Model for an exciton on a carbon nanotube in the presence of an impurity

T. C. Dorlas
Dublin Institute for Advanced Studies
School of Theoretical Physics
10 Burlington Road, Dublin 4, Ireland.
Email: dorlas@stp.dias.ie

P. Duclos
Centre de physique théorique
Luminy, Marseille, France.
Email: duclos@univ-tln.fr and duclos@cpt.univ-mrs.fr

July 29, 2008

Abstract

We analyse the spectrum of a model of an exciton on a carbon nanotube in the presence of a fixed impurity potential.

1 Proof of the existence of at least one bound state

Theorem 1.1 *There is at least one bound state in the domain* $\{(\theta, z) : 0 \leq \theta \leq \pi/4, \quad 0 \leq z \leq 1/\sqrt{2}\}$.

Proof. We consider the skeleton $S(k)$ and apply to a two-component vector $\psi = (\psi_1, \psi_2)$:

$$\begin{aligned} \langle \psi \,|\, S(k)\psi \rangle &= \langle \psi_1 \,|\, (g_2^{-1}k + T_0 - D_1(k))\psi_1 \rangle \\ &\quad + 2\Re\langle \psi_1 \,|\, (T_\theta - D_2(k))\psi_2 \rangle + \langle \psi_2 \,|\, (g_3^{-1}k + T_0 - D_3(k))\psi_2 \rangle. \end{aligned} \tag{1.1}$$

Here

$$D_1(k) = T_{\pi/2}(g_1^{-1}k + T_0)^{-1}T_{\pi/2}, \tag{1.2}$$

$$D_2(k) = T_{\pi/2}(g_1^{-1}k + T_0)^{-1}T_{\pi/2-\theta}, \tag{1.3}$$

$$D_3(k) = T_{\pi/2-\theta}(g_1^{-1}k + T_0)^{-1}T_{\pi/2-\theta} \tag{1.4}$$

and

$$T_\theta(p,q) = \frac{1}{\pi}\frac{\sin(\theta)}{p^2 + q^2 + 2pq\cos(\theta) + 2\sin^2(\theta)}. \tag{1.5}$$

In the region where $0 < z \le 1/\sqrt{2}$ and $0 \le \theta \le \pi/4$, $g_1 = z/\cos(\theta)$, $g_2 = -z/\sin(\theta)$ and $g_3 = -1$, and want to show that there exists ψ such that $\langle \psi \,|\, S(k_*)\psi \rangle > 0$, where $k_* = \frac{1}{\sqrt{2}}$. Thus, we want to show that

$$\begin{aligned} \langle \psi \,|\, S(k_*)\psi \rangle &= \langle \psi_1 \,|\, (-\frac{\sin(\theta)}{\sqrt{2}z} + T_0 - D_1(k_*))\psi_1 \rangle \\ &\quad + 2\Re\langle \psi_1 \,|\, (T_\theta - D_2(k_*))\psi_2 \rangle \\ &\quad + \langle \psi_2 \,|\, (-\frac{1}{\sqrt{2}} + T_0 - D_3(k_*))\psi_2 \rangle > 0. \end{aligned} \tag{1.6}$$

We first extract the dominant terms from this expression for small z, where we may assume that $\psi_1 = O(z)$. These are:

$$-\frac{\sin(\theta)}{\sqrt{2}z}||\psi_1||^2 + 2\Re\langle \psi_1 \,|\, T_\theta\psi_2 \rangle - \langle \psi_2 \,|\, (\frac{1}{\sqrt{2}} - T_0)\psi_2 \rangle - 2z\langle \psi_2 \,|\, T_{\pi/2-\theta}^2\psi_2 \rangle. \tag{1.7}$$

We now note that if $\theta = \pi/4$ then this can be written as

$$-\frac{1}{2z}||\psi_1 - 2zT_{\pi/4}\psi_2||^2 - \langle \psi_2 \,|\, (\frac{1}{\sqrt{2}} - T_0)\psi_2 \rangle. \tag{1.8}$$

Clearly, this has to vanish, so we need to take $\psi_1 = 2zT_{\pi/4}\psi_2$ and ψ_2 has to be an approximation of the eigenvector of T_0 with eigenvalue $1/\sqrt{2}$. We put

$$\psi_2 = \frac{1}{2\epsilon}1_{[-\epsilon,\epsilon]}. \tag{1.9}$$

In the general case, we put $\psi_1 = 2zT_\theta\psi_2$. Now,

$$(T_\theta\psi_2)(p) \approx \frac{\sqrt{2\epsilon}}{\pi}\frac{\sin(\theta)}{p^2 + 2\sin^2(\theta)}. \tag{1.10}$$

Hence

$$\langle T_\theta\psi_2 \,|\, T_\theta\psi_2\rangle \approx \frac{2\epsilon}{\pi^2}\int dp \frac{\sin^2(\theta)}{(p^2 + 2\sin^2(\theta))^2} = \frac{\epsilon}{2\sqrt{2}\pi\sin(\theta)}, \tag{1.11}$$

and

$$\begin{aligned}\langle T_{\pi/2-\theta}\psi_2 \,|\, T_\theta\psi_2\rangle &\approx \frac{2\epsilon}{\pi^2}\int dp \frac{\sin(\theta)\cos(\theta)}{(p^2 + 2\sin^2(\theta))(p^2 + 2\cos^2(\theta))} \\ &= \frac{\epsilon}{\sqrt{2}\pi(\sin(\theta) + \cos(\theta))}.\end{aligned} \tag{1.12}$$

