Functional treatment of solitons in polyacetylene

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Abstract. In this paper we apply functional methods to the study of polyacetylene. We represent the polyacetylene free energy as a functional determinant ratio, obtain the uniform dimerization equation and calculate the soliton creation energy in some limiting cases.

1. Introduction

Polyacetylene, $(CH)_n$, is the simplest linear conjugated polymer of the CH group. In the ground state the polymer is made of alternating single and double bonds and said to be dimerized. A theoretical model which describes the dimerization of this polymer has been proposed by Su, Schrieffer and Heeger (SSH) [1]. They showed that the lattice deformation energy due to dimerization (the charge density wave of wavenumber $2k_F$) is overcome by the change in the electronic energy and that the ground state of the system is a dimerized one with two CH groups in a unit cell. They have also shown that the system admits a soliton solution and that the soliton exhibit very peculiar electronic properties.

In the analysis of SSH the lattice is treated as discrete, which makes mathematical analysis rather complicated. To avoid this difficulty Takayama, Lin-Liu and Maki (TLM) [2] constructed a continuum version of the model. Here the Hamiltonian of the system is represented by a $(1+1)$-dimensional Dirac operator with a position dependent mass and the velocity of light replaced by the Fermi velocity v_F. With the continuum model one can carry out the mathematical analysis easily and also make use of the results obtained for relativistic quantum field theoretic models.

In the present work we study polyacetylene from a functional integral point of view. We carry out the direct evaluation of the functional integrals for the effective action (the free energy) and obtain the gap equation and soliton creation energy. To simplify some computations we employ the Schwinger proper time formalism. Although our analysis here is exact, we point out that it is also suitable for a systematic approximation if the system under consideration does not admit exact evaluation of the functional integrals.

In the next section we represent the free energy in terms of a functional determinant. In section 3 we write down the exact formula for the soliton free energy. In section 4 the soliton free energy is evaluated in various limits. Section 5 is devoted to conclusion and discussion. In appendix A some technical points concerning integration over Grassmann variables and functional determinants are presented. In appendix B we

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comment on the high-energy different cut-off procedures. In appendix C we derive the 'magic formula' for functional determinants. Finally, in appendix D we construct an alternative integral representation for the soliton free energy.

2. Expressing the free energy in terms of a functional determinant ratio

In this work we model polyacetylene as a continuum field theory of fermions moving in one spatial dimension (labelled by x) and coupled to a static dimerization field [2]. In terms of a Euclidean action S depending on independent Grassmann fields ψ and $\bar{\psi}$ the model can be written as [3]

$$S = \int_0^\beta L \, d\tau + \beta \frac{\omega_Q^2}{2g^2} \int dx \, \Delta^2 \qquad (2.1a)$$

$$L = \int dx \, \bar{\psi}(\partial_\tau + H)\psi \qquad (2.1b)$$

$$H = -iv_F \partial_x \sigma^3 + \Delta \sigma^1 \qquad (2.1c)$$

where β is the reciprocal of the temperature T and τ is a Euclidean time variable. The quantity Δ is the static dimerization field (in the present work it depends only on x and not τ) and ω_Q and g are effective spring and coupling constants for the dimerization. The Fermi velocity is denoted by v_F and σ^k ($k = 1, 2, 3$) are the Pauli matrices which describe the physics in the problem associated with electrons moving at $\pm v_F$ (they do not describe the spin which plays an almost passive role in what follows and merely results in a factor of two appearing; we shall point out where this occurs below).

