^{\mathrm{i}py/\hbar} = -\mathrm{i}\hbar \int_{-\infty}^{\infty} \mathrm{d}y\, \delta'(y)e^{\mathrm{i}py/\hbar} \\
=& -\mathrm{i}\hbar \left(e^{\mathrm{i}py/\hbar}\right)'\Big|_{y=0} = p.
\end{aligned}$$

Lemma 1. *For any operators $\hat{A}(\hat{q},\ \hat{p})$ and $\hat{B}(\hat{q},\ \hat{p})$, $aA_{\mathrm{W}} + bB_{\mathrm{W}} = (aA + bB)_{\mathrm{W}}$, where $a,\ b$ are any complex numbers.*

Proof. Note that

$$\begin{aligned}
A_{\mathrm{W}} =& \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{A}|q + y/2\rangle\, e^{\mathrm{i}py/\hbar}, \\
B_{\mathrm{W}} =& \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{B}|q + y/2\rangle\, e^{\mathrm{i}py/\hbar}, \\
(aA + bB)_{\mathrm{W}} =& \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|aA + bB|q + y/2\rangle\, e^{\mathrm{i}py/\hbar} \\
=& \int_{-\infty}^{\infty} \mathrm{d}y \left(a\, \langle q - y/2|\hat{A}|q + y/2\rangle + b\, \langle q - y/2|\hat{B}|q + y/2\rangle\right) e^{\mathrm{i}py/\hbar} \\
=& a \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{A}|q + y/2\rangle\, e^{\mathrm{i}py/\hbar} + b \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{B}|q + y/2\rangle\, e^{\mathrm{i}py/\hbar} \\
=& aA_{\mathrm{W}} + bB_{\mathrm{W}}.
\end{aligned}$$

□

Lemma 2. $(\hat{q}^n)_{\mathrm{W}} = q^n$*,* $(\hat{p}^n)_{\mathrm{W}} = p^n$*.*

Proof.

$$\begin{aligned}
(\hat{q}^n)_{\mathrm{W}} =& \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{q}^n|q + y/2\rangle\, e^{\mathrm{i}py/\hbar} \\
=& \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x - q + y/2)(q + y/2)^n\delta(x - q - y/2)e^{\mathrm{i}py/\hbar} \\
=& \int_{-\infty}^{\infty} \mathrm{d}y\, (q + y/2)^n\delta(y)e^{\mathrm{i}py/\hbar} = q^n,
\end{aligned}$$

and

$$\begin{aligned}
(\hat{p}^n)_{\mathrm{W}} =& \int_{-\infty}^{\infty} \mathrm{d}y\ \langle q - y/2|\hat{p}^n|q + y/2\rangle\, e^{\mathrm{i}py/\hbar} \\
=& \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x - q + y/2)(\mathrm{i}\hbar)^n\frac{\partial^n}{\partial x^n}\delta(x - q - y/2)e^{\mathrm{i}py/\hbar} \\
=& (\mathrm{i}\hbar)^n \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x - q + y/2)\delta^{(n)}(x - q - y/2)e^{\mathrm{i}py/\hbar} \\
=& (\mathrm{i}\hbar)^n \int_{-\infty}^{\infty} \mathrm{d}y\, \delta^{(n)}(-y)e^{\mathrm{i}py/\hbar} = (-\mathrm{i}\hbar)^n \int_{-\infty}^{\infty} \mathrm{d}y\, \delta^{(n)}(y)e^{\mathrm{i}py/\hbar} \\
=& (-\mathrm{i}\hbar)^n \left(e^{\mathrm{i}py/\hbar}\right)^{(n)}\Big|_{y=0} = p^n.
\end{aligned}$$