Moreover,

$$\langle \psi_2 \,|\, (\frac{1}{\sqrt{2}} - T_0)\psi_2\rangle \approx \frac{1}{2\epsilon}\int_{-\epsilon}^{\epsilon} \frac{p^2}{4\sqrt{2}} dp = \frac{\epsilon^2}{12\sqrt{2}} = O(\epsilon^2). \tag{1.13}$$

Therefore

$$\begin{aligned}&-\frac{\sin(\theta)}{\sqrt{2}z}||\psi_1||^2 + 2\Re\langle\psi_1 \,|\, T_\theta\psi_2\rangle \\ &\quad -\langle\psi_2 \,|\, (\frac{1}{\sqrt{2}} - T_0)\psi_2\rangle - 2z\langle\psi_2 \,|\, T^2_{\pi/2-\theta}\psi_2\rangle \\ &= -2\sqrt{2}z\sin(\theta)||T_\theta\psi_2||^2 + 4z||T_\theta\psi_2||^2 - 2z||T_{\pi/2-\theta}\psi_2||^2 + O(\epsilon^2) \geq O(\epsilon^2).\end{aligned} \tag{1.14}$$

Here we use that $\sin(\theta) \leq 1/\sqrt{2}$ and $\cos(\theta) \geq \sin(\theta)$.

We now write the remaining terms in the case $\theta = \pi/4$:

$$
\begin{aligned}
&\langle \psi_1 \,|\, T_0 - D_1 \,|\, \psi_1 \rangle - 2\,\Re\,\langle \psi_1 \,|\, D_2 \,|\, \psi_2 \rangle \qquad (1.15)\\
&-\langle \psi_2 \,|\, D_3 \,|\, \psi_2 \rangle + 2z \langle \psi_2 \,|\, T_{\pi/4}^2 \psi_2 \rangle \\
&= 4z^2 \langle T_{\pi/4}\psi_2 \,|\, T_0 T_{\pi/4}\psi_2 \rangle - 4z\,\Re\,\langle T_{\pi/4}\psi_2 \,|\, D_2 \psi_2 \rangle \\
&\quad -4z^2 \langle T_{\pi/4}\psi_2 \,|\, T_{\pi/2} \left(\frac{1}{2z} + T_0 \right)^{-1} T_{\pi/2} T_{\pi/4}\psi_2 \rangle \\
&\quad +4z^2 \langle T_{\pi/4}\psi_2 \,|\, T_0 (1 + 2zT_0)^{-1} T_{\pi/4}\psi_2 \rangle + \\
&= 4z^2 \langle T_{\pi/4}\psi_2 \,|\, T_0 (1 + (1 + 2zT_0)^{-1}) T_{\pi/4}\psi_2 \rangle \\
&\quad -4z\,\Re\,\langle T_{\pi/4}\psi_2 \,|\, T_{\pi/2} \left(\frac{1}{2z} + T_0 \right)^{-1} T_{\pi/4}\psi_2 \rangle \\
&\quad -4z^2 \langle T_{\pi/4}\psi_2 \,|\, T_{\pi/2} \left(\frac{1}{2z} + T_0 \right)^{-1} T_{\pi/2} T_{\pi/4}\psi_2 \rangle \\
&= 8z^2 \langle T_{\pi/4}\psi_2 \,|\, (T_0 - T_{\pi/2}) T_{\pi/4}\psi_2 \rangle \\
&\quad -4z^2 \Big\{ \langle T_{\pi/4}\psi_2 \,|\, T_0 (\frac{1}{2z} + T_0)^{-1} T_0 T_{\pi/4}\psi_2 \rangle \\
&\quad -2\,\Re\,\langle T_{\pi/4}\psi_2 \,|\, T_{\pi/2} (\frac{1}{2z} + T_0)^{-1} T_0 T_{\pi/4}\psi_2 \rangle \\
&\quad + \langle T_{\pi/4}\psi_2 \,|\, T_{\pi/2} (\frac{1}{2z} + T_0)^{-1} T_{\pi/2} T_{\pi/4}\psi_2 \rangle \Big\} \\
&= 8z^2 \langle T_{\pi/4}\psi_2 \,|\, (T_0 - T_{\pi/2}) T_{\pi/4}\psi_2 \rangle \\
&\quad -4z^2 \langle T_{\pi/4}\psi_2 \,|\, (T_0 - T_{\pi/2}) (\frac{1}{2z} + T_0)^{-1} (T_0 - T_{\pi/2}) T_{\pi/4}\psi_2 \rangle .
\end{aligned}
\tag{1.16}
$$

Inserting (1.9) we have

$$
\begin{aligned}
(T_0 - T_{\pi/2}) T_{\pi/4}\psi_2 &\approx \frac{\sqrt{\epsilon}}{\pi} \left(\frac{1}{p^2+1} \frac{1}{\sqrt{p^2+2}} - \frac{1}{\pi} \int \frac{dq}{(q^2+1)(p^2+q^2+2)} \right) \\
&= \frac{\sqrt{\epsilon}}{\pi} \frac{1}{p^2+1} \left\{ \frac{2}{\sqrt{p^2+2}} - 1 \right\} .
\end{aligned}
\tag{1.17}
$$

