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.

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I. WIGNER CRYSTAL

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look.

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Note:

this is a note, neat isn't it?

II. PATH INTEGRAL FORMALISM

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

A. Free Particle

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B. Harmonic Oscillator

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C. One Particle Tunneling

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1. One Particle Hamiltonian

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2. Action Integral Calculation

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3. Tunneling calculation in quartic potentials

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III. EXPERIMENTAL CONSIDERATIONS

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A. Modeling the Potential and Fitting

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B. Polarization data

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C. Scaling

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IV. MANY BODY TUNNELING CALCULATIONS - INSTANTON

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A. Quartic Hamiltonian model

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1. Rescaling and Dimensionless Hamiltonian

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B. Milnikov method

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C. Classical Equilibrium Positions

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D. Harmonic Oscillator Eigenfrequencies adn Eigenmodes

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E. Trajectory Calculation

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F. Arc Lengt Paramterization

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G. Egzact Diagonalization (ED)

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V. POLARIZATION

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A. Classical Polarization Calculation

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B. Polarization using ED

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VI. OPEN QUESTIONS

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Appendix A: Mathematics

1. Gaussian Integrals

Problem A.1 (Purely quadratic case).

$$I_{\text{pure gauss.}}(a) = \int_{-\infty}^{\infty} dx \, e^{ax^2} \qquad (A.1)$$

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.

$$I(a)^2 = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 e^{ax_1^2} e^{ax_2^2} \qquad (A.2)$$

$$= \iint_{-\infty}^{\infty} dx_1 dx_2 \, e^{a(x_1^2 + x_2^2)} \qquad (A.3)$$

Now one can go from $dx_1 dx_2$ to $drd\phi$, 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

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

$$I(a)^2 = \int_0^{\infty} dr \int_0^{2\pi} d\phi \, re^{a(r^2)} \qquad (A.5)$$

$$= 2\pi \int_0^{\infty} dr \, re^{a(r^2)} \qquad (A.6)$$

It is convinient to make another substitution $q = -r^2 \to dq = -2rdr$.

$$I(a)^2 = -2\pi \int_0^{\infty} dq \, \frac{1}{2} e^{-aq} \qquad (A.7)$$

$$= \frac{\pi}{-a} \qquad (A.8)$$

$$\boxed{\int_{-\infty}^{\infty} dx \, e^{ax^2} = \sqrt{\frac{\pi}{-a}}} \qquad (A.9)$$

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

Problem A.2 (General Gaussian Integral).

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

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

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

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 $y = x + \frac{b}{2a}$ $(dy = dx)$

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

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

$$\boxed{\int_{-\infty}^{\infty} dx \, e^{ax^2 + bx + c} = e^{c - \frac{b^2}{4a^2}} \sqrt{\frac{\pi}{-a}}} \qquad (A.13)$$

2. Cauchy's Resiude Theorem

3. Besel Problem

Prove the following equality

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

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

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

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

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

$$a_n = \frac{2}{L} \int_{-\pi}^{\pi} dx \, f(x) \cos\left(\frac{n\pi 2x}{L}\right) \qquad (A.17)$$

$$= \frac{2}{\pi} \left(\frac{x^2 \sin(nx)}{n} \right)\Big|_0^{\pi} - \frac{2}{\pi} \int_0^{\pi} dx \, \frac{2x \sin(nx)}{n}$$

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

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

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

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

Choose x^2 to be equal to 0,

$$\pi^2 = \frac{\pi^2}{3} + \sum_{n=1}^{\infty} \frac{4}{n^2}. \quad \text{(A.19)}$$

Then subtract the a_0 term and devide by 4

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} \quad \text{(A.20)}$$

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

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

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

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

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:

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

and from the 2nd order pole:

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

Writing now Cauchy's residue theorem A 2

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

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

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

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

$$= \frac{3}{4} \sum_{n=1}^{\infty} \frac{1}{n^2} \quad \text{(A.29)}$$

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2} \quad \text{(A.30)}$$

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.