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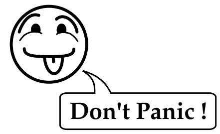


Quantum Mechanics I 7th Oct. '02.

1st Midterm Exam Solutions T. Hübsch

DISCLAIMER: This solution set presents more detail than was required of the Student, and is meant as an additional resource for learning. Please *do* study not just the solutions as presented, but try also to understand the rationale behind the approach.

1. Given two state vectors, $|u_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\1\end{bmatrix}$, and $|u_2\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\1\end{bmatrix}$,

a. determine a linearly independent $|u_3\rangle$ and prove that $\{|u_i\rangle\,, i=1,2,3\}$ form a complete and normalized (albeit not orthonormal) basis for 3-dimensional vectors.

Solution____________________.

For linear independence, we need to find (x,y,z) such that

$$\frac{c_1}{\sqrt{2}}\begin{bmatrix}1\\0\\1\end{bmatrix}+\frac{c_2}{\sqrt{2}}\begin{bmatrix}0\\1\\1\end{bmatrix}+c_3\begin{bmatrix}x\\y\\z\end{bmatrix}=0\;,\qquad\Rightarrow\qquad\begin{bmatrix}1&0&\sqrt{2}\,x\\0&1&\sqrt{2}\,y\\1&1&\sqrt{2}\,z\end{bmatrix}\begin{bmatrix}c_1\\c_2\\c_3\end{bmatrix}=0\;.$$

would hold only if all $c_i=0$. Thus

$$0\overset{!}{\neq}\begin{vmatrix}1&0&\sqrt{2}\,x\\0&1&\sqrt{2}\,y\\1&1&\sqrt{2}\,z\end{vmatrix}=\sqrt{2}(z-x-y)\;,\qquad\Rightarrow\qquad z\neq x+y\;. \qquad (*)$$

Clearly, there are many "nice" solutions to this inequality, *e.g.*:

$$\begin{bmatrix}1\\0\\0\end{bmatrix},\quad\begin{bmatrix}0\\1\\0\end{bmatrix},\quad\begin{bmatrix}0\\0\\1\end{bmatrix},\quad\tfrac{1}{\sqrt{2}}\begin{bmatrix}1\\1\\0\end{bmatrix},\quad\tfrac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\1\end{bmatrix},\quad\textit{etc.}$$

For reasons of symmetry, we'll pick the fourth choice here. [=5pt]

b. Construct the $\langle u_i|$, $i=1,2,3$ and show that this basis it not orthonormal.

Solution____________________.

For the $\langle u_i|$ to act on the column-vectors $|u_i\rangle$ and to produce (in general, complex) numbers, they must be hermitian-conjugate row-vectors:

$$\langle u_1| = \tfrac{1}{\sqrt{2}}[1,0,1]\;,\quad \langle u_1| = \tfrac{1}{\sqrt{2}}[0,1,1]\;,\quad \langle u_1| = \tfrac{1}{\sqrt{2}}[1,1,0]\;.$$

Non-orthogonality is proven by finding $\langle u_i|u_j\rangle \neq 0$ for any $i\neq j$; in this case, this is true for all three pairs:

$$\langle u_i|u_j\rangle = \tfrac{1}{2}(1+\delta_{i,j})\;,\qquad i,j=1,2,3\;.$$

Since $\langle u_i|u_j\rangle \neq 0$ when $i\neq j$, this basis, albeit complete and 'nicely' symmetric (which may be the reason for using it in some particular application), is not orthogonal. [=5pt]

c. Starting with $|v_1\rangle = |u_1\rangle$, and $|v_2\rangle = b_1\,|u_1\rangle + b_2\,|u_2\rangle$, construct an orthonormal basis $\{|v_i\rangle\,, i = 1, 2, 3\}$.

Solution____.