Thus

$$
\begin{aligned}
\langle T_{\pi/4}\psi_2 \,|\, (T_0 - T_{\pi/2}) T_{\pi/4}\psi_2 \rangle &= \frac{\epsilon}{\pi^2} \int \frac{1}{(p^2+1)^2} \left\{ \frac{2}{\sqrt{p^2+2}} - 1 \right\} dp \\
&= \frac{\epsilon}{\pi^2} \left(2 - \frac{\pi}{2} \right)
\end{aligned}
\tag{1.18}
$$

and

$$
\begin{aligned}
&\langle T_{\pi/4}\psi_2 \,|\, (T_0 - T_{\pi/2})(\frac{1}{2z} + T_0)^{-1}(T_0 - T_{\pi/2})T_{\pi/4}\psi_2\rangle \\
&\approx \quad \frac{\epsilon}{\pi^2}\int \frac{dp}{(p^2+1)^2}\left(\frac{2}{\sqrt{p^2+2}}-1\right)^2\left(\frac{1}{2z}+\frac{1}{\sqrt{p^2+2}}\right)^{-1} \\
&\leq \quad 2z\frac{\epsilon}{\pi^2}\int \frac{dp}{(p^2+1)^2}\left(\frac{2}{\sqrt{p^2+2}}-1\right)^2 \\
&= \quad \frac{\epsilon}{\pi^2}((4\sqrt{2}-3)\pi - 8)z. \qquad (1.19)
\end{aligned}
$$

We now consider the general case $0 \leq \theta < \pi/4$. This is less elegant. We compute the individual terms. We need the following integrals:

$$
\begin{aligned}
&\int \frac{1}{(p^2+2\sin^2(\theta))^2}\frac{dp}{\sqrt{p^2+2}} = \\
&= \quad \frac{1}{4}\int_{-\pi/2}^{\pi/2}\frac{\cos^3(\alpha)d\alpha}{(\sin^2(\alpha)+\sin^2(\theta)\cos^2(\alpha))^2} \\
&= \quad \frac{1}{4}\int_{-1}^{1}\frac{(1-u^2)du}{(u^2\cos^2(\theta)+\sin^2(\theta))^2} \\
&= \quad \frac{1}{8\sin^2(\theta)\cos^2(\theta)}\int_{-1}^{1}du\left\{\frac{\cos^2(\theta)-\sin^2(\theta)}{\cos^2(\theta)u^2+\sin^2(\theta)}+\frac{\sin^2(\theta)-u^2\cos^2(\theta)}{(u^2\cos^2(\theta)+\sin^2(\theta))^2}\right\} \\
&= \quad \frac{1}{2\sin^2(2\theta)}\left\{\frac{\cos(2\theta)}{\sin^2(\theta)}\tan(\theta)\int_{-\cot(\theta)}^{\cot(\theta)}\frac{dz}{z^2+1}+\frac{u}{u^2\cos^2(\theta)+\sin^2(\theta)}\Big|_{-1}^{1}\right\} \\
&= \quad \frac{1}{\sin^2(2\theta)}\left\{1+\frac{(\pi-2\theta)\cos(2\theta)}{\sin(2\theta)}\right\} \qquad (1.20)
\end{aligned}
$$

and by transformation $\theta \to \frac{\pi}{2} - \theta$,

$$
\int \frac{1}{(p^2+2\cos^2(\theta))^2}\frac{dp}{\sqrt{p^2+2}} \quad = \quad \frac{1}{\sin^2(2\theta)}\left\{1-\frac{2\theta}{\tan(2\theta)}\right\}. \qquad (1.21)
$$

We also need

$$
\begin{aligned}
\left(T_{\pi/2}T_\theta\psi_2\right)(p) \quad &\approx \quad \frac{\sqrt{2\epsilon}}{\pi^2}\int \frac{dq}{p^2+q^2+2}\frac{\sin(\theta)}{q^2+2\sin^2(\theta)} \\
&= \quad \frac{\sqrt{2\epsilon}}{\pi}\frac{1}{p^2+2\cos^2(\theta)}\left\{\frac{1}{\sqrt{2}}-\frac{\sin(\theta)}{\sqrt{p^2+2}}\right\}. \qquad (1.22)
\end{aligned}
$$

Thus we have

$$
\begin{aligned}
\langle \psi_1 \,|\, T_0 \,|\, \psi_1 \rangle &= 4z^2 \langle T_\theta \psi_2 \,|\, T_0 \,|\, T_\theta \psi_2 \rangle \\
&\approx 8 \frac{\epsilon z^2}{\pi^2} \sin^2(\theta) \int \frac{dp}{(p^2 + 2\sin^2(\theta))^2 \sqrt{p^2+2}}. \qquad (1.23)
\end{aligned}
$$

