Modern Quantum Chemistry, Szabo & Ostlund
HW

wsr

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Contents

7 The 1-Particle Many-body Green's Function

7.1 Green's Function in Single-Particle Systems

Ex 7.1

$$\mathbf{V} = \mathbf{G}_0(E)^{-1} - \mathbf{G}(E)^{-1} \tag{7.1.1}$$

thus

$$\begin{aligned}\mathbf{G}_0(E)\mathbf{V}\mathbf{G}(E) &= \mathbf{G}_0(E)[\mathbf{G}_0(E)^{-1} - \mathbf{G}(E)^{-1}]\mathbf{G}(E) \\ &= \mathbf{G}(E) - \mathbf{G}_0(E)\end{aligned} \tag{7.1.2}$$

i.e.

$$\mathbf{G}(E) = \mathbf{G}_0(E) + \mathbf{G}_0(E)\mathbf{V}\mathbf{G}(E) \tag{7.1.3}$$

Ex 7.2

a. When $x = 0$,

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}x^2}|x|\bigg|_{x=0} &= \lim_{\epsilon\to 0}\frac{\frac{\mathrm{d}|x|}{\mathrm{d}x}\Big|_{x=\epsilon} - \frac{\mathrm{d}|x|}{\mathrm{d}x}\Big|_{x=-\epsilon}}{2\epsilon} \qquad (\epsilon > 0) \\ &= \lim_{\epsilon\to 0}\frac{1-(-1)}{2\epsilon} \\ &= \infty\end{aligned} \tag{7.1.4}$$

otherwise,

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}x^2}|x| &= \frac{\mathrm{d}^2}{\mathrm{d}x^2}[x\ \mathrm{sgn}(x)] \\ &= \frac{\mathrm{d}}{\mathrm{d}x}[1\times\mathrm{sgn}(x) + x\times 0] \\ &= 0\end{aligned} \tag{7.1.5}$$

b.

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{\mathrm{d}^2}{\mathrm{d}x^2}|x|\mathrm{d}x &= \int_{-\infty}^{\infty}\mathrm{d}\left(\frac{\mathrm{d}}{\mathrm{d}x}|x|\right) \\ &= \frac{\mathrm{d}}{\mathrm{d}x}|x|\bigg|_{-\infty}^{\infty} \\ &= 1-(-1) \\ &= 2\end{aligned} \tag{7.1.6}$$

thus

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}|x| = 2\delta(x) \tag{7.1.7}$$

c.

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}x^2}a(x) &= \frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{1}{2}\int_\alpha^\beta \mathrm{d}x'|x-x'|b(x') \\ &= \frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{1}{2}\int_\alpha^x \mathrm{d}x'(x-x')b(x') + \frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{1}{2}\int_x^\beta \mathrm{d}x'[-(x-x')]b(x') \\ &= \frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{2}\int_\alpha^x \mathrm{d}x'b(x') - \frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{2}\int_x^\beta \mathrm{d}x'b(x') \\ &= \frac{1}{2}b(x) - \frac{1}{2}[-b(x)] \\ &= b(x)\end{aligned} \tag{7.1.8}$$

Ex 7.3

$$\begin{aligned}
\left(E+\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)G_0(x,x',E) &= \left(E+\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\frac{1}{\mathrm{i}(2E)^{1/2}}\,\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|} \\
&= \frac{E}{\mathrm{i}(2E)^{1/2}}\,\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}+\frac{1}{2}\frac{1}{\mathrm{i}(2E)^{1/2}}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|} \\
&= \frac{E}{\mathrm{i}(2E)^{1/2}}\,\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}+\frac{1}{2}\frac{1}{\mathrm{i}(2E)^{1/2}}\frac{\mathrm{d}}{\mathrm{d}x}\left[\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}\,\mathrm{i}(2E)^{1/2}\frac{\mathrm{d}}{\mathrm{d}x}|x-x'|\right] \\
&= \frac{E}{\mathrm{i}(2E)^{1/2}}\,\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}+\frac{1}{2}\left[\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}\,\mathrm{i}(2E)^{1/2}\left(\frac{\mathrm{d}}{\mathrm{d}x}|x-x'|\right)^2+\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}\,\frac{\mathrm{d}^2}{\mathrm{d}x^2}|x-x'|\right] \\
&= \frac{E}{\mathrm{i}(2E)^{1/2}}\,\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}+\frac{1}{2}\,\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}\left[\mathrm{i}(2E)^{1/2}\times 1+2\delta(x-x')\right] \\
&= \mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}\left[\frac{E}{\mathrm{i}(2E)^{1/2}}+\frac{-E}{\mathrm{i}(2E)^{1/2}}+\delta(x-x')\right] \\
&= \mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}\,\delta(x-x') \\
&= \delta(x-x')
\end{aligned} \tag{7.1.9}$$

