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Configuration entropy for N-Dirac fermions with dissipation and external field: An effective-mass phase transition

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Abstract – Dirac fermions in solid state are defined through a homogeneous dispersion relation of degree one. Consequently, the group velocity, having a superior bound, becomes invariant under spatial scaling. This fact allows considering the dynamics of a family or set of Dirac fermions at different spatial dimensions and subjected to an external field and dissipation. From the degeneration of the stationary states, the non-Hermitian dynamics allows defining the configuration entropy. With the applied external field being the control parameter, an inflection point becomes associated with entropy. Consequently, an effective-mass phase transition is conjectured including the usual Dirac fermions in a graphene sheet. The critical field and the critical angle are analytically calculated.

Introduction. – Over the last decade, it became clear that the hermiticity of operators is not a requirement for real spectra [1–10]. And although the subject has proliferated during these years, it has been known for far longer. For instance, Galitski *et al.* [11] described some simple cases and mentioned the non-orthogonality of eigenfunctions. This matter is also related to *PT*-symmetry in the sense that non-Hermitian systems exhibiting *PT*-symmetry are good candidates for a real spectrum in some regions —a topic also applied to Rabi oscillations [12]. Additionally, dissipative Caldirola-Kanai theory [13–20] is related to a time-dependent quantum Hamiltonian, where formally the Planck constant diminishes exponentially with time in the full (time-dependent) Schrödinger equation. It is connected to dissipation and comparable to the approach developed in this article (eqs. (3), (4)).

The present work is devoted to generic Dirac fermion dynamics with dissipation. For frequency ω, in spatial dimension D, consider the homogeneous dispersion relation of degree one

$$\omega = v_f \left(|\vec{k}_x|^n + |\vec{k}_T|^n \right)^{1/n}, \qquad (1)$$

where n is a real number and v_f becomes the so-called Fermi velocity[1]. The wave vector is partitioned as

$$\vec{k} = \vec{k}_x + \vec{k}_T \qquad (2)$$

and direction x is privileged in advance since a fixed external field $F\hat{x}$ will be considered. For convenience, the angle between the two vectors is defines as $\tan(\theta) = k_T/k_x$.

Equation (1) is not a prerequisite for more broad homogeneous dispersion relations of degree one. Indeed, any function $\omega(\vec{k})$ of degree one satisfied a relation like $\omega = v_f k_x$ (Dirac fermions) in direction x when the wave vector transversal component is zero ($\vec{k}_T = 0$). I use eq. (1) because of its simplicity to consider dissipation plus an external field, which is the focus of this work.

A physical example of dispersion equation (1) is graphene [21–27] where $n = 2$ and which has spatial dimension $D = 2$. Similarly, the case $n = 1$ with $D = 1$ has been strongly employed such as carbon-nanotubes. More all-purpose materials similar to graphene, and including gaps, have also been considered in solid state [28].

Figure 1 shows different Dirac cones for values $n = -2$; $n = 2$ and $n = 6$. The figure in the middle corresponds to the usual graphene sheet.

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[1]Under the non-canonic transformation $|\vec{k}_x| = x^{2/n}$; $|\vec{k}_T| = y^{2/n}$ and $E^2 = \omega^n$, eq. (1) is transformed into $E = v_f\sqrt{x^2 + y^2}$ corresponding to usual Dirac fermions structure.
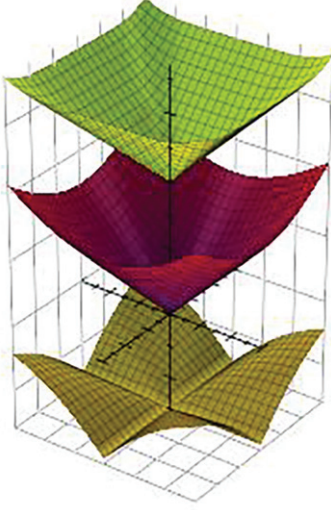

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Fig. 1: Three Dirac cones at spatial dimension $D = 2$ related to frequencies spectrum eq. (1) and corresponding to parameter values $n = -2$; $n = 2$ and $n = 6$ (from bottom to top, respectively). Figures are shifted from $(0, 0)$ to improve the visual aspect. Graphene corresponds to the middle figure (*i.e.*, $D = 2$ and $n = 2$).

