HW2
PHYS4240: Solid State Physics

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February 6, 2025

Question 1. The Delta Function Potential

I have no idea how much you want us to show, so I showed quite a bit just in case!

In the case of the delta function potential, the case of interest for this problem is scattering states where $E > 0$. With this, the Hamiltonian for a particle of mass m is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \lambda\delta(x). \tag{1}$$

In the regions $x < 0$ and $x > 0$, the potential term vanishes due to the delta function, and we are left with:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{2}$$

so the Schrödinger equation looks like

$$\hat{H}\psi(x) = E\psi(x) \quad \rightarrow \quad -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x). \tag{3}$$

This is something we have seen on a number of occasions. Defining $k \equiv \sqrt{2mE}/\hbar$, our solutions are complex exponentials:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0, \\ Ce^{ikx} + De^{-ikx} & x > 0. \end{cases} \tag{4}$$

The usual boundary conditions at $\pm\infty$ don't apply here, i.e. we can't eliminate one term due to it blowing up, since these are complex exponentials. But, intuitively, since there is no other boundary past the delta function potential, we would expect that the term proportional to D, involving a wave propagating from the right on the right side of the potential, should be zero. Thus $D = 0$.

The next boundary condition we can consider is imposing that $\psi(x)$ be continuous at $x = 0$, meaning that we have

$$A + B = C. \tag{5}$$

The last condition we can consider is that the first derivative of $\psi(x)$ must also be continuous at $x = 0$, except at points where the potential is not, which is exactly what we have here. In this case, we can use the prescription that

$$\Delta\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right) = \lim_{\epsilon\to 0}\left(\left.\frac{\mathrm{d}\psi}{\mathrm{d}x}\right|_{+\epsilon} - \left.\frac{\mathrm{d}\psi}{\mathrm{d}x}\right|_{-\epsilon}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{+\epsilon} V(x)\psi(x)\,\mathrm{d}x. \tag{6}$$

For us, since we have a delta function, we don't need to actually do the integral and we have

$$\Delta\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right) = \frac{2m\lambda}{\hbar^2}\psi(0). \tag{7}$$

Now,

$$\left.\frac{\mathrm{d}\psi}{\mathrm{d}x}\right|_{-\epsilon} = \left[ik(Ae^{ikx} - Be^{-ikx})\right]_{-\epsilon} = ik(A - B), \tag{8}$$

$$\left.\frac{\mathrm{d}\psi}{\mathrm{d}x}\right|_{\epsilon} = \left[ik(Ce^{ikx})\right]_{\epsilon} = ikC, \tag{9}$$

$$\tag{10}$$

so

$$ik(A - B - C) = \frac{2m\lambda}{\hbar^2}(A + B). \tag{11}$$

Doing some rearranging, we find

$$A\left(1+2i\frac{m\lambda}{\hbar^2 k}\right)-B\left(1-2i\frac{m\lambda}{\hbar^2 k}\right)=C. \tag{12}$$

Defining $\alpha \equiv \hbar^2/(m\lambda)$, we can say

$$A\left(1+\frac{2i}{k\alpha}\right)-B\left(1-\frac{2i}{k\alpha}\right)=C. \tag{13}$$

I'll leave out the tedious algebra; we find that

$$B=\frac{i/k\alpha}{1-(i/k\alpha)}A, \quad \text{and} \quad C=\frac{1}{1-(i/k\alpha)}. \tag{14}$$

Intuitively, based on the fact that the wavefunction is normalized, the coefficients are almost like probabilities, or relative sizes of the corresponding propagating waves, so we can treat their ratios with A to determine relative probabilities that the forward propagating wave either transmits or reflects. For the former case, this is

$$T=\frac{|C|^2}{|A|^2}=\frac{1}{1+1/(k\alpha)^2}=\boxed{\frac{(k\alpha)^2}{1+(k\alpha)^2},} \tag{15}$$

and for the latter case, this is

$$R=\frac{|B|^2}{|A|^2}=\frac{1/(k\alpha)^2}{1+1/(k\alpha)^2}=\boxed{\frac{1}{1+(k\alpha)^2}.} \tag{16}$$

The determine the unit of k, we consider that the quantity in an exponential must be unitless, so the units of k and x must cancel, so $[k]=\mathrm{m}^{-1}$ (meters). The transmission/reflection coefficients must also be unitless, since all ratios are, meaning that the units of α are the inverse of k, so $[\alpha]=m$. Lastly, since the units of potential must be the same as those of energy, then λ has units of energy.