Further,

$$
\begin{aligned}
&\langle \psi_1 \,|\, D_1 \,|\, \psi_1 \rangle = \\
&\quad = 4z^2 \langle T_\theta \psi_2 \,|\, T_{\pi/2} \left(\frac{\cos(\theta)}{\sqrt{2}z} + T_0 \right)^{-1} T_{\pi/2} T_\theta \psi_2 \rangle \\
&\quad = \frac{8\epsilon z^2}{\pi^2} \int \left(\frac{1}{\sqrt{2}} - \frac{\sin(\theta)}{\sqrt{p^2+2}} \right)^2 \left(\frac{\cos(\theta)}{\sqrt{2}z} + \frac{1}{\sqrt{p^2+2}} \right)^{-1} \frac{dp}{(p^2 + 2\cos^2(\theta))^2}. \qquad (1.24)
\end{aligned}
$$

and

$$
\begin{aligned}
&2\Re \langle \psi_1 \,|\, D_2 \,|\, \psi_2 \rangle = \\
&\quad = 4z\, \Re \langle T_\theta \psi_2 \,|\, T_{\pi/2} \left(\frac{\cos(\theta)}{\sqrt{2}z} + T_0 \right)^{-1} T_{\pi/2-\theta} \psi_2 \rangle \\
&\quad = \frac{4\sqrt{2}z^2}{\cos(\theta)} \Big\{ \langle T_\theta \psi_2 \,|\, T_{\pi/2} T_{\pi/2-\theta} \psi_2 \rangle \\
&\qquad - \langle T_\theta \psi_2 \,|\, T_{\pi/2} \left(\frac{1}{2z} + T_0 \right)^{-1} T_0 T_{\pi/2-\theta} \psi_2 \rangle \Big\}. \\
&\quad = \frac{8\sqrt{2}\epsilon z^2}{\pi^2} \int \left\{ \frac{1}{\sqrt{2}} - \frac{\sin(\theta)}{\sqrt{p^2+2}} \right\} \frac{dp}{(p^2 + 2\cos^2(\theta))^2} \\
&\qquad - \frac{8\sqrt{2}\epsilon z^2}{\pi^2} \int \left\{ \frac{1}{\sqrt{2}} - \frac{\sin(\theta)}{\sqrt{p^2+2}} \right\} \frac{1}{\sqrt{p^2+2}} \\
&\qquad\quad \times \left(\frac{\cos(\theta)}{\sqrt{2}z} + \frac{1}{\sqrt{p^2+2}} \right)^{-1} \frac{dp}{(p^2 + 2\cos^2(\theta))^2}. \qquad (1.25)
\end{aligned}
$$

Finally,

$$
\begin{aligned}
-\langle \psi_2 \,|\, D_3 \,|\, \psi_2 \rangle + \frac{\sqrt{2}z}{\cos(\theta)} \langle \psi_2 \,|\, T^2_{\pi/2-\theta} \psi_2 \rangle = \\
&= \frac{\sqrt{2}z}{\cos(\theta)} \langle T_{\pi/2-\theta}\psi_2 \,|\, T_0 \left(\frac{\cos(\theta)}{\sqrt{2}z} + T_0 \right)^{-1} T_{\pi/2-\theta}\psi_2 \rangle \\
&= \frac{2z^2}{\cos^2(\theta)} \Big\{ \langle T_{\pi/2-\theta}\psi_2 \,|\, T_0 T_{\pi/2-\theta}\psi_2 \rangle \\
&\quad - \langle T_{\pi/2-\theta}\psi_2 \,|\, T_0 \left(\frac{\cos(\theta)}{\sqrt{2}z} + T_0 \right)^{-1} T_0 T_{\pi/2-\theta}\psi_2 \rangle \Big\} \\
&= \frac{4\epsilon z^2}{\pi^2} \int \frac{1}{\sqrt{p^2+2}} \frac{dp}{(p^2 + 2\cos^2(\theta))^2} \\
&\quad - \frac{4\epsilon z^2}{\pi^2} \int \frac{1}{p^2+2} \left(\frac{\cos(\theta)}{\sqrt{2}z} + \frac{1}{\sqrt{p^2+2}} \right)^{-1} \frac{dp}{(p^2 + 2\cos^2(\theta))^2}. \qquad (1.26)
\end{aligned}
$$

We first consider the $O(z^2)$ terms. They add up to

$$
\begin{aligned}
& \frac{8\epsilon z^2}{\pi^2} \sin^2(\theta) \int \frac{dp}{\sqrt{p^2+2}\,(p^2 + 2\sin^2(\theta))^2} \\
& - \frac{8\sqrt{2}\epsilon z^2}{\pi^2} \int \left(\frac{1}{\sqrt{2}} - \frac{\sin(\theta)}{\sqrt{p^2+2}} \right) \frac{dp}{(p^2 + 2\cos^2(\theta))^2} \\
& + \frac{4\epsilon z^2}{\pi^2} \int \frac{1}{\sqrt{p^2+2}} \frac{dp}{(p^2 + 2\cos^2(\theta))^2} \\
= \;& \frac{4\epsilon z^2}{\pi^2} \left\{ \frac{\pi \cos(2\theta)}{\sin^3(2\theta)} - \frac{\pi}{2\sqrt{2}\cos^3(\theta)} + \frac{(\sqrt{2}\sin(\theta)+1)^2}{\sin^2(2\theta)} \left(1 - \frac{2\theta}{\tan(2\theta)} \right) \right\}.
\end{aligned}
\qquad (1.27)
$$

To prove that this expression is positive, we change to the new variable $x = \frac{\pi}{4} - \theta$:

$$
\begin{aligned}
\frac{4\epsilon z^2}{\pi^2} \Big\{ & \frac{\pi \sin(2x)}{\cos^3(2x)} - \frac{\pi}{(\cos(x)+\sin(x))^3} \\
& + \frac{(\cos(x) - \sin(x) + 1)^2}{\cos^2(2x)} \left(1 - \left(\frac{\pi}{2} - 2x \right) \tan(2x) \right) \Big\}.
\end{aligned}
\qquad (1.28)
$$