We start with the $|v_i\rangle$, $i = 1, 2$ as instructed, require orthogonality:

$$0 \stackrel{!}{=} \langle v_1|v_2\rangle = \langle u_1|\Big(b_1\,|u_1\rangle + b_2\,|u_2\rangle\Big) = b_1 + \tfrac{1}{2}b_2\ , \quad \Rightarrow \quad |v_1\rangle = \frac{b_1}{\sqrt{2}}\begin{bmatrix}1\\-2\\-1\end{bmatrix}\ ,$$

and then normalize:

$$1 \stackrel{!}{=} \langle v_2|v_2\rangle = \frac{|b_1|^2}{2}[1,-2,-1]\begin{bmatrix}1\\-2\\-1\end{bmatrix} = |b_1|^2{\cdot}3, \quad \Rightarrow \quad |v_2\rangle = \frac{1}{\sqrt{6}}\begin{bmatrix}1\\-2\\-1\end{bmatrix}\ .$$

Then, we introduce

$$|v_3\rangle = \begin{bmatrix}x\\y\\z\end{bmatrix}\ , \quad \text{such that} \quad \langle v_i|v_3\rangle = \delta_{i,3}\ , \quad i = 1, 2, 3\ .$$

These three conditions, listed in turn, uniquely fix x, y, z: [=10pt]

$$\left.\begin{aligned} x + z &= 0\\ x - 2y - z &= 0\\ x^2 + y^2 + z^2 &= 1\end{aligned}\right\} \quad \Rightarrow \quad |v_1\rangle = \frac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\-1\end{bmatrix}\ .$$

d. Construct the projection operators $\hat{\mathsf{P}}_i = |v_i\rangle\,\langle v_i|$ and prove that $\sum_{i=1}^{3}\hat{\mathsf{P}}_i = \mathbb{1}$, and that $\hat{\mathsf{P}}_i\hat{\mathsf{P}}_j = \delta_{ij}\hat{\mathsf{P}}_j$, $\forall\, i, j = 1, 2, 3$. (Neither of these holds for $\hat{\P}_i = |u_i\rangle\,\langle u_i|$.)

Solution____.

Straightforwardly:

$$\hat{\mathsf{P}}_1 = |v_1\rangle\,\langle v_1| = \tfrac{1}{2}\begin{bmatrix}1\\0\\1\end{bmatrix}[1,0,1] = \begin{bmatrix}{}^1\!/_2 & 0 & {}^1\!/_2\\ 0 & 0 & 0\\ {}^1\!/_2 & 0 & {}^1\!/_2\end{bmatrix}\ ,$$

and

$$\hat{\mathsf{P}}_2 = \begin{bmatrix}{}^1\!/_6 & -{}^1\!/_3 & -{}^1\!/_6\\ -{}^1\!/_3 & {}^2\!/_3 & {}^1\!/_3\\ -{}^1\!/_6 & {}^1\!/_3 & {}^1\!/_6\end{bmatrix}\ , \quad \hat{\mathsf{P}}_3 = \begin{bmatrix}{}^1\!/_3 & {}^1\!/_3 & -{}^1\!/_3\\ {}^1\!/_3 & {}^1\!/_3 & -{}^1\!/_3\\ -{}^1\!/_3 & -{}^1\!/_3 & {}^1\!/_3\end{bmatrix}\ .$$

And, with these, indeed:

$$\begin{bmatrix}{}^1\!/_2 & 0 & {}^1\!/_2\\ 0 & 0 & 0\\ {}^1\!/_2 & 0 & {}^1\!/_2\end{bmatrix} + \begin{bmatrix}{}^1\!/_6 & -{}^1\!/_3 & -{}^1\!/_6\\ -{}^1\!/_3 & {}^2\!/_3 & {}^1\!/_3\\ -{}^1\!/_6 & {}^1\!/_3 & {}^1\!/_6\end{bmatrix} + \begin{bmatrix}{}^1\!/_6 & -{}^1\!/_3 & -{}^1\!/_6\\ -{}^1\!/_3 & {}^2\!/_3 & {}^1\!/_3\\ -{}^1\!/_6 & {}^1\!/_3 & {}^1\!/_6\end{bmatrix} = \begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}\ ,$$

and, similarly, $\hat{\mathsf{P}}_i\hat{\mathsf{P}}_i = \hat{\mathsf{P}}_i$ for $i = 1, 2, 3$ but $\hat{\mathsf{P}}_i\hat{\mathsf{P}}_j = 0$ if $i \neq j$. These matrix calculations are clearly lengthy and were best left for the take-home part. [=15pt]

2. An observable of the system in problem 1 is represented by $\hat{F} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{bmatrix}$.

a. Determine all possible results of (single attempts of) measuring $\hat{F}$.

