Theoretical modeling of the collective tunneling of a Wigner necklace

Dominik szombathy

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A Mathematics

In this appendix I will write down some useful mathematical expressions, proofs or identities that are used in the discussion above

A.1 Gaussian Integrals

A.2 Besel Problem

Fourier Way Let's consider first an arbitrary function $f(x)$. The fourier series of this function is:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left\{ a_n \cos\left(\frac{n\pi l}{L}\right) + b_n \sin\left(\frac{n\pi l}{L}\right) \right\} \tag{A.1}$$

where $l \in [l_i, l_f]$ and $L = l_f - l_i$

let $f(x) = x^2$ and $l_i = -l_f = -\pi$ so that $L = 2\pi$

Now the coefficients can be calculated:

$$a_0 = \frac{2}{L} \int_{-\pi}^{\pi} f(x)dx \tag{A.2}$$

$$= \frac{2}{\pi} \int_{0}^{\pi} dx\, x^2 \tag{A.3}$$

$$= \frac{2}{3}\pi^2 \tag{A.4}$$

$$a_n = \frac{2}{L} \int_{-\pi}^{\pi} dx\, f(x) \cos\left(\frac{n\pi 2x}{L}\right) \tag{A.5}$$

$$= \frac{2}{\pi} \left(\frac{x^2 \sin(nx)}{n}\right)\Bigg|_0^{\pi} - \frac{2}{\pi} \int_0^{\pi} dx\, \frac{2x \sin(nx)}{n} \tag{A.6}$$

$$= \text{another partial integration later} \tag{A.7}$$

$$= \frac{4(-1)^n}{n^2} \tag{A.8}$$

$b_n = 0$ because x^2 is even. So the function now looks like this:

$$x^2 = \frac{2\pi^2}{3 \cdot 2} + \sum_{n=1}^{\infty} \frac{4(-1)^n}{n^2} \cos\left(\frac{2n\pi x}{L}\right) \tag{A.9}$$

$$= \frac{\pi^2}{3} + \sum_{n=1}^{\infty} \frac{4(-1)^n}{n^2} (-1)^n \tag{A.10}$$

now choose x^2 tob e equal to 0:

$$\pi^2 = \frac{\pi^2}{3} + \sum_{n=1}^{\infty} \frac{4}{n^2} \tag{A.11}$$

subtract the a_0 term and devide by 4:

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{A.12}$$

Complex Integral Way consider the following integral:

$$I = \int_C \frac{1}{z^2} f(z) dz \tag{A.13}$$

let $f(z)$ be the Fermi function:

$$f(z) = \frac{1}{1 + e^{i\pi z}} \tag{A.14}$$

we have several first order poles at $z = \pm(2n+1) = p_n$ and a second order pole at $z = 0$.

The residue from the 1st order poles:

$$Res(f(z), p_n) = \lim_{z \to p_n} (z - p_n) f(z) = \frac{i}{\pi p_n^2} \tag{A.15}$$

rom the 2nd order pole:

$$Res(f(z), 0) = \lim_{z \to 0} \frac{d}{dz}(z^2 f(z)) = \frac{-\pi i}{4} \tag{A.16}$$

$$\int_C g(z) dz = 2\pi i \sum Res(g(z)) \tag{A.17}$$

$$\int_C f(z) dz = 2\pi i \left(\frac{-\pi i}{4} \right) + 2\pi i \sum_{n=0}^{\infty} \frac{2i}{\pi(2n+1)^2} = 0 \tag{A.18}$$

$$\frac{\pi i}{4} = \sum_{n=0}^{\infty} \frac{2i}{\pi(2n+1)^2} \tag{A.19}$$

$$\frac{\pi^2}{8} = \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \tag{A.20}$$

$$= \frac{3}{4} \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{A.21}$$

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{A.22}$$

B Algorithms and Methods

B.1 Monte Carlo and Simulated Annealing

B.2 Minimalization by Nelder-Mead algorithm