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Quantization of the Coulomb Chain in an External Focusing Field*

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Abstract

With the appropriate choice of parameters and sufficient cooling, charged particles in a circular accelerator are believed to undergo a transition to a highly-ordered crystalline state[1]. The simplest possible crystalline configuration is a one-dimensional chain of particles. In this paper, we write down the quantized version of its dynamics. We show that in a low-density limit, the dynamics is that of a theory of interacting phonons. There is an infinite sequence of n-phonon interaction terms, we write down the first orders, which involve phonon scattering and decay processes. The quantum formulation developed here can serve as a first step towards a quantum-mechanical treatment of the system at finite temperatures.

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1 Higher-Order Dynamics of the Coulomb Chain

We consider an ensemble of charged point particles forced into an one-dimensional setup by an external focusing field. In equilibrium, the particles will be equidistant longitudinally. We treat the limit of an infinite, but periodic, chain. The problem will be treated in the rest frame of an orbiting particle, curvature and retardation effects will be neglected.

The kinetic, potential and Coulomb interaction Lagrangian are, respectively

$$\begin{aligned}
\mathcal{L}_k &= \frac{1}{2m}\sum_{\mu} \dot{\boldsymbol{x}}_{\boldsymbol{\mu}} \cdot \dot{\boldsymbol{x}}_{\boldsymbol{\mu}} \\
\mathcal{L}_p &= -\frac{m\omega_{ext,x}^2}{2}\sum_{\mu}(x_\mu^1)^2 - \frac{m\omega_{ext,y}^2}{2}\sum_{\mu}(x_\mu^2)^2 \\
\mathcal{L}_i &= \frac{1}{2}\sum_{\mu\neq\nu}\mathcal{L}_{\mu\nu} = \frac{e^2}{2}\sum_{\mu\neq\nu}\frac{1}{\sqrt{(\boldsymbol{x}_\mu - \boldsymbol{x}_\nu + (\mu-\nu)\boldsymbol{\lambda})^2}} \quad ,
\end{aligned} \tag{1}$$

where we have introduced local coordinates around each particle's equilibrium position. The sums run over all lattice sites. $\boldsymbol{\lambda}$ is the lattice vector, we use a coordinate system where $\boldsymbol{\lambda} = (0, 0, \lambda)$. The particle has mass m, and the external focusing strengths are given by $\omega_{ext,x}^2, \omega_{ext,y}^2$ and are assumed to be constant along the ring. We are using natural units with $\hbar = c = 1$.

We expand (1) in x_μ, that is, we write

$$\mathcal{L}_{\mu\nu} =_{p=0}^{\infty} \sum_{i_1,\ldots,i_p=1}^{3} \sum_{\mu_1,\ldots,\mu_p=1}^{\infty} \frac{1}{p!}\sum \mathcal{L}_{\mu\nu}^{(p),\mu_1\cdots\mu_p} x_{\mu_1}^{i_1}\cdots x_{\mu_p}^{i_p} \quad . \tag{2}$$

$\mathcal{L}_i^{(0)}$ diverges, but is irrelevant here; $\mathcal{L}_i^{(1)} = 0$, as the coördinates are expanded around their equilibrium. For the first interesting orders, we get

$$\left.\begin{aligned}
\mathcal{L}_{\mu\nu}^{(2),\mu_1\mu_2} &= \frac{\Delta^1\Delta^2}{\lambda^3\left|\mu-\nu\right|^3}\left(3\delta^{i_1 3}\delta^{i_2 3} - \delta^{i_1 i_2}\right) \\
\mathcal{L}_{\mu\nu}^{(3),\mu_1\mu_2\mu_3} &= \frac{\Delta^1\Delta^2\Delta^3(\mu-\nu)}{\lambda^3\left|\mu-\nu\right|^5}\sum_{\Pi(i)}\delta^{i_1 3}\left(\frac{3}{2}\delta^{i_2 i_3} - \frac{5}{2}\delta^{i_1 i_2 i_3}\right) \\
\mathcal{L}_{\mu\nu}^{(4),\mu_1\cdots\mu_4} &= \frac{\Delta^1\Delta^2\Delta^3\Delta^4}{\lambda^5\left|\mu-\nu\right|^5}\sum_{\Pi(i)}\left(\frac{3}{8}\delta^{i_1 i_2}\delta^{i_3 i_4} - \frac{15}{4}\delta^{i_1 i_2}\delta^{i_3 3}\delta^{i_4 3}\right. \\
&\quad \left. + \frac{35}{8}\delta^{i_1 3}\delta^{i_2 3}\delta^{i_3 3}\delta^{i_4 3}\right)
\end{aligned}\right\} \quad , \tag{3}$$