It is convenient to calculate not the full free energy of the system but rather the difference in free energy between the system of interest and an appropriately chosen reference system (denoted by a subscript 0). Thus, following standard methods we determine $F - F_0$ from a functional integral over Grassmann fields ψ and $\bar{\psi}$ that are antiperiodic in τ over β:

$$e^{-\beta(F-F_0)} = \left[\int d[\bar{\psi}] \, d[\psi] \exp(-S) \right]$$

$$\times \left[\int d[\bar{\psi}] \, d[\psi] \exp(-S_0) \right]^{-1}. \qquad (2.2)$$

and S_0 follows from S with the replacement $\Delta \to \Delta_0$. The free energy difference $F - F_0$ follows from this equation however its physical value follows by treating Δ as a variational field and minimizing $F - F_0$ with respect to parameters appearing in Δ. We shall say more on this in later sections where various choices will be made for Δ and Δ_0. On carrying out the functional integrations we obtain a ratio of two functional determinants; some technical points associated with this are discussed in appendix A. We obtain

$$e^{-\beta(F-F_0)} = \left(\frac{\det(\partial_\tau + H)}{\det(\partial_\tau + H_0)} \right)^2 \exp\left(-\beta \frac{\omega_Q^2}{2g^2} \int dx(\Delta^2 - \Delta_0^2) \right) \qquad (2.3)$$

where the index 2 follows from the two spin species each contributing a factor of a determinant ratio and the determinants are evaluated on eigenfunctions which are

antiperiodic in τ over β. As is discussed in appendix A it is possible to express $\det[\partial_\tau + H]$ as $\sqrt{\det[-\partial_\tau^2 + H^2]}$ thus we can write

$$F - F_0 = -\frac{1}{\beta} \ln\left(\frac{\det[-\partial_\tau^2 + H^2]}{\det[-\partial_\tau^2 + H_0^2]}\right) + \frac{\omega_Q^2}{2g^2} \int dx(\Delta^2 - \Delta_0^2). \tag{2.4}$$

3. Soliton creation energy

As has been discussed in section 1, the dimerization field of polyacetylene is capable of supporting topological solitons.

In this section we shall consider the case of a single soliton and calculate its creation energy, i.e. the zero temperature limit of $F - F_0$ where F_0 is the free energy of a soliton-free uniform system with dimerization

$$\Delta_0 \approx W \exp\left(-\frac{\pi v_F \omega_Q^2}{2g^2}\right) \tag{3.1}$$

(a derivation of this may be found at the beginning of appendix B). We take the soliton profile, $\Delta(x)$, to be

$$\Delta(x) = \Delta_0 \tanh(x/\xi) \tag{3.2}$$

where ξ is a parameter to be determined by requiring that the free energy is at a minimum when ξ is at its physical value.

From section 2 we have

$$F - F_0 = -\frac{1}{\beta} \ln\left(\frac{\det[-\partial_\tau^2 + H^2])}{\det[-\partial_\tau^2 + H_0^2]}\right) + \frac{\omega_Q^2}{2g^2} \int dx(\Delta^2(x) - \Delta_0^2). \tag{3.3}$$

Using the form for H given by (2.1c) it follows that $(\Delta'(x) = \partial_x \Delta(x))$

$$H^2 = -v_F^2 \partial_x^2 + \Delta^2(x) + \sigma^2 v_F \Delta'(x) \tag{3.4a}$$

$$H_0^2 = -v_F^2 \partial_x^2 + \Delta_0^2. \tag{3.4b}$$

Within the determinant ratio we diagonalize both $-\partial_\tau^2$ and σ^2 (eigenvalues $\omega_n^2 = (\pi(2n+1)/\beta)^2$ and $\sigma = \pm 1$ respectively) to obtain

$$\frac{\det[-\partial_\tau^2 + H^2]}{\det[-\partial_\tau^2 + H_0^2]} = \prod_{n=-\infty}^{\infty} \prod_{\sigma} \frac{\det[\omega_n^2 + \Delta_0^2 - v_F^2 \partial_x^2 - (\Delta_0^2 + \sigma v_F \Delta_0/\xi) \operatorname{sech}^2(x/\xi)]}{\det[\omega_n^2 + \Delta_0^2 - v_F^2 \partial_x^2]}. \tag{3.5}$$

The determinants on the RHS of this equation are taken in a space with no matrix structure where $-\partial_x^2$ etc operates.