Furthermore, in the field direction, assume the particle is subjected to dissipation $-\gamma v_g$ related to group velocity v_g with a non-negative dissipation coefficient $\gamma \geq 0$. Formally, the system of equations [29–32] corresponding to this non-reversible motion becomes

$$v_g(\vec{k}) = \frac{\partial \omega}{\partial k_x}, \tag{3}$$

$$\hbar \frac{dk_x}{dt} = -\gamma v_g(\vec{k}) + F \tag{4}$$

with the main interest in the stationary solution. The group velocity, in direction x, is given explicitly by

$$v_g{}^2 = v_f{}^2 \left(1 + \frac{|\vec{k}_T|^n}{|\vec{k}_x|^n}\right)^{\frac{2}{n}(1-n)} \tag{5}$$

which is a homogeneous function of degree zero as expected and, consequently, invariant under spatial scaling and requiring $D \geq 2$. Importantly, eq. (5) depends only on the polar angle in dimension three. Further, the condition for which the Fermi velocity is an upper bound provides a constraint on parameter n:

$$|v_g| \leq v_f \iff (n < 0 \text{ or } n \geq 1). \tag{6}$$

This work emphasizes a possible phase transition correlated to eqs. (1)–(5). This transition is not (apparently) related to aggregation of matter and is studied in the out-of-equilibrium context [32–35]. Therefore, the concept of configuration entropy will be used as a practical tool and the transition will be associated with an existing entropy inflection point. The control parameter is the external field F and there is a definite critical field related to the inflection point.

Configuration entropy. – In principle, I shall consider boundary conditions on all transverse spatial dimensions (*i.e.*, on $\vec{k}_T$). In the field direction, from eq. (4), the dissipative stationary states are given by the simple condition

$$v_g(\vec{k}) = F/\gamma \tag{7}$$

which defines, using eq. (5) in k's space, a hyper-sphere of radius R ($n \neq 1$):

$$R = \left(\left(\frac{F}{\gamma v_f}\right)^{\frac{n}{1-n}} - 1\right)^{1/n}. \tag{8}$$

Note that the surface of a hyper-sphere in spatial dimension α is given by the expression $\left(2\pi^{\alpha/2}/\Gamma(\alpha/2)\right) R^{\alpha-1}$ where Γ denotes the gamma function. Importantly, in the case of eq. (5) α corresponds to $D - 1$.

Degeneration N of the system is assumed proportional to the hyper-sphere surface [36–40] and becomes

$$N = A \left(\left(\frac{F}{\gamma v_f}\right)^{\frac{n}{1-n}} - 1\right)^{(D-2)/n}, \tag{9}$$

where $A = A(D)$ is related to the Gamma function and does not depend on n. This term generates a residual entropy, S_o, which is irrelevant for the following developments, *i.e.*, the effective entropy corresponds to the difference ΔS. Remark, degeneration N depends on the spatial dimension where $D \geq 2$ is assumed.

The configuration entropy S is given by $S = K \times \ln(N)$ and its dependence on an external field F becomes

$$\Delta S = K \left(\frac{D-2}{n}\right) \times \ln \left(\left(\frac{F}{\gamma v_f}\right)^{\frac{n}{1-n}} - 1\right). \tag{10}$$

Figure 2(a) shows entropy equation (10) as a function of the (quadratic) external field F for different positive values of n with $D > 2$ (explicitly $n = 1.5; 2; 3; 6$). Remark, as a function of the angle, $\Delta S \propto \ln(\tan^n(\theta))$.

Entropy diminishes when the external field rises, *i.e.*, an ordered situation becomes expected when $F \to \gamma v_f$. This is analogous to a thermodynamic system reaching an energy upper bound and related to negative temperatures [37,38]. Indeed, the first derivative of entropy ΔS is negative (fig. 2(b)). From the point of view of dissipation, and reasonably comprehensively, entropy diminishes when dissipation also diminishes (fig. 2(a)).

Still related to fig. 2, there is an inflection point for the entropy (fig. 2(c)). It will be considered in detail in the next section, but such points are connected in thermodynamic to phase transitions [36–40].

