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Thermodynamic Quantum Time-Space Crystal: Spontaneous Breaking of Time-Translation Invariance

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Konstantin. B. Efetov

[1]*Ruhr University Bochum, Faculty of Physics and Astronomy, Bochum, 44780, Germany*
[2]*National University of Science and Technology MISiS, Moscow, 119049, Russia*
[3]*International Institute of Physics, UFRN, 59078-400 Natal, Brazil*
E-mail: Konstantin.B.Efetov@ruhr-uni-bochum.de

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Abstract. We suggest and study a model of interacting fermions demonstrating existence of a thermodynamically stable quantum time-space crystal. An order parameter characterizing this state is periodic in both real and imaginary times. The imaginary-time dependence is used for calculation of the free energy of the system, while the real-time dependence leads to non-decaying oscillation of correlation functions of two- and more times. Single-time physical quantities do not depend on time. The oscillation of correlation functions at different time scan in principle be observed in scattering experiments.

Keywords: thermodynamic quantum time crystal, time-dependent order parameter, instanton-anti-instanton lattice.

1. Introduction

Many materials have stable crystalline structures that are periodic in space but not in time. Are thermodynamic states with a periodic time dependence of physical quantities forbidden by fundamental laws of nature? This question was raised by Wilczek [1] who proposed a concept of quantum time crystals using a model that possessed a state with a current oscillating in time. The publication has attracted a great attention but a more careful consideration of the model [2] has led to the conclusion that this was not an equilibrium state. More general arguments against thermodynamically stable macroscopic quantum time crystals have been proposed later [3]. As a result, a consensus has been achieved that thermodynamically macroscopic quantum time crystals could not exist although slowly decaying oscillations in systems out of equilibrium were not forbidden. At present, the term 'Quantum Time Crystal' is used for non-equilibrium systems.

Here, considering a model of interacting fermions it is demonstrated, that the system can undergo a phase transition into a state with an order parameter oscillating in both imaginary τ and real t time. The period of the oscillations in the imaginary time τ equals $(mT)^{-1}$, where T is temperature and m is an integer, as required by boundary conditions for bosonic fields. The periodic real time oscillations can be observed in scattering cross sections or other quantities containing correlation functions of two or more order parameters but there are no oscillations in single time quantities. Thermodynamic quantum time crystal (TQTC) proposed here can exist in an arbitrarily large volume and is a novel type of ordered states of matter. A more detailed discussion can be found in Refs. [4,5].

2. Model and calculation of the free energy

Although being rather general, the model considered here has been originally introduced in a form of a spin-fermion model with overlapping hot spots (SFMOHS) for description of under doped superconducting cup rates [6,7,8]. In the language of SFMOHS, the new TQTC state is characterized by a loop currents order parameter oscillating both in space and time. The phase of the oscillations in time is arbitrary, and one should integrate over the phase at the end of calculations. It is very important that the average of the order parameter equals zero. As a result, the time reversal symmetry is broken but nomagnetic moments appear. These features may correspond to the still mysterious pseudogap state in superconducting cup rates [9,10,11]. Hamiltonian of a simplified model used here can be written in a form

$$\hat{H} = \sum_p c_p^+ \left(\varepsilon_p^+ + \varepsilon_p^- \Sigma_3 \right) c_p + \frac{1}{4V} \left[\tilde{U}_0 \left(\sum_p c_p^+ \Sigma_1 c_p \right)^2 - U_0 \left(\sum_p c_p^+ \Sigma_2 c_p \right)^2 \right] \tag{1}$$

The Hamiltonian $\hat{H}$, Eq. (1),describes interacting fermions of two bands *1* and *2*, while p stands for both the momentum **p**and spin of the fermions. The energies $\varepsilon_p^{\pm} = \left(\varepsilon_1(p) \pm \varepsilon_2(p) \right)/2$ are determined by the energy spectra $\varepsilon_{1,2}(p)$ of the bands *1* and *2*, the interaction constants U_0 and $\tilde{U}_0$ are positive, whereas V is the volume of the system. Two-component vectors $c_p = \left\{ c_p^1, c_p^2 \right\}$ contain as components annihilation operators of the fermions in the bands *1* and *2*. The matrices $\Sigma_1, \Sigma_2, \Sigma_3$ are Pauli matrices in the space of the band numbers *1* and *2*.

Hamiltonian $\hat{H}$ resembles the Bardeen-Cooper-Schrieffer (BCS) [12] Hamiltonian for Cooper pairs but contains a long-range interaction of electron-hole pairs instead of the interaction of electron-electron pairs. Usually, such a form of the interaction makes BCS-like mean field theories exact. However, the Hamiltonian $\hat{H}$ contains both the inter-band attraction (term with Σ_2) and repulsion (term with Σ_1). Neglecting the repulsion leads in the language of SFMOHS to emergence of static loop currents oscillating in space with the double period of the lattice [8]. This corresponds to a hypothetical d-density wave (DDW) state [13]. It is the repulsion term with Σ_1 that can eventually make the thermodynamic states yielding correlation functions oscillating in time energetically more favorable than conventional ones.

