

Ballistic transport in classical and quantum integrable systems

Xenophon Zotos

*Institut Romand de Recherche Numérique en Physique des Matériaux,
PPH-Ecublens, CH-1015 Lausanne, Switzerland*

In this essay, we first sketch the development of ideas on the extraordinary dynamics of integrable classical nonlinear and quantum many body Hamiltonians. In particular, we comment on the state of mathematical techniques available for analyzing their thermodynamic and dynamic properties.

Then, we discuss the unconventional finite temperature transport of integrable systems using as example the classical Toda chain and the toy model of a quantum particle interacting with a fermionic bath in one dimension; we focus on the singular long time asymptotic of current-current correlations, we introduce the notion of the Drude weight and we emphasize the role played by conservation laws in establishing the ballistic character of transport in these systems.

PACS numbers: 71.27.+a, 05.45, 72.10.-d

1. INTRODUCTION

The extraordinary stability of solitons upon collisions in integrable nonlinear systems was first discovered in a numerical simulation of the Korteweg-de-Vries evolution equation, a system commonly studied in hydrodynamics and plasma physics¹. This discovery was soon followed by the development of a beautiful mathematical theory - the Inverse Scattering Method (ISM) - that allows the analytical evaluation of the time evolution of an initial pulse configuration using linear operations²; this is the analogue of the Fourier Transform for linear systems. These seminal works opened the new and still rapidly expanding field of nonlinear physics, with developments ranging from mathematical physics to applications³.

Here, we should point out that there is a fundamental distinction between *integrable systems* (mostly one dimensional) characterized by the pres-

X. Zotos

ence of “mathematical solitons” and those with “topological solitons”. On the one hand, the stability of mathematical solitons is guaranteed by a subtle interplay between dispersion and nonlinearity; this interplay is expressed by the existence of a macroscopic number of *conservation laws* constraining the dynamical evolution. On the other hand, the stability of topological solitons is enforced by a topological constraint; of course there are examples, like the sine-Gordon field theory, which possess topological solitons but they are also integrable. In this work we will focus on the transport properties of integrable systems.

Due to the presence and stability upon scattering of nonlinear excitations, integrable systems are expected to show unconventional finite temperature transport properties, as ideal thermal, charge or spin conductivities, ballistic rather than diffusive transport. Within the traditional framework of linear response theory, the finite temperature dynamic correlations characterize the transport behavior and they are directly linked to experimental observations. However, although integrable models are considered as exactly soluble, meaning that the initial value problem can be exactly analyzed using the ISM, rather little progress has been done in the evaluation of dynamic correlations which remains at best technically very involved.

In the quantum domain, parallel to developments on the analysis of classical integrable nonlinear systems, in the early 80’s it was realized that the exact solution of a certain class of one dimensional quantum models by the Bethe ansatz (BA) method was equivalent to a quantum version of the ISM⁴. In this class belong well known prototype systems as the Hubbard or spin-1/2 Heisenberg model, commonly used for the description of (quasi) one-dimensional electronic or magnetic materials. The BA method provides the exact eigenfunctions and eigenvalues and by a certain procedure (and assumptions) the exact thermodynamic properties and excitation spectrum. Similarly to their classical counterparts, the quantum systems possess a macroscopic number of conservation laws, characteristic of their integrability. It should therefore come as no surprise the proposition that quantum integrable systems should also exhibit unconventional transport⁵. The situation however is similar to the one of classical systems; although the exact eigenfunctions and eigenvalues are known, the calculation of finite temperature dynamic correlations is still out of reach for most of the models.

In the following, we discuss two simple examples, one classical and one quantum, in order to show the ideal conducting properties of integrable systems. Our strategy is to focus on the *long time* asymptotic value of the current correlations in order to demonstrate the ballistic transport instead of attempting to evaluate the full frequency dependence of the conductivity (or mobility). Furthermore, instead of linking the ideal conductivity to the

Ballistic transport

dynamics of soliton excitations, not very transparent for quantum many body systems, we directly relate it to the conservation laws characterizing integrable systems.

First, we present a study of the energy current - current correlations (related to the thermal conductivity) for the classical Toda chain. Second, we introduce the notion of the *Drude weight* as a criterion of ideal conductivity and evaluate it exactly using the Bethe ansatz method in the context of the mobility for a toy model describing a quantum particle interacting with a fermionic bath.