In brief, and this is the core of this work, in the system described for the frequency spectrum eq. (1) and dissipation equations (3), (4), a kind of transition could be anticipated at some critical external field (control parameter).
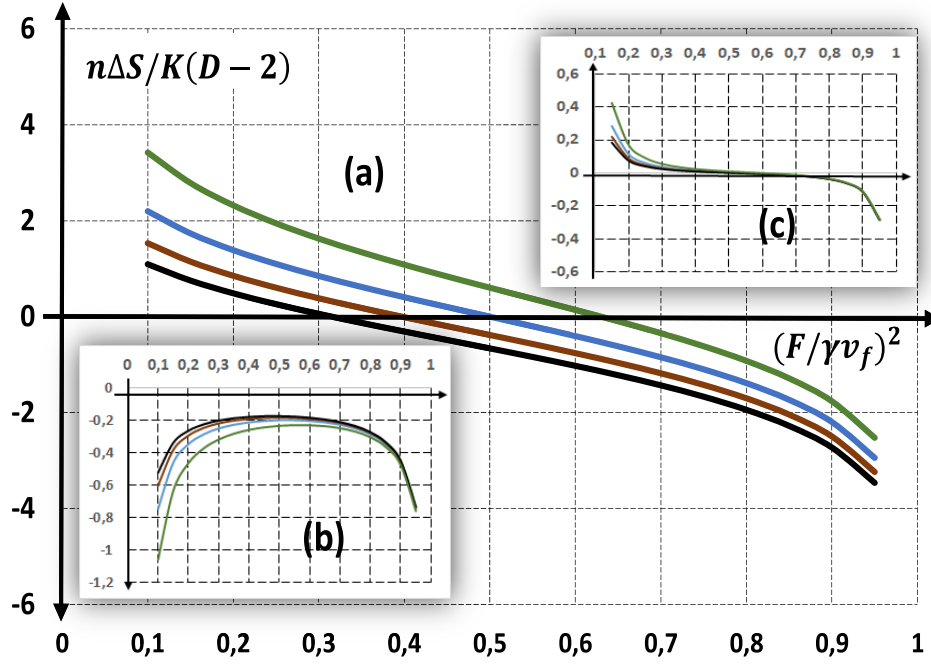
Fig. 2: (a) Main graph, configuration entropy ΔS for $n = 1.5; 2; 3;$ and 6 from top to bottom, respectively, and as a function of the (quadratic) dimensionless external field $F/\gamma v_f$ for spatial dimension $D > 2$ (remark, if γ reduces also ΔS). (b) The inferior inner figure shows the first derivative of the entropy, as a function of F^2, being negative and equivalent to the concept of negative temperature in thermodynamics. (c) The second derivative of entropy is also shown as a function of F^2. For every curve in (a), there is an inflection point (a zero) at some critical field F_c (eq. (11)). An entropy inflection point can be correlated with a phase transition. The superior constraint $|F/\gamma v_f| \leq 1$ for the field comes from eqs. (6), (7).

Entropy inflection point: Critical field and polar angle. – For clarity, I make derivatives with respect to the quadratic external field (*i.e.*, d/dF^2) since the quadratic-group velocity and F^2 are expected to be proportional to kinetic energy.

The second derivative of entropy ΔS (eq. (10)) has a zero at the critical point F_c. This critical field is analytically given by

$$\left(\frac{F_c}{\gamma v_f}\right)^2 = \left(\frac{3n - 2}{2(n - 1)}\right)^{\frac{2(1-n)}{n}}. \qquad (11)$$

When $n = 2$ then, $F_c/\gamma v_f = 1/\sqrt{2}$ as previously studied [41]. In general terms, the critical point F_c does not depend on the spatial dimension as expected from a mean-field theory. Figure 3 shows the critical field eq. (11) as a function of n. Formally, in the limit $n \to \pm\infty$, then $F_c/\gamma v_f = 2/3$.

From the expression for group velocity in eq. (3), which is connected to the critical field by eq. (7), the transition is likewise related to the angle θ between $\vec{k}_T$ and $\vec{k}_x$. Namely, the critical angle θ_c is given by the expression

$$1 + |\tan(\theta_c)|^n = \frac{3n - 2}{2(n - 1)}. \qquad (12)$$

The inner graph in fig. 3 shows this critical angle as a function of parameter n ($n < 0$ and $n \geq 1$). For $n = 2$, *i.e.*, graphene, the angle is ~ 0.78 ($= \pi/4$).
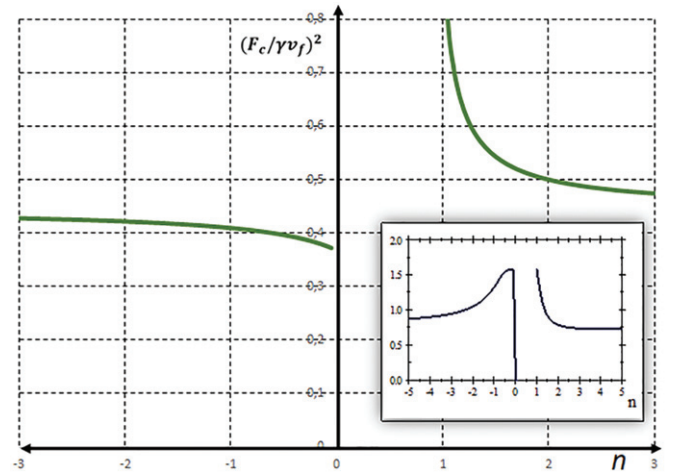

Fig. 3: Dimensionless critical field (green) as a function of parameter n for Dirac fermions described by eq. (1) and dissipation. The inner figure is the (positive) critical angle θ_c, eq. (12), between $\vec{k}_T$ and $\vec{k}_x$ also as a function of parameter n. This angle can be related to the effective mass ratio between both directions (appendix).

