

Origin of conical dispersion relations

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A mechanism that produces conical dispersion relations is presented. A Kronig Penney one dimensional array with two different strengths delta function potentials gives rise to both the gap closure and the dispersion relation observed in graphene and other materials. The Schrödinger eigenvalue problem is locally invariant under the infinite dimensional Virasoro algebra near conical dispersion points in reciprocal space, thus suggesting a possible relation to string theory.

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1. Introduction

Dirac massless fermions dispersion relations have been observed in graphene and other materials. In spite of the extensive literature published on the subject, see for instance [1–5] and references therein, there does not seem to exist a cogent understanding of the essence of this remarkable feature.

Materials in which this dispersion relation arises have different structures and their symmetry groups do not match but share a common feature: They all have more than one lattice point per unit cell. Although this feature seems to be necessary it does not appear to be sufficient.

Here we present a mechanism that produces conical dispersion relations. A modified Dirac-Kronig-Penney one dimensional array with two different strengths delta function potentials gives rise to both the gap closure and the dispersion relation observed in graphene and other materials. The condition that the (first neighbors) structure factor vanishes defines the position of the conical dispersion points in reciprocal space and produces both the gap closure and conical dispersion relations.

The Schrödinger eigenvalue problem is locally invariant under the infinite dimensional Virasoro algebra near conical dispersion points in reciprocal space, thus suggesting a relation to string theory.

2. The Model

Consider the usual Dirac-Kronig-Penney problem (use the notation defined in [7]) described by the potential $V_{DKP}(x)$

$$V_{DKP}(x) = U \sum_{n=-\infty}^{n=+\infty} \delta(x - na). \quad (1)$$

The associated Schrödinger equation is

$$-\frac{\hbar^2}{2m} \psi'' + V_{DKP}(x) \psi = E \psi. \quad (2)$$

In this case, as it is well known, the translational symmetry transformation is

$$x' = x + a \quad (3)$$

The eigenvalue problem implies the following dispersion relation

$$\cos ka - \cos qa - \frac{m U a \sin qa}{\hbar^2 qa} = 0, \quad (4)$$

where

$$q \equiv \frac{\sqrt{2mE}}{\hbar}. \quad (5)$$

It is convenient to define the functions $f_1(k, a)$ and $g_1(q, a, U)$ by

$$f_1(k, a) \equiv \cos ka, \quad (6)$$

and

$$g_1(q, a, U) \equiv \cos qa + \frac{m U a \sin qa}{\hbar^2 qa}, \quad (7)$$

respectively, so that the dispersion relation (4) may be equivalently written as

$$f_1(k, a) = g_1(q, a, U). \quad (8)$$

It is very well known that (8) gives rise to energy gaps due to the fact that while $-1 \leq f_1(k, a) \leq +1$, there are local minima of $g_1(q, a, U)$ which are inferior to -1 and local maxima that exceed $+1$. We could therefore say that there are two kind of energy gaps, “maxima gaps” and “minima gaps”.

Consider now the modified potential $V_M(x)$, defined by

$$V_M(x) = \sum_{n=-\infty}^{n=+\infty} (U \delta(x - 2na) + V \delta(x - (2n+1)a)). \quad (9)$$

The associated Schrödinger equation is

$$-\frac{\hbar^2}{2m} \psi'' + V_M(x) \psi = E \psi. \quad (10)$$

In this case, clearly, the translational symmetry transformation is

$$x' = x + 2a \tag{11}$$

The dispersion relation, in this case, turns out to be

$$\begin{aligned} \cos 2ka - \cos 2qa - \frac{m U a \sin 2qa}{\hbar^2 qa} - \frac{m V a \sin 2qa}{\hbar^2 qa} \\ - \frac{2m^2 UV a^2 (\sin qa)^2}{\hbar^4 q^2 a^2} = 0 \end{aligned} \tag{12}$$

