Wigner Crystal Collective tunneling - A theoretical investigation

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The documentation of the title's topic, Wigner crystal collective tunneling. Motivated by experiments, where in an effectively one dimensional system a wigner crystal for up to 7 electrons were observed. This work aims to investigate the phenomena from a theoreitcal point of view using ED, Instanton and DMRG techniques.

Usage: This note aims to document every major developement in the project, explain the necessary 'new' physics (at least new for me), derive or proof mathematical concepts that the investigation is dependent upon, and be a somewhat self-contained material for me and possibly others during the research process.

Structure: The structure is as follows: Starting from elementary physics concepts that describes the environment that we are trying to understand, then developing the path integral tools along Feynman's book and Milnikov's work, these are followed by Monte-Carlo simulations, ED calculations and Polarization calculations,then ends with open quaestions, hopefully with some answers. The notes ends with the Appendix containing the necessary math, programming and other important materials.

CONTENTS

I. WIGNER CRYSTAL

Note:
this is a note, neat isn't it?

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II. PATH INTEGRAL FORMALISM

A. Free Particle

B. Harmonic Oscillator

C. One Particle Tunneling

1. *One Particle Hamiltonian*

2. *Action Integral Calculation*

3. *Tunneling calculation in quartic potentials*

III. EXPERIMENTAL CONSIDERATIONS

A. Modeling the Potential and Fitting

B. Polarization data

C. Scaling

IV. MANY BODY TUNNELING CALCULATIONS - INSTANTON

A. Quartic Hamiltonian model

1. *Rescaling and Dimensionless Hamiltonian*

B. Milnikov method

C. Classical Equilibrium Positions

D. Harmonic Oscillator Eigenfrequencies adn Eigenmodes

E. Trajectory Calculation

F. Arc Lengt Paramterization

G. Egzact Diagonalization (ED)

V. POLARIZATION

A. Classical Polarization Calculation

B. Polarization using ED

VI. OPEN QUESTIONS

Appendix A: Mathematics

1. Gaussian Integrals

Problem A.1 (Purely quadratic case)**.**

$$I_{\text{pure gauss.}}(a) = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{ax^2} \tag{A.1}$$

A way to solve this integral is to intorduce $I(a)^2$, go to a polar coordinate representation by a simple substitution, then integrate over the polar angle ϕ and finally take the square root of the result.

$$I(a)^2 = \int_{-\infty}^{\infty} \mathrm{d}x_1 \int_{-\infty}^{\infty} \mathrm{d}x_2 e^{ax_1^2} e^{ax_2^2} \tag{A.2}$$

$$= \iint_{-\infty}^{\infty} \mathrm{d}x_1 \mathrm{d}x_2\, e^{a(x_1^2+x_2^2)} \tag{A.3}$$

Now one can go from $\mathrm{d}x_1\mathrm{d}x_2$ to $\mathrm{d}r\mathrm{d}\phi$, by the $x_1 = r\cos(\phi)$ and $x_2 = r\sin(\phi)$. Meaning that $x_1^2 + x_2^2 = r^2$ replaces the exponent. Calculating the Jacobian for the change of the metric

$$J = \begin{vmatrix} \frac{\partial x_1}{\partial r} & \frac{\partial x_1}{\partial \phi} \\ \frac{\partial x_2}{\partial r} & \frac{\partial x_2}{\partial \phi} \end{vmatrix} = \begin{vmatrix} \cos(\phi) & -r\sin(\phi) \\ \sin(\phi) & r\cos(\phi) \end{vmatrix} = r \tag{A.4}$$

$$I(a)^2 = \int_0^{\infty} \mathrm{d}r \int_0^{2\pi} \mathrm{d}\phi\, r e^{a(r^2)} \tag{A.5}$$

$$= 2\pi \int_0^{\infty} \mathrm{d}r\, r e^{a(r^2)} \tag{A.6}$$

It is convinient to make another substitution $q = -r^2 \rightarrow \mathrm{d}q = -2r\mathrm{d}r$.

$$I(a)^2 = -2\pi \int_0^{\infty} \mathrm{d}q\, \frac{1}{2} e^{-a\,q} \tag{A.7}$$

$$= \frac{\pi}{-a} \tag{A.8}$$

$$\boxed{\int_{-\infty}^{\infty} \mathrm{d}x\, e^{ax^2} = \sqrt{\frac{\pi}{-a}}} \tag{A.9}$$

assuming that $\mathbb{R}(a) \leq 0$

Problem A.2 (General Gaussian Integral)**.**

$$I_{\text{Gen.gauss.}}(a,b,c) = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{ax^2+bx+c} \tag{A.10}$$