For the first term we have:

$$\frac{\sin(x)}{\cos^3(x)} \geq x + \frac{4}{3}x^3 \tag{1.29}$$

as can be easily checked by differentiation. For the second term, we have

$$\frac{1}{(\cos(x)+\sin(x))^3} \leq 1 - 3x + \frac{15x^2}{2(1+2x)}. \tag{1.30}$$

Indeed, $\cos(x) + \sin(x) \geq 1 + x - \frac{1}{2}x^2 - \frac{1}{6}x^3$, so it suffices to prove that

$$1 + 2x \leq ((1-3x)(1+2x) + \frac{15}{2}x^2)(1 + x - \frac{1}{2}x^2 - \frac{1}{6}x^3)^3.$$

Expanding the right-hand side we get

$$1 + 2x + \frac{1}{2}x^3 + 3x^4 - \frac{5}{4}x^5 - \frac{35}{12}x^6 + \frac{5}{8}x^7 + \frac{11}{16}x^8 - \frac{11}{432}x^9 - \frac{25}{432}x^{10} - \frac{1}{144}x^{11}.$$

Clearly, for $x \leq 1$, the last 3 terms are less than $\frac{13}{144}x^8$. Thus it remains to show that

$$f_2(x) = \frac{1}{2} + 3x - \frac{5}{4}x^2 - \frac{35}{12}x^3 + \frac{5}{8}x^4 + \frac{43}{72}x^5 \geq 0.$$

This follows easily by differentiation:

$$f_2''(x) = -\frac{5}{2} - \frac{35}{2}x + \frac{15}{2}x^2 + \frac{215}{18}x^3 < 0,$$

so f_2' is decreasing. But $f_2'(0) = 3$ and $f_2'(1) = 3 - \frac{5}{2} - \frac{35}{4} + \frac{5}{2} + \frac{215}{72} < 0$. Therefore f_2 is first increasing, then decreasing. But $f_2(0) = \frac{1}{2}$ and $f_2(1) = \frac{1}{2} + 3 - \frac{5}{4} - \frac{35}{12} + \frac{5}{8} + \frac{43}{72} = \frac{5}{9}$.

As to the third term, we first prove that

$$\frac{1 - (\frac{\pi}{2} - 2x)\tan(2x)}{\cos^2(2x)} \geq 1 - \pi x + \frac{7x^2}{1+2x}. \tag{1.31}$$

Clearly, both sides are 1 at $x = 0$. We now differentiate both sides, replacing $2x$ by x:

$$\frac{d}{dx}\frac{1 - (\frac{\pi}{2} - x)\tan(x)}{\cos^2(x)} = \frac{3\sin(x)\cos(x) - (\frac{\pi}{2} - x)(1 + 2\sin^2(x))}{\cos^4(x)} \tag{1.32}$$

and

$$\frac{d}{dx}\left(1-\frac{\pi}{2}x+\frac{7x^2/4}{1+x}\right)=-\frac{\pi}{2}+\frac{7}{4}\frac{2x+x^2}{(1+x)^2}. \tag{1.33}$$

Both expressions are easily seen to be negative for $x \in [0, \frac{\pi}{2}]$. It therefore suffices to prove that

$$3\sin(x)\cos(x)-(\frac{\pi}{2}-x)(1+2\sin^2(x)) > -\frac{\pi}{2}+\frac{7}{4}\frac{2x+x^2}{(1+x)^2}.$$

Consider first the case $0 \le x \le \frac{\pi}{4}$. Using the fact that $\sin(x)\cos(x) = \frac{1}{2}\sin(2x) > x - \frac{2}{3}x^3$, it then suffices if

$$(4x-\pi x^2)(1+x)^2 > \frac{7}{4}x(2+x).$$

Now, if $f_3(x) = \frac{1}{2}+(\frac{25}{4}-\pi)x-(2\pi-4)x^2-\pi x^3$, then $f_3'(x) = \frac{25}{4}-\pi-2(2\pi-4)x-3\pi x^2$ and $f_3''(x) < 0$, so f_3' is decreasing. Since $f_3'(0) = \frac{25}{4}-\pi > 0$ and $f_3'(\frac{\pi}{4}) = \frac{25}{4}-\pi-(\pi-2)\pi-\frac{3}{16}\pi^3 < 0$, f_3 is first increassing, then decreasing. We thus only need to check that $f_3(\frac{\pi}{4}) > 0$. In fact, $f_3(\frac{\pi}{4}) = \frac{1}{2}+(\frac{25}{4}-\pi)\frac{\pi}{4}-(\pi-2)\frac{\pi^2}{8}-\frac{\pi^4}{64} = 0.01$. For $x > \frac{\pi}{4}$, we change variables to $u = \frac{\pi}{2}-x$. Then we need to prove that

$$3\sin(u)\cos(u)+\frac{\pi}{2}-u-2u\cos^2(u) > \frac{7}{4}(\frac{\pi}{2}-u)\frac{2+\frac{\pi}{2}-u}{(1+\frac{\pi}{2}-u)^2}.$$

Again, $3\sin(u)\cos(u) > 3u-2u^3$. Moreover, $\cos^2(u) = \frac{1}{2}(1+\cos(2u)) < 1-u^2+\frac{1}{3}u^4$. It thus suffices to prove that

$$(\frac{\pi}{2}-\frac{2}{3}u^5)(1+\frac{\pi}{2}-u)^2 > \frac{7}{4}(\frac{\pi}{2}-u)(2+\frac{\pi}{2}-u).$$