□

Therefore, if $\hat{T}$ and $\hat{W}$ converge to their Taylor series, then

$$
\begin{aligned}
H_{\mathrm{W}} =&(T(p)+V(q))_{\mathrm{W}} = \left(\sum_{n=0}^{\infty}\frac{1}{n!}\frac{\mathrm{d}^n T}{\mathrm{d}p^n}p^n + \sum_{n=0}^{\infty}\frac{1}{n!}\frac{\mathrm{d}^n V}{\mathrm{d}q^n}q^n\right)_{\mathrm{W}} \\
=&\sum_{n=0}^{\infty}\frac{1}{n!}\frac{\mathrm{d}^n T}{\mathrm{d}p^n}p^n_{\mathrm{W}} + \sum_{n=0}^{\infty}\frac{1}{n!}\frac{\mathrm{d}^n V}{\mathrm{d}q^n}q^n_{\mathrm{W}} = \sum_{n=0}^{\infty}\frac{1}{n!}\frac{\mathrm{d}^n T}{\mathrm{d}p^n}p^n + \sum_{n=0}^{\infty}\frac{1}{n!}\frac{\mathrm{d}^n V}{\mathrm{d}q^n}q^n = T(p)+V(q) = H(q,\ p).
\end{aligned}
$$

(ii) For a pure state, $\hat{\rho} = |\psi\rangle\langle\psi|$, and

$$
\begin{aligned}
\rho_{\mathrm{W}} =&\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}y\ \langle q-y/2|\hat{\rho}|q+y/2\rangle\, e^{\mathrm{i}py/\hbar} \\
=&\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}y\, \psi(q+y/2)^*\psi(q-y/2)e^{\mathrm{i}py/\hbar},
\end{aligned}
$$

Then,
(TBF)

(iii) We need the following lemma.

Lemma 3. *For any operator $\hat{A}(\hat{q},\ \hat{p})$, $(A^\dagger)_{\mathrm{W}} = (A_{\mathrm{W}})^*$.*

Proof. Note that

$$
\begin{aligned}
(A^\dagger)_{\mathrm{W}} =& \int_{-\infty}^{\infty}\mathrm{d}y\ \langle q-y/2|\hat{A}^\dagger|q+y/2\rangle\, e^{\mathrm{i}py/\hbar} \\
=&\int_{-\infty}^{\infty}\mathrm{d}y\ \langle q+y/2|\hat{A}|q-y/2\rangle^*\, e^{\mathrm{i}py/\hbar} \\
=&\int_{-\infty}^{\infty}\mathrm{d}y\ \langle q-y/2|\hat{A}|q+y/2\rangle^*\, e^{-\mathrm{i}py/\hbar} \\
=&(A_{\mathrm{W}})^*
\end{aligned}
$$

□

$$
\begin{aligned}
\frac{\mathrm{d}\left(\hat{O}_H\right)_{\mathrm{W}}}{\mathrm{d}t} =&\left(-\frac{\mathrm{i}}{\hbar}\left[\hat{O}_H, \hat{H}_H\right]\right)_{\mathrm{W}} \\
=&-\frac{\mathrm{i}}{\hbar}((\hat{O}_H\hat{H}_H)_{\mathrm{W}} - (\hat{H}_H\hat{O}_H)_{\mathrm{W}}) \\
=&-\frac{\mathrm{i}}{\hbar}((\hat{O}_H\hat{H}_H)_{\mathrm{W}} - ((\hat{O}_H\hat{H}_H)_{\mathrm{W}})^*).
\end{aligned}
$$

Recall that $\left(\hat{A}\hat{B}\right)_{\mathrm{W}} = A_{\mathrm{W}}e^{-\frac{\mathrm{i}\hbar}{2}\overleftrightarrow{\Lambda}}B_{\mathrm{W}}$, where $\overleftrightarrow{\Lambda} = \frac{\overleftarrow{\partial}}{\partial p}\frac{\overleftarrow{\partial}}{\partial q} - \frac{\overrightarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}$, therefore,