Solution____.

Possible outcomes of single measurements are the eigenvalues of $\hat{F}$. These we obtain by solving the secular equation:

$$0 \stackrel{!}{=} \det[\hat{F} - f\mathbb{1}] = \begin{vmatrix} -f & 1 & 0 \\ 1 & -(f{+}1) & 1 \\ 0 & 1 & -f \end{vmatrix} = -f^2(f+1) + 2f = -f(f{+}2)(f{-}1) ,$$

so the possible single measurement results are $f = -2, 0, 1$. [=5pt]

b. Determine all eigenvectors of $\hat{F}$.

Solution____.

Writing $\hat{F}\,|f\rangle = f\,|f\rangle$ as $[\hat{F} - f\mathbb{1}]\,|f\rangle = 0$, we calculate

$$0 \stackrel{!}{=} [\hat{F} + 2\mathbb{1}]\,|{-2}\rangle = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} , \quad \Rightarrow \quad \left.\begin{aligned} 2x{+}y &= 0 \\ x{+}y{+}z &= 0 \\ y{+}2z &= 0 \end{aligned}\right\} \quad \Rightarrow \quad |{-2}\rangle = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} .$$

$$0 \stackrel{!}{=} [\hat{F} - 0\mathbb{1}]\,|0\rangle = \begin{bmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} , \quad \Rightarrow \quad \left.\begin{aligned} y &= 0 \\ x{-}y{+}z &= 0 \\ y &= 0 \end{aligned}\right\} \quad \Rightarrow \quad |0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} .$$

$$0 \stackrel{!}{=} [\hat{F} - 1\mathbb{1}]\,|1\rangle = \begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} , \quad \Rightarrow \quad \left.\begin{aligned} -x{+}y &= 0 \\ x{-}2y{+}z &= 0 \\ y{-}z &= 0 \end{aligned}\right\} \quad \Rightarrow \quad |1\rangle = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} .$$

[=10pt]

c. Calculate the expectation value of $\hat{F}$ in the pure state u_1.

Solution____.

This probability equals $\mathrm{Tr}[\hat{\rho}_{u_1}\hat{F}] = \langle u_1|\hat{F}|u_1\rangle$, and we can calculate it directly:

$$\langle\hat{F}\rangle_{u_1} = \mathrm{Tr}\left[\begin{bmatrix} 1/2 & 0 & 1/2 \\ 0 & 0 & 0 \\ 1/2 & 0 & 1/2 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{bmatrix}\right] = \mathrm{Tr}\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} = 0 ,$$

or [=5pt]

$$\langle\hat{F}\rangle_{u_1} = \tfrac{1}{2}[1,0,1] \begin{bmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \tfrac{1}{2}[1,0,1] \begin{bmatrix} 0 \\ 2 \\ 0 \end{bmatrix} = 0 ,$$

d. Calculate the probability that the measurement of the observable $\hat{F}$ in the system in state pure state u_1 would turn out to be 1.

Solution

As given in the text, and used in the homework solution, $\text{Prob}(\hat{F}{=}f|\hat{\rho}) = \text{Tr}[\hat{\rho}\,\hat{\mathsf{P}}_f]$. Since $\hat{\mathsf{P}}_f \stackrel{\text{def}}{=} |f\rangle\langle f|$, and for the pure state $\hat{\rho}_{u_1} = |u_1\rangle\langle u_1|$, we have that

$$\text{Prob}(\hat{F}{=}f|\hat{\rho}) = \text{Tr}\big[\hat{\rho}\,|f\rangle\langle f|\,\big] = \langle f|\hat{\rho}|f\rangle\ , \quad = \text{Tr}\big[\,|u_1\rangle\langle u_1|\,\hat{\mathsf{P}}_f\big] = \langle u_1|\hat{\mathsf{P}}_f|u_1\rangle$$

that is,

$$\text{Prob}(\hat{F}{=}f|\hat{\rho}) = \text{Tr}\big[\,|u_1\rangle\langle u_1|\,|f\rangle\langle f|\,\big] = \langle f|u_1\rangle\langle u_1|f\rangle = \big|\langle u_1|f\rangle\big|^2\ .$$

Alternatively (as done in other texts focusing on the wave-functions), we expand $|u_1\rangle = c_{-2}|{-2}\rangle + c_0|0\rangle + c_1|1\rangle$, use the orthonormalization of the $|f\rangle$ to obtain that $\langle 1|u_1\rangle = c_1$ is the probability amplitude, and deduce that $\text{Prob}(\hat{F}{=}f|\hat{\rho}) = |c_f|^2 = \big|\langle f|u_1\rangle\big|^2$, in agreement with the above, more direct calculation.