Expanding again, we need

$$\begin{aligned} f_4(u) \quad = \quad & -\frac{5}{4}\pi+\frac{1}{16}\pi^2+\frac{1}{8}\pi^3+\left(\frac{7}{2}+\frac{3}{4}\pi-\frac{1}{2}\pi^2\right)u-\frac{7}{4}u^2+\frac{1}{2}\pi u^2 \\ & -\frac{2}{3}u^5-\frac{2}{3}\pi u^5-\frac{1}{6}\pi^2u^5+\frac{4}{3}u^6+\frac{2}{3}\pi u^6-\frac{2}{3}u^7 > 0. \end{aligned}$$

By successive differentiations it is seen that this function is first increasing, then decreasing. Indeed, $f_4^{(5)}$ and $f_4^{(4)}$ change sign from negative to positive. Then $f_4''' < 0$ and $f_4'' < 0$, and f_4' changes from positive to negative. Since f_4

is positive at both ends, it is positive everywhere on the interval $[0, \frac{\pi}{4}]$. This completes the proof of (1.31).

We now use the inequality $\cos(x) - \sin(x) \geq 1 - x - \frac{1}{2}x^2$ to deduce (for $x \in [0, \frac{\pi}{4}]$)

$$(\cos(x) - \sin(x) + 1)^2 \frac{1 - (\frac{\pi}{2} - 2x)\tan(2x)}{\cos^2(2x)} \geq 4 - 4x - 4\pi x + \frac{35x^2}{1 + 2x}. \quad (1.34)$$

To see this, we compute $(2 - x - \frac{1}{2}x^2)^2((1 - \pi x)(1 + 2x) + 7x^2) - 4(1 - x - \pi x)(1 + 2x) = 27x^2 + 4\pi x^2 - 29x^3 + 9\pi x^3 - \frac{19}{4}x^4 + \pi x^4 + \frac{15}{2}x^5 - \frac{9}{4}\pi x^5 + \frac{7}{4}x^6 - \frac{\pi}{2}x^6$. The $O(x^6)$ and $O(x^5)$ terms are clearly positive and can be omitted. Since $x < 1$, in the remaining expression, $0 \leq (\frac{19}{4} - \pi)x^4 < (5 - \pi)x^3$ and $29x^3 - 9\pi x^3 + (5 - \pi)x^3 < (34 - 10\pi)x^2$, so that the whole expression is greater than $(14\pi - 7)x^2 > 35x^2$.

We finally put it all together to find

$$\begin{aligned} & \frac{\pi \sin(2x)}{\cos^3(2x)} - \frac{\pi}{(\cos(x) + \sin(x))^3} \\ & \qquad + \frac{(\cos(x) - \sin(x) + 1)^2}{\cos^2(2x)} \left(1 - \left(\frac{\pi}{2} - 2x\right)\tan(2x)\right) \\ \geq\ & 2\pi x + \frac{32}{3}\pi x^3 - \pi + 3\pi x - \frac{15\pi x^2}{2(1 + 2x)} + 4(1 - x - \pi x) + \frac{35x^2}{1 + 2x} \\ =\ & (4 - \pi)(1 - x) + \frac{32}{3}x^3 + 5\frac{(7 - \frac{3}{2}\pi)x^2}{1 + 2x} \geq 0. \qquad (1.35) \end{aligned}$$

The graph of the left-hand side and the lower bound on the right-hand side is illustrated in Figure 1, which is probably more convincing than the above argument:

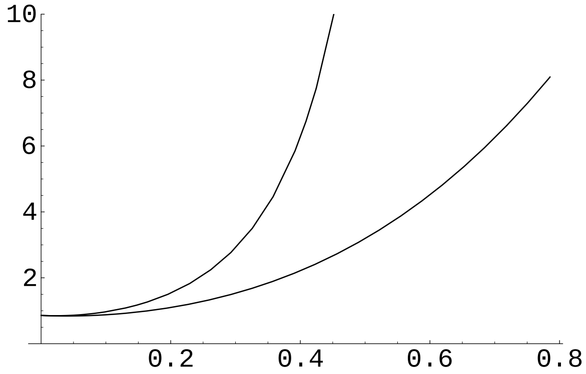

Figure 1. The order-z^2 terms and the lower bound (1.35) as a function of θ.

The $O(z^3)$ terms add up to (we omit a minus sign)