Question 2. Position and Momentum Basis

a) Of course, $\hat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle=\boldsymbol{p}\,|\boldsymbol{p}\rangle$, so we can easily see that $\langle\boldsymbol{x}|\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle=\boldsymbol{p}\,\langle\boldsymbol{x}|\boldsymbol{p}\rangle$. Another way to interpret it is that this is the position representation of the momentum operator acting on a momentum state, which, in three-dimensions, is the gradient (times $-i\hbar$), meaning that also $\langle\boldsymbol{x}|\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle=-i\hbar\hat{\boldsymbol{\nabla}}\,\langle\boldsymbol{x}|\boldsymbol{p}\rangle$. Therefore, doing a teeny bit of reshuffling, we can see that

$$\frac{i\boldsymbol{p}}{\hbar}\,\langle\boldsymbol{x}|\boldsymbol{p}\rangle=\hat{\boldsymbol{\nabla}}\,\langle\boldsymbol{x}|\boldsymbol{p}\rangle\,. \tag{17}$$

b) The above result is a simple differential equation, which becomes clear when we express $\psi_{\boldsymbol{p}}(\boldsymbol{x})=\langle\boldsymbol{x}|\boldsymbol{p}\rangle$, and the result is something we have seen many times; it's an exponential (times a constant):

$$\psi_{\boldsymbol{p}}(\boldsymbol{x})=Ae^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}. \tag{18}$$

As a complex exponential, we can't use the ordinary normalization condition $|\psi_{\boldsymbol{p}}(\boldsymbol{x})|^2=1$, but we can use Dirac orthonormality, i.e. that $\langle\boldsymbol{p}'|\boldsymbol{p}\rangle=\delta^3(\boldsymbol{p}-\boldsymbol{p}')$. Inserting the identity, we find

$$\int \mathrm{d}^3x\;\langle\boldsymbol{p}'|\boldsymbol{x}\rangle\,\langle\boldsymbol{x}|\boldsymbol{p}\rangle=|A|^2\int \mathrm{d}^3x\; e^{-i\boldsymbol{p}'\cdot\boldsymbol{x}/\hbar}e^{-\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}=|A|^2\int \mathrm{d}^3x\; e^{i(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{x}/\hbar}. \tag{19}$$

However we know that

$$\delta(x)=\frac{1}{2\pi}\int \mathrm{d}k\; e^{ikx}, \tag{20}$$

so the lefthand side is really just the delta function, with a factor of $(2\pi\hbar)^3$, meaning we have

$$|A|^2(2\pi\hbar)^3\delta^3(\boldsymbol{p}'-\boldsymbol{p}) = \delta^3(\boldsymbol{p}-\boldsymbol{p}'), \tag{21}$$

meaning

$$A = \frac{1}{(2\pi\hbar)^{3/2}}, \tag{22}$$

so,

$$\boxed{\psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle \boldsymbol{x}|\boldsymbol{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}.} \tag{23}$$

c) Since $\boldsymbol{p} = \hbar\boldsymbol{k}$, then of course $\boldsymbol{p}/\hbar = \boldsymbol{k}$, which has the effect of getting rid of all the $\hbar$'s in our result, so this one is easy:

$$\boxed{\psi_{\boldsymbol{k}}(\boldsymbol{x})\,\langle \boldsymbol{k}|\boldsymbol{x}\rangle = \frac{1}{(2\pi)^{3/2}}e^{i\boldsymbol{k}\cdot\boldsymbol{x}}.} \tag{24}$$

Question 3. The Harmonic Oscillator

a) The ladder operators are defined like

$$\hat{a}_\pm \equiv \frac{1}{\sqrt{2m\omega\hbar}}(\mp i\hat{p} + m\omega\hat{x}). \tag{25}$$