2. A classical system: the Toda chain

The classical Toda lattice is a prototype model for studying the physics of nonlinear excitations⁶. It is one of the first models analyzed using the Inverse Scattering method⁷, the conservation laws characterizing this system⁸ have been presented and it has even been invoked in attempts to describe nonlinear transport in DNA molecules⁹. As we mentioned above, although the initial value problem and the thermodynamic properties can be analytically studied, there is no clear picture on the finite temperature dynamic correlations¹⁰.

A physical quantity of interest in an anharmonic chain is the heat conductivity. In a generic case, it is expected that the energy current correlations decay to zero at long times and the decay is fast enough so that a transport coefficient can be defined. This behavior seems rather difficult to observe in several one dimensional systems^{11,12}, where the currents decay to zero but often too slowly, leaving the issue of diffusive transport controversial.

For an integrable model, ideal conducting behavior is expected with current correlations decaying to a finite value at long times. To quantify the contribution of nonlinear excitations, different ingenious methods have been devised⁹ (soliton counting procedures). Here, we will use the long time asymptotic value of current correlations as a measure of ideal transport, related in integrable systems to the existence of conservation laws.

To establish this relation, we will use an inequality proposed by Mazur¹³, linking the long time asymptotic of dynamic correlations functions to the presence of conservation laws:

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle A(t)A \rangle dt \geq \sum_n \frac{\langle A Q_n \rangle^2}{\langle Q_n^2 \rangle}. \quad (1)$$

Here $\langle \rangle$ denotes thermodynamic average, the sum is over a set of conserved quantities Q_n , orthogonal to each other $\langle Q_n Q_m \rangle = \langle Q_n^2 \rangle \delta_{n,m}$ and we suppose that $\langle A \rangle = 0$.

X. Zotos

The classical Toda Hamiltonian for a chain of L sites with periodic boundary conditions is given in reduced units by:

$$H = \sum_{l=1}^L \frac{p_l^2}{2} + e^{-q_l} \quad (2)$$

where p_l is the momentum of particle l , x_l its position and $q_l = x_{l+1} - x_l$.

The energy current for a system of interacting particles is given by¹⁴:

$$j^E = \sum_{l=1}^L p_l h_l + \frac{(p_{l+1} + p_l)}{2} q_l e^{-q_l} \quad (3)$$

where $h_l = \frac{p_l^2}{2} + \frac{1}{2}(e^{-q_l} + e^{-q_{l-1}})$.

We consider dynamic correlation functions in the fixed temperature-pressure thermodynamic ensemble:

$$\langle A(t)A \rangle = Z^{-1} \int \prod_{l=1}^L dp_l dq_l A(t) A e^{-\beta(H+PL)} \quad (4)$$

where $Z = \int \prod_{l=1}^L dp_l dq_l e^{-\beta(H+PL)}$, $L = \sum_{l=1}^L q_l$, P is the pressure and β the inverse of the temperature.

In this thermodynamic ensemble, equal time correlation functions can be calculated analytically. For instance the average distance is given by:

$$\langle q \rangle = \ln(\beta) - \Psi(\beta P) \quad (5)$$

where $\Psi(z)$ is the digamma function.

The classical Toda lattice is characterized by a macroscopic number of conservation laws. The first few ones are:

$$Q_1 = \sum_{l=1}^L p_l \quad (6)$$

$$Q_2 = \sum_{l=1}^L \frac{p_l^2}{2} + e^{-q_l} \quad (7)$$

$$Q_3 = \sum_{l=1}^L \frac{p_l^3}{3} + (p_l + p_{l+1})e^{-q_l} \quad (8)$$

$$Q_4 = \sum_{l=1}^L \frac{p_l^4}{4} + (p_l^2 + p_l p_{l+1} + p_{l+1}^2)e^{-q_l} + \frac{1}{2}e^{-2q_l} + e^{-q_l} e^{-q_{l+1}} \quad (9)$$

$$Q_5 = \sum_{l=1}^L \frac{p_l^5}{5} + (p_l^3 + p_l^2 p_{l+1} + p_l p_{l+1}^2 + p_{l+1}^3)e^{-q_l} \quad (10)$$

$$+ (p_l + p_{l+1})e^{-2q_l} + (p_l + 2p_{l+1} + p_{l+2})e^{-q_l} e^{-q_{l+1}} \dots \quad (11)$$