With the introduction of the dimensionless variables

$$y = x/\xi \tag{3.6a}$$

$$\lambda = \Delta_0 \xi / v_F \tag{3.6b}$$

$$a_n = \lambda \left(1 + \frac{\omega_n^2}{\Delta_0^2}\right)^{1/2} \tag{3.6c}$$

we can re-express the RHS of (3.5) as

$$\text{RHS} = \prod_{n=-\infty}^{\infty} \prod_{\sigma} \frac{\det[a_n^2 - \partial_y^2 - \lambda(\lambda + \sigma) \operatorname{sech}^2 y]}{\det[a_n^2 - \partial_y^2]}. \tag{3.7}$$

In appendix C we present a derivation of a known 'magic result' for functional determinants [4]:

$$\frac{\det[-\partial_y^2 - \lambda(\lambda+1)\,\mathrm{sech}^2\,y - z]}{\det[-\partial_y^2 - z]} = \frac{\Gamma(1+\sqrt{-z})\Gamma(\sqrt{-z})}{\Gamma(1+\lambda+\sqrt{-z})\Gamma(\sqrt{-z}-\lambda)}. \tag{3.8}$$

With this result we can write

$$\frac{\det[-\partial_\tau^2 + H^2]}{\det[-\partial_\tau^2 + H_0^2]} = \prod_{n,\sigma} \frac{\Gamma(1+a_n)\Gamma(a_n)}{\Gamma(1+a_n+\sigma\lambda)\Gamma(a_n-\sigma\lambda)}. \tag{3.9}$$

Hence the free energy difference of (3.3) can be written (we have evaluated the elementary integral over x involving the dimerization)

$$F - F_0 = -1/\beta \sum_{n,\sigma} \ln \frac{\Gamma(1+a_n)\Gamma(a_n)}{\Gamma(1+a_n+\sigma\lambda)\Gamma(a_n-\sigma\lambda)} - \lambda\Delta_0 v_F \frac{\omega_Q^2}{g^2}. \tag{3.10}$$

In the limit of zero temperature $F - F_0 \to E - E_0$, the soliton creation energy and $1/\beta \sum_n \to \int_{-\infty}^{\infty} \mathrm{d}\omega/2\pi$. Note however that the finite bandwidth of the electronic spectrum $W = 2v_F p_F$ ($p_F =$ Fermi momentum) has not been taken into account in the evaluation of the functional determinant ratio in (3.9). We would normally expect to implement this in, for example, momentum integrals however as is discussed in appendix B it can, quite equivalently, be made in the frequency integral. Thus, taking into account the evenness of the integrand, we have $\int_{-\infty}^{\infty} \mathrm{d}\omega/2\pi \to \int_0^{W/2} \mathrm{d}\omega/\pi$. We now make the change of variables

$$u = (1 + \omega^2/\Delta_0^2)^{1/2} \tag{3.11}$$

use $\Gamma(z+1) = z\Gamma(z)$ and carry out the sum over σ. We obtain

$$\frac{E - E_0}{\Delta_0} = -\frac{1}{\pi} \int_1^\Lambda \frac{u\,\mathrm{d}u}{(u^2-1)^{1/2}} \ln\left[\frac{u^2}{u^2-1} \frac{\Gamma^4(\lambda u)}{\Gamma^2(\lambda u + \lambda)\Gamma^2(\lambda u - \lambda)}\right] - \lambda v_F \frac{\omega_Q^2}{g^2} \tag{3.12}$$

where

$$\Lambda = (1 + W^2/4\Delta_0^2)^{1/2}. \tag{3.13}$$

An interesting feature of (3.12) is that the RHS is well approximated by allowing $\Delta_0/W \to 0$ (we shall loosely term this the 'no cut-off limit'). As a result (3.12) leads, to a good approximation, to a universal function depending only on λ. To see this we use the 'gap equation' (3.1) to eliminate the second term on the RHS of (3.12).
We have

$$-\lambda v_F \frac{\omega_Q^2}{g^2} = -\frac{\lambda}{\pi} \ln\left[\left(\frac{W}{\Delta_0}\right)^2\right]. \tag{3.14}$$