where we used the shorthand notation $\Delta^i = (\delta_{\mu_i m} - \delta_{\mu_i n})$.

Doing the summation over m, n, we get

$$\left.\begin{aligned}
\mathcal{L}^{(2)}_{\mu_1\mu_2} &= \left(2\delta^{\mu^1\mu^2}\sum_{\pm k=1}^{\infty}\Phi^{(3)}_{k_0} - 2\Phi^{(3)}_{\mu_1\mu_2}\right)\delta^{i_1 i_2}(3\delta^{i_1 3}-1) \\
\mathcal{L}^{(3)}_{\mu_1\mu_2\mu_3} &= \sum_{\Pi(\mu)}\left(-\delta^{\mu_1\mu_2}\Phi^{(4)}_{\mu_1\mu_3}\right)\sum_{\Pi(i)}\delta^{i_1 3}\left(\frac{3}{2}\delta^{i_2 i_3} - \frac{5}{2}\delta^{i_1 i_2 i_3}\right) \\
\mathcal{L}^{(4)}_{\mu_1\cdots\mu_4} &= \sum_{\Pi(\mu)}\left(\frac{1}{12}\delta^{\mu_1\mu_2\mu_3\mu_4}\sum_{\pm k=1}^{\infty}\Phi^{(5)}_{k0} - \frac{1}{3}\delta^{\mu_1\mu_2\mu_3}\Phi^{(5)}_{\mu_1\mu_4}\right. \\
&\quad \left.+\frac{1}{4}\delta^{\mu_1\mu_2}\delta^{\mu_3\mu_4}\Phi^{(5)}_{\mu_1\mu_4}\right) \\
&\quad \times\sum_{\Pi(i)}\delta^{i_1 i_2}\delta^{i_3 i_4}\left(\frac{3}{8} + \delta^{i_4 3}\left(-\frac{15}{4} + \frac{35}{8}\delta^{i_1 3}\right)\right)
\end{aligned}\right\} \quad , \tag{4}$$

where $\Phi^{(n)}_{\mu\nu} = \frac{1}{2}e^2\lambda^{-n}(\mathrm{sgn}(\mu-\nu))^{n-1}\left|\mu-\nu\right|^{-n}\Big|_{\mu\neq\nu}$ and $\Phi^{(n)}_{\mu\mu} = 0$ and Π denotes all permutations of a set of indices.

The sums over Φ_{k0} give

$$\sum_{k=1}^{\infty}\Phi^{(n)}_{k0} = \frac{1}{2}e^2\lambda^{-n}\zeta(n) \tag{5}$$

for odd n and vanish for even n. ($\zeta(3) \approx 1.202, \zeta(5) \approx 1.037$).

As the interaction is translationally invariant, we proceed by Fourier transformation:

$$\left.\begin{aligned}
x^m_\mu &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ik\mu}\xi^m(k) \\
\xi^m(k) &= \sum_{\mu=-\infty}^{\infty} e^{ik\mu}x^m_\mu
\end{aligned}\right\} \tag{6}$$

We write down the interaction Lagrangian in this basis. For convenience, we introduce vertex functions

$$F^{(p)}_{i_1\ldots i_2} = \frac{1}{(2\pi)^{p-1}}\int\delta^{2\pi}\left(\sum_{i=1}^{p}k_i\right)\tilde{\Phi}^{(p+1)}(k_{i_1}+\cdots+k_{i_n})\mathrm{d}^p k \quad . \tag{7}$$

