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Transition in the fermion determinant of a polymer model†

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Abstract. We calculate the one-dimensional fermion determinant associated with a polymer model with a soliton. The model exhibits a curious transition, which corresponds to the disappearance of a normalised zero mode as one of its parameters varies. The calculation is done on the whole real axis, so as to preserve the topology of the background, by using the scattering data of a steplike potential.

1. Introduction

Determinants appear naturally in quantum field theory when formulated in the path integral approach. In a semiclassical approximation, the first quantum correction leads to the calculation of determinants of differential operators (fluctuation determinants). As a rule, they are divergent and it is necessary to introduce a regularisation procedure. The infinities appear because one has an infinite number of ever-increasing eigenvalues (ultraviolet divergences) which may even be continuous. Typically, one discretises those eigenvalues by putting the system in a large box and then applies standard methods (i.e. zeta function regularisation) to deal with the infinite product (Camperi and Gamboa Saraví 1984). However, in the case of fermions in the presence of a topological background, this procedure does not preserve the asymptotic properties responsible for topological effects, unless the compactification is performed with extreme care (i.e. stereographic projections are usually involved). We have thus chosen to calculate determinants on the whole real axis and this led us to a scattering problem.

In fact, determinants can be used as a tool to analyse scattering processes and yield spectral properties and phase shifts (Baker 1958). They are naturally related to scattering data via Jost functions (de Vega 1981). As many QFT models display interesting properties related to the appearance of fermionic zero modes (Niemi and Semenoff 1986) in the presence of non-trivial topological backgrounds, we were led to investigate the behaviour of one such determinant in a model in $1+1$ dimensions.

Recently, these models have attracted the attention and research efforts of field theoreticians due to their possible applications in condensed matter physics. In particular, the physics of quasi-one-dimensional polymers offers not only conceptual but also rich phenomenological possibilities for the realisation of ideas common to high-energy models.

These applications are based on a continuum limit approach to Hamiltonians defined on a lattice, whose prototype is the Su-Schieffer-Heeger model (Yu-Lu 1987).

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It describes the interaction of lattice vibrations with π electrons through hopping terms. Linearisation of the dispersion relation of π electrons around the Fermi level (Jackiw and Semenoff 1983) yields a continuum limit electron-phonon Hamiltonian identical to a relativistic Dirac model with interacting fermion and boson fields. It has the general form:

$$H = \begin{pmatrix} \varepsilon & D \\ D^+ & -\varepsilon \end{pmatrix}$$

where $D \equiv -d/dx + \phi(x)$, and $\phi(x)$ is related to the dimerisation parameter.

This Hamiltonian exhibits interesting properties when $\phi(x)$ is considered as an external field with non-trivial topology (i.e. a soliton or structural defect): fermion number fractionisation, supersymmetry and appearance of localised states. Fermion number fractionisation is connected with topology through the existence of normalisable zero modes of H . The spectral properties of H can be investigated 'globally' by means of an associated one-dimensional Schrödinger determinant which contains its scattering data. As the fermion determinant can also be calculated through the scattering data of the Dirac operator (Dashen *et al* 1975) we reduce its computation to the Schrödinger problem.

In this paper we discuss the behaviour of a determinant of that type, which appears in the continuum limit of a generalised polymer model, as a function of a variable mass parameter μ (measuring the hopping asymmetry). Recent work indicates the occurrence of a curious transition of the fermion number in this process, corresponding to the disappearance of zero modes.

2. One-dimensional determinants

In one dimension, it is well established (Fuentes 1987) that one can calculate determinants of Schrödinger operators through eigenfunctions obeying suitable boundary conditions in the interval $[-L, L]$. The idea is to consider operators like $\hat{D} = -\partial_x^2 + U(x)$, $U(x)$ bounded below, and analyse the eigenvalue problem:

$$(-\partial_x^2 + U(x) - \tau)f(x) = 0$$

imposing periodic boundary conditions, $f(-L) = f(L) = 0$. This amounts to putting the system in a box so that \hat{D} has a discrete infinite spectrum, bounded below. If $\tau = \tau_0$ coincides with one of these eigenvalues, then the shifted operator $\hat{D} - \tau_0$ has a zero mode and therefore its determinant vanishes. Alternatively, if we consider the function $g_{U,\tau}(x)$ defined as the unique solution of the initial-value problem:

$$\begin{aligned} (-\partial_x^2 + U(x) - \tau)g(x) &= 0 \\ g(-L) &= 0 \quad g'(-L) = 1 \end{aligned}$$

we see that τ will be an eigenvalue of \hat{D} if and only if $g_{U,\tau}(L) = 0$. When this happens, $g_{U,\tau}(x)$ is, in fact, the associated eigenfunction.

