Exact Solution of a Nonlinear Eigenvalue Problem in One Dimension

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An exact solution of the eigenvalue problem

$$\{-d^2/dx^2 + \Delta[1 - a_0\rho(x)]\}\psi_n(x) = E_n\psi_n(x)$$

with $\rho(x) = \sum_{n=1}^{N}|\psi_n(x)|^2$ and with periodic boundary condition is presented. The solution gives rise to a density wave with $[\text{const} - \rho(x)]$ proportional to $\text{sn}^2[(x/\lambda)|m]$ for suitable values of the parameters λ and m. The solution rests upon some remarkable properties of the solutions of Lamé's equation.

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The present work is concerned with an exact solution of a Hartree-like nonlinear eigenvalue problem (the N-component nonlinear Schrödinger equation) in one dimension,

$$\{-d^2/dx^2 + \Delta[1 - a_0\rho(x)]\}\psi_n(x) = E_n\psi_n(x), \quad (1)$$

where $0 \leq x \leq L$, $1 \leq n \leq N$, $a_0 = L/N$, Δ is a coupling constant,

$$\rho(x) = \sum_{n=1}^{N}|\psi_n(x)|^2 \quad (2)$$

and ψ_n's are orthonormal and obey periodic boundary conditions $\psi_n(x+L) = \psi_n(x)$.

This problem has been considered approximately in various contexts earlier. In the context of the nuclear many-body problem[1] Eqs. (1) appear as Hartree's equations for N spinless fermions constrained to a box of size L, interacting through a two-body attractive δ-function potential with strength Δ. In an important paper entitled "Structure of Nuclear Matter" Overhauser[1] presented a

weak-coupling theory ($\Delta \to 0$) and showed that there exist solutions with broken translation invariance, in addition to the trivial solutions $\psi(x) \sim \exp(iKx)$, which are always lower in (total) energy. Overhauser found that the fermion density develops a sinusoidal shape with an amplitude that depends nonanalytically on the coupling Δ as $\Delta \to 0$. These "charge-density waves" have found wide application in condensed-matter physics. Exact solutions of the equations do not appear to be known for large N, although the time-dependent version of the problem with boundary conditions

$$\psi_n(x) \xrightarrow[x \to \pm \infty]{} 0$$

seems to be better understood.[2]

These equations may be viewed as the Hartree-Fock (HF) equations for a system of $2N$ spin-$\frac{1}{2}$ fermions on a ring with an attractive δ-function interaction, which is of course a celebrated exactly solvable many-body problem.[3,4] Lieb and

de Llano (LL) have studied the HF theory for this case rigorously.[5] The following results of LL are important in the present context: (a) HF theory exists in the sense that the total HF energy attains its minimum for orbitals which satisfy the HF equations. (b) For the case of $2N$ fermions, the optimal orbitals are solutions of the restricted HF equations which reduce essentially to Eqs. (1). (c) All the orbitals are real in the ground state. In addition LL solve Eqs. (1) for the case $N = 1$ and 2.

The motivation for the study of this problem was in yet another context. Equations (1) are

related to the problem of Peierls distortion of the linear chain. Here one considers fermions (spinless for convenience) in a linear chain coupled to the lattice within the adiabatic approximation. This system was shown by Peierls to be unstable with respect to the formation of a periodic lattice distortion accompanied by the opening of a gap in the spectrum at the Fermi level.[6] In the limit of low concentration, the kinetic energy may be taken to be quadratic in momentum and the contiuum limit for the lattice leads to the physical system modeled by Eqs. (1). Consider the energy functional

$$E[\{\psi_n(x)\}, V(x)] = \int_0^L dx \left[\sum_n |\psi_n'(x)|^2 + V(x)\rho(x) + (2\Delta a_0)^{-1} V^2(x)\right]. \tag{3}$$

Here $V(x)$ represents the strain field and extremizing E with respect to $V(x)$ [subject to $\int dx V(x) = 0$] and $\psi_n(x)$ yields Eqs. (1). Sutherland and the present author studied a simplified version of the problem wherein the potential V was determined by solving a single-component version of Eqs. (1) exactly.[7] This study gave the functional form of $V(x)$ [and hence $\rho(x)$] involving Jacobian elliptic functions and led in a natural way to Lamé's equation[8-10] (with $n = 1$ in the notation of Ref. 8). The equations solved in Ref. 7 may be obtained by replacing the sum over different orbitals in Eq. (3) by N times the Fermi orbital and then extremizing with respect to V, a process which clearly generates an upper bound to E. In the limit $\Delta \to \infty$ the different orbitals are degenerate and hence the bound is expected to be saturated. The analytical form is then determined in the strong-coupling limit.

The present work is inspired by the results of Ref. 7 and is best viewed as an $Ansatz$ for the functional dependence of $V(x)$. Firstly scale the coordinate thus: $u = x/\lambda$. The $Ansatz$ is

$$\lambda^2 \Delta[1 - \rho(u)a_0] = 2m \operatorname{sn}^2(u|m) + 2(E/K - 1). \tag{4}$$