The large u part of the integral in (3.12) accurately cancels with the logarithmic term (3.14) (with power-law corrections in the small quantity Δ_0/W). Evidence for this follows by replacing the gamma functions in the integral by their large argument asymptotic forms and evaluating the resulting integral. If we use the leading term in the asymptotic series this leads to

$$\frac{\Gamma^4(\lambda u)}{\Gamma^2(\lambda u + \lambda)\Gamma^2(\lambda u - \lambda)} \approx \frac{u^2-1}{u^2}\,\mathrm{e}^{-2\lambda/u} \tag{3.15}$$

The integral that results in (3.12) from this is

$$\frac{2\lambda}{\pi} \int_1^\Lambda \frac{\mathrm{d}u}{(u^2-1)^{1/2}} \approx \frac{\lambda}{\pi} \ln\left[\left(\frac{W}{\Delta_0}\right)^2\right] \tag{3.16}$$

and this is quickly shown to cancel (with power-law corrections in the small quantity Δ_0/W) with the final, logarithmic term, in (3.12). Thus assuming the power-law corrections in Δ_0/W are neglectable in the formula for the soliton creation energy, we do the following. We re-represent the second term in (3.12) as minus the integral appearing in (3.16). Then combining this with the first integral in (3.12) and taking the upper limit of the integrals to be infinity we obtain the universal function of λ

$$\frac{E-E_0}{\Delta_0} = -\frac{1}{\pi} \int_1^\infty \mathrm{d}u \frac{u}{(u^2-1)^{1/2}} \ln\left[\frac{u^2}{u^2-1} \frac{\Gamma^4(\lambda u)^{1/2} \, e^{2\lambda/u}}{\Gamma^2(\lambda u+\lambda)\Gamma^2(\lambda u-\lambda)}\right]. \tag{3.17}$$

In appendix D we derive an alternative but equivalent integral representation for $(E-E_0)/\Delta_0$.

4. Evaluation of the formula for various values of λ

Formula (3.17) for the creation energy of the soliton (in units of Δ_0, the zero-temperature dimerization) does not, to our knowledge, have a simple form for general values of λ. In the case where λ is zero or a positive integer analytic expressions can be obtained as we shall demonstrate in this section. As it will turn out this discrete set includes the physical value of λ (i.e. the one that minimizes the energy) namely $\lambda = 1$.

To proceed we distinguish two separate cases:

Case (a). $\lambda = 0$. This corresponds to a discontinuous jump in the dimerization. In this limit the gamma functions are replaced by the reciprocal of their argument and we quickly obtain the result

$$\frac{E-E_0}{\Delta_0} = 1. \tag{4.1}$$

Case (b). $\lambda =$ positive integer. This case is more complicated than the previous one. We need to use the identities

$$\Gamma(a+\lambda) = \left(\prod_{j=1}^\lambda (a+\lambda-j)\right)\Gamma(a) \tag{4.2a}$$

$$\Gamma(a) = \left(\prod_{j=1}^\lambda (a-j)\right)\Gamma(a-\lambda). \tag{4.2b}$$

Using these within the equation for the soliton creation energy, (3.17), employing the identity $u/(u^2-1)^{1/2} \equiv (\mathrm{d}/\mathrm{d}u)(u^2-1)^{1/2}$ and integrating by parts we obtain:

$$\frac{E-E_0}{\Delta_0} = \frac{2}{\pi} \int_1^\infty \mathrm{d}u (u^2-1)^{1/2} \left(\frac{1}{u^2-1} + 2\lambda \sum_{j=1}^{\lambda-1} \frac{j}{(\lambda u)^2-j^2} - \frac{\lambda}{u^2}\right). \tag{4.3}$$