Writing the combination $\hat{a}_+\hat{a}_-$:

$$\begin{aligned}
\hat{a}_+\hat{a}_- &= \frac{1}{2m\omega\hbar}\left(\hat{p}^2 - im\omega\hat{p}\hat{x} + im\omega\hat{x}\hat{p} + (m\omega\hat{x})^2\right) &(26)\\
&= \frac{1}{2m\omega\hbar}\left(\hat{p}^2 + (m\omega\hat{x})^2 + im\omega[\hat{x},\hat{p}]\right). &(27)
\end{aligned}$$

The commutator $[\hat{x},\hat{p}] = i\hbar$, so

$$\hat{a}_+\hat{a}_- = \frac{1}{\omega\hbar}\left[\frac{1}{2m}(\hat{p}^2 + (m\omega\hat{x})^2)\right] + \frac{i}{2\hbar}(i\hbar). \tag{28}$$

The first term is just the Hamiltonian, and the second is $-1/2$:

$$\hat{a}_+\hat{a}_- = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2}, \tag{29}$$

$$\boxed{\hat{H} = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right).} \tag{30}$$

Or, we also associate the “raising” operator with the “creation” operator which we typically denote $\hat{a}^\dagger$, where the annihilation operator is its Hermitian conjugate $\hat{a}$, so our Hamiltonian can also be written like so:

$$\boxed{\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right).} \tag{31}$$

b) The number operator is defined as $\hat{N} \equiv \hat{a}^\dagger \hat{a}$, meaning we could write the Hamiltonian yet another way:

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right) . \tag{32}$$

The Hamiltonian is now constructed with the number operator and constant terms. Since the number operator obviously commutes with itself and any constant, it must also commute with the Hamiltonian. Therefore, there must be a set of simultaneous eigenstates between them.

c) With the Hamiltonian written with the number operator, the eigenvalues of the kets $|n\rangle$ are trivial:

$$\hat{H} |n\rangle = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) |n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |n\rangle = E_n |n\rangle , \tag{33}$$

so $E_n = \hbar\omega(n + \frac{1}{2})$.

d) Let's consider $\hat{a} |n\rangle = A_n |n-1\rangle$, where A_n is the eigenvalue we are trying to find. We know that if we create a sandwich with the number operator:

$$\langle n|\hat{a}^\dagger \hat{a}|n\rangle \to \langle \hat{a}n|\hat{a}n\rangle = |A_n|^2 \langle n-1|n-1\rangle . \tag{34}$$

However, obviously, since it's the number operator, we also have

$$\langle n|\hat{a}^\dagger \hat{a}|n\rangle = n \langle n|n\rangle , \tag{35}$$

meaning we have

$$|A_n|^2 \langle n-1|n-1\rangle = n \langle n|n\rangle . \tag{36}$$

Via Dirac orthonormality, this becomes $|A_n|^2 = n$, so $A_n = \sqrt{n}$ since n is positive/real.
Next, we consider $\hat{a}^\dagger |n\rangle = B_n |n+1\rangle$. In this case, we make the sandwich $\langle n|\hat{a}\hat{a}^\dagger|n\rangle$, which is

$$\langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle \hat{a}^\dagger n|\hat{a}^\dagger n\rangle = |B_n|^2 \langle n+1|n+1\rangle . \tag{37}$$

Now, since $[\hat{a}, \hat{a}^\dagger] = 1$, this is also

$$\langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle n|\hat{N} + 1|n\rangle = (n+1) \langle n|n\rangle . \tag{38}$$

Therefore, $B_n = \sqrt{n+1}$, so

$$\boxed{\hat{a} |n\rangle = \sqrt{n} |n-1\rangle ,} \quad \text{and} \tag{39}$$

$$\boxed{\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle .} \tag{40}$$

e) Writing a few terms, we find

$$|1\rangle = \frac{1}{\sqrt{1}} \hat{a}^\dagger |0\rangle , \tag{41}$$

$$|2\rangle = \frac{1}{\sqrt{2}} \hat{a}^\dagger |1\rangle = \frac{1}{\sqrt{2 \cdot 1}} (\hat{a}^\dagger)^2 |0\rangle . \tag{42}$$

$$|2\rangle = \frac{1}{\sqrt{3}} \hat{a}^\dagger |2\rangle = \frac{1}{\sqrt{3 \cdot 2 \cdot 1}} (\hat{a}^\dagger)^3 |0\rangle , \tag{43}$$

and so on. Clearly, this is just

$$\boxed{|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n |0\rangle\,.} \tag{44}$$