$$
\begin{aligned}
\frac{\mathrm{d}\left(\hat{O}_H\right)_{\mathrm{W}}}{\mathrm{d}t} =&-\frac{\mathrm{i}}{\hbar}\left((\hat{O}_H)_{\mathrm{W}}e^{-\frac{\mathrm{i}\hbar}{2}\overleftrightarrow{\Lambda}}(\hat{H}_H)_{\mathrm{W}} - \left((\hat{O}_H)_{\mathrm{W}}e^{-\frac{\mathrm{i}\hbar}{2}\overleftrightarrow{\Lambda}}(\hat{H}_H)_{\mathrm{W}}\right)^*\right) \\
=&-\frac{\mathrm{i}}{\hbar}\left((\hat{O}_H)_{\mathrm{W}}e^{-\frac{\mathrm{i}\hbar}{2}\overleftrightarrow{\Lambda}}(\hat{H}_H)_{\mathrm{W}} - (\hat{O}_H)^*_{\mathrm{W}}e^{\frac{\mathrm{i}\hbar}{2}\overleftrightarrow{\Lambda}}(\hat{H}_H)^*_{\mathrm{W}}\right) \\
=&-\frac{2}{\hbar}(\hat{O}_H)_{\mathrm{W}}\sin\frac{\hbar\overleftrightarrow{\Lambda}}{2}(\hat{H}_H)_{\mathrm{W}}.
\end{aligned}
$$

In the last step we have applied the fact that $(\hat{O}_H)_{\mathrm{W}}$ is real for any Hermitian $\hat{O}_H$ since $(\hat{O}_H)_{\mathrm{W}} = (\hat{O}_H^\dagger)_{\mathrm{W}} = ((\hat{O}_H)_{\mathrm{W}})^*$.

(iv) When $\hbar \to 0$, $(\hat{O}_H)_{\mathrm{W}} = O^c + \hbar O_1 + o(\hbar)$, $(\hat{H}_H)_{\mathrm{W}} = H^c + \hbar H_1 + o(\hbar)$, and $\sin\frac{\hbar\overleftrightarrow{\Lambda}}{2} = \frac{\hbar\overleftrightarrow{\Lambda}}{2} + o(\hbar)$, then,

$$\begin{aligned}
\frac{\mathrm{d}\left(\hat{O}_H\right)_{\mathrm{W}}}{\mathrm{d}t} &= -\frac{2}{\hbar}(\hat{O}_H)_{\mathrm{W}} \sin\frac{\hbar\overleftrightarrow{\Lambda}}{2}(\hat{H}_H)_{\mathrm{W}} \\
\Rightarrow \frac{\mathrm{d}O^c}{\mathrm{d}t} + o(1) &= -2O^c\frac{\overleftrightarrow{\Lambda}}{2}H^c + o(1) \\
\Rightarrow \frac{\mathrm{d}O^c}{\mathrm{d}t} &= \{H^c, O^c\}_P + o(1),
\end{aligned}$$

where $\{\cdot,\cdot\}_P$ is the Poisson bracket.

(v) When we use the wigner representation and take the limit of $\hbar \to 0$ then we recover the classical mechanics, which means that the classical mechanics is a specific representation of quantum mechanics under the limit that Planck constant is small enough.

From 5iv we know that as $\hbar \to 0$, the dynamics of the physical operator in the Wigner representation coincide with the equation of motion in classical mechanics.

(The density operator in the Wigner representation should has the same formalism of the volume element in the phase space in classical mechanics.)

6. Code is available at `https://github.com/vINyLogY/QD-hw2`.

(A) (i) Here we only need to focus on monitoring the eigenstate with $n = 100$. Therefore the dimensionality of the grid basis should be at least 101 (assume we start counting n from 0). We choose an overkill (checked convergence by simply increasing these parameters) dimensionality 1001 and $q_0 = 25$, and the results are showed in Figure 4.