Note that momentum conservation is only up to integer multiples of 2π. After some Fourier

gymnastics, we have

$$\left.\begin{aligned}
\mathcal{L}^{(2)} &= 2\left(F^{(2)} - F_1^{(2)}\right)\delta^{i_1 i_2}(3\delta^{i_1 3} - 1) \\
\mathcal{L}^{(3)} &= \sum_{\Pi(k)} F_1^{(3)} \sum_{\Pi(i)} \delta^{i_1 3}\left(\frac{3}{2}\delta^{i_2 i_3} - \frac{5}{2}\delta^{i_1 i_2 i_3}\right) \\
\mathcal{L}^{(4)} &= \sum_{\Pi(k)}\left(\frac{1}{12}F^{(4)} - \frac{1}{3}F_{123}^{(4)} + \frac{1}{4}F_{12}^{(4)}\right) \\
&\quad \sum_{\Pi(i)} \delta^{i_1 i_2}\delta^{i_3 i_4}\left(\frac{3}{8} + \delta^{i_4 3}\left(\frac{35}{8}\delta^{i_1 3} - \frac{15}{4}\right)\right)
\end{aligned}\right\} \quad . \tag{8}$$

2 Quantization

The quadratic terms of the total Lagrangian describe an ensemble of harmonic oscillators with coördinate variables $\xi_i(k), \xi_i^*(k) = \xi_i(-k)$. We introduce momenta variables $\pi_i(k), \pi_i^*(k) = \pi_i(-k)$ obeying the usual commutation relations.

Quantization is straightforwardly done by defining creation and annihilation operators $a_i(k), a_i^+(k)$ by

$$\sqrt{2\Omega(k)}a_j(k) = \Omega(k)\xi_j(k) + i\pi_j(-k) \quad , \tag{9}$$

with oscillator frequencies $\Omega(k)$ defined below. These oscillator eigenmodes describe phononic (particle displacement waves) excitations of our system.

We write the full Lagrangian (8) in terms of the operators $a_i(k), a_i^+(k)$. The momentum-independent terms in (8) are disposed of by absorbing them into the Fourier transform of the potential: $\tilde{\Phi}(k) \to \tilde{\Phi}(k) - \tilde{\Phi}(0)$.

Inspecting (8), one notices that the terms can be interpreted diagrammatically:

1. $F_1^{(2)}$ gives the one-particle propagator, i. e., it gives the dispersion relation $\Omega^2(k)$ for the phonons (Fig. 1)

2. $F_1^{(3)}$ describes a decay process: one incoming phonon decays into two outgoing ones (Fig. 2)

3. $F_{123}^{(4)}$ describes a decay process: one incoming phonon decays into three outgoing ones (Fig. 3)

4. $F_{12}^{(4)}$ describes a scattering: two incoming phonons exchange momentum (Fig. 4)

Note that our diagrams are in terms of the spatial coördinates ξ, ξ^*. If we want to draw the diagrams in terms of phononic eigenmodes, we have to use $\xi, \xi^* \propto a^+ \pm a$ and draw all 8 possible three-point and 32 possible four-point diagrams: Each leg in any of the diagrams can be flipped over to make an outgoing particle an ingoing one while changing the sign of its momentum.

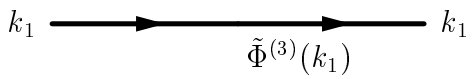

Figure 1: Free two-point function

Also, we have to multiply each diagram by the polarization tensors, i. e. the totally symmetric i_i dependent terms in (8). With an obvious notation for transverse and longitudinal polarizations, these are given in Table 1; contributions with index configurations not given in the table vanish.