Question 4. The Translation Operator

a) We know that the position operator transforms under the translation operator like so:

$$\hat{T}^\dagger(a)\hat{x}\hat{T}(a) = \hat{x} + a. \tag{45}$$

Acting on both sides with $\hat{T}(a)$ cancels the $\hat{T}^\dagger(a)$ on the left since the translation operator is unitary, so

$$\hat{x}\hat{T}(a) = \hat{T}(a)\hat{x} + a\hat{T}(a) \quad \rightarrow \boxed{[\hat{x}, \hat{T}(a)] = a\hat{T}(a).} \tag{46}$$

b) We are considering now the how $\langle \hat{x} \rangle$ and how it compares to $\langle \hat{x}' \rangle$. First, from the commutator:

$$\hat{x}\hat{T}(a) - \hat{T}(a)\hat{x} = a\hat{T}(a). \tag{47}$$

Acting with $\hat{T}^\dagger(a)$:

$$\hat{T}^\dagger(a)\hat{x}\hat{T}(a) - \hat{x} = a, \quad \rightarrow \quad \hat{x'} = \hat{T}^\dagger(x)\hat{x}\hat{T}(a) = \hat{x} + a. \tag{48}$$

Thus,

$$\langle \hat{x}' \rangle = \langle x|\hat{x} + a|x\rangle = \boxed{\langle x \rangle + a.} \tag{49}$$

Question 5. The Born-Oppenheimer Approximation

We begin by writing the Hamiltonian for this system; it's just the combination of the kinetic and potential energies:

$$\hat{H} = \frac{\hat{p}_1^2}{2M} + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}k_1\hat{x}_1^2 + \frac{1}{2}k_2\hat{x}_2^2 + \frac{1}{2}k_{12}(\hat{x}_1 - \hat{x}_2)^2. \tag{50}$$

To start with the Born-Oppenheimer approximation, we first make the assumption that the heavier particle is so much heavier that we can neglect its motion compared to the lighter particle. In this case, this means that its kinetic energy is significantly smaller than that of the lighter particle. We also recognize that the Hamiltonian can be split up into three parts: $\hat{H} = \hat{H}_1 + \hat{H}_{12} + \hat{H}_2$ where $\hat{H}_i$ is the Hamiltonian of the ith particle and $\hat{H}_{12}$ is the interaction part containing the last potential term. With our assumption, we have that $\hat{H}_1 << \hat{H}_{12} + \hat{H}_2$, so we solve the latter:

$$(\hat{H}_{12} + \hat{H}_2)\,|\psi_n\rangle = (E_2)_n\,|\psi_n\rangle\,, \tag{51}$$

where $|\psi_n\rangle$ is the nth eigenket for the light particle. This is something that we can solve. Writing out this new Hamiltonian, we have

$$\hat{H}_{12} + \hat{H}_2 = \frac{\hat{p}_2^2}{2m} + \frac{1}{2}k_2x_2^2 + \frac{1}{2}k_{12}(\hat{x}_1 - \hat{x}_2)^2. \tag{52}$$

We can complete the square here and get a decently simple equation:

$$
\begin{aligned}
\hat{H}_{12} + \hat{H}_2 &= \frac{\hat{p}_2^2}{2m} + \frac{1}{2}k_2 x_2^2 + \frac{1}{2}k_{12}x_1^2 - k_{12}x_1 x_2 + \frac{1}{2}k_{12}x_2^2 && (53)\\
&= \frac{\hat{p}_2^2}{2m} + \frac{1}{2}(k_2 + k_{12})x_2^2 - k_{12}x_1 x_2 + \frac{1}{2}k_{12}x_1^2 && (54)\\
&= \frac{\hat{p}_2^2}{2m} + \frac{1}{2}(k_2 + k_{12})\left[x_2^2 - \left(\frac{2k_{12}}{k_2 + k_{12}x_1}x_2 + \frac{k_{12}}{k_2 + k_1 2}x_1^2\right)\right]. && (55)
\end{aligned}
$$