For our case at hand, [=10pt]

$$\text{Prob}(\hat{F}{=}1|\hat{\rho}_{u_1}) = \big|\langle u_1|1\rangle\big|^2 = \left|\tfrac{1}{\sqrt{2}}[1,0,1]\tfrac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\1\end{bmatrix}\right|^2 = \tfrac{1}{6}\,|2|^2 = \frac{2}{3}\ .$$

e. Calculate the expectation value of $\hat{F}$ in the impure state with $\hat{\rho} = \frac{1}{4}\hat{\mathsf{P}}_1 + \frac{3}{4}\hat{\mathsf{P}}_2$.

Solution

Doing the straightforward matrix algebra:

$$\hat{\rho} = \tfrac{1}{4}\hat{\mathsf{P}}_1 + \tfrac{3}{4}\hat{\mathsf{P}}_2 = \tfrac{1}{4}\begin{bmatrix}1/2 & 0 & 1/2\\ 0 & 0 & 0\\ 1/2 & 0 & 1/2\end{bmatrix} + \tfrac{3}{4}\begin{bmatrix}1/6 & -1/3 & -1/6\\ -1/3 & 2/3 & 1/3\\ -1/6 & 1/3 & 1/6\end{bmatrix} = \begin{bmatrix}1/4 & -1/4 & 0\\ -1/4 & 1/2 & 1/4\\ 0 & 1/4 & 1/4\end{bmatrix}\ ,$$

we have that

$$\langle\hat{F}\rangle_\rho = \text{Tr}\left[\begin{bmatrix}1/4 & -1/4 & 0\\ -1/4 & 1/2 & 1/4\\ 0 & 1/4 & 1/4\end{bmatrix}\begin{bmatrix}0 & 1 & 0\\ 1 & -1 & 1\\ 0 & 1 & 0\end{bmatrix}\right] = \text{Tr}\begin{bmatrix}-1/4 & 1/2 & -1/4\\ 1/2 & -1/2 & 1/2\\ 1/4 & 0 & 1/4\end{bmatrix} = -\frac{1}{2}\ .$$

Alternatively, using the linearity of Tr[ ], we have that

$$\begin{aligned}\langle\hat{F}\rangle_\rho &= \text{Tr}[(\tfrac{1}{4}\hat{\mathsf{P}}_1 + \tfrac{3}{4}\hat{\mathsf{P}}_2)\hat{F}] = \tfrac{1}{4}\,\text{Tr}[\hat{\mathsf{P}}_1\hat{F}] + \tfrac{3}{4}\,\text{Tr}[\hat{\mathsf{P}}_2\hat{F}]\ ,\\ &= \tfrac{1}{4}\langle v_1|\hat{F}|v_1\rangle + \tfrac{3}{4}\langle v_2|\hat{F}|v_2\rangle = \tfrac{1}{4}(0) + \tfrac{3}{4}(-\tfrac{2}{3}) = -\tfrac{1}{2}\ .\end{aligned}$$

[=10pt]

f. Calculate the probability that the measurement of the observable $\hat{F}$ in the system in impure state with $\hat{\rho} = \frac{1}{4}\hat{\mathsf{P}}_1 + \frac{3}{4}\hat{\mathsf{P}}_2$ would turn out to be 1.

Solution.

