then the minima is given by

$$\frac{dL_{ABC}}{d\theta} = -\left(\frac{\vec{A}}{\sqrt{\vec{A}^2 + \vec{B}^2 - 2\vec{A}\cdot\vec{B}}} + \frac{\vec{C}}{\sqrt{\vec{C}^2 + \vec{B}^2 - 2\vec{C}\cdot\vec{B}}} \right) \cdot \vec{B}'(\theta) = 0.$$

The minima can then be found using a bisection algorithm or using Newton-Raphson. A simpler way is to observe that $\vec{B}'(\theta)$ is orthogonal to $\vec{B}(\theta)$ so that the vector

$$\vec{D} = \frac{\vec{A}}{\sqrt{\vec{A}^2 + \vec{B}^2 - 2\vec{A}\cdot\vec{B}}} + \frac{\vec{C}}{\sqrt{\vec{C}^2 + \vec{B}^2 - 2\vec{C}\cdot\vec{B}}}$$

will be proportional to $\vec{B}$. This then provides an iterative sequence for finding $\vec{B}$

- *Starting from your current guess for $\vec{B}$ calculate $\vec{D}$*
- *Put $\vec{B} = a\vec{D}/|\vec{D}|$*
- *Repeat the first step until you converge.*

At each iteration of the improvement cycle the total length of the orbit is measured. The minimization is complete when the path length stops improving. Although this algorithm is not as fast as the Newton-Raphson method, it nevertheless converges very rapidly.

(Adam Prügel-Bennet)

Chapter 24

Solution 24.1: Green's function. *The Laplace transform of the (time-dependent) quantum propagator*

$$K(q, q', t) = \sum_n \phi_n(q) e^{-iE_n t/\hbar} \phi_n^*(q')$$

is the (energy-dependent) Green's function

$$\begin{aligned} G(q, q', E + i\varepsilon) &= \frac{1}{i\hbar} \int_0^\infty dt\, e^{\frac{i}{\hbar}Et - \frac{\varepsilon}{\hbar}t} \sum_n \phi_n(q) e^{-iE_n t/\hbar} \phi_n^*(q') \\ &= \frac{1}{i\hbar} \sum_n \phi_n(q)\phi_n^*(q') \int_0^\infty dt\, e^{\frac{i}{\hbar}(E - E_n + i\varepsilon)t} \\ &= -\sum_n \phi_n(q)\phi_n^*(q') \frac{1}{E - E_n + i\varepsilon} e^{-\frac{\varepsilon}{\hbar}t} e^{i(E-E_n)t/\hbar} \Big|_{t=0}^{t=\infty} . \end{aligned}$$

When ε is positive, $e^{-\frac{\varepsilon}{\hbar}\infty} = 0$, so

$$G(q, q', E + i\varepsilon) = \sum_n \frac{\phi_n(q)\phi_n^*(q')}{E - E_n + i\varepsilon} .$$

(Bo Li)

Solution 24.2: Lorentzian representation of the Dirac delta function. *General hint: read up on principal parts, positive and negative frequency parts of the Dirac delta function, perhaps the Cauchy theorem, in any good quantum mechanics textbook.*

To see that (24.18) satisfies properties of the delta function,

$$\delta(E - E_n) = -\lim_{\varepsilon \to 0} \frac{1}{\pi} \mathrm{Im} \frac{1}{E - E_n + i\varepsilon} ,$$

start by expressing explicitely the imaginary part:

$$\begin{aligned} -\mathrm{Im} \frac{1}{E - E_n + i\varepsilon} &= -\mathrm{Im} \frac{E - E_n - i\varepsilon}{(E - E_n + i\varepsilon)(E - E_n - i\varepsilon)} \\ &= \frac{\varepsilon}{(E - E_n)^2 + \varepsilon^2} . \end{aligned}$$

This is a Lorenzian of width ϵ, with a peak at $E = E_n$. It has the correct normalization for the delta function,

$$\begin{aligned} \frac{1}{\pi} \int_{-\infty}^{\infty} dE \frac{\varepsilon}{(E - E_n)^2 + \varepsilon^2} &= \frac{1}{\pi} \frac{\varepsilon}{\varepsilon} \arctan \frac{E - E_n}{\varepsilon} \bigg|_{-\infty}^{\infty} \\ &= \frac{1}{\pi} (\pi/2 - (-\pi/2)) = 1 , \end{aligned}$$

so

$$\frac{1}{\pi} \int_{-\infty}^{\infty} dE \frac{\epsilon}{(E - E_n)^2 + \epsilon^2} = 1 , \tag{O.22}$$

independently of the width ϵ.