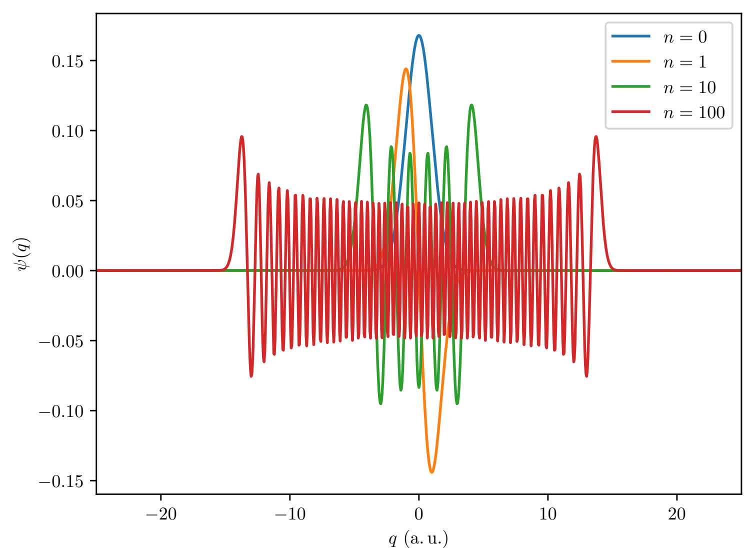


Figure 4: $\psi(x)$ for a harmonic oscillator.

The following results are focused with $q_0 = 25$.

(ii) See Figure 5.

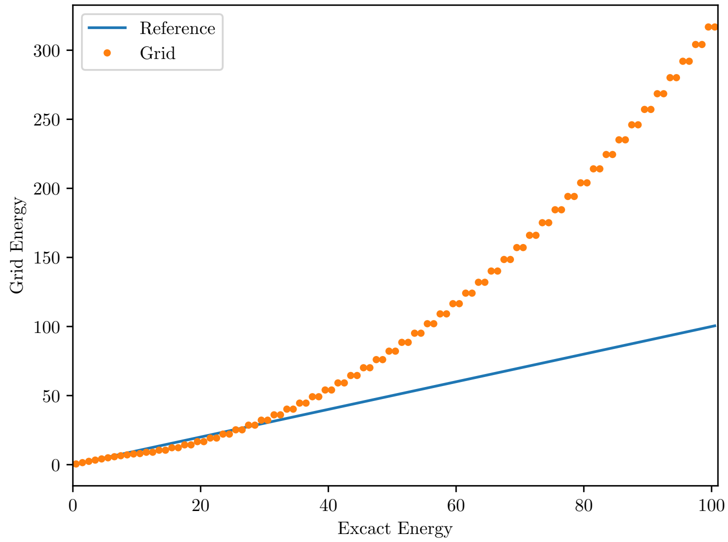


Figure 5: Energy of each eigenstates for a harmonic oscillator.

Note that the grid method only gets the exact answer for those states with small eigenvalues. This is because for the excited states with large energy, the wavefunction oscillates crazy as showed in Figure 4, and hence we need more dense grid to characterize the wavefunction.

(iii) We need to change the dimensionality of grid basis in this case. For the eigenstate $n = 32$, we need at least 33 grids. We calculated the energy difference between the one from the grid representation and the exact one, change the dimensionality of grid basis, *i. e.*, different Δq. See Figure 6.

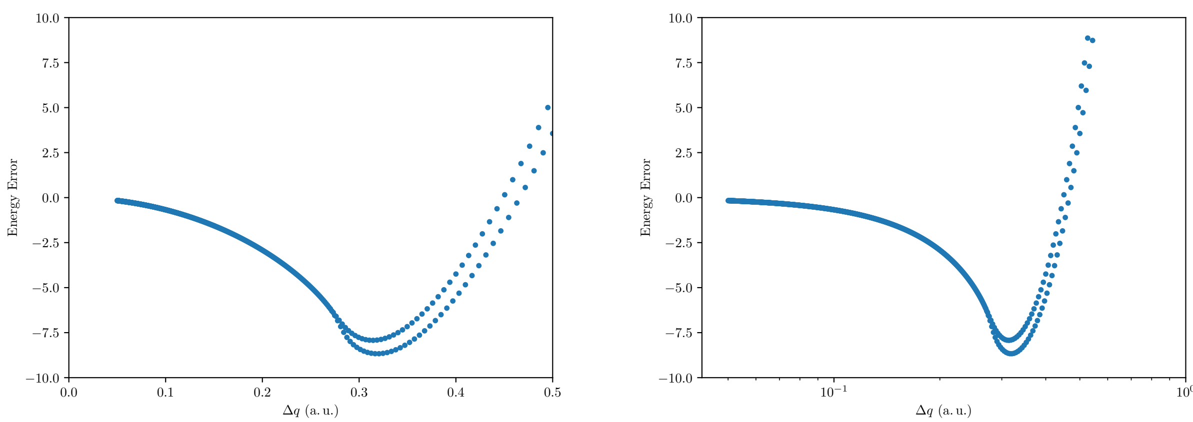


Figure 6: Energy error vs. Δq.