$$\begin{aligned}
&\frac{4\epsilon z^2}{\pi^2}\int\frac{dp}{(p^2+2\cos^2(\theta))^2}\left(\frac{\cos(\theta)}{\sqrt{2}z}+\frac{1}{\sqrt{p^2+2}}\right)^{-1}\times\\
&\times\left\{2\left(\frac{1}{\sqrt{2}}-\frac{\sin(\theta)}{\sqrt{p^2+2}}\right)^2\right.\\
&\qquad\left.-2\sqrt{2}\left(\frac{1}{\sqrt{2}}-\frac{\sin(\theta)}{\sqrt{p^2+2}}\right)\frac{1}{\sqrt{p^2+2}}+\frac{1}{p^2+2}\right\}\\
=\;&\frac{4\epsilon z^2}{\pi^2}\int\frac{dp}{(p^2+2\cos^2(\theta))^2}\left(\frac{\cos(\theta)}{\sqrt{2}z}+\frac{1}{\sqrt{p^2+2}}\right)^{-1}\left\{1-\frac{\sqrt{2}\sin(\theta)+1}{\sqrt{p^2+2}}\right\}^2\\
\leq\;&\frac{4\sqrt{2}\epsilon z^3}{\pi^2\cos(\theta)}\int\frac{dp}{(p^2+2\cos^2(\theta))^2}\left\{1-\frac{\sqrt{2}\sin(\theta)+1}{\sqrt{p^2+2}}\right\}^2\\
=\;&\frac{4\sqrt{2}\epsilon z^3}{\pi^2\cos(\theta)}\left\{\frac{\pi}{4\sqrt{2}\cos^3(\theta)}-2\frac{\sqrt{2}\sin(\theta)+1}{\sin^2(2\theta)}\left(1-\frac{2\theta}{\tan(2\theta)}\right)\right.\\
&\qquad\left.+\frac{(\sqrt{2}\sin(\theta)+1)^2\pi}{8\sqrt{2}\cos^3(\theta)}\,\frac{1+2\cos(\theta)}{(1+\cos(\theta))^2}\right\}. \qquad (1.36)
\end{aligned}$$

We shall prove that the contribution of these terms, while negative, is small.

For this, we again change variables to $x = \frac{\pi}{4} - \theta$. Then the expression becomes

$$\frac{4\epsilon z^3}{\pi^2 \cos(\theta)} \left\{ \frac{\pi}{\sqrt{2}(\cos(x) + \sin(x))^3} \right.$$
$$-2\sqrt{2}\frac{\cos(x) - \sin(x) + 1}{\cos^2(2x)} \Big(1 - (\frac{\pi}{2} - 2x)\tan(2x)\Big)$$
$$\left. + \frac{\sqrt{2}(\cos(x) - \sin(x) + 1)^2 \pi}{(\cos(x) + \sin(x))^3} \frac{1 + \sqrt{2}(\cos(x) + \sin(x))}{(\sqrt{2} + \cos(x) + \sin(x))^2} \right\}. \tag{1.37}$$

For the first two terms we can use the same estimates as before. In the third term, we have

$$\frac{1 + \sqrt{2}(\cos(x) + \sin(x))}{(\sqrt{2} + \cos(x) + \sin(x))^2} \leq \sqrt{2} - 1, \tag{1.38}$$

and

$$\frac{(\cos(x) - \sin(x) + 1)^2}{(\cos(x) + \sin(x))^3} \leq 4\left(1 - 3x + \frac{7x^2}{1 + 2x}\right). \tag{1.39}$$

The first inequality is elementary. The second follows as before: Using $\cos(x) - \sin(x) \leq 1 - x + \frac{1}{6}x^3$ and $\cos(x) + \sin(x) \geq 1 + x - \frac{1}{2}x^2 - \frac{1}{6}x^3$, it suffices to prove that

$$(1 + 2x)(1 - x + \frac{1}{6}x^3)^2 \leq 4(1 - x + x^2)(1 + x - \frac{1}{2}x^2 - \frac{1}{6}x^3)^3.$$

Expanding the difference yields

$$4x + 5x^2 - \frac{20}{3}x^3 + 8x^4 + \frac{2}{3}x^5 - \frac{295}{36}x^6 + \frac{17}{18}x^7 + \frac{11}{6}x^8 - \frac{1}{54}x^9 - \frac{4}{27}x^{10} - \frac{1}{54}x^{11}.$$

This is easily seen to be positive for $x \leq 1$ by cancelling terms from the left. Thus, the sum of the negative $O(x^9)$, $O(x^{10})$ and $O(x^{11})$ terms is smaller than the $O(x^8)$ term. The $O(x^6)$ term is cancelled by the all previous terms, as $4 + 5 - \frac{20}{3} + 8 + \frac{2}{3} > \frac{295}{36}$.

We now have

$$
\begin{aligned}
& \frac{\pi}{\sqrt{2}(\cos(x)+\sin(x))^3} \\
& \qquad -2\sqrt{2}\frac{\cos(x)-\sin(x)+1}{\cos^2(2x)}\Big(1-(\frac{\pi}{2}-2x)\tan(2x)\Big) \\
& \qquad +\frac{(\cos(x)-\sin(x)+1)^2\pi}{\sqrt{2}(\cos(x)+\sin(x))^3}\,\frac{1+\sqrt{2}(\cos(x)+\sin(x))}{(\sqrt{2}+\cos(x)+\sin(x))^2} \\
\leq\ & \frac{\pi}{\sqrt{2}}\left(1-3x+\frac{15x^2}{2(1+2x)}\right)+2\sqrt{2}(\sqrt{2}-1)\pi\left(1-3x+\frac{7x^2}{1+2x}\right) \\
& \quad -2\sqrt{2}(2-x-\frac{1}{2}x^2)\left(1-\pi x+\frac{7x^2}{1+2x}\right). \qquad (1.40)
\end{aligned}
$$