Finally we make the variable change $v = (u^2 - 1)^{1/2}$, employ twice the elementary identity $u^2/(u^2 + a^2) \equiv 1 - a^2/(u^2 + a^2)$ and use

$$1 - \lambda + \frac{2}{\lambda} \sum_{j=1}^{\lambda-1} j \equiv 0 \tag{4.4}$$

$$\int_0^\infty \frac{dv}{\sqrt{1+v^2}} \frac{1}{a^2 + v^2} = \frac{1}{\sqrt{a^2(1-a^2)}} \tan^{-1} \left(\frac{\sqrt{1-a^2}}{a^2} \right) \tag{4.5}$$

to obtain

$$\frac{E - E_0}{\Delta_0} = \frac{2}{\pi} \left[\lambda - \frac{2}{\lambda} \sum_{j=1}^{\lambda-1} (\lambda^2 - j^2)^{1/2} \tan^{-1} \left(\frac{j}{\sqrt{\lambda^2 - j^2}} \right) \right] \qquad \lambda = 1, 2, 3, \ldots. \tag{4.6}$$

As noted at the beginning of this section the physical value of λ corresponds to $\lambda = 1$. This may be verified directly by showing that (3.17) has an extremum at $\lambda = 1$ (alternatively the result of appendix D may be used to show this). That this point is a minimum follows from the convex nature of the free energy (we imagine that Δ_0 is held fixed and varying λ corresponds to varying the variational length scale ξ). Numerical analysis explicitly verifies the correctness of this. We thus have from (4.6) the physical soliton creation energy corresponding to $\lambda = 1$:

$$E - E_0 = \frac{2\Delta_0}{\pi}. \tag{4.7}$$

5. Conclusion

In this work we have studied solitons in polycetylene using functional methods. We have represented the soliton creation energy in terms of a functional determinant ratio and have provided an integral representation for the creation energy. This has avoided any phase shift analysis [2] and is an efficient method of tackling the problem. Out of this analysis we have shown that the soliton creation energy, $(E - E_0)/\Delta_0$, is rather accurately a universal function of $\lambda = \Delta_0 \xi/v_F$. We have also given some discussion to alternative ways of implementing cut-offs in the theory.

The motivation for presenting the analysis given lies in work to be presented in future publications. In these we will use the results derived above to test an approximation method for the calculation of free energies of fermionic systems involving extended structures (solitons).

These investigations will furnish us with a solid foundation for the approximate treatment of more complicated systems, where exact calculations have not yet been performed.

Acknowledgments

Appendix A

In this appendix we shall discuss several technical points concerning Grassmann functional integrals and their relationship to functional determinant ratios. Factors of two associated with spin will be neglected in this appendix.

In section 2 of this work we encountered functional integrals over Grassmann fields (which were antiperiodic in τ over β) of the form

$$I = \int d[\bar{\psi}] \, d[\psi] \exp\left(-\int \bar{\psi}(\partial_\tau + H)\psi\right) \tag{A.1}$$

and we asserted that

$$\ln(I/I_0) = \ln\left(\frac{\det[-\partial_\tau + H]}{\det[-\partial_\tau + H_0]}\right). \tag{A.2}$$

The integral I is usually taken to represent $\mathrm{Tr}[\exp(-\beta\hat{H})]$ where $\hat{H} = \int dx \, \bar{\psi}H\psi$, ψ is a Fermion field operator and Tr denotes a trace over the many particle Hilbert space. As has been pointed out by Faddeev [5] a number of operations not consistent with the definition of the functional integrals have been used to obtain the result (A.2). To see under what conditions (A.2) leads to the correct result we shall assume H (the first quantized Hamiltonian) is diagonalizable and has eigenvalues ε_k. By explicit calculation we have

$$\ln(I/I_0) = \sum_k \ln\left(\frac{1 + \exp(-\beta\varepsilon_k)}{1 + \exp(-\beta\varepsilon_k^0)}\right)$$

$$\equiv \sum_k \ln\left(\frac{\cosh(\beta\varepsilon_k/2)}{\cosh(\beta\varepsilon_k^0/2)}\right) - \beta/2 \sum_k (\varepsilon_k - \varepsilon_k^0). \tag{A.3}$$