Using this, one can show that

$$\frac{\det(-\partial_x^2 + V(x) - \tau)}{\det(-\partial_x^2 + W(x) - \tau)} = \frac{g_{V,\tau}(L)}{g_{W,\tau}(L)}$$

as a consequence of the identity between two functions of complex variable τ which have the same zeros and poles (Coleman 1985, Felgason 1981). The reason for taking

a quotient of determinants is to ensure convergence (in general $W(x)$ is taken as a constant free potential).

These results are valid for an interval $[-L, L]$. However, in physics we are interested in operators defined on the whole real axis. The simplest one can try is, therefore, to consider a sufficiently large box and, after the calculation, proceed to the limit $L \rightarrow +\infty$, hoping to obtain a convergent and sensible result. With this in mind we consider the equation:

$$-\psi'' + V(x)\psi = k^2\psi$$

with $V(x)$ bounded below and such that $\lim_{x \rightarrow \pm\infty} V(x) = 0$. Then, we take the linear combination:

$$\psi(x) = A\psi_1(x) + B\psi_2(x)$$

where $\psi_1(x)$ and $\psi_2(x)$ are independent solutions of the corresponding scattering problem. Their asymptotic behaviour is given by

$$\psi_1(x, k) \sim \exp(ikx) + R(k) \exp(-ikx) \quad x \rightarrow -\infty$$

$$\psi_1(x, k) \sim T(k) \exp(ikx) \quad x \rightarrow +\infty$$

$$\psi_2(x, k) \sim T(k) \exp(-ikx) \quad x \rightarrow -\infty$$

$$\psi_2(x, k) \sim \exp(ikx) + R'(k) \exp(ikx) \quad x \rightarrow +\infty.$$

The justification for taking these scattering solutions is to avoid divergences in the $L \rightarrow +\infty$ limit which would appear had we taken combinations of bound states. Then we follow the recipe of the method above. Imposing the conditions

$$\psi_{-\infty}(-L/2) = 0 \quad \partial_x \psi_{-\infty}(-L/2) = 1$$

we determine A and B . Then we can find $\psi_{+\infty}(L/2)$ and, therefore, in the box

$$\begin{aligned} \det\left(\frac{-\partial_x^2 + V(x) - k^2}{-\partial_x^2 - k^2}\right) &= \frac{\psi_{+\infty}(L/2)}{\psi_{+\infty}^{(0)}(L/2)} \\ &= \frac{1}{1 - \exp(-2ikL)} \left(T - \frac{1}{T} [\exp(-2ikL) + RR' + (R + R') \exp(-ikL)] \right). \end{aligned}$$

To proceed to the $L \rightarrow +\infty$ limit, we make an 'analytic continuation' to the upper half-plane: $k = i\chi$, $\chi > 0$. Returning to real k we obtain

$$\det\left(\frac{-\partial_x^2 + V(x) - k^2}{-\partial_x^2 - k^2}\right) = \frac{1}{T(k)}.$$

We then see that the determinant *defined on the whole axis* is directly associated with the scattering data, namely the transmission coefficient. (We observe that the hypothesis $\lim_{x \rightarrow \pm\infty} V(x) = 0$ is essential to ensure a convergent result.)

