Theoretical modeling of the collective tunneling of a Wigner necklace

Dominik szombathy

December 13, 2022

Abstract

Contents

1	Wi	gner Crystals	4		
2	Pat	h Integral Formalism	4		
	2.1	Free Particle	4		
	2.2	Harmonic Oscillator	4		
	2.3	One particle tunneling	4		
		2.3.1 One Particle Hamiltonian	4		
		2.3.2 Action Integral Calculation	4		
		2.3.3 Tunneling calculation in quartic potentials	4		
3	Exp	perimental Considerations	4		
	3.1	Modeling the Potential and Fitting	4		
	3.2	Polarization data	4		
	3.3	Scaling	4		
4	Many Body Tunneling Calculations - Instanton				
	4.1	Quartic Hamiltonian model	4		
		4.1.1 Rescaling and Dimensionless Hamiltonian	4		
	4.2	Milnikov method	4		
	4.3	Classical Equilibrium Positions	4		
	4.4	Harmonic Oscillator Eigenfrequencies adn Eigenmodes	4		
	4.5	Trajectory Calculation	4		
	4.6	Arc Lengt Paramterization	4		
	4.7	Egzact Diagonalization (ED)	4		
5	Pol	arization	4		
	5.1	Classical Polarization Calculation	4		
	5.2	Polarization using ED	4		

6	Open Questions	4		
\mathbf{A}	Mathematics			
	A.1 Gaussian Integrals	Ę		
	A.2 Cauchy's Residue Theorem	Ę		
	A.3 Besel Problem	Ę		
\mathbf{B}	Algorithms and Methods			
	B.1 Monte Carlo and Simulated Annealing	(
	B.2 Minimalization by Nelder-Mead algorithm	(
\mathbf{C}	Links, Data and other stuff	6		

- 1 Wigner Crystals
- 2 Path Integral Formalism
- 2.1 Free Particle
- 2.2 Harmonic Oscillator
- 2.3 One particle tunneling
- 2.3.1 One Particle Hamiltonian
- 2.3.2 Action Integral Calculation
- 2.3.3 Tunneling calculation in quartic potentials
- 3 Experimental Considerations
- 3.1 Modeling the Potential and Fitting
- 3.2 Polarization data
- 3.3 Scaling
- 4 Many Body Tunneling Calculations Instanton
- 4.1 Quartic Hamiltonian model
- 4.1.1 Rescaling and Dimensionless Hamiltonian
- 4.2 Milnikov method
- 4.3 Classical Equilibrium Positions
- 4.4 Harmonic Oscillator Eigenfrequencies adn Eigenmodes
- 4.5 Trajectory Calculation
- 4.6 Arc Lengt Paramterization
- 4.7 Egzact Diagonalization (ED)
- 5 Polarization
- 5.1 Classical Polarization Calculation
- 5.2 Polarization using ED
- 6 Open Questions

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 Cauchy's Residee Theorem

A.3 Besel Problem

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \tag{A.3.1}$$

Fourier Way Let's consider first an arbitrary function f(x). One could wirte the fourier series of this function as

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left\{ a_n \cos\left(\frac{n\pi l}{L}\right) + b_n \sin\left(\frac{n\pi l}{L}\right) \right\},\tag{A.3.2}$$

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 $L = 2\pi$. The coefficients can be calculated as

$$a_0 = \frac{2}{L} \int_{-\pi}^{\pi} f(x) dx = \frac{2}{\pi} \int_{0}^{\pi} dx \, x^2 = \frac{2}{3} \pi^2$$
 (A.3.3)

$$a_{n} = \frac{2}{L} \int_{-\pi}^{\pi} dx \, f(x) \cos\left(\frac{n\pi 2x}{L}\right)$$

$$= \frac{2}{\pi} \left(\frac{x^{2} \sin(nx)}{n}\right) \Big|_{0}^{\pi} - \frac{2}{\pi} \int_{0}^{\pi} dx \, \frac{2x \sin(nx)}{n}$$

$$= \frac{4(-1)^{n}}{n^{2}}.$$
(A.3.4)

Considering the problem at hand, consider the function as x^2 , so $b_n = 0$ because x^2 is even. The Fourier series then takes the form

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

$$= \frac{\pi^{2}}{3} + \sum_{n=1}^{\infty} \frac{4(-1)^{n}}{n^{2}} (-1)^{n}.$$
(A.3.5)

Choose x^2 to be equal to 0,

$$\pi^2 = \frac{\pi^2}{3} + \sum_{n=1}^{\infty} \frac{4}{n^2}.$$
 (A.3.6)

Then subtract the a_0 term and devide by 4

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{A.3.7}$$

Complex Integral Way Consider the following integral:

$$I = \int_C \frac{1}{z^2} f(z) dz. \tag{A.3.8}$$

Let f(z) be the Fermi function:

$$f(z) = \frac{1}{1 + e^{i\pi z}},\tag{A.3.9}$$

then 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:

$$Res(f(z), p_n) = \lim_{z \to p_n} (z - p_n) f(z) = \frac{i}{\pi p_n^2},$$
 (A.3.10)

and from the 2nd order pole:

$$Res(f(z), 0) = \lim_{z \to 0} \frac{d}{dz}(z^2 f(z)) = \frac{-\pi i}{4}.$$
 (A.3.11)

Writing now Cauchy's residue theorem A.2

$$\int_{C} g(z)dz = 2\pi i \sum Res(g(z))$$
(A.3.12)

$$\int_{C} f(z)dz = 2\pi i \left(\frac{-\pi i}{4}\right) + 2\pi i \sum_{n=0}^{\infty} \frac{2i}{\pi (2n+1)^{2}} = 0$$
 (A.3.13)

$$\frac{\pi i}{4} = \sum_{n=0}^{\infty} \frac{2i}{\pi (2n+1)^2} \tag{A.3.14}$$

$$\frac{\pi^2}{8} = \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2}$$
 (A.3.15)

$$=\frac{3}{4}\sum_{n=1}^{\infty}\frac{1}{n^2}\tag{A.3.16}$$

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{A.3.17}$$

B Algorithms and Methods

- **B.1** Monte Carlo and Simulated Annealing
- B.2 Minimalization by Nelder-Mead algorithm
- C Links, Data and other stuff

[?], [?]

References

- $[1]\,$ Anna Anderegg, 2022, Example 1.
- $[2]\,$ Brenda Bradshaw, 2021, Example 2.