Ballistic transport

with Q_1 the total momentum, of course present in all translationally invariant systems, integrable or not, as also Q_2 the total energy. According to the standard Green-Kubo formulation of transport theory¹⁴ “subtracted fluxes” should be used in the dynamic correlation functions determining the transport coefficients. So in the case of energy transport we will study the decay of the “subtracted” energy current¹⁵:

$$\tilde{j}^E = j^E - \frac{\langle Q_1 j^E \rangle}{\langle Q_1^2 \rangle} Q_1 \quad (12)$$

We see that the use of a subtracted flux is equivalent to removing the contribution of Q_1 in the long time asymptotic bound¹³ for $\langle j^E(t) j^E \rangle$.

We will now calculate a bound on the long time asymptotic value of $\langle j^E(t) j^E \rangle$ by the Mazur inequality eq.(1) using the first m conservation laws. We should note that Q_3 has a structure very similar to the energy current, so we expect a large contribution from this term; actually in some quantum models like the spin-1/2 Heisenberg chain or the t-J model, the energy current is identical to a conservation law, directly implying a non-decaying energy current and thus infinite thermal conductivity¹⁶. Here, Q'_n s with $n = \text{even}$ do not couple to \tilde{j}^E so we will consider only $Q_n, n = 3, 5, 7$. Higher Q'_n s can of course be included but the calculations become rather cumbersome. Orthogonalizing the conserved quantities which appear in the right hand side of eq.(1) is equivalent to evaluating the expression:

$$C_{j^E j^E}^m = \langle \tilde{j}^E | Q \rangle \langle Q | Q \rangle^{-1} \langle Q | \tilde{j}^E \rangle \quad (13)$$

where $\langle Q | Q \rangle$ is the $m \times m$ overlap matrix of Q'_n s and $\langle Q | \tilde{j}^E \rangle$ the overlap vector of \tilde{j}^E with the Q'_n s.

In Fig.1 we show the temperature dependence of $C_{j^E j^E}^m / \langle \tilde{j}^E \rangle^2$ for $m = 1$ ($n = 3$), $m = 2$ ($n = 3, 5$) and $m = 3$ ($n = 3, 5, 7$). At low T the behavior is linear with slope $\frac{3}{35}$ for $m = 2$ and $\frac{4}{63}$ for $m = 3$. It is interesting that this value is comparable to the value for the density of solitons¹⁷ $N_s/N = \ln(2)/\pi^2 T$. So, we find that the long time asymptotic value of the subtracted energy current correlations is finite and most interestingly that it increases with temperature. This trend we can interpret as evidence for an increasing contribution of thermally excited nonlinear excitations on the ballistic transport.

The idea presented here provides, on the one hand a conceptual understanding of the role played by the conservation laws on the finite temperature dynamic correlations and on the other hand a simple analytical method for evaluating, or at least giving bounds on their long time asymptotic value. A similar analysis can be carried out for quantum integrable systems¹⁶ al-

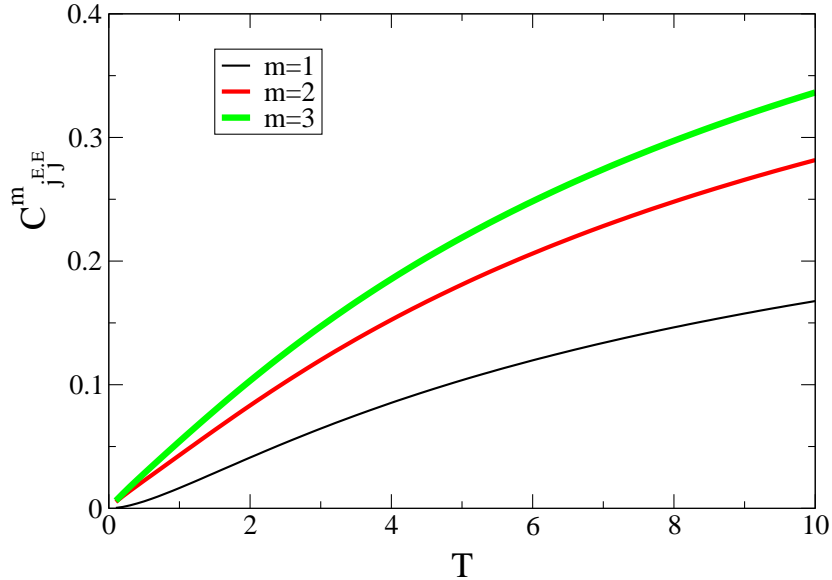


Fig. 1. Lower bounds on the long time asymptotic value of energy current correlations.

though the complexity of the quantum conservation laws renders their wide use rather limited.