We have that $\text{Prob}(\hat{F}{=}f|\hat{\rho}) = \langle f|\hat{\rho}|f\rangle$ is:

$$\text{Prob}(\hat{F}{=}1|\hat{\rho}) = \tfrac{1}{3}[1,1,1]\begin{bmatrix} {}^1\!/_4 & -{}^1\!/_4 & 0 \\ -{}^1\!/_4 & {}^1\!/_2 & {}^1\!/_4 \\ 0 & {}^1\!/_4 & {}^1\!/_4 \end{bmatrix}\begin{bmatrix}1\\1\\1\end{bmatrix} = \frac{1}{3}\ .$$

We could have also calculated this using the linearity of Tr[ ]:

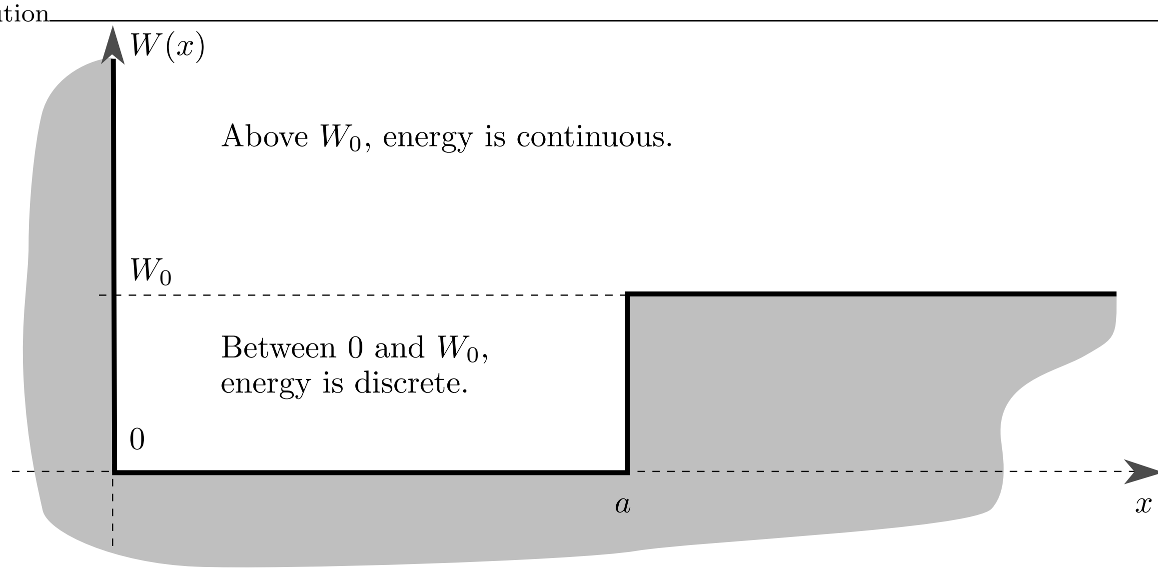
$$\begin{aligned}\text{Prob}(\hat{F}{=}f|\hat{\rho}) &= \text{Tr}[(\tfrac{1}{4}\hat{\mathsf{P}}_1 + \tfrac{3}{4}\hat{\mathsf{P}}_2)\hat{\mathsf{P}}_f] = \tfrac{1}{4}\,\text{Tr}[\hat{\mathsf{P}}_1\hat{\mathsf{P}}_f] + \tfrac{3}{4}\,\text{Tr}[\hat{\mathsf{P}}_2\hat{\mathsf{P}}_f]\ ,\\ &= \tfrac{1}{4}\big|\langle v_1|f\rangle\big|^2 + \tfrac{3}{4}\big|\langle v_2|f\rangle\big|^2 \end{aligned}$$

Thus, $\text{Prob}(\hat{F}{=}1|\hat{\rho}) = \frac{1}{4}\big|\langle v_1|1\rangle\big|^2 + \frac{3}{4}\big|\langle v_2|1\rangle\big|^2 = \frac{1}{4}\big|\frac{1}{\sqrt{2\cdot3}}(2)\big|^2 + \frac{3}{4}\big|\frac{1}{\sqrt{6\cdot3}}(-2)\big|^2 = \frac{1}{3}$. [=15pt]

3. Consider a particle under the influence of the potential: $W(x) = +\infty$ for $x < 0$, $W(x) = 0$ for $0 < x < a$, and $W(x) = W_0$ for $a < x$, with $W_0, a > 0$.

a. Sketch potential and determine the energy spectrum: which values are discrete and which are continuous.

Solution.



[=3pt]

b. State/specify all boundary conditions for stationary states with $0 < E < W_0$.