Introduce now the functions $f_2(k, a)$ and $g_2(q, a, U, V)$ defined by

$$f_2(k, a) \equiv \cos 2ka, \tag{13}$$

and

$$\begin{aligned} g_2(q, a, U, V) \equiv \cos 2qa + \frac{m U a \sin 2qa}{\hbar^2 qa} \\ + \frac{m V a \sin 2qa}{\hbar^2 qa} + \frac{2m^2 UV a^2 (\sin qa)^2}{\hbar^4 q^2 a^2} \end{aligned} \tag{14}$$

respectively, so that the dispersion relation (12) may be equivalently written as

$$f_2(k, a) = g_2(q, a, U, V). \tag{15}$$

It is interesting to note that

$$f_2(k, a) = 2[f_1(k, a)]^2 - 1, \tag{16}$$

while

$$g_2(q, a, U, V) = 2g_1(q, a, U)g_1(q, a, V) - 1. \tag{17}$$

3. The V=U case

We will study the dispersion relation (15), in general, but it is convenient to start the analysis by considering the case $V = U$ (which is inadequate from a physical standpoint because in that case the symmetry translation vector is given by (3) instead of (11)).

In this case,

$$g_2(q, a, U, U) = 2[g_1(q, a, U)]^2 - 1. \tag{18}$$

Therefore, the dispersion relation (8) implies that

$$f_2(k, a) = g_2(q, a, U, U), \tag{19}$$

is satisfied. The converse statement is false.

It is, of course, clear that both $f_2(k, a) \geq -1$ and $g_2(q, a, U, U) \geq -1$. Therefore, -1 is the minimum value attained by both functions.

The minimum values are reached for $f_2(k, a)$ when

$$f_1(k_r, a) = 0, \tag{20}$$

and for $g_2(q, a, U, U)$ when

$$g_1(q_s, a, U) = 0, \tag{21}$$

at points $(k_r = (2r + 1)\pi/2a, q_s)$.

Therefore, some ‘‘minima gaps’’ disappear in this scheme. The dispersion relation at generic minima points (k_r, q_s) defined by

$$f_2(k_r, a) = g_2(q_s, a, U, U) = -1, \tag{22}$$

is degenerate because both the functions *and* their derivatives coincide at points (k_r, q_s) . In fact, the functions derivatives vanish at those points, due to the fact that the equality is reached at the minima of the functions, *i.e.*, we have that at the points (k_r, q_s)

$$\frac{df_2(k, a)}{dk} \Big|_{k=k_r} = 4 \frac{df_1(k, a)}{dk} f_1(k, a) \Big|_{k=k_r} = 0 \tag{23}$$

and

$$\begin{aligned} \frac{dg_2(q, a, U, U)}{dq} \Big|_{q=q_s} \\ = 4 \frac{dg_1(q, a, U)}{dq} g_1(q, a, U) \Big|_{q=q_s} = 0, \end{aligned} \tag{24}$$

also.

This degeneracy gives rise to local invariance under the Virasoro algebra at the conical dispersion relations points (k_r, q_s) , in reciprocal space (k -space, see below). This feature is discussed in Sec. 5.

Therefore, the dispersion relations in the vicinity of the minima read

$$\begin{aligned} \frac{d^2 f_2(k, a)}{dk^2} \Big|_{k=k_r} (k - k_r)^2 \\ = \frac{d^2 g_2(q, a, U, U)}{dq^2} \Big|_{q=q_s} (q - q_s)^2, \end{aligned} \tag{25}$$

Note that both

$$\frac{d^2 f_2(k, a)}{dk^2} \Big|_{k=k_r} = 4a^2 > 0 \tag{26}$$

and

$$\begin{aligned} \frac{d^2 g_2(q, a, U, U)}{dq^2} \Big|_{q=q_s} = 4 \\ \times \left(\frac{dg_1(q, a, U)}{dq} \right)^2 \Big|_{q=q_s} > 0 \end{aligned} \tag{27}$$

because the points (k_r, q_s) define both functions minima.