3. A quantum system: the “heavy particle” model

The Drude weight D (or charge stiffness) was introduced as a criterion of an ideal conducting or insulating state at zero temperature¹⁸ and recently extended as a measure of ideal transport at finite temperatures⁵. Within linear response theory, it is essentially the prefactor of the low frequency reactive part of the conductivity, $\sigma'' = 2D/\omega|_{\omega \rightarrow 0}$, a finite D implying a freely accelerating system. For a normal, diffusive system the Drude weight is zero at any finite temperature in the thermodynamic limit; according to the standard scenario the weight at zero frequency spreads to a “Drude peak” with width proportional to the inverse of the collision time. As we will see below, in integrable systems the Drude weight remains finite at all temperatures indicative of ballistic rather than diffusive transport.

The Drude weight can be conveniently evaluated¹⁸ as the thermal average of curvatures of energy levels ϵ_n of the system subject to a fictitious flux ϕ ,

Ballistic transport

$$D = \frac{1}{2L} \sum_n p_n \frac{\partial^2 \epsilon_n}{\partial \phi^2} \Big|_{\phi \rightarrow 0} \quad (14)$$

where p_n are the Boltzmann weights and the sum is over all eigenstates of the system. It is also equal to the long time asymptotic value of the current-current correlations¹⁶,

$$D = \frac{\beta}{2L} \langle j(t)j \rangle \Big|_{t \rightarrow \infty} = \frac{\beta}{2L} \sum_n p_n |\langle n|j|n \rangle|^2 \quad (15)$$

so useful bounds on D can be obtained using the Mazur inequality following the same formulation as in the previous example.

For integrable quantum many body models it can be evaluated exactly following recent developments in the Bethe ansatz technique, thus providing essential information on the transport properties of these systems without requiring the full calculation of the frequency dependence of the conductivity. This type of analysis, still under discussion as it is technically involved, has been carried out for several one dimensional integrable quantum models as the Hubbard chain, the spin 1/2 Heisenberg and the nonlinear- σ model^{20,21,22}. These calculations show that in most of the cases the Drude weight is finite at all temperatures implying ideal thermal, charge or spin conductivity. Recently, investigation of the finite temperature of these systems was also carried out by a semiclassical approach²³ and within the Luttinger liquid description^{24,25}.

Here, we will demonstrate the idea behind this type of Bethe ansatz analysis by evaluating the Drude weight related to the mobility of a quantum particle interacting with a bath of fermions in a one dimensional system¹⁹. A similar analysis was carried out for a particle moving on a lattice⁵ but the case discussed below is simpler and shows a qualitatively new behavior.

We consider a particle with coordinate y moving on a system of length L with periodic boundary conditions and interacting with a set of N fermions described by the coordinates x_j via a δ -function interaction of strength c ,

$$H = - \sum_j \frac{\partial^2}{\partial x_j^2} - \frac{\partial^2}{\partial y^2} + 2c \sum_j \delta(x_j - y). \quad (16)$$

When the mass of the “heavy particle” is equal to the mass of the fermions the model is integrable and so we expect a ballistic behavior of the mobility and therefore a finite Drude weight. To evaluate D using eq. (14), we consider the dependence of the energy levels on a flux ϕ acting only on the heavy particle. The momenta k_j and the collective coordinate Λ describing the Bethe ansatz wavefunctions are then given by the following standard equations obtained by applying periodic boundary conditions,

X. Zotos

$$Lk_j = 2\pi I_j + \theta(k_j - \Lambda), \quad j = 1, \dots, N+1, \quad (17)$$

$$\theta(p) = -2 \tan^{-1}(2p/c), \quad (18)$$

$$L \sum_{j=1}^{N+1} k_j = 2\pi \sum_{j=1}^{N+1} I_j + 2\pi J + L\phi. \quad (19)$$

The eigenstates are characterized by the quantum numbers (I_j, J) and their energy is given by:

$$E = \sum_{j=1}^{N+1} \epsilon(k_j) = \sum_{j=1}^{N+1} k_j^2. \quad (20)$$

These equations can be solved to order $1/L$ as we consider the effect of the one particle on the ensemble of fermions.