Calculation of the partition function Z can be performed using the imaginary-time formalism with τ in the interval $(0,1/T)$ [14]. Writing the partition function Z as

$$Z = Tr \exp\left[-\hat{H}/T \right] \tag{2}$$

we decouple the interaction terms in the Hamiltonian $\hat{H}$ using a Hubbard-Stratonovich transformation. This allows one to compute the trace Tr over fermion operators and represent the free energy F in a form of a functional integral over boson fields $b(\tau)$ and $b_1(\tau)$ as

$$F = -T \ln \int \exp\left[-\mathcal{F}\left[b, b_1\right]/T\right] DbDb_1 \tag{3}$$

where the free energy functional $\mathcal{F}\left[b, b_1\right]$ equals

$$\frac{\mathcal{F}}{T} = \int_0^{1/T} \left[-2\sum_{\mathbf{p}} tr\left[\ln h(\tau, \mathbf{p})\right]_{\tau,\tau} + V\left(\frac{b^2(\tau)}{U_0} + \frac{b_1^2(\tau)}{\tilde{U}_0}\right)\right] d\tau, \tag{4}$$

and

$$h(\tau, \mathbf{p}) = \partial_\tau + \varepsilon^+(\mathbf{p}) + \varepsilon^-(\mathbf{p})\Sigma_3 - b(\tau)\Sigma_2 - ib_1(\tau)\Sigma_1 \tag{5}$$

The boson fields $b(\tau)$ and $b_1(\tau)$ obey bosonic boundary conditions

$$b(\tau) = b(\tau + 1/T), \quad b_1(\tau) = b_1(\tau + 1/T). \tag{6}$$

In the limit $V \to \infty$, the form of the interaction between the electron-hole pairs in Eq.(1) allows one to calculate the integral over the fields $b(\tau)$ and $b_1(\tau)$ using the saddle point-method. Both the terms in the functional $\mathcal{F}\left[b, b_1\right]$ are proportional to the volume V, and one can obtain the physical free energy F, Eq.(2), simply minimizing $\mathcal{F}\left[b, b_1\right]$ with respect to $b(\tau)$ and $b_1(\tau)$. Although the minimum at

$$b(\tau) = \gamma, \quad b_1(\tau) = 0 \tag{7}$$

found previously [8] is a minimum of $\mathcal{F}\left[b, b_1\right]$, there is a region of parameters where the absolute minimum is reached at $\tau-$dependent functions $b(\tau)$ and $b_1(\tau)$.

Non-trivial extrema of $\mathcal{F}\left[b, b_1\right]$ exist even at $b_1(\tau) = 0$. Varying the functional $\mathcal{F}\left[b, 0\right]$ one comes to the following equation

$$b(\tau) = -U_0 \mathrm{tr} \int \Sigma_2 \left[h_0^{-1}(\tau, \mathbf{p})\right]_{\tau,\tau} \frac{d\mathbf{p}}{(2\pi)^2} \tag{8}$$

In Eq. (8), $h_0(\tau, \mathbf{p})$ is obtained from $h(\tau, \mathbf{p})$, Eq. (5), by putting $b_1(\tau) = 0$.

Equation (7) describes the static solutions of Eq. (8). Although Eq. (8) is generally quite non-trivial due to a possible dependence of $b(\tau)$ on τ, solutions $b_0(\tau)$ can be written exactly in terms of a Jacobi double-periodic elliptic function $sn(x|k)$,

$$b_0(\tau) = k\gamma \mathrm{sn}\left(\gamma(\tau - \tau_0)|k\right), \tag{9}$$

where the parameter k, $0 < k < 1$, is the modulus, γ is an energy, and τ_0 is an arbitrary shift of the imaginary time in the interval $0 < \tau_0 < 1/T$. In the limit $k \to 1$, the function $b_0(\tau)$ has an

asymptotic behavior $sn(x|k) \to \pm \tanh(x)$, while in the limit $k \ll 1$ one obtains $sn(x|k) \to \sin x$.