Ex 7.4

$$\begin{aligned}
\phi_n(x)\phi_n^*(x') &= \lim_{E\to E_n}(E-E_n)\frac{1}{\mathrm{i}(2E)^{1/2}}\left[\mathrm{e}^{\mathrm{i}(2E)^{1/2}|x-x'|}-\frac{\mathrm{e}^{\mathrm{i}(2E)^{1/2}(|x|+|x'|)}}{1+\mathrm{i}(2E)^{1/2}}\right] \\
&= \lim_{E\to -1/2}(E+1/2)\frac{1}{-1}\left[\mathrm{e}^{-|x-x'|}-\frac{\mathrm{e}^{-(|x|+|x'|)}}{1+\mathrm{i}(2E)^{1/2}}\right] \\
&= -\lim_{E\to -1/2}(E+1/2)\,\mathrm{e}^{-|x-x'|}+\lim_{E\to -1/2}(E+1/2)\frac{\mathrm{e}^{-(|x|+|x'|)}}{1+\mathrm{i}(2E)^{1/2}} \\
&= 0+\lim_{E\to -1/2}(E+1/2)\frac{\mathrm{e}^{-(|x|+|x'|)}(1-\mathrm{i}(2E)^{1/2})}{(1+\mathrm{i}(2E)^{1/2})(1-\mathrm{i}(2E)^{1/2})} \\
&= \lim_{E\to -1/2}(E+1/2)\frac{\mathrm{e}^{-(|x|+|x'|)}(1-\mathrm{i}(2E)^{1/2})}{1+2E} \\
&= \frac{1}{2}\,\mathrm{e}^{-(|x|+|x'|)}(1-(-1)) \\
&= \mathrm{e}^{-(|x|+|x'|)}
\end{aligned} \tag{7.1.10}$$

Let $x=x'$,

$$\phi_n^2(x)=\mathrm{e}^{-2|x|} \tag{7.1.11}$$

thus

$$\phi_n(x)=\mathrm{e}^{-|x|} \tag{7.1.12}$$

Ex 7.5

$$\begin{aligned}
\mathscr{H}\,\phi &= \left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}-\delta(x)\right]\mathrm{e}^{-|x|} \\
&= -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left[\mathrm{e}^{-|x|}\left(-\frac{\mathrm{d}}{\mathrm{d}x}|x|\right)\right]-\delta(x)\,\mathrm{e}^{-|x|} \\
&= \frac{1}{2}\left[-\mathrm{e}^{-|x|}(\frac{\mathrm{d}}{\mathrm{d}x}|x|)^2+\mathrm{e}^{-|x|}\,\frac{\mathrm{d}^2}{\mathrm{d}x^2}|x|\right]-\delta(x)\,\mathrm{e}^{-|x|} \\
&= \frac{1}{2}\left[-\mathrm{e}^{-|x|}+\mathrm{e}^{-|x|}\times 2\delta(x)\right]-\delta(x)\,\mathrm{e}^{-|x|} \\
&= -\frac{1}{2}\,\mathrm{e}^{-|x|}
\end{aligned} \tag{7.1.13}$$

thus the eigenvalue is $-\dfrac{1}{2}$.

Ex 7.6

$$\begin{aligned} \mathrm{i}\,\frac{\partial}{\partial t}\phi(x,t) &= \mathrm{i}\int \mathrm{d}x'\,\frac{\partial G(x,x',t)}{\partial t}\psi(x') \\ &= \end{aligned} \tag{7.1.14}$$