Define

$$g'_1 \equiv \frac{dg_1(q, a, U)}{dq} \Big|_{q=q_s}, \tag{28}$$

$$f_2'' \equiv \frac{d^2 f_2(k, a)}{dk^2} \Big|_{k=k_r} (= 4a^2), \tag{29}$$

$$g_2'' \equiv \frac{d^2 g_2(q, a, U, U)}{dq^2} \Big|_{q=q_s} = 4(g_1')^2, \tag{30}$$

$$\Delta k \equiv k - k_r, \tag{31}$$

$$\Delta E \equiv \frac{\hbar^2 q^2}{2m} - \frac{\hbar^2 q_s^2}{2m}, \tag{32}$$

to get the conical dispersion relation

$$\begin{aligned} \Delta E &= \pm \sqrt{\frac{f_2''}{g_2''} \frac{\hbar^2 q_s}{m}} \Delta k \\ &= \pm \frac{a}{g_1'} \frac{\hbar^2 q_s}{m} \Delta k = \pm \hbar v_F \Delta k, \end{aligned} \tag{33}$$

where the Fermi velocity v_F is given by

$$v_F \equiv \sqrt{\frac{f_2''}{g_2''} \frac{\hbar q_s}{m}} = \frac{a}{g_1'} \frac{\hbar q_s}{m}. \tag{34}$$

4. The general case

Note that for $V \neq U$, one may write

$$\begin{aligned} g_2(q, a, U, V) &\equiv g_2(q, a, U, U) \\ &+ \frac{2m(V - U)a \sin qa}{\hbar^2} g_1(q, a, U), \end{aligned} \tag{35}$$

therefore

$$\begin{aligned} g_2(q_s, a, U, V) &= g_2(q_s, a, U, U) \\ &= f_2(k_r, a) = -1, \end{aligned} \tag{36}$$

It is interesting to realize that the corresponding condition $g_1(q'_s, a, V) = 0$ (exchanging V and U) also implies $g_2(q'_s, a, U, V) = -1$, as it should. In what follows, we write everything in terms of the the $g_1(q_s, a, U) = 0$ condition only, understanding that similar results are reached in points (k_r, q_s) and points (k_r, q'_s) .

The function $g_2(q, a, U, V)$ does not, in general, attain a minimum at the points q_s . In fact,

$$\begin{aligned} \frac{dg_2(q, a, U, V)}{dq} \Big|_{q=q_s} &= \frac{2m(V - U)a \sin q_s a}{\hbar^2} \frac{dg_1(q, a, U)}{dq} \Big|_{q=q_s} \\ &= \frac{2m(V - U)a^2}{\hbar^2 q_s a} \left(-1 + \frac{\sin 2q_s a}{2q_s a} \right) \neq 0, \end{aligned} \tag{37}$$

in general. We nonetheless get conical dispersion relations both for low energies $q_s a \rightarrow 0$ and for high energies (as compared to the potential strength difference) $\frac{2m(V-U)a^2}{\hbar^2 q_s a} \ll 1$.

The tight binding approach ($\frac{mUa}{\hbar^2} \gg 1$ and $\frac{mVa}{\hbar^2} \gg 1$) also yields interesting results. In fact, in that case one may

study the behavior of $g_1(q_n, a, U)=0$ (or $g_1(q'_n, a, V)=0$) near the zeroes of $(\sin qa/qa)$ [7], i.e., at the points $q_n a = n\pi + (-1)^n \delta_n, n \in \{\mathbb{Z} - \{0\}\}$

$$g_1(q_n, a, U) = (-1)^n + \frac{mUa}{\hbar^2} \frac{\delta_n}{n\pi}. \tag{38}$$

The requirement $g_1(q_n, a, U) = 0$ implies

$$\delta_n = (-1)^{n+1} \frac{n\pi \hbar^2}{mUa}, \tag{39}$$

while for $g_1(q'_n, a, V) = 0$ one gets

$$\delta'_n = (-1)^{n+1} \frac{n\pi \hbar^2}{mVa}. \tag{40}$$

Note that due to the tight binding condition both $\delta_n \ll 1$ and $\delta'_n \ll 1$. Therefore, for $U \sim V$ the difference $(\delta_n - \delta'_n)$ is of the order δ_n^2 , i.e., to first order, $q_n = q'_n$, which means that $g_2(q_n, a, U, V) = -1$, thus $g_2(q_n, a, U, V)$ attains minima at $q = q_n$ in the tight binding approximation, giving rise to conical dispersion relations at those points.