Index Structure	Weight
$(\perp,\perp)$	-1
$(\|,\|)$	$+2$
$(\|,\|,\|)$	-6
$(\|,\perp,\perp)$	-2
$(\perp,\perp,\perp,\perp)$	$+9$
$(\perp,\perp,\perp',\perp')$	$+3$
$(\perp,\perp,\|,\|)$	-12
$(\|,\|,\|,\|)$	$+24$

Table 1: Weight factors of different polarizations

Looking at the coefficient of the two-particle diagram, we can write down the oscillator frequencies due to the internal degrees of freedom:

$$\Omega_k^2 = \frac{e^2}{m\lambda^3}\sum_{\mu=1}^{\infty}\mu^{-3}(1-\cos(k\mu)) \quad . \tag{10}$$

The explicit form of this dispersion relation involves generalized Zeta functions and is not too enlightening. However, we can write down the energy of the π mode, which is easily seen to be the highest energy mode (see Fig. 6):

$$\Omega_\pi^2 = \frac{e^2}{m\lambda^3}\sum_{\mu=1}^{\infty}\mu^{-3}(1-(-1)^\mu) = \frac{7e^2}{8m\lambda^3}\zeta(3) \quad . \tag{11}$$

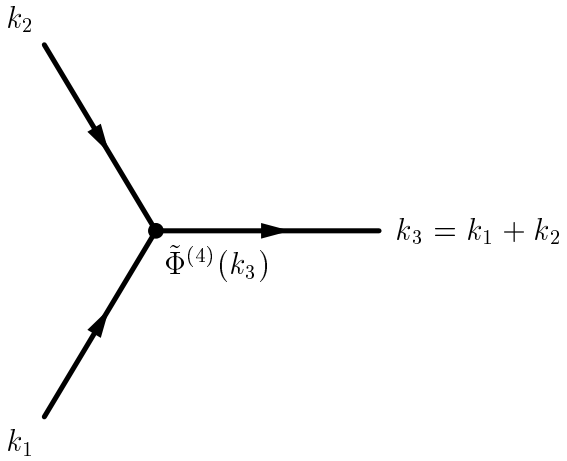

Figure 2: Decay diagram

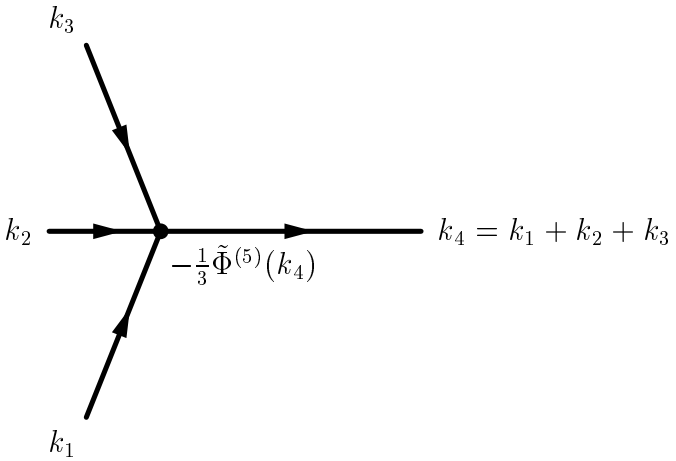

Figure 3: Decay diagram

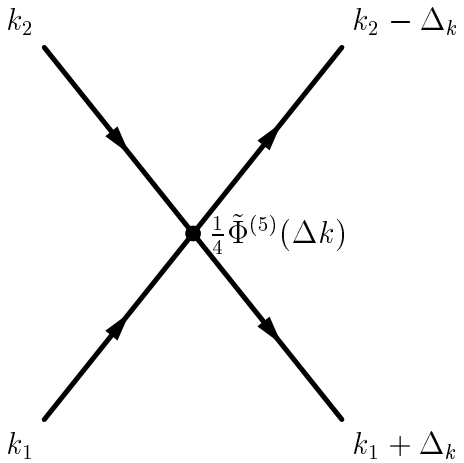

Figure 4: Scattering diagram

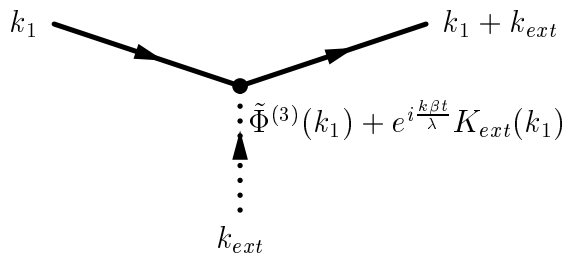

Figure 5: Momentum insertion by the external lattice

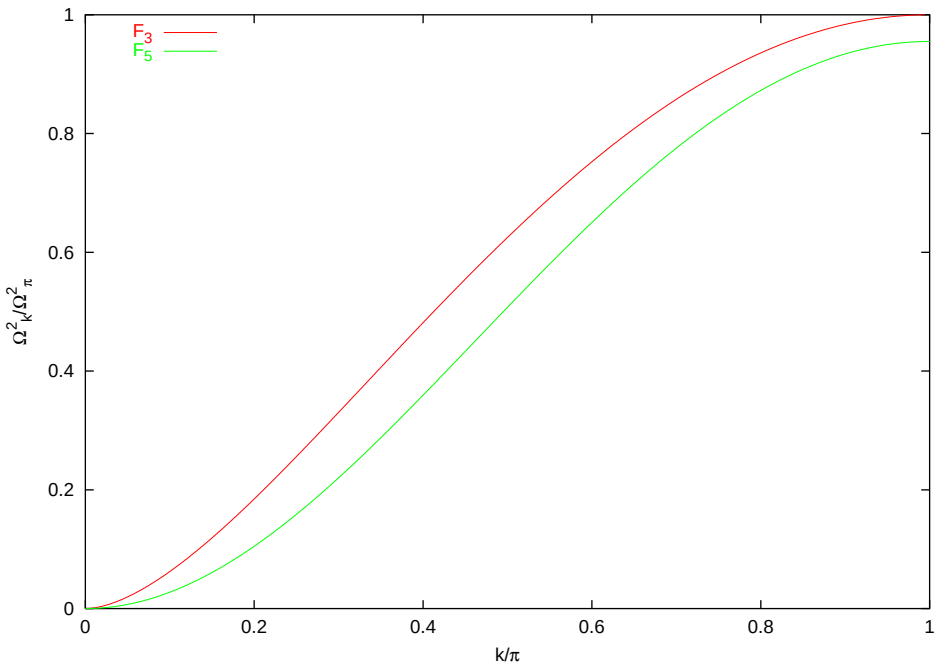

Figure 6: Spectrum and interaction strength of the infinite coulomb chain

One reads off that $\Omega^2_{\perp,k} = -\Omega^2_k$ and $\Omega^2_{\|,k} = 2\Omega^2_k$, that is, in the absence of external forces the transverse motion is unstable. This has to be counteracted by an external focusing field with a field gradient greater than Ω^2_π. In real-world situations, this field will be position-dependent, i.e., our