Therefore, $\Delta q < 0.1$ a. u. is an adequate choice.

(B) (i) Use Sine-DVR[1] here. As the concerns in grid basis, we choose the dimensionality to be 999 and $q_0 = 25$. See Figure 7.

[1] See `https://www.pci.uni-heidelberg.de/tc/usr/mctdh/lit/NumericalMethods.pdf`.

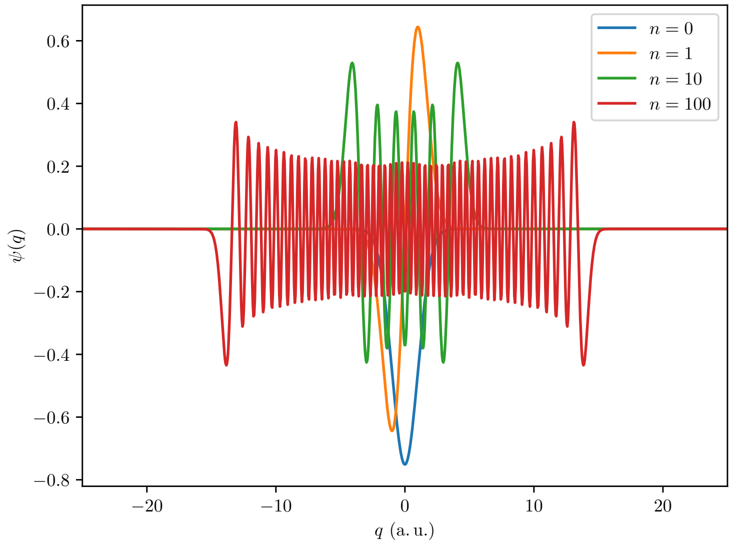


Figure 7: Energy of each eigenstates for a harmonic oscillator.

Note that the $\psi(q)$ has up to a different phase from the results by grid basis.

(ii) See Figure 8.

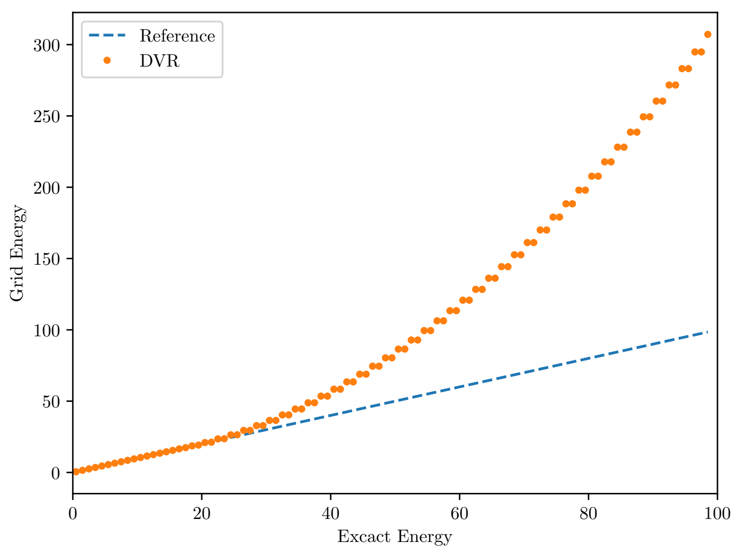


Figure 8: Energy of each eigenstates for a harmonic oscillator.

Similarly, the DVR method only gets the exact answer for those states with small eigenvalues. This is because for the excited states with large energy, they need the basis includes the functions that corresponding to larger momentum, therefore, we need more dimensionality for the finite basis representation, or smaller grid interval, to represent such high-energy states.

(iii) We need to change the dimensionality of grid basis in this case. For the eigenstate $n = 32$, we need at least 33 grids. We calculated the energy difference between the one from the grid representation and the exact one, change the dimensionality of grid basis, *i. e.*, different Δq. See Figure 9.