The energy spectrum is readily computed, to get

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \left(1 - \frac{\hbar^2}{mUa} \right)^2 \tag{41}$$

or

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \left(1 - \frac{\delta_1}{\pi} \right)^2 \simeq \frac{n^2 \pi^2 \hbar^2}{2ma^2} \left(1 - 2 \frac{\delta_1}{\pi} \right) \tag{42}$$

to first order in δ_1 .

5. Local Virasoro invariance in reciprocal space

Define $F(k, q, a, U, V)$ by

$$F(k, q, a, U, V) \equiv f_2(k, a) - g_2(q, a, U, V). \tag{43}$$

The function $F(k, q, a, U, V)$ and its first derivatives with respect to k and q vanish at $(k_r = (2r + 1)\pi/2a, q_s)$ ($(k_r = (2r + 1)\pi/2a, q'_s)$) whenever the conditions for conical dispersion relations are met (see Secs. 3 and 4). As a matter of fact, (k_r, q_s) and (k_r, q'_s) define saddle points for the function $F(k, q, a, U, V)$.

For conical dispersion relations $F(k_r + \Delta k, q_s + \Delta q, a, U, V)$ may be written as

$$\begin{aligned} &F(k_r + \Delta k, q_s + \Delta q, a, U, V) \\ &\simeq \frac{\partial^2 F}{\partial k^2} \Big|_{k=k_r} \Delta k^2 + \frac{\partial^2 F}{\partial q^2} \Big|_{q=q_s} \Delta q^2, \end{aligned} \tag{44}$$

because the function and its first derivatives vanish at those points. Moreover, the product of the second derivatives of F is negative.

Therefore, the eigenvalue equation $F(k, q, a, U, V) = 0$ in the vicinity of conical points $(k_r = (2r + 1)\pi/2a, q_s)$ reduces to

$$\frac{\partial^2 F}{\partial k^2} \Big|_{k=k_r} \Delta k^2 + \frac{\partial^2 F}{\partial q^2} \Big|_{q=q_s} \Delta q^2 = 0, \quad (45)$$

which defines a two dimensional “light” cone associated to the Fermi velocity v_F . The Fermi velocity is proportional to the (square root) of the (negative of) the ratio of the second derivatives of the function $F(k, q, a, U, V)$ at the conical points as showed in (34). A conformally invariant metric near the conical points may be defined in terms of v_F . Two dimensional conformal transformations leave the dispersion relation (45) near conical points invariant.

It is a widely known fact that such structures are invariant under the action of the (infinite dimensional) Virasoro algebra [8]. This symmetry gives rise to local gauge invariance of the Schrödinger wave function around conical points. This fact encourages the search of a relationship of this problem to string theory.

In three dimensional models (two space dimensions) [6], the symmetry is reduced to the (ten generators) three dimensional conformal algebra.

6. Conclusions

I have presented a mechanism that produces conical dispersion relations consistent with behavior observed in graphene and other materials [1–5]. The mechanism assumes the existence of more than one lattice point per unit cell. The condition to achieve conical dispersion relations is equivalent to require that the nearest neighbors structure factor vanish [6]. The Schrödinger eigenvalue problem near conical points happens to be invariant under the Virasoro algebra which hints a relationship between this problem and string theory. In a forthcoming paper [6], a bidimensional generalization which includes Hubbard model (tight binding) calculations, the ideas presented here are explored and extended. The invariance near conical points, in two dimensional arrays, is reduced to the ten dimensional conformal group in three (spacetime) dimensions.

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