We can interpret the result by referring to the well known dispersion relation for the scattering data of the problem

$$\begin{aligned} -\psi''(x) + V(x)\psi &= k^2\psi \\ \int_{-\infty}^{+\infty} (1 + |x|) |V(x)| dx &< \infty. \end{aligned}$$

Under such conditions, one can show (Fadeev 1967) that $T(k)$ (the $S_{11}(k)$ S -matrix element) is a meromorphic function on the upper half-plane for $k \neq 0$, whose poles are given by $k_n = i\chi_n$, $n = 1, \dots, N_B$, $\chi_n > 0$ associated with the bound states of the potential. Then

$$T(k) = \prod_{i=1}^{N_B} \left(\frac{k + i\chi_i}{k - i\chi_i} \right) \exp\left(\frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{\ln|T(q)|}{q - k} dq \right)$$

for $\text{Im } k > 0$, $k \neq 0$ and $T(k) = \lim_{\epsilon \rightarrow \infty} T(k + i\epsilon)$, $\text{Im } k = 0$. Thus, we can clearly distinguish the contribution of the discrete and continuum parts of the spectra. In particular, we see that the determinant vanishes whenever k passes through a normalisable bound state of $-\partial_x^2 + V(x)$ or, equivalently, a zero mode of $-\partial_x^2 + V(x) - k^2$.

An often cited example is the Pöschl-Teller potential:

$$V(x) = -\frac{\hbar^2}{2m} \alpha^2 \lambda (\lambda - 1) \text{sech}^2 \alpha x \quad \lambda > 1$$

which is an exactly solvable potential (Flügge 1971). We obtain

$$\det\left(\frac{-\partial_x^2 - \alpha^2 \lambda (\lambda - 1) \text{sech}^2 \alpha x - k^2}{-\partial_x^2 - k^2} \right) = \frac{\Gamma(-ik/\alpha)\Gamma(1-ik/\alpha)}{\Gamma(\lambda - ik/\alpha)\Gamma(1 - \lambda - ik/\alpha)}$$

This potential appears in the Jackiw-Rebbi model, a ϕ^4 model with Yukawa coupling, describing the interaction of a real scalar field $\phi(x)$ and spinor $\psi(x)$. When the fermions are in a soliton background $\phi(x) = \hat{\phi} \tanh(\hat{\phi}x)$, the Dirac Hamiltonian possesses a normalisable zero mode in the middle of the gap. This means that one of the Schrödinger equations obtained has a zero mode. In fact, the equation is

$$(-\partial_x^2 - 2\hat{\phi}^2 \text{sech}^2(\hat{\phi}x) + \hat{\phi}^2)\psi(x) = \hat{D}\psi = E^2\psi$$

and \hat{D} has a zero mode. Therefore its determinant must vanish. Comparing with the formula above we get $\lambda = 2$, $\alpha = \hat{\phi}$ and $k^2 = -\hat{\phi}^2$. Then

$$\det\left(\frac{-\partial_x^2 - 2\hat{\phi}^2 \text{sech}^2(\hat{\phi}x) + \hat{\phi}^2}{-\partial_x^2 + \hat{\phi}^2} \right) = \frac{\Gamma(1)\Gamma(2)}{\Gamma(3)\Gamma(0)} \rightarrow 0$$

as expected.

3. A curious transition

The phenomenon of fermion number fractionisation is connected with the spectral properties of Dirac operators, in particular the appearance of zero modes. In field theory models for polymers in the presence of soliton-like (kink) structural defects, the fermion number is related to properties such as conductivity, magnetic susceptibility and optical absorption of the π electrons of the polymer.

In recent work (Aragão de Carvalho and Pureza 1988) the occurrence of a curious transition in a generalised polymer model was observed whose hopping amplitude for the electron-phonon interaction is of the form:

$$t_{n+1,n} = \begin{cases} t_1 - \gamma(y_{n+1} - y_n) & n \text{ odd} \\ t_2 - \gamma(y_{n+1} - y_n) & n \text{ even.} \end{cases}$$

Here, y_n is the position of the n th atom of the chain and we define the parameter $\mu = (t_1 - t_2)/2$. The continuum limit yields a relativistic quantum field model whose Dirac Hamiltonian is

$$\hat{H} = \begin{pmatrix} 0 & \hat{D}(\mu) \\ \hat{D}^+(\mu) & 0 \end{pmatrix} = \alpha \hat{p} + \beta(\phi + \mu)$$

where $\hat{D} = d/dx + \phi(x) + \mu$, so that μ corresponds to a mass term for the fermions.