$$k_j = k_j^0 + \frac{1}{L}\theta(k_j - \Lambda), \quad k_j^0 = \frac{2\pi I_j}{L} \quad (21)$$

Thus the total energy can be written as,

$$E = \sum_j \epsilon(k_j^0) + \frac{2}{L} k_j^0 \theta(k_j^0 - \Lambda), \quad (22)$$

$$\frac{1}{L} \sum_j \theta(k_j^0 - \Lambda) = \frac{2\pi J}{L} + \phi. \quad (23)$$

Going to the continuum limit we obtain:

$$E(\rho(k), \Lambda) = \frac{L}{2\pi} \int dk \rho(k) (k^2 + \frac{2}{L} k \theta(k - \Lambda)), \quad (24)$$

$$P + \phi = \frac{1}{2\pi} \int dk \rho(k) \theta(k - \Lambda), \quad P = \frac{2\pi J}{L}. \quad (25)$$

Now we can define a correlation energy $\epsilon_c(\Lambda)$ assuming that the distribution of the fermion momenta is not affected by the presence of the extra particle and replacing the density $\rho(k)$ by the Fermi-Dirac distribution $f(k)$,

$$\epsilon_c(\Lambda) = \frac{1}{2\pi} \int dk f(k) 2k \theta(k - \Lambda). \quad (26)$$

Using this formulation and the definition of the Drude weight eq.(14) we obtain:

$$D = \frac{1}{2\pi Z_\Lambda} \int d\Lambda g(\Lambda) w(\Lambda) \frac{1}{2} \frac{\partial^2 \epsilon_c(\Lambda)}{\partial \phi^2} \quad (27)$$

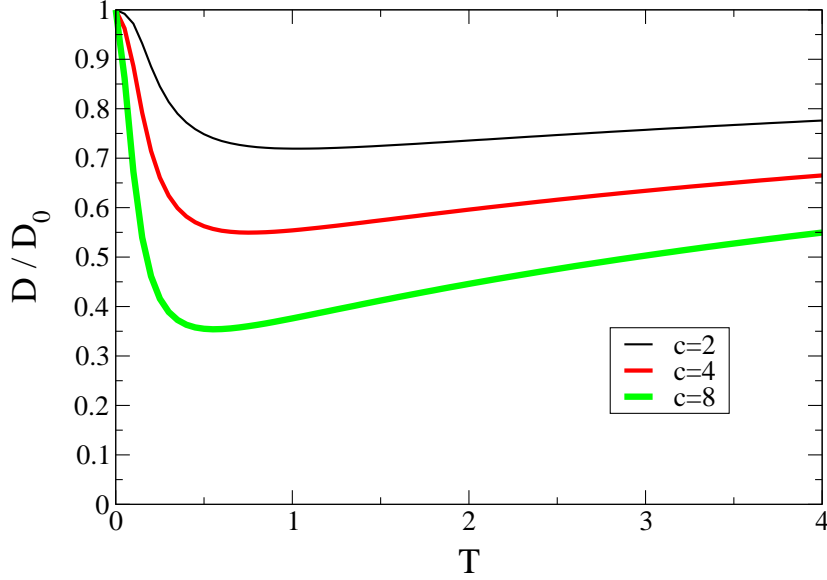


Fig. 2. Drude weight of the “heavy particle”.

where,

$$g(\Lambda) = \frac{\partial P}{\partial \Lambda} = \frac{1}{2\pi} \int dk f(k) \frac{\partial \theta(k - \Lambda)}{\partial \Lambda}, \quad (28)$$

$$Z_\Lambda = \frac{1}{2\pi} \int d\Lambda g(\Lambda) w(\Lambda), \quad w(\Lambda) = e^{-\beta \epsilon_c(\Lambda)}. \quad (29)$$