The period of the oscillations for an arbitrary k equals $4K(k)/\gamma$, where $K(k)$ is the elliptic integral of the first kind, and therefore the condition

$$\gamma = 4K(k)mT \tag{10}$$

with integer *m*, is satisfied to fulfill equations (6). In the most interesting limit of small $1-k$, the period $4K(k)/\gamma$ of $b_0(\tau)$ grows logarithmically as $(1/2)ln\left((8/(1-k))\right)$, and the solution $b_0(\tau)$ consists of *2m* well separated alternating instantons and anti-instantons with the shape $\pm\gamma \tanh(\gamma\tau)$. It is important that the integral over the period of the oscillations in Eq. (9) equals zero. Integration over the position τ_0 of the instant on gives zero as well

$$\overline{b_0(\tau)} = 0. \tag{11}$$

The existence of the non-trivial local minima of $\mathcal{F}[b,0]$ at $b_0(\tau)$ has been established previously [15,16] starting from a different model. Generally, there can be many solutions corresponding to different minima of $\mathcal{F}[b,0]$ depending on the number m of instanton-antiinstanton pairs (IAP). However, the lowest value of the functional $\mathcal{F}[b,0]$ is reached at $m=0$ corresponding to the static order [4,5,17].

Although putting $b_1(\tau)=0$ leads to the correct static solution (7) for $b(\tau)$, the first order of expansion in $b_1(\tau)$ of logarithm in Eq. (4) yields an interaction $\mathcal{F}[b,b_1]$ between the fields $b_0(\tau)$ and $b_1(\tau)$

$$\frac{\mathcal{F}_1[b_0,b_1]}{VT} = -2J\int_0^{1/T} \frac{\partial b_0(\tau)}{\partial \tau} b_1(\tau)\, d\tau \tag{12}$$

where J is a constant. Eq. (12) shows that the field $b_1(\tau)$ linearly couples to the time derivative of $b_0(\tau)$, Eq. (9). The functional $\mathcal{F}_1[b_0,b_1]$ is real for $\tilde{U}_0 > 0$. It is this interaction that can destabilize the minimum at static *b*, Eq. (7). Writing

$$\mathcal{F}[b,b_1] \approx \mathcal{F}[b_0,0] + \mathcal{F}_1[b_0,b_1], \tag{13}$$

substituting $\mathcal{F}[b,b_1]$, Eq. (13), into Eq. (4), and calculating the Gaussian integral over $b_1(\tau)$ one obtains an effective instanton-instanton attraction described by the negative contribution

$$\mathcal{F}_{II}[b_0,0] = -\tilde{U}_0 J^2 \int_0^{1/T} \dot{b}_0^2(\tau)\, d\tau \tag{14}$$

that should be added to $\mathcal{F}[b_0,0]$. The negative sign in Eq. (14) favors formation of $\tau-$dependent

structures.

Calculation of the free energy simplifies in the limit of low temperatures T, when one expects large number of IAP in the system, and of small $1-k$ corresponding to a large period of the IAP lattice. In this limit, the difference ΔF between the total free energy F and the free energy of the system with the static order parameter is proportional to $2m$. The case $\Delta F/(TV)>0$ corresponds to the state with the static order, while in the region of parameters where $\Delta F/(TV)<0$ one can expect a chain of alternating instantons and anti-instantons.

In the limit $k\to 1$, one can write for $\Delta F/V(2mT)$ using Eqs. (4), (13), (14)

$$\Delta F = F_{\text{inst}} + F_{\text{II}} \tag{15}$$

In Eq. (15), F_{inst} is the free energy of the instantons calculated at $b_1(\tau)=0$, while the contribution F_{II} originates from the term $\mathcal{F}_{\text{II}}[b_0,0]$, Eq. (14), of the free energy functional. A detailed analysis presented in Refs. [4,5] leads to the conclusion that a region of parameters of the model, Eq. (1), exists where $\Delta F<0$. This means that the state with the static order parameter, Eq. (7), is unstable in this region. As a result, one can expect there a structure with an imaginary-time-dependent order parameter.

3. Correlation functions of real time. Operator order parameter

The periodic structure described by the Jacobi elliptic function $b_0(\tau)$, Eq.(9), is actually double periodic in the complex plane of τ and, hence, is periodic in real time *t*. Remarkably, $b_0(it)$ still satisfies Eq. (8) after the rotation $\tau\to it$. Formally, real-time correlation function can be calculated using the functional integrals formalism. One should simply replace $\tau\to it$ and integrate over t from $-\infty$ to ∞ in the expression for the action. Repeating the steps made within the imaginary-time representation one should integrate over functions $B(t)$, $B_1(t)$, instead of $b(\tau)$, $b_1(\tau)$. Then, minimizing the action one comes to real-time order parameters $B(t)$ and $B_1(t)$ periodic in time and related to $b(\tau)$ and $b_1(\tau)$ as

$$iB(t)=b_0(it),\quad B_1(t)=b_1(it) \tag{16}$$

Again, if $B(t)$ and $B_1(t)$ provide the extremum of the action, so do $B(t-t_0)$ and $B_1(t-t_0)$ for an arbitrary shift t_0. The Jacobi elliptic function $sn(iu|k)$ of an imaginary argument iu is related to an elliptic function $sc(u|k)$ with the period $2K(k)$ as

$$\mathrm{sn}(iu|k)=i\mathrm{sc}(u|k'),\ k^2+k'^2=1, \tag{17}$$

and one obtains for $B(t)$

$$B(t)=\gamma k\mathrm{sc}\left(\gamma(t-t_0)|k'\right), \tag{18}$$

where t_0 is an arbitrary shift of time.