Defining $a \equiv k_{12}/(k_2 + k_{12})$ to make things simpler, we have

$$
\begin{aligned}
\hat{H}_{12} + \hat{H}_2 &= \frac{\hat{p}_2^2}{2m} + \frac{1}{2}(k_2 + k_{12})\left[x_2^2 - 2ax_1x_2 + ax_1^2\right] && (56)\\
&= \frac{\hat{p}_2^2}{2m} + \frac{1}{2}(k_2 + k_{12})\left[(x_2 - ax_1)^2 + a(1-a)x_1^2\right] && (57)\\
&= \frac{\hat{p}_2^2}{2m} + \frac{1}{2}(k_2 + k_{12})(x_2 - ax_1)^2 + k_{12}(1-a)x_1^2. && (58)
\end{aligned}
$$

We have recovered a normal simple harmonic oscillator Hamiltonian, but with $k_2' = k_2 + k_{12}$ and a constant term. The constant term won't do anything but sum the normal simple harmonic oscillator solutions. So:

$$
(E_2)_0 = \hbar\omega_2'\left(n + \frac{1}{2}\right) + k_{12}(1-a)x_1^2 = \hbar\omega_2'\left(n + \frac{1}{2}\right) + x_1^2\left(\frac{k_2 k_{12}}{k_2 + k_{12}}\right), \tag{59}
$$

where $\omega_2' = \sqrt{k_2'/m} = \sqrt{(k_2 + k_{12})/m}$.

We now adopt the product ansätz, that is, that we express the total wavefunction as a product of the heavier and lighter particle wavefunctions:

$$
|\Psi\rangle = |\psi\rangle\,|\phi\rangle\,, \quad \text{or} \quad \Psi(x_1, x_2) = \psi(x_1)\phi(x_2). \tag{60}
$$

To look at the wavefunction for the heavier particle, we make another assumption: the lighter particle remains in the same state as the system progresses. If this is the case, we can just place it in the ground state without loss of generality. Now, we act on the total wavefunction with $\hat{H}_{12} + \hat{H}_2$. It will ignore the heavy part since this combined light operator sees it as essentially constant. This leaves us with:

$$
(\hat{H}_{12} + \hat{H}_2)\,|\Psi\rangle = (E_2)_0\,|\psi\rangle\,|\phi\rangle\,. \tag{61}
$$

Now if we act with $\hat{H}_1$ on this Hamiltonian, we can first consider the kinetic term:

$$
\begin{aligned}
\hat{p}_1^2\,|\psi\rangle\,|\phi\rangle = (-\hbar^2\partial_{x_1}^2\,|\psi\rangle)\,|\phi\rangle + |\psi\rangle\,(\hat{p}_1^2\,|\phi\rangle) && (62)\\
- 2i\hbar(\partial_{x_1}|\psi\rangle)(\hat{p}_1\,|\phi\rangle) && (63)
\end{aligned}
$$

If we just define $U_1(x_1) \equiv kx_1^2/2$, then the entire $\hat{H}_1$ term acting on the total wavefunction looks like

$$
\begin{aligned}
\hat{H}_1\,|\Psi\rangle = \left(-\frac{\hbar^2}{2M}\partial_{x_1}^2\,|\psi\rangle\right)|\phi\rangle + |\psi\rangle\left(\frac{\hat{p}_1^2}{2M}\,|\phi\rangle\right) && (64)\\
- \frac{i\hbar}{m}(\partial_{x_1}|\psi\rangle)(\hat{p}_1\,|\phi\rangle) + |\psi\rangle\,U(x_1)\,|\phi\rangle\,. && (65)
\end{aligned}
$$

So, adding this with the light-particle solution (which is just the energy eigenvalues) we get the action of the total Hamiltonian on the total wavefunction:

$$\hat{H}\,|\Psi\rangle = |\psi\rangle\left[-\frac{\hbar^2}{2M}\partial_{x_1}^2 + U_1(x_1) + (E_2)_0\right]|\phi\rangle \tag{66}$$

$$-\left[\frac{i\hbar}{M}(\partial_{x_1}|\psi\rangle)\hat{p}_1 + \frac{\hbar^2}{2M}\partial_{x_1}^2|\psi\rangle\right]|\phi\rangle\,. \tag{67}$$