Solution.

Besides the mathcing condition at $x = a$:

$$\lim_{\epsilon\to0}\psi(a-\epsilon) = \lim_{\epsilon\to0}\psi(a+\epsilon)\ , \quad \text{and} \quad \lim_{\epsilon\to0}\psi'(a-\epsilon) = \lim_{\epsilon\to0}\psi'(a+\epsilon)\ ,$$

we also have that $\psi(0) = 0$ and $\lim_{x\to\infty}\psi(x) = 0$. [=5pt]

c. Find the equation that determines E when $0 < E < W_0$.

Solution

Since $\psi(0) = 0$ and $E > W(x)$ in the first region ($0 < x < a$), here we write $\psi_{(1)}(x) = A\sin(kx)$, where $k = \sqrt{2ME}/\hbar$. In the second region, we use the requirement that $\lim_{x\to\infty}\psi(x) = 0$ and that now $E < W(x)$, so that we write $\psi_{(2)}(x) = Ce^{-\kappa x}$, where $\kappa = \sqrt{2M(W_0 - E)}/\hbar$. The matching conditions then become

$$A\sin(ka) = Ce^{-\kappa a} \ , \quad \text{and} \quad kA\cos(ka) = -\kappa Ce^{-\kappa a} \ .$$

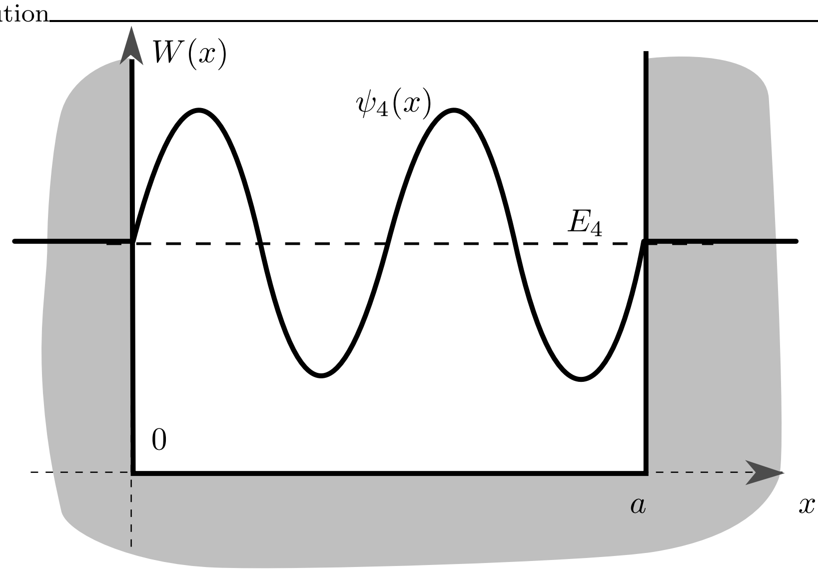
Dividing the second with the first, we obtain

$$k\cot(ka) = -\kappa \ , \quad \textit{i.e.} \quad \tan\Big(\frac{a}{\hbar}\sqrt{2ME}\Big) = -\sqrt{\frac{E}{W_0 - E}} \ ,$$

which is the transcendental equation determining E. [=15pt]

d. Sketch the potential and a wave-function when $W_0 \to \infty$;

Solution



Note that all $\psi(x) \equiv 0$ for $x < 0$ and $x > a$.

[=2pt]

e. Find the allowed values of E when $W_0 \to \infty$.

Solution

The allowed values can be obtained from the result of part c., by letting $W_0 \to \infty$. Then we have

$$\tan\Big(\frac{a}{\hbar}\sqrt{2ME}\Big) = 0 \ , \quad \textit{i.e.} \quad \sin\Big(\frac{a}{\hbar}\sqrt{2ME}\Big) = 0 \ ,$$

which happens for the select values of energy, E_n:

$$\frac{a}{\hbar}\sqrt{2ME_n} = n\pi \ , \quad \text{so} \quad E_n = \frac{\hbar^2\pi^2n^2}{2Ma^2} \ ,$$

which agrees with the result obtained in class, using that for the infinite potential well, as we have it here, with boundary conditions: $\psi(0) = 0 = \psi(a)$. [=5pt]