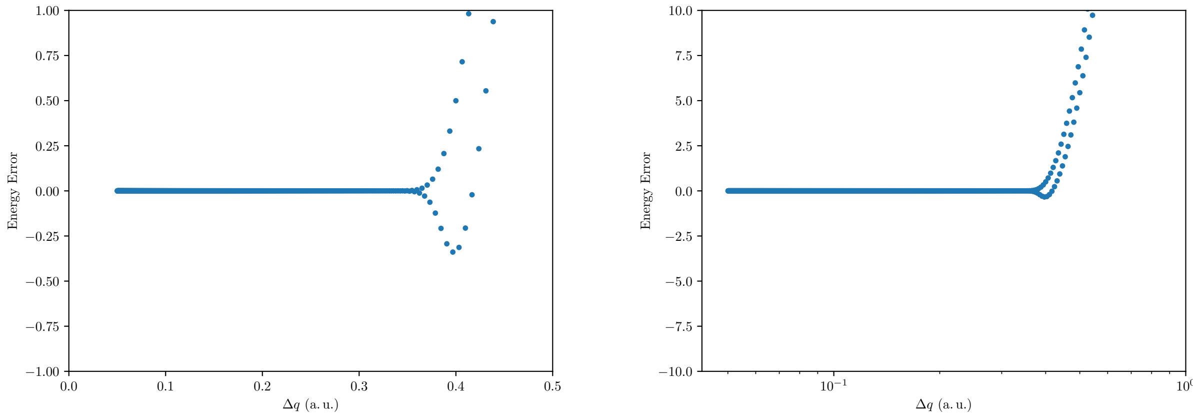


Figure 9: Energy error vs. Δq.

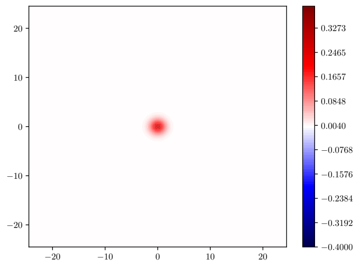
Therefore, $\Delta q < 0.1$ a. u. is an adequate choice.

(iv) From Figure 5 and Figure 8 we can find that DVR can get exact energy for states with relatively larger energy when compared to grid method. Also, from Figure 6 and Figure 9 we can find that DVR can get exact energy with a relatively small dimensionality, or larger grid interval.

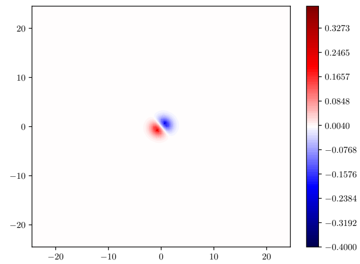
(C) (i) Suppose under 1-D DVR basis $\{|\chi_i\rangle\}$ the kinetic matrix in one dimension i is T_i, the potential matrix in one dimension i is V_i, then the kinetic matrix of 2-D is $T_1 \otimes T_2$, and the potential matrix is a diagonal matrix $V_1 \otimes V_2$. Hence we can diagonalize the hamiltonian in the 2-D basis.

(ii) See Figure 10. It is clear that for such a system, the exact eigenenergies are $E = \hbar\omega(n+1)$, where $n = n_a + n_b$, and $n_a,\ n_b \in \mathbb{N}$. This means that for $E = \hbar\omega$, the degeneracy is 1 ($n = 0 + 0$); for $E = 2\hbar\omega$, the degeneracy is 2 ($n = 1 + 0 = 0 + 1$); for $E = 3\hbar\omega$, the degeneracy is 3 ($n = 2 + 0 = 0 + 2 = 1 + 1$); for $E = 4\hbar\omega$, the degeneracy is 4 ($n = 3 + 0 = 0 + 3 = 1 + 2 = 2 + 1$); and so on. From Figure 10 we can also find that the parameters (upper and lower bound are both 25 and -25 for each dimension; the dimensionality of basis for each degrees of freedom is 99) is sufficient for the lowest 10 eigenstates.