We can now integrate out the light-particle degrees of freedom by acting on the left with $\langle\psi|$:

$$\langle\psi|\hat{H}|\Psi\rangle = \langle\psi|\left[-\frac{\hbar^2}{2M}\partial_{x_1}^2 + U_1(x_1) + (E_2)_0\right]|\phi\rangle \tag{68}$$

$$-\left[\frac{i\hbar}{m}(\langle\psi|\partial_{x_1}|\psi\rangle\,\hat{p}_1 + \frac{\hbar^2}{2M}(\langle\psi|\partial_{x_1}^2|\psi\rangle)\right]|\phi\rangle\,. \tag{69}$$

We know from class that the two terms in the second line are zero; the first is zero due to time-reversal symmetry, the second is proportional to the kinetic energy of the lighter particle divided by the mass of the large particle, which in our approximation, we can take to zero. Thus,

$$\langle\psi|\hat{H}|\Psi\rangle = \langle\psi|\left[\frac{\hat{p}_1^2}{2M} + U_1(x_1) + (E_2)_0\right]|\phi\rangle\,, \tag{70}$$

hence, we can define an effective Hamiltonian for the heavy particle:

$$\hat{H}_{1,\mathrm{eff}} = \frac{\hat{p}_1^2}{2M} + U_1(x_1) + (E_2)_0 = \frac{\hat{p}_1^2}{2M} + \frac{1}{2}k_1x_1^2 + (E_2)_0. \tag{71}$$

This is an easily Hamiltonian to solve. First, the ground state of the lighter particle has

$$(E_2)_0 = \frac{\hbar\omega_2'}{2} + x_1^2\left(\frac{k_2k_{12}}{k_2+k_{12}}\right), \tag{72}$$

which leads to

$$\hat{H}_{1,\mathrm{eff}} = \frac{\hat{p}_1^2}{2M} + \frac{1}{2}\left(k_1 + \frac{2k_2k_{12}}{k_2+k_{12}}\right)x_1^2 + \frac{\hbar\omega_2'}{2}. \tag{73}$$

This is just another SHO with a constant term. So, defining k_1' as the stuff inside the parentheses, we have

$$(E_1)_n = \hbar\omega_1'\left(n+\frac{1}{2}\right) + \frac{\hbar\omega_2'}{2}, \tag{74}$$

where $\omega_1' = \sqrt{k_1'/M}$.

At this point, we have solved this problem in the Born-Oppenheimer approximation. The next order of business would be to solve it exactly, i.e. without any approximations. This is something I still don't quite understand, so I will just recap my very basic understanding. First, we can better express this in matrix form like so:

$$H = \frac{1}{2}\mathbf{P}^\intercal\mathbf{M}^{-1}\mathbf{P} + \frac{1}{2}\mathbf{X}^\intercal\mathbf{K}\mathbf{X}, \tag{75}$$

where $\mathbf{P} = \begin{pmatrix}\hat{p}_1 & \hat{p}_2\end{pmatrix}$, $\mathbf{M}$ is a positive-definite, diagonal mass matrix, $\mathbf{X} = \begin{pmatrix}x_1 & x_2\end{pmatrix}$, and

$$\mathbf{K} = \begin{pmatrix}k_1+k_{12} & -k_{12}\\ -k_{12} & k_1+k_{12}\end{pmatrix}. \tag{76}$$

(The next half-page or so is overexplained, but I am doing it in hopes that by explaining it thoroughly on paper, it will become more clear to me. It will also make it easier for you to point out where I inevitably went wrong somewhere.) The idea is to diagonalize $\mathbf{K}$, since that way we would have two decoupled harmonic oscillators, whose energies we can very easily solve for (it'd just be a sum of the two). However, we can't just diagonalize $\mathbf{K}$, since we are in essence doing a coordinate transformation, meaning the momentum matrices would have to be transformed non-trivially as well. In doing so, in order for the kinetic part of the Hamiltonian to remain diagonal, the coefficients must have mass-dependence.