Let us choose as our background field a topological kink, $\phi(x) = \phi_0 \tanh(\phi_0 x)$. A model with asymmetrical hopping amplitudes is more suitable to mirror the *cis* polymer variety because of the position of the hydrogen atoms in the chain. Such a variety does not possess a degenerate ground state (as *trans* polymers do). Therefore, it is not expected to support a kink-like defect. However, recent work (Aragão de Carvalho 1988) indicates the possibility that even a *cis* polymer might admit a kink defect. Besides, samples of *cis* polymers are always contaminated with *trans*, where a soliton might occur. Thus, the above choice might not be merely academic if one could alter the value of μ without destroying the defect itself (e.g. chemically).

To analyse the spectral properties one considers the iterated Hamiltonian:

$$\hat{H}^2 = \begin{pmatrix} \hat{D}(\mu)\hat{D}^+(\mu) & 0 \\ 0 & \hat{D}^+(\mu)\hat{D}(\mu) \end{pmatrix}$$

so that we have to solve the one-dimensional Schrödinger problems:

$$[\hat{D}^+(\mu)\hat{D}(\mu)]\xi = E\xi \quad [\hat{D}(\mu)\hat{D}^+(\mu)]\chi = E\chi.$$

These involve Morse-Rosen (Morse and Feshbach 1953) potentials:

$$\hat{L} = -\frac{d^2}{dx^2} + C_0 + C_1 \tanh(\phi_0 x) + \left(\frac{C_2}{C_3}\right) \text{sech}^2(\phi_0 x)$$

where

$$C_0 = \phi_0^2 + \mu^2$$

$$C_1 = 2\mu\phi_0$$

$$C_2 = 0$$

$$C_3 = -2\phi_0^2.$$

It can be shown that the problem:

$$[-d^2/dx^2 + (\phi_0^2 + \mu^2) + 2\mu\phi_0 \tanh(\phi_0 x) - 2\phi_0^2 \text{sech}^2(\phi_0 x)]\xi = k^2\xi$$

where $V(x) = (\phi_0^2 + \mu^2) + 2\mu\phi_0 \tanh(\phi_0 x) - 2\phi_0^2 \text{sech}^2(\phi_0 x)$, admits a normalisable zero mode for $0 < \mu < \phi_0$. It can also be shown that, as we vary the parameter $r \equiv \mu/\phi_0$, there occurs a transition in which this zero mode, present when $\mu < \phi_0$, is swallowed up by the continuum and eventually disappears as the gap reopens for $\mu > \phi_0$.

The disappearance of the zero mode when $\mu > \phi_0$ results in an abrupt transition of the fermion number (the system admits charge conjugation invariance)

$$N = \pm \frac{1}{2} \theta(\mu - \phi_0)$$

where $\theta(x)$ is the Heaviside function.

It would be interesting to investigate the behaviour of the determinant in this process, as the disappearance of a zero mode would correspond to an abrupt change in its value, from zero to a finite amount.

We then want to calculate the determinant of a one-dimensional step-like Schrödinger potential. If we tried to apply the given method we would have to choose

$$\psi(x) = A\psi_1(x) + B\psi_2(x)$$

where now

$$\begin{aligned} \psi_1(x, k) &\sim \exp(ik'x) + R_- \exp(-ik'x) & x \rightarrow -\infty \\ \psi_1(x, k) &\sim T_- \exp(ik''x) & x \rightarrow +\infty \\ \psi_2(x, k) &\sim \exp(ik''x) + R_+ \exp(-ik''x) & x \rightarrow +\infty \\ \psi_2(x, k) &\sim T_+ \exp(ik'x) & x \rightarrow -\infty \end{aligned}$$

and $k' = [k^2 - (\phi_0 + \mu)^2]^{1/2}$; $k'' = [k^2 - (\phi_0 - \mu)^2]^{1/2}$.