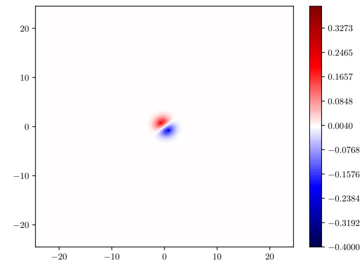
(iii) See Figure 11.



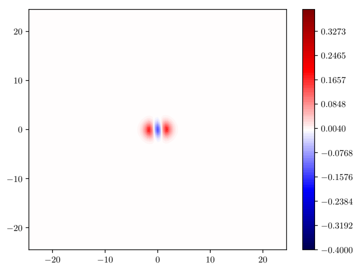
$E = 0.99999999999999889$



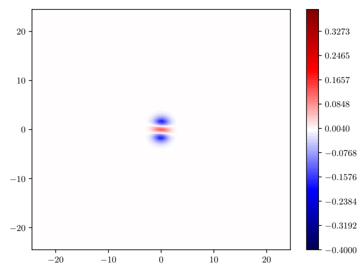
$E = 1.999999999999758860$



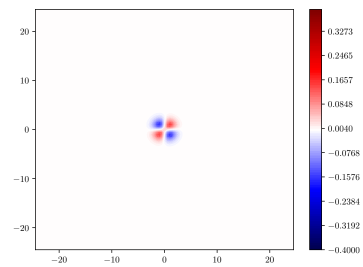
$E = 1.999999999999908962$



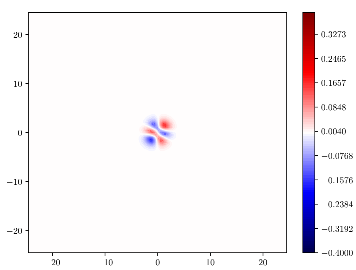
$E = 2.999999999999794387$



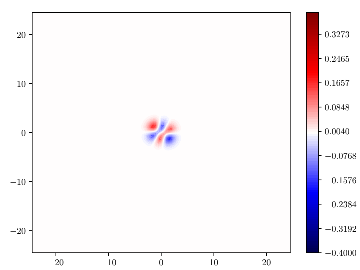
$E = 2.999999999999797939$



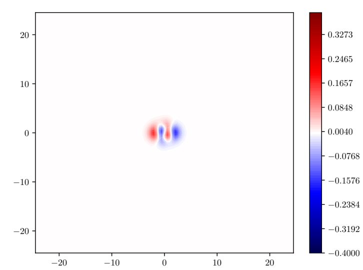
$E = 2.999999999999895195$



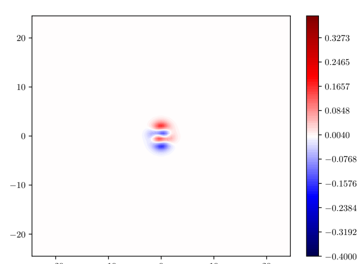
$E = 3.999999999999648281$



$E = 3.999999999999723332$

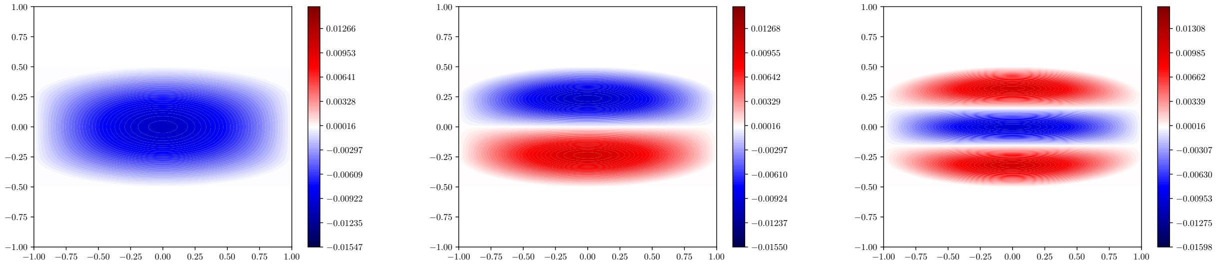


$E = 4.000000000003303136$