The second order polinomial in the exponent can be written as a square: $\alpha(x+\beta)^2 - \gamma = ax^2 + bx + c$. Identifying the coefficients on the l.h.s. we find that $\alpha = a$; $\beta = \frac{b}{2a}$; and $\gamma = c - \frac{b^2}{4a^2}$. Now rewrite the integral using the squared form of the polynomial

$$I(a,b,c) = \int \mathrm{d}x\, e^{a(x+\frac{b}{2a})^2 + c - \frac{b^2}{4a^2}} \tag{A.11}$$

where the last two terms in the exponent are just constant factors which can be placed outside of the integral, leaving the $a(x+\frac{b}{2a})^2$ term. Substitute in $y = x + \frac{b}{2a}$ ($\mathrm{d}y = \mathrm{d}x$)

$$I(a,b,c) = e^{c-\frac{b^2}{4a^2}} \int_{-\infty}^{\infty} \mathrm{d}y\, e^{ay^2}. \tag{A.12}$$

Integral on the l.h.s. is the same as in problem A.1, giving the answer as

$$\boxed{\int_{-\infty}^{\infty} \mathrm{d}x\, e^{ax^2+bx+c} = e^{c-\frac{b^2}{4a^2}} \sqrt{\frac{\pi}{-a}}} \tag{A.13}$$

2. Cauchy's Resiude Theorem

3. Besel Problem

Prove the following equality

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \tag{A.14}$$

Problem A.3 (Basel problem - Fourier series way)**.** Let's consider first an arbitrary function $f(x)$. One could wirte the fourier series of this function as

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left\{ a_n \cos\left(\frac{n\pi l}{L}\right) + b_n \sin\left(\frac{n\pi l}{L}\right) \right\}, \tag{A.15}$$

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

$$a_0 = \frac{2}{L} \int_{-\pi}^{\pi} f(x)dx = \frac{2}{\pi} \int_0^{\pi} dx\, x^2 = \frac{2}{3}\pi^2 \tag{A.16}$$

$$\begin{aligned} a_n &= \frac{2}{L} \int_{-\pi}^{\pi} dx\, f(x) \cos\left(\frac{n\pi 2x}{L}\right) \\ &= \frac{2}{\pi} \left(\frac{x^2 \sin(nx)}{n} \right)\Bigg|_0^{\pi} - \frac{2}{\pi} \int_0^{\pi} dx\, \frac{2x \sin(nx)}{n} \\ &= \frac{4(-1)^n}{n^2}. \end{aligned} \tag{A.17}$$

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

$$\begin{aligned} x^2 &= \frac{2\pi^2}{3 \cdot 2} + \sum_{n=1}^{\infty} \frac{4(-1)^n}{n^2} \cos\left(\frac{2n\pi x}{L}\right) \\ &= \frac{\pi^2}{3} + \sum_{n=1}^{\infty} \frac{4(-1)^n}{n^2} (-1)^n. \end{aligned} \tag{A.18}$$

Choose x^2 to be equal to 0,

$$\pi^2 = \frac{\pi^2}{3} + \sum_{n=1}^{\infty} \frac{4}{n^2}. \tag{A.19}$$

Then subtract the a_0 term and devide by 4

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{A.20}$$

Problem A.4 (Complex Integral way)**.** Consider the following integral:

$$I = \int_C \frac{1}{z^2} f(z) dz. \tag{A.21}$$

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

$$f(z) = \frac{1}{1 + e^{i\pi z}}, \tag{A.22}$$

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:

$$Res(f(z), p_n) = \lim_{z \to p_n} (z - p_n) f(z) = \frac{i}{\pi p_n^2}, \tag{A.23}$$

and from the 2nd order pole:

$$Res(f(z), 0) = \lim_{z \to 0} \frac{d}{dz} (z^2 f(z)) = \frac{-\pi i}{4}. \tag{A.24}$$

Writing now Cauchy's residue theorem A 2

$$\int_C g(z)dz = 2\pi i \sum Res(g(z)) \tag{A.25}$$

$$\int_C f(z)dz = 2\pi i \left(\frac{-\pi i}{4} \right) + 2\pi i \sum_{n=0}^{\infty} \frac{2i}{\pi(2n+1)^2} = 0 \tag{A.26}$$

$$\frac{\pi i}{4} = \sum_{n=0}^{\infty} \frac{2i}{\pi(2n+1)^2} \tag{A.27}$$

$$\frac{\pi^2}{8} = \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \tag{A.28}$$

$$= \frac{3}{4} \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{A.29}$$

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{A.30}$$

Appendix B: Algorithms and Methods

1. Monte Carlo and Simulated Annealing

2. Minimalization by Nelder-Mead algorithm

Appendix C: Links, Data and other stuff

[1], [2]

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