This can be seen by considering the kinetic part only. If we were to do a coordinate transformation, we end up with:

$$\frac{1}{2}\mathbf{P}^{\intercal}\mathbf{M}^{-1}\mathbf{P} \quad \rightarrow \quad \frac{1}{2}\mathbf{P}^{\intercal}\mathbf{U}^{-1}\mathbf{M}^{-1}\mathbf{U}\mathbf{P}. \tag{77}$$

Expressing elements of $\mathbf{U}$ generally as u_{ij} and elements of $\mathbf{U}_{-1}$ generally as u_{ij}^{-1}, we find that an off-diagonal component of the final matrix sandwiched between the momentum vectors would look like:

$$\left(\mathbf{U}^{-1}\mathbf{M}^{-1}\mathbf{U}\right)_{12} = \frac{u_{11}^{-1}u_{12}}{m_1} + \frac{u_{12}^{-1}u_{22}}{m_2}. \tag{78}$$

Without any mass dependence, there is no way for these terms to cancel. Hence, we can consider splitting the mass matrix up into $\mathbf{U}^{-1}\mathbf{M}^{-1/2}\mathbf{M}^{-1/2}\mathbf{U}$, such that $\mathbf{U}^{-1}\mathbf{M}^{-1/2}$ and $\mathbf{M}^{-1/2}\mathbf{U}$ are the two transformations, and in this way, the kinetic term remains trivially diagonal and we can look to the potential term to make any determinations. Under these transformations, the potential term will look $\mathbf{x}^{\intercal}\mathbf{U}^{-1}\mathbf{M}^{-1/2}\mathbf{K}\mathbf{M}^{-1/2}\mathbf{U}\mathbf{x}$. At the end of the day, then, we are looking to diagonalize not $\mathbf{K}$ but $\mathbf{M}^{-1/2}\mathbf{K}\mathbf{M}^{-1/2}$:

$$\mathbf{M}^{-1/2}\mathbf{K}\mathbf{M}^{-1/2} = \begin{pmatrix} \frac{k_1+k_{12}}{M} & -\frac{k_{12}}{\sqrt{Mm}} \\ -\frac{k_{12}}{\sqrt{Mm}} & \frac{k_1+k_{12}}{m} \end{pmatrix}. \tag{79}$$

I don't want to type everything out here, but by diagonalizing this and using the ever-wonderful quadratic formula, we arrive the eigenvalues, which are the two frequencies (squared) of the normal modes:

$$\omega_{\pm}^2 = \frac{-\frac{k_{12}(M+m)+mk_1+Mk_2}{Mm} \pm \sqrt{\left(\frac{k_{12}(M+m)+mk_1+Mk_2}{Mm}\right)^2 - 4\left(\frac{k_1k_{12}+k_1k_2+k_{12}k_2}{Mm}\right)}}{2}. \tag{80}$$

Since we have $m << M$, we can simplify the term outside the square root (and the identical term that's squared inside the square root and get

$$\omega_{\pm}^2 = \frac{-\frac{k_{12}+k_2}{m} \pm \sqrt{\left(\frac{k_{12}+k_2}{m}\right)^2 - 4\left(\frac{k_1k_{12}+k_1k_2+k_{12}k_2}{Mm}\right)}}{2}. \tag{81}$$

Further, if we multiply top and bottom by m, we get

$$\omega_{\pm}^2 = \frac{-(k_{12}+k2) \pm \sqrt{(k_{12}+k_2)^2 - 4\frac{m}{M}(k_1k_{12}+k_1k_2+k_{12}k_2)}}{2m}, \tag{82}$$

and the second term in brackets vanishes. If we then take the limiting case $k_{12} << k_1, k_2$, the $\pm$ gives two terms, one of which is zero, and all we get left is $\omega = \sqrt{k_2/m}$ (taking the positive root), which gives us energy levels which makes complete sense! If one particle is super heavy and doesn't move much compared to the other, and they hardly interact, then we essentially just have the one oscillator, which is exactly what we just got.

We also see pretty easily that the same occurs for our approximation case.