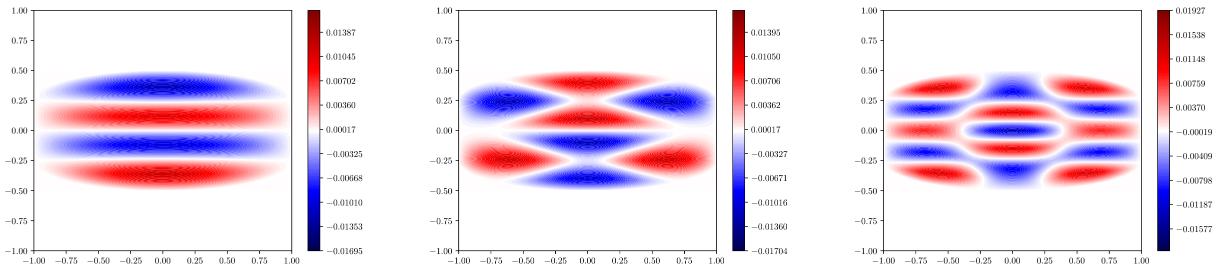


$E = 4.000000000003453238$

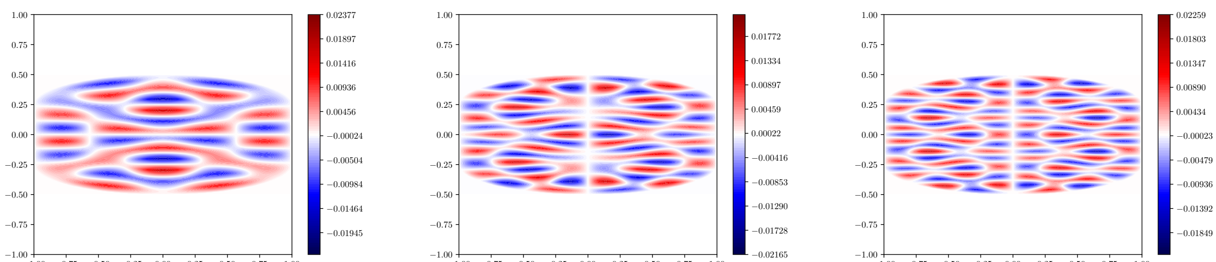
Figure 10: Eigenstates and their eigenenergies for a 2-D harmonic oscillator.



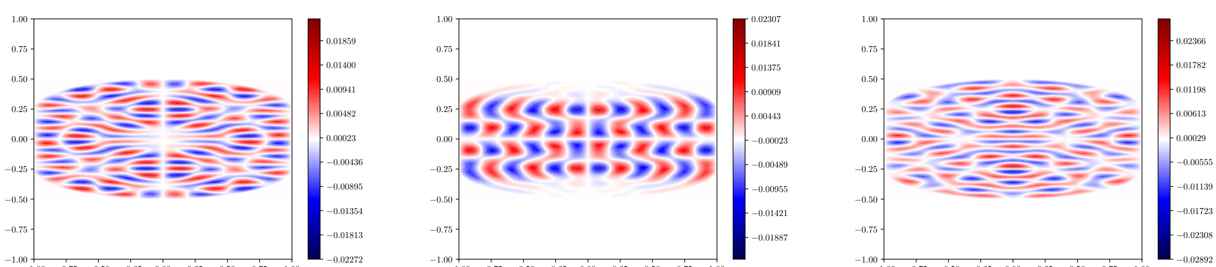
$E_0 = 6.369778636492784$ $E_1 = 10.604723421874684$ $E_2 = 17.49625007137572$



$E_5 = 26.818961595179772$ $E_{10} = 50.75276012770485$ $E_{20} = 87.88823005740137$



$E_{50} = 204.00943730722977$ $E_{100} = 394.4271319580347$ $E_{150} = 578.41848374364$



$E_{195} = 735.5352784543273$ $E_{198} = 755.8825724428713$ $E_{199} = 757.6928364999236$

Figure 11: Eigenstates and their eigenenergies for a 2-D potential well.