The functional determinant ratio, by contrast, leads only to the first sum in (A.3). Thus only in circumstances where the second sum vanishes identically is it valid to use the functional determinant ratio. Perhaps the most important case where the second sum in (A.3) vanishes is when the spectra of both H and H_0 are symmetric, that is, there is a pairing such that for each non-zero eigenvalue there exists precisely one eigenvalue of the opposite sign. A detailed analysis is possible in the case of polycetylene where the boundary conditions and eigenvalues are known [6]. In the thermodynamic limit ($L \to \infty$) it can be verified that the pairing noted above does occur (for both the no-soliton and one-soliton sectors) and hence the determinant ratio is correct in this case. It should be said that a simple inspection of the first quantized hamiltonian H is not, on the face of it, sufficient to determine the pairing property since the spectrum depends also on the boundary conditions. It may be, however, that in the thermodynamic limit pairing (or its absence) may simply follow from the form of H and is insensitive to the precise boundary conditions; we suspect this to be so, however, we know of no proof of this.

A second point we wish to note in this appendix is that

$$\det[-\partial_\tau + H] = \sqrt{\det[-\partial_\tau^2 + H^2]}. \tag{A.4}$$

This holds simply because the eigenvalues of $-\partial_\tau$ are $i\omega_n$ where

$$\omega_n = (2n + 1)\pi/\beta \tag{A.5}$$

Thus multiplying the terms in the determinant with $i\omega_n$ and $-i\omega_n$ leads to a factor $\omega_n^2 + H^2$. This is a single factor from $\det[-\partial_\tau^2 + H^2]$ and the square root allows us to allow ω_n to cover its full range. (This elementary analysis also indicates that the ratio of functional determinants will be non-negative.) More generally, (A.4) follows from an operator, say Q having a real (and positive) determinant. Then $\det[Q] = \sqrt{\det[QQ^\dagger]}$.

Appendix B

In this appendix we will show the equivalence of three different cut-off procedures for the calculation of the polyacetylene free energy for uniform systems at zero temperature. With some work the results of this appendix can be extended to polyacetylene with a soliton present.

The uniform system consists of a half-filled conduction band of electrons. The occupied states have energies ranging from $-v_F p_F$ to 0 (measured relative to the Fermi energy) and the energy bandwidth is $W = 2v_F p_F$. We shall express cut-off quantities in terms of W. Thus momentum integrals are bounded by $|p| \leq W/2v_F$. We calculate the free energy of a uniform (dimerized) system of length L relative to the free energy of an undimerized system being given by (the limit $\beta \to \infty$ is implicit in what follows). Using in (2.4) the identity $\ln \det \equiv \mathrm{Tr} \ln$ and employing the Schwinger 'proper time' integral for the logarithms [7]: $\ln(A/B) = -\int_0^\infty \mathrm{d}s/s \, (\mathrm{e}^{-sA} - \mathrm{e}^{-sB})$ we have

$$
\begin{aligned}
F - F_0 &= -\frac{1}{\beta} \mathrm{Tr} \ln \left(\frac{-\partial_\tau^2 + H_0^2}{-\partial_\tau^2 - v_F^2 \partial_x^2} \right) + \frac{\omega_Q^2}{2g^2} \Delta_0^2 L \\
&= 2L \int_0^\infty \frac{\mathrm{d}s}{s} \int \frac{\mathrm{d}\omega}{2\pi} \int_{|p| \leq W/2v_F} \frac{\mathrm{d}p}{2\pi} \mathrm{e}^{-s(\omega^2 + v_F^2 p^2)} (\mathrm{e}^{-s\Delta_0^2} - 1) + \frac{\omega_Q^2}{2g^2} \Delta_0^2 L \\
&= \frac{2L}{\pi} \int_0^{W/2v_F} \mathrm{d}p (v_F p - \sqrt{\Delta_0^2 + v_F^2 p^2}) + \frac{\omega^2}{2g^2} \Delta_0^2 L.
\end{aligned}
\tag{B.1}
$$

Expanding the integrals in powers of Δ_0/W and neglecting corrections $O(\Delta_0/W)^n$, $n > 1$, gives

$$
\frac{F - F_0}{L} \approx -\frac{\Delta_0^2}{2\pi v_F} \left(1 - 2 \ln \left(\frac{2\Delta_0}{W} \right) \right) + \frac{\omega_Q^2}{2g^2} \Delta_0^2.
\tag{B.2}
$$

Minimizing $F - F_0$ with respect to Δ_0 results in the zero-temperature dimerization equation (3.1).