Next we show that in the $\epsilon \to \infty$ limit the support of the Lorentzian is concentrated at $E = E_n$. When $E = E_n$,

$$\lim_{\varepsilon \to 0} \frac{1}{\pi} \left(\frac{\varepsilon}{(E - E_n)^2 + \varepsilon^2} \right) = \lim_{\varepsilon \to 0} \frac{1}{\pi} \frac{1}{\varepsilon} = \infty ,$$

and when $E \neq E_n$,

$$\lim_{\varepsilon \to 0} \frac{1}{\pi} \frac{\varepsilon}{(E - E_n)^2 + \varepsilon^2} = 0$$

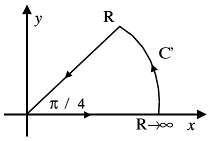
Providing that a function convolved with $\delta(s)$, $\int f(E)\delta(E - E_n)dE$ has a continuous first derivative at $E = E_n$ and falls of sufficiently rapidly as $E \to \pm\infty$, this is a representation of the delta function.

(R. Paskauskas, Bo Li)

Chapter 25

Solution 25.2: Fresnel integral. *Start by re-expressing the integral overthe infinite half-line:*

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2ia}} = \frac{2}{\sqrt{2\pi}} \int_0^{\infty} dx\, e^{-\frac{x^2}{2ia}}, \qquad a \in \mathbb{R}, \quad a \neq 0.$$

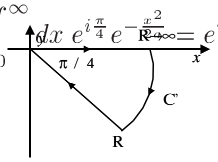
When $a > 0$, the contour 

vanishes, as it contains no pole:

$$\begin{aligned} \oint_C dz\, e^{-z^2/2ia} &= \int_0^{\infty} dx\, e^{-\frac{x^2}{2ia}} + \int_{C'} + \int_{\infty}^{0} e^{i\frac{\pi}{4}} e^{-\frac{x^2}{2a}} dx = 0 \\ \int_{C'} &= \int_0^{\frac{\pi}{4}} e^{iR^2 e^{i2\phi}/2a} R e^{i\phi} i d\phi = 0 \,. \end{aligned} \tag{O.23}$$

So

$$\frac{2}{\sqrt{2\pi}} \int_0^{\infty} dx\, e^{-\frac{x^2}{2ia}} = \frac{2}{\sqrt{2\pi}} \int_0^{\infty} dx\, e^{i\frac{\pi}{4}} e^{-\frac{x^2}{2a}} = e^{i\frac{\pi}{4}} \sqrt{a} = \sqrt{ia}$$

In the $a < 0$ case take the contour 

$$\begin{aligned} \oint_C dz\, e^{-z^2/2ia} &= \int_0^{\infty} dx\, e^{-\frac{x^2}{2ia}} + \int_{C'} + \int_{\infty}^{0} e^{-i\frac{\pi}{4}} e^{\frac{x^2}{2a}} dx \\ &= \int_0^{\infty} dx\, e^{-\frac{x^2}{2ia}} - e^{-i\frac{\pi}{4}} \int_0^{\infty} dx\, e^{\frac{x^2}{2a}} = 0 \,. \end{aligned}$$

Again

$$\frac{2}{\sqrt{2\pi}} \int_0^{\infty} dx\, e^{-\frac{x^2}{2ia}} = e^{-i\frac{\pi}{4}} \sqrt{|a|} \,,$$

and, as one should have perhaps intuited by analyticity arguments, for either sign of a *we have the same Gaussian integral formula*

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\; e^{-\frac{x^2}{2ia}} = |a|^{1/2} e^{i\frac{\pi}{4}\frac{a}{|a|}} = \sqrt{ia}\,.$$

The vanishing of the C' *contour segment (O.23) can be proven as follows: Substitute* $z = Re^{i\phi}$ *into the integral*

$$I_R = \int_0^{\frac{\pi}{4}} e^{iR^2 e^{i2\phi}/2a} Re^{i\phi} i d\phi = \int_0^{\frac{\pi}{4}} e^{iR^2(\cos 2\phi + i\sin 2\phi)/2a} Re^{i\phi} i d\phi\,.$$

Then

$$|I_R| \leq R\int_0^{\frac{\pi}{4}} e^{-R^2\sin 2\phi/2a} d\phi = \frac{R}{2}\int_0^{\frac{\pi}{2}} e^{-R^2\sin\theta/2a} d\theta\,.$$

In the range $[0, \pi/2]$ *we can replace* $\frac{2}{\pi}\theta \leq \sin\theta$ *, obtain a bound*

$$|I_R| \leq \frac{R}{2}\int_0^{\frac{\pi}{2}} e^{-R^2\theta/\pi a} d\theta = \frac{R}{2}\frac{1 - e^{-R^2/2a}}{R^2/a\pi}\,,$$

so

$$\lim_{R\to\infty} |I_R| = 0\,.$$

(Bo Li)