In Fig. 2 we show the normalized Drude weight D/D_0 for different values of the interaction c as a function of temperature, with $D_0 = D(T = 0) = (\pi/2)(\tan^{-1}(2k_F/c) - (2k_F/c)/(1+(2k_F/c)^2))/\tan^{-1}(2k_F/c)^2$ and $k_F = \pi n$. The chemical potential is chosen so that we consider density $n = 1$; upon scaling $n \rightarrow nc, \beta \rightarrow \beta/c^2$ the Drude weight D remains the same. We note that the behavior of D is not monotonic, initially decreasing at low temperatures because of the interaction and then tending to the free particle value at high temperatures. This is in contrast to the Drude weight of systems on a lattice (tight binding models) where D goes always to zero as β at high temperatures. The difference in behavior can be attributed to the bounded spectrum in lattice models in contrast to the unbounded one for continuous models. Furthermore, numerical calculations on this model show that, the Drude weight vanishes at any finite temperature when the mass of the “heavy particle” is not equal to that of fermions, as expected for any normal system. In conclusion, the presented analysis demonstrates the basic features of the generic finite temperature ballistic transport behavior of integrable quantum many body systems.

X. Zotos

ACKNOWLEDGMENTS

It is my honor and pleasure to dedicate this paper to Professor Peter Wölfle on the occasion of his 60th birthday. This research was supported by the Swiss National Science Foundation, the University of Fribourg and Neuchâtel. I would also like to thank P. Prelovšek, H. Castella and F. Naef for our collaboration in the development of the ideas here presented.

REFERENCES

1. N. J. Zabusky and M. D. Kruskal, *Phys. Rev. Lett.* **15**, 240 (1965).
2. C. S. Gardner, J. M. Greene, M. D. Kruskal and R. M. Miura, *Phys. Rev. Lett.* **19**, 1095 (1967).
3. “Optical solitons: theoretical challenges and industrial perspectives”, editors: V.E. Zakharov and S. Wabnitz, *Les Houches Workshop*, Springer (1998).
4. “Quantum Inverse Scattering Method and Correlation Functions”, V.E. Korepin, N.M. Bogoliubov and A.G. Izergin, *Cambridge Univ. Press* (1993).
5. H. Castella, X. Zotos, P. Prelovšek, *Phys. Rev. Lett.* **74**, 972 (1995).
6. M. Toda, “Theory of Nonlinear Lattices”, *Springer Series in Solid-State Sciences 20*, Springer-Verlag, (1981).
7. H. Flaschka, *Phys. Rev.* **B9**, 1924 (1974).
8. M. Henon, *Phys. Rev.* **B9**, 1921 (1974).
9. V. Muto, A.C. Scott and P.L. Christiansen, *Physica* **D44**, 75 (1990).
10. See for instance: T. Schneider and E. Stoll, *Phys. Rev. Lett.* **45**, 997 (1980); A. Cuccoli et al., *Phys. Rev.* **B47**, 7859 (1993); N. Theodorakopoulos and M. Peyrard, *Phys. Rev. Lett.* **83**, 2293 (1999).
11. C. Giardina et al., *Phys. Rev. Lett.* **84**, 2144 (1998).
12. See however the system analyzed in, M. Garst and A. Rosch, *Eur. Lett.* **55**, 66 (2001).
13. P. Mazur, *Physica* **43**, 533 (1969); M. Suzuki, *Physica* **51**, 277 (1971).
14. J.A. McLennan, “Introduction to non equilibrium statistical mechanics”, *Prentice-Hall Advanced Reference Series*, (1989).
15. Basically equivalent to the entropic component, N.W. Ashcroft and N.D. Mermin, “Solid State Physics”, *Holt, Rinehart and Winston*, p. 253 (1976).
16. X. Zotos, F. Naef and P. Prelovšek, *Phys. Rev.* **B55**, 11029 (1997).
17. F.G. Mertens and H. Büttner, *Phys. Lett.* **84A**, 335 (1981).
18. W. Kohn, *Phys. Rev.* **A171**, 133 (1964).
19. J. B. McGuire, *J. Math. Ph.* **6**, 432 (1965); C. N. Yang, *Phys. Rev. Lett.* **19**, 1312 (1967).
20. S. Fujimoto and N. Kawakami, *J. Phys. A.* **31**, 465 (1998).
21. S. Fujimoto, *J. Phys. Soc. Jpn.* **68**, 2810 (1999).
22. X. Zotos, *Phys. Rev. Lett.* **82**, 1764 (1999).
23. K. Damle and S. Sachdev, *Phys. Rev.* **B57**, 8307 (1998).
24. T. Giamarchi and A. J. Millis, *Phys. Rev.* **B46**, 9325 (1992).
25. A. Rosch and N. Andrei, *Phys. Rev. Lett.* **85**, 1092 (2000).