Lagrangian ceases to be diagonal in the Fourier basis. Instead, we have a convolution with the Fourier decomposition of the lattice focusing. Diagrammatically, this means that the two-point functions can get injected momentum from the magnetic lattice (Fig. 5), the $K_{ext}(0)$ contribution just being the average focusing strength.

Also, $\Omega(k)$ determines the validity of our quantization procedure. Instead of quantizing the fermionic particles, we have quantized their collective phononic excitations, which we obtained by expanding the classical Lagrangian around the classical equilibrium (cf. [2, 3]). Obviously, the particles have to be localized even in the quantum-mechanical domain for this procedure to be valid.

We have seen the particles behave oscillator-like to lowest nontrivial order. Thus, we can estimate their wave functions' longitudinal extension; the ground state of an harmonic oscillator has

$$\sigma^2 = \frac{1}{m\omega} \tag{12}$$

as its extension. For a point-particle expansion to be valid, we have to require

$$\frac{1}{m\Omega_\pi} \ll \lambda^2 \quad , \tag{13}$$

or, with (11)

$$\frac{1}{e^2 m} = r_{Bohr} \ll \frac{8\lambda}{7\zeta(3)} \approx \lambda \quad , \tag{14}$$

(which is the one-dimensional version of the $r_s \gg 1$ condition known from Wigner crystal theory[4, 5]), so the quantization procedure is valid for low particle densities. As the condition is expressed in the rest frame (so $\lambda = \gamma\lambda_{Lab}$), the condition can easily be fulfilled in realistic setups.

3 Acknowledgments

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