Alternatively one can introduce a cut-off in the integral over frequencies; $|\omega| \leq W/2$, leading to the same result. This is clear from the second of equations (B.1) where the integrand is symmetric in ω and $v_F p$.

A third method of putting in a cut-off comes from the observation that small values of the proper time, s, corresponds to large energies. Consequently cutting off the small s part of the integral is equivalent to cutting off the large momenta or frequencies. Let us introduce a cut-off as follows

$$
\begin{aligned}
F - F_0 &= 2L \int_{1/\tilde{W}^2}^\infty \frac{\mathrm{d}s}{s} \int \frac{\mathrm{d}p}{2\pi} \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-s(v_F^2 p^2 + \omega^2)} (\mathrm{e}^{-\Delta_0^2 s} - 1) + \frac{\omega_Q^2}{2g^2} \Delta_0^2 L \\
&= \frac{L \Delta_0^2}{2\pi v_F} \int_{(\Delta_0/\tilde{W})^2}^\infty \frac{\mathrm{d}s}{s^2} (\mathrm{e}^{-s} - 1) + \frac{\omega_Q^2}{2g^2} \Delta_0^2 L.
\end{aligned}
\tag{B.3}
$$

Expanding again in powers of $\Delta_0 / \tilde{W}$ we find

$$\frac{F - F_0}{L} \approx \frac{\Delta_0^2}{2\pi v_F} \left(\ln \left(\frac{\Delta_0}{\tilde{W}} \right)^2 + \gamma - 1 \right) + \frac{\omega_Q}{2g^2} \Delta_0^2 \tag{B.4}$$

where γ is Euler's constant.

This leads to the same dimerization equation as found previously provided we make the identification $\tilde{W} = e^{\gamma/2} W/2$.

Appendix C

In this appendix we derive the determinant formula (4.8) using a theorem of scattering theory. Let

$$H = -\frac{d^2}{dx^2} + U(x) \tag{C.1}$$

be a Hamiltonian such that $\lim_{x \to \pm\infty} U(x) = a^2$ and let

$$H_0 = -\frac{d^2}{dx^2} + a^2. \tag{C.2}$$

Now take a scattering state eigenfunction $f(x, z)$ of H such that

$$\lim_{x \to +\infty} f(x, z) e^{-ikx} = 1 \tag{C.3}$$

for $k^2 = z - a^2 > 0$. Then the general form for $f(x, z)$ at $x \to -\infty$ is

$$\lim f(x, z) = e^{-ikx} A(z) + e^{ikx} F(z). \tag{C.4}$$

Then it can be shown that [3]

$$\frac{\det(H - z)}{\det(H_0 - z)} = F(z). \tag{C.5}$$

For our Hamiltonian the scattering wavefunction satisfying the condition (C.3) is

$$f(x, z) = 2^{ik}(1 - \eta^2)^{-ik/2} F(-ik - \lambda, -ik + \lambda + 1, -ik + 1, \tfrac{1}{2}(1 - \eta)) \tag{C.6}$$

where $\eta = \tanh x$, $k^2 = z$ and $F(\alpha, \beta, \gamma, z)$ is the Gauss hypergeometric function. The asymptotic form of (C.6) for $x \to \infty$ is

$$f(x, z) \to i \frac{\sin \pi\lambda}{\sinh \pi k} e^{-ikx} + \frac{\Gamma(-ik)\Gamma(1 - ik)}{\Gamma(-ik - \lambda)\Gamma(-ik + \lambda + 1)} e^{ikx} \tag{C.7}$$

from which it follows that

$$\frac{\det[-d^2/dx^2 - \lambda(\lambda + 1) \operatorname{sech}^2 x - z]}{\det[-d^2/dx - z]} = \frac{\Gamma(-ik)\Gamma(1 - ik)}{\Gamma(-ik - \lambda)\Gamma(-ik + \lambda + 1)}. \tag{C.8}$$