Imposing our conditions, we would have

$$\begin{aligned} \psi_{+\infty}(L/2) &= \frac{1}{2ik'} \left(T_- \exp[(k' + k'')L/2] \right. \\ &\quad - \frac{1}{T_+} \{ \exp[-(k' + k'')L/2] + \exp[i(k' - k'')L/2]R_- \\ &\quad \left. + \exp[-i(k' + k'')L/2]R_+ + \exp[i(k' + k'')L/2]R_+R_- \right). \end{aligned}$$

For the free case, we choose $\psi_{+\infty}^{(0)}(L/2) = \sin(\bar{k}L)/\bar{k}$ ($\bar{k} = (k^2 - \phi_0^2)^{1/2}$). But then the identification:

$$\det \left(\frac{-\partial_x^2 + V(x) - k^2}{-\partial_x^2 + \phi_0^2 - k^2} \right) = \frac{\psi_{+\infty}(L/2)}{\psi_{+\infty}^{(0)}(L/2)}$$

does not converge in the $L \rightarrow +\infty$ limit (after the analytic continuation $k = i\chi$, $\chi > 0$). But if we observe that

$$\begin{aligned} \det \left(\frac{-\partial_x^2 + V(x) - k^2}{-\partial_x^2 + \phi_0^2 - k^2} \right) &= \frac{\det(-\partial_x^2 + V(x) - k^2)}{\det(-\partial_x^2 - \mathbb{K}^2)} \frac{\det(-\partial_x^2 - \mathbb{K}^2)}{\det(-\partial_x^2 + \phi_0^2 - k^2)} \\ &= \left(\frac{\psi_{+\infty}(L/2)}{\bar{\psi}_{+\infty}^{(0)}(L/2)} \right) \left(\frac{\bar{\psi}_{+\infty}^{(0)}(L/2)}{\psi_{+\infty}^{(0)}(L/2)} \right) \end{aligned}$$

where $\mathbb{K}^2 = ((k' + k'')/2)^2$ and $\bar{\psi}_{+\infty}^{(0)}(L/2) = \sin(\mathbb{K}L)/\mathbb{K}$, we would obtain

$$\begin{aligned} \frac{\psi_{+\infty}(L/2)}{\bar{\psi}_{+\infty}^{(0)}(L/2)} &= \left(\frac{k' + k''}{2k'} \right) \frac{1}{\exp(i\mathbb{K}L) - \exp(-i\mathbb{K}L)} \left(T_- \exp(i\mathbb{K}L) - \frac{1}{T_+} \right. \\ &\quad \times \{ \exp(-i\mathbb{K}L) + \exp[i(k' - k'')L/2]R_- + \exp[-i(k' - k'')L/2]R_+ \\ &\quad \left. + \exp(i\mathbb{K}L)R_+R_- \right). \end{aligned}$$

This expression converges in the $L \rightarrow +\infty$ limit:

$$\frac{\psi_{+\infty}(L/2)}{\bar{\psi}_{+\infty}^{(0)}(L/2)} \xrightarrow{L \rightarrow +\infty} \left(\frac{k' + k''}{2k'} \right) \frac{1}{T_+(k)}$$

after analytic continuation.

Now, it can be shown that (Cohen and Kappeler 1985)

$$k'T_+ = k''T_-$$

where T_- is the transmission coefficient for a plane wave incident from $-\infty$ to $+\infty$, and is given by (Khare and Sukhatme 1988)

$$T_-(k) = \frac{\Gamma(1 - ik'/2\phi_0 - ik''/2\phi_0)\Gamma(2 - ik'/2\phi_0 - ik''/2\phi_0)}{\Gamma(-ik'/\phi_0)\Gamma(1 - k''/\phi_0)}.$$

Note that for $\mu = 0$, $k' = k''$ and we recover the Pöschl-Teller case: $V(x) = \phi_0^2 - 2\phi_0^2 \operatorname{sech}^2(\phi_0 x)$.

We want to analyse the $k = 0$ case (zero mode) while $r = \mu/\phi$ varies. In this case $\mathbb{K}^2(k = 0) = -\phi_0^2$, so that the quotient of free determinants is

$$\det\left(\frac{-\partial_x^2 - \mathbb{K}^2}{-\partial_x^2 + \phi_0^2 - k^2}\right)_{k=0} = \det\left(\frac{-\partial_x^2 + \phi_0^2}{-\partial_x^2 + \phi_0^2}\right) = 1.$$

We then have the following.