We need to show that this is smaller than (1.35). We write the difference as a sum of two expressions:

$$
\begin{aligned}
h_1(x) &= (4-\pi)(1-x)+\frac{32}{3}x^3-\frac{\pi}{\sqrt{2}}(1-3x)-2\sqrt{2}(\sqrt{2}-1)\pi(1-3x) \\
&\qquad +2\sqrt{2}(2-x-\frac{1}{2}x^2)(1-\pi x) \\
&= 4+4\sqrt{2}-5\pi+\frac{3}{2}\pi\sqrt{2}-\left(4+2\sqrt{2}-13\pi+\frac{17}{2}\pi\sqrt{2}\right)x \\
&\qquad +\sqrt{2}(2\pi-1)x^2+\left(\frac{32}{3}+\sqrt{2}\pi\right)x^3 \qquad (1.41)
\end{aligned}
$$

and

$$
\begin{aligned}
& h_2(x) = \\
&= \left[5(7-\frac{3}{2}\pi)-\frac{15\pi}{2\sqrt{2}}-14\sqrt{2}(\sqrt{2}-1)\pi+14\sqrt{2}(2-x-\frac{1}{2}x^2)\right]\frac{x^2}{1+2x} \\
&= \left[35+28\sqrt{2}-\frac{71}{2}\pi+\frac{41}{4}\sqrt{2}\pi-14\sqrt{2}x-7\sqrt{2}x^2\right]\frac{x^2}{1+2x}. \qquad (1.42)
\end{aligned}
$$

These two expressions are plotted in Figure 2.

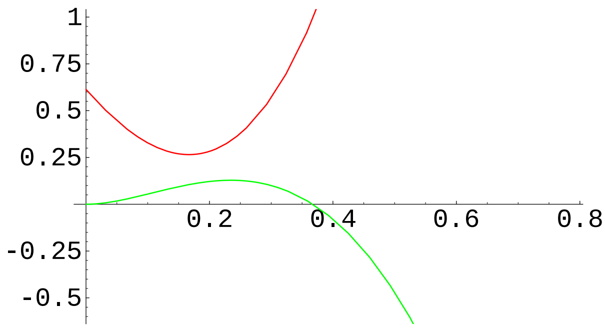

Figure 2.

It is clear that both are positive for small x. Indeed, the quadratic in brackets in $h_2(x)$ is numerically given by $8.61-19.8x-9.9x^2$, which is positive for $x < 0.3674$. On the other hand, $h_1(x) > 0$ for all $x > 0$. This is easy to deduce by removing the positive x^3-term. For $x > 0.3674$ we can write

$$h_2(x) > \frac{1}{2}x\left(35 + 28\sqrt{2} - \frac{71}{2}\pi + \frac{41}{4}\sqrt{2}\pi - 14\sqrt{2}x - 7\sqrt{2}x^2\right)$$

and hence

$$\begin{aligned}
&h_1(x) + h_2(x) \\
&\quad > \left(\frac{32}{3} + \sqrt{2}\pi - \frac{7}{2}\sqrt{2}\right)x^3 + \left(2\sqrt{2}\pi - 8\sqrt{2}\right)x^2 \\
&\quad - \left(4 + 2\sqrt{2} - 13\pi + \frac{17}{2}\pi\sqrt{2} - \frac{1}{2}\left(35 + 28\sqrt{2} - \frac{71}{2}\pi + \frac{41}{4}\sqrt{2}\pi\right)\right)x \\
&\quad +4 + 4\sqrt{2} - 5\pi + \frac{3}{2}\pi\sqrt{2} \\
&= 10.16x^3 - 2.43x^2 + 0.55x + 0.61.
\end{aligned}$$

This is easily seen to be positive.

Figure 3 shows graphs of the $O(z^2)$ (red) and $O(z^3)$ expressions, as well as the corresponding lower and upper bounds (blue and purple).

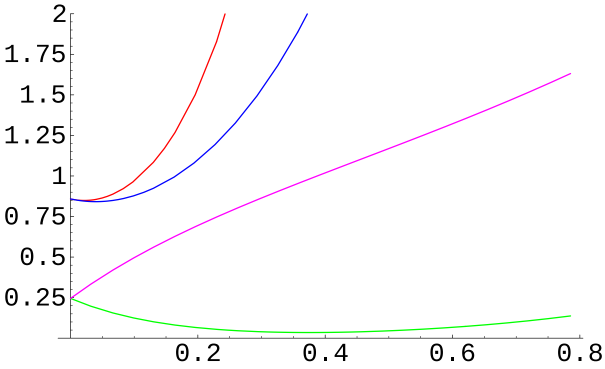

Figure 3.

Remark. Looking at your notes, I now realise that in the region $z \le 1/\sqrt{2}$ and $\theta \le \pi/4$, we do not always have $k_* = \frac{1}{\sqrt{2}}$. Apparently,

$$k_* = \frac{1}{\sqrt{2}} \max\left\{\frac{z}{\sin(\theta)}, 1\right\}.$$

We therefore have to consider separately the case $z > \sin(\theta)$. I also note that for $z > \sin(\theta)$,

$$\begin{aligned}\langle\psi\,|\,S(k_*)\psi\rangle &= \langle\psi_1\,|\,(-\frac{1}{\sqrt{2}} + T_0 - D_1^*)\psi_1\rangle \\ &\quad +2\Re\langle\psi_1\,|\,(T_\theta - D_2^*)\psi_2\rangle + \langle\psi_2\,|\,(-\frac{z}{\sqrt{2}\sin(\theta)} + T_0 - D_3^*)\psi_2\rangle,\end{aligned} \tag{1.43}$$

where D_1^* etc. are independent of z! It follows that for large z, $\psi_2 = O\left(\frac{1}{\sqrt{z}}\right)$. The second term is then negligible and the entire expression is negative. I conclude that there *is* a critical value for large z.