For $z < 0$ the analytical continuation is carried out by making the replacement $k \to i\sqrt{-z}$ and we finally obtain

$$\frac{\det[-d^2/dx^2 - \lambda(\lambda + 1) \operatorname{sech}^2 x - z]}{\det[-d^2/dx^2 - z]} = \frac{\Gamma(\sqrt{-z})\Gamma(1 + \sqrt{-z})}{\Gamma(\sqrt{-z} - \lambda)\Gamma(\sqrt{-z} + \lambda + 1)}. \tag{C.9}$$

Appendix D

In this appendix we derive an alternative integral representation for the soliton creation energy to the one obtained in section 3. The form presented here makes it manifestly obvious that $(E - E_0)/\Delta_0$ has an extremum at $\lambda = 1$ and may have advantages in numerical evaluation of this quantity.

We use the integral representation for $\ln \Gamma(z)$ [8]

$$\ln \Gamma(z) = \int_0^\infty \frac{dt}{t} \left(\frac{e^{-zt} - e^{-t}}{1 - e^{-t}} + (z - 1) e^{-t} \right) \tag{D.1}$$

Using this in (3.17) leads to

$$\frac{E - E_0}{\Delta_0} = -\frac{1}{\pi} \int_1^\infty du \frac{u}{(u^2 - 1)^{1/2}} \left(\ln\left(\frac{u^2}{u^2 - 1} \right) + \frac{2\lambda}{u} \right.$$
$$\left. + \int_0^\infty \frac{dt}{t} \frac{(2e^{-\lambda ut} - e^{-\lambda(u+1)t} - e^{-\lambda(u-1)t})}{1 - e^{-t}} \right). \tag{D.2}$$

The integral involving the logarithm may be evaluated exactly and has the value -1. For the integral over t we write

$$e^{-\lambda ut} = -\frac{1}{\lambda u} \frac{d}{dt} e^{-\lambda ut} \tag{D.3}$$

and use this to integrate by parts. We obtain

$$\frac{E - E_0}{\Delta_0} = -1 - \frac{2}{\lambda \pi} \int_1^\infty du \frac{1}{(u^2 - 1)^{1/2}} \int_0^\infty dt \, e^{-\lambda ut} \frac{d}{dt} \left(\frac{2 - e^{-\lambda t} - e^{\lambda t}}{t(1 - e^{-t})} \right) \tag{D.4}$$

Using the integral representation of the Bessel function $K_0(z)$ [8]

$$K_0(z) = \int_1^\infty \frac{e^{-zt}}{(t^2 - 1)^{1/2}} dt \tag{D.5}$$

enables the u integration to be performed and leads, after a rescaling of the integration variable, to the alternative integral representation for $(E - E_0)/\Delta_0$:

$$\frac{E - E_0}{\Delta_0} = -1 - \frac{2}{\pi} \int_0^\infty dt \, K_0(t) \frac{d}{dt} \left(\frac{2 - e^{-t} - e^t}{t(1 - e^{-t/\lambda})} \right) \tag{D.6}$$

As pointed out above the advantage of this representation appears when we differentiate with respect to λ. We obtain

$$\frac{d}{d\lambda} \left(\frac{E - E_0}{\Delta_0} \right) = \frac{2}{\pi \lambda^2} \int_0^\infty dt \, K_0(t) \frac{d}{dt} \left(\frac{\sinh^2(t/2)}{\sinh^2(t/2\lambda)} \right) \tag{D.7}$$

which makes it clear that there is an extremum at $\lambda = 1$. A numerical evaluation of the second derivitive indicates that $\lambda = 1$ is a minimum; as we would expect from convexity of the free energy.

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