(i) $\mu < \phi_0$; $k = 0 \Rightarrow k' = i(\phi_0 + \mu)$; $k'' = i(\phi_0 - \mu)$:

$$\begin{aligned} T_-(0) &= \frac{\Gamma[-1 + (\phi_0 + \mu)/2\phi_0 + (\phi_0 - \mu)/2\phi_0]\Gamma[2 + (\phi_0 + \mu)/2\phi_0 + (\phi_0 - \mu)/2\phi_0]}{\Gamma((\phi_0 + \mu)/\phi_0)\Gamma(1 + (\phi_0 - \mu)/\phi_0)} \\ &= \frac{\Gamma(0)\Gamma(3)}{\Gamma(1 + \mu/\phi_0)\Gamma(2 - \mu/\phi_0)} \rightarrow +\infty \end{aligned}$$

so that the determinant vanishes, as expected, for the zero mode is present.

(ii) $\mu = \phi_0$:

$$\begin{aligned} k''T_-(k) &= \frac{k\Gamma(-1 - i(k^2 - 4\phi_0^2)^{1/2}/2\phi_0 - ik/2\phi_0)\Gamma(2 - i(k^2 - 4\phi_0^2)^{1/2}/2\phi_0 - ik/2\phi_0)}{\Gamma(-i(k^2 - 4\phi_0^2)^{1/2}/\phi_0)\Gamma(1 - ik/\phi_0)} \\ &\xrightarrow{k \rightarrow \infty} 2i\phi_0(-ik/\phi_0) \frac{\Gamma(-ik/2\phi_0)\Gamma(3)}{\Gamma(2)\Gamma(1)} = 2i\phi_0 \frac{\Gamma(1)\Gamma(3)}{\Gamma(2)\Gamma(1)} = 4i\phi_0 \end{aligned}$$

(we used $z\Gamma(z) = \Gamma(z+1) \Rightarrow$ as $z \rightarrow 0$, $z\Gamma(z) \rightarrow \Gamma(1)$). Then

$$\det\left(\frac{-\partial_x^2 + V(x)}{-\partial_x^2 - \phi_0^2}\right) = \frac{1}{4}.$$

(iii) $\mu > \phi_0$:

$$\begin{aligned} \det\left(\frac{-\partial_x^2 + V(x)}{-\partial_x^2 - \mu^2}\right) &= \frac{2i\mu}{2i(\mu - \phi_0)} \frac{\Gamma(1 + \mu/\phi_0)\Gamma(\mu/\phi_0)}{\Gamma(-1 + \mu/\phi_0)\Gamma(2 + \mu/\phi_0)} \\ &= \frac{(-1 + \mu/\phi_0)}{(1 - \phi_0/\mu)(1 + \mu/\phi_0)} \\ &= \frac{r}{1+r} \quad (r = \mu/\phi_0). \end{aligned}$$

We note that, as $r \rightarrow 1$, we have

$$\det \begin{pmatrix} -\partial_x^2 + V(x) \\ -\partial_x^2 - \phi_0^2 \end{pmatrix} = \frac{1}{2}$$

and not $\frac{1}{4}$ as we have obtained in case (ii).

We then see that the determinant jumps from zero to a finite value $\mu > \phi_0$, in agreement with the intuitive idea suggested by the disappearance of the zero mode. Curiously, the value at $\mu = \phi_0$ is the average of the values for $\mu < \phi_0$ and $\mu > \phi_0$.

4. Conclusion

One-dimensional Schrödinger determinants can be calculated for a class of step-like potentials on the whole real axis. According to general results, they are directly related to scattering data. We saw, in an example borrowed from polymers physics, that, although not a topological invariant, the determinant is sensitive to the disappearance of zero modes. In this way, it has a complementary behaviour to fermion number. A similar analysis could probably be made for problems in higher dimensions with spherical symmetry, for instance in two dimensions in the presence of vortices. In these cases, however, the analysis is probably more subtle due to the existence of resonant states.

We could thus treat the problem directly in a non-compact space and take account of the topological properties involved. We stress that, since fermionic determinants may sometimes be written in terms of scattering data, our method might lead to other interesting applications in problems where topological backgrounds are present.

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