As the minimum of the action is degenerate, one should integrate over t_0 when using the saddle point approximation. As a result, the averaged order parameter vanishes

$$\overline{B(t)} = 0. \tag{19}$$

In Eq. (19) the bar stands for averaging over the period of $B(t)$.
In order to calculate a 2-times correlation function

$$N(t) = \overline{B(t)B(0)} \tag{20}$$

one can use a Fourier series for the function $sc(u|k)$ [18]. Integration over t_0 gives in the limit $1-k \ll 1$ [4,5]

$$N(t) \approx 2\gamma^2 \sum_{n=1}^{\infty} f_n^2 cos(2\gamma nt), \quad f_n = [1-(1/2)(((1-k)/8))^{2n}]. \tag{21}$$

Function $N(t)$ shows an oscillating behavior with the frequencies $2\gamma n$. The energy 2γ is the energy of the breaking of electron-hole pairs, and one can interpret the form of $N(t)$ as oscillations between the static order and normal state. The contribution of high harmonics n does not decay with n but apparently this is a consequence of the approximations used.

The order parameter $B(t-t_0)$ appears when calculating fermionic quantum averages corresponding to the loop currents, and therefore Eq. (19) shows that physical currents are equal to zero at any time t. Non-vanishing oscillations of two-times correlation function $N(t)$ allow us to classify the physical state found here as thermodynamic quantum time-space crystal.

The correlation function $N(t)$, Eq. (21), has been obtained after integration over the position t_0. Remarkably, the same results for correlation functions can be obtained considering a Hamiltonian $\hat{H}_{TC}$ of a harmonic oscillator

$$\hat{H}_{TC} = 2\gamma(a^+a + 1/2), \tag{22}$$

where a^+ and a are bosonic creation and annihilation operators. Using the Hamiltonian $\hat{H}_{TC}$ one can write the correlation function $N(t_1-t_2)$ in the form

$$N(t) = \gamma^2(<0|A(t)A^+(0)|0> + <0|A(0)A^+(t)|0>, \tag{23}$$

where

$$A^+(t) = e^{i\hat{H}_{TC}t}A^+e^{-i\hat{H}_{TC}t}, \quad A^+ = \sum_{n=1}^{\infty} \frac{f_n(a^+)^n}{\sqrt{n!}}.$$

and $|0>$ stands for the wave function of the ground state of the Hamiltonian $\hat{H}_{TC}$, Eq.(22). At

the same time, quantum averages of the operators A and A^+ vanish

$$\langle 0|A(t)|0\rangle = \langle 0|A^+(t)|0\rangle = 0.$$

The operator order parameter A extends the variety of conventional order parameters like scalars, vectors, matrices used in theoretical physics. The non-decaying time oscillations is an important property for designing qubits.

Possibility of an experimental observation depends on systems described by the Hamiltonian (1). For cup rates, inelastic polarized neutron spectroscopy can be a proper tool for observations. The Fourier transform $N(\omega)$ of the function $N(t)$ can be compared with the one for the hypothetical time-independent DDW result $2\pi\gamma^2\delta(\omega)$. As a result, one can write at low temperatures the ratio of the responses at (π,π) for these two states as

$$\chi(\omega,\mathbf{q}) = \chi_0 \sum_{n=1}^{\infty} f_n \delta(\omega - 2n\gamma)\delta(\mathbf{q}-\mathbf{Q}_{AF}). \tag{24}$$

In Eq. (24) the static susceptibility χ_0 is proportional to the response χ_{DDW} of the DDW state, $\chi_{DDW}(\omega) = \chi_0\delta(\omega)$. Equation(24) demonstrates that the elastic scattering cannot lead to any signal expected for DDW. Actually, anisotropic magnetic (π,π) excitations have been observed [19] in $YBa_2Cu_3O_{6.9}$ but more detailed experiments are necessary to clarify their origin**.**

4. Conclusion

The main conclusion of the present study is that the quantum time-space crystals may exist as a thermodynamically stable state in macroscopic systems. The order parameter of TQTC is periodic in both real and imaginary times, but its average over the phase of the oscillations vanishes. The non-decaying oscillations can be seen, e.g., in two- or more times correlation functions. This leads to a natural generalization of the notion of the space long-range order to the time-space one. Two-times correlation functions determine cross-section in inelastic scattering experiments. The frequency of the oscillations remains finite in the limit of infinite volume, $V \to \infty$. One can expect various experimental consequences and, in particular, one can suppose that the time crystal may be a good candidate for the pseudogap state in superconducting cuprates.

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