The dimensionless critical field eq. (11) is a function of parameter n, also valid for a critical dissipation coefficient γ_c. Namely, eq. (11) likewise is valid for $F/\gamma_c v_f$ for a fixed arbitrary external field. From this point of

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view, it is natural that entropy diminished when the dissipation coefficient also decreased (fig. 2). This approach is semi-classical [29–32]. Nevertheless, Chen [42] proposed a full quantum dynamics for a fermionic environment.

In brief, an ordered phase is expected when $F > F_c$ (or $\gamma < \gamma_c$). The physics related to this phase transition remains elusive. Nevertheless, the ratio between the transverse and longitudinal effective mass also comprises the angle θ between $\vec{k}_T$ and $\vec{k}_x$. Consequently, the transition is possibly related to the effective mass behavior (see appendix).

As long as the (inverse) mass tensor is related to the angle θ with two eigenvectors (appendix), these vectors can be also related to the order parameter. Namely, the transition seems operative when the system goes from one eigenvector to the other.

Conclusions. – This work has considered a set of homogeneous dispersion relations of degree one, Dirac fermions, indexed by a parameter n (for electrons in graphene $n = 2$).

The usual motion equations of solid-state physics were applied to the set for a given external field and dissipation. Degeneration exists since the dissipative stationary solution is depending only on the ratio between the magnitude of the transverse and longitudinal component of the wave vector. Namely, in dimension three, the solution depends on the polar angle, not the azimuthal one.

Degeneration allowed evaluating the configuration entropy as a function of the dimensionless external field (control parameter) and different values of n in the set (fig. 2). In every case, the entropy had an inflection point at some critical field calculated explicitly (fig. 3). Usually, as occurs in thermodynamics, an entropy inflection point stays related to a phase transition.

In brief, for the non-Hermitian set of Dirac fermions here considered (eqs.(1)–(4)), a phase transition was conjectured in some critical external field (eq. (11)). The physics of this transition is related to the effective mass alteration (appendix). Beyond the small wave vector approximation, the spectrum for graphene is not isotropic [43],

$$\hbar\omega = t \left| e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_1} + e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_2} + e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_3} \right|, \tag{13}$$

with $\boldsymbol{\delta}_1 = \frac{a}{2}(1,\sqrt{3})$; $\boldsymbol{\delta}_2 = \frac{a}{2}(1,-\sqrt{3})$; $\boldsymbol{\delta}_3 = -a(1,0)$. It is an open question to determine, or not, a mass phase transition in this case.

Finally, concerning eq. (1), a more symmetric homogeneous dispersion relation (degree one) is

$$\omega = v_f \left(\sum_{i=1}^{D} \left| \vec{k}_i \right|^n \right)^{1/n} \tag{14}$$

which does not privilege in advance a direction. For $n = 2$ and $D = 2$, both expressions in eqs. (1) and (14) coincide.

With dissipation and an external field, a phase transition is also expected in this highly symmetric case of N-Dirac fermions.

Data availability statement: No new data were created or analysed in this study.

APPENDIX

The dispersion relation eq. (1) becomes associated with the so-called (inverse) effective mass tensor $1/M$ constructed through second derivatives [29–32]. For $n = 2$, and two dimensions (graphene), this tensor is

$$\frac{\hbar}{M} = \frac{v_F}{\left(k_x{}^2 + k_y{}^2\right)^{3/2}} \begin{pmatrix} k_y{}^2 & -k_x k_y \\ -k_x k_y & k_x{}^2 \end{pmatrix},$$

with eigenvalues 0 and $v_F{}^2/\omega$ (formally similar to $E = mc^2$). The ratio between diagonal masses becomes $M_{xx}/M_{yy} = k_y{}^2/k_x{}^2 \; (= \tan^2(\theta))$ and is related to the critical angle eq. (12). It suggests a transition related to the effective mass.

In polar coordinates, $k_x = k\cos(\theta)$ and $k_y = k\sin(\theta)$, the tensor is

$$\frac{k\hbar}{v_F M} = \begin{pmatrix} \sin^2(\theta) & -\sin(\theta)\cos(\theta) \\ -\sin(\theta)\cos(\theta) & \cos^2(\theta) \end{pmatrix}$$

being the matrix a projector with eigenvalues 0 and 1 and eigenvectors $(\cos(\theta),\sin(\theta))$ and $(-\sin(\theta),\cos(\theta))$, respectively. Formally, for a given force $\vec{F} = (F,0)$, the acceleration $\vec{a} = \frac{1}{M}\vec{F}$ becomes

$$\vec{a} = \frac{v_F}{\hbar k} F \begin{pmatrix} \sin^2(\theta) \\ -\frac{1}{2}\sin(2\theta) \end{pmatrix}$$

and a_y is extreme at $\theta = \pm\pi/4$.

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