Equations (3) and (4) contain two unknown parameters λ and m and the constant term in the right-hand side of Eq. (4) is picked so that the average of the right-hand side is zero.[11] Equation (4) transforms Eqs. (1) into the standard form for Lamé's equation,[8-10]

$$[-d^2/du^2 + 2m \operatorname{sn}^2(u|m)]\psi_n(u) = \epsilon_n \psi_n(u), \tag{5}$$

with

$$E_n = \lambda^{-2}\left\{\epsilon_n + 2E/K - 2\right\}. \tag{6}$$

Equation (5) is in the form of a Bloch-like periodic-potential problem with a period $2K(m)$ which should correspond to the mean particle separation a_0 (i.e., commensurate) and hence we set

$$2K(m)\lambda = a_0. \tag{7}$$

I now show that the $Ansatz$ is self-consistent. To this end note that Eq. (5) admits one (and only one) band gap leading to a single "valence band" and a single "conduction band." The valence-band wave functions may be written in the form[12]

$$\psi_p(u) \propto \frac{\theta_1(u + ip)}{\theta(u)} \exp\left\{iu\left[\frac{\pi p}{2KK'} + Z(p|m_1)\right]\right\} \tag{8}$$

with eigenvalue

$$\epsilon_p = 1 - m_1 \operatorname{cn}^2(p|m_1). \tag{9}$$

Here $m_1 = 1 - m$, $K \equiv K(m)$, $K' = K(m_1)$, θ and Z are Jacobi's theta and zeta functions with parameter m, $\theta_1(u) = \theta(u + K)$, and p is the quantum number, necessarily real to ensure bounded solutions. It should be noted that distinct solutions correspond to $-K' < p \leq K'$ since P and $p + 2K'$ lead to essentially the same solution. In order to compute $|\psi_p(u)|^2$ we use the addition theorem of Jacobi,

$$\theta_1(u + ip)\theta_1(u - ip) = [\pi/2K(m_1)^{1/2}][\theta^2(u)\theta_1^2(ip) - H^2(u)H_1^2(ip)], \tag{10}$$

where H is the eta function. On dividing by $\theta^2(u)$, using the definition $H^2(u)/\theta^2(u) = m^{1/2} \operatorname{sn}^2(u|m)$ and

Jacobi's imaginary transformation we find

$$|\psi_p(u)|^2 = n_p[\mathrm{dn}^2(p\,|\,m_1) - m\,\mathrm{sn}^2(u\,|\,m)]. \qquad (11)$$

The remarkable factorization of $|\psi_p(u)|^2$ in Eq. (11) into a space part independent of p [$\mathrm{sn}^2(u\,|\,m)$] and a p-dependent prefactor ensures that the *Ansatz* in Eq. (4) is functionally satisfied. Normalization yields

$$n_p^{-1} = L\,[\mathrm{dn}^2(p\,|\,m_1) + E/K - 1], \qquad (12)$$

where $E \equiv E(m)$.

The total density is obtained by summing (11) over occupied p's, and on comparing with Eq. (4) we find the self-consistency equation

$$\sum_{p \in \mathrm{occ}} n_p = 2/\lambda^2 \Delta a_0. \qquad (13)$$

Turning to the determination of the allowed p's, we apply periodic boundary conditions $\psi_p(u) = \psi_p(u + L/\lambda)$ to Eq. (8) which leads to the condition

$$\pi p/K' + 2KZ(p\,|\,m_1) = ka_0, \qquad (14)$$

where $k = (2\pi/L) \times (\text{integer})$. The relation (14) is particularly simple in the limit $m \to 1$ (strong coupling) where $KZ(m_1) \to 0$ and we get $p \sim (ka_0/2)$. In the limit $L \to \infty$, p's form a continuum. I denote by $L\sigma(p)dp$ the number of p's between p and

$p + dp$, with $\sigma(p) = (2\pi)^{-1}dk/dp$. By differentiating (14) and using

$$\frac{dZ(p\,|\,m_1)}{dp} = \mathrm{dn}^2(p\,|\,m_1) - E'/K' \qquad (15)$$

and Legendre's relation $E'K + EK' - KK' = \pi/2$, we find

$$\sigma(p) = (2\pi\lambda)^{-1}[\mathrm{dn}^2(p\,|\,m_1) + E/K - 1]. \qquad (16)$$

The limits on p are from $-K'$ to $+K'$ (corresponding to $-\pi/a_0 < k \leq \pi a_0$) and it is readily checked from Eq. (16) that

$$L \int_{-K'}^{K'} \sigma(p)dp = N,$$

thereby ensuring that the valence band can accommodate N fermions. Combining Eqs. (12) and (16) with (13) we get

$$2/\lambda^2\Delta = (a_0/\pi\lambda)K'. \qquad (17)$$

Eliminating λ between Eqs. (7) and (17) we get the remarkably simple final result

$$K'/K = 4\pi/\Delta a_0^2. \qquad (18)$$

Equation (18) may also be written in terms of the "nome" $q = \exp(-4\pi^2/\Delta a_0^2)$, a form which is very useful for actual computations. The total energy per particle can be found from Eqs. (3), (6), (9), and (16) (with $s = E/K - 1$):

$$E_{\mathrm{tot}}/N = (2/\lambda^2)(s + m_1) - (2/\lambda^2\pi)[E'E + K'K(s + m_1)s - \tfrac{1}{3}E'K(2m_1^2 - 7m_1 + 3) - \tfrac{2}{3}EK'(1 - m_1^2)], \qquad (19)$$

and may be verified to be always lower than the trivial Hartree result $(\pi^2/3a_0^2)$.

The features of the solution are summarized in the following remarks. (1) The density has a periodic variation in space so that the particles experience a periodic potential. (2) The periodic potential is in Lamé's form and has only one band gap; the valence band is completely filled and the conduction band empty. (3) In the weak-coupling limit $\Delta \to 0$, we have $K' \to \infty$ and from Eq. (18) $m \to 16\exp(-4\pi^2/\Delta a_0^2)$ leading to a sinusoidal density variation with an amplitude $(2m\pi^2/a_0^2\Delta)$ which is nonanalytic in Δ. This agrees with the result of Overhauser.[1] (4) In the strong-coupling limit $\Delta \to \infty$, we have $K \to \infty$ and from Eq. (18) $m \to 1 - 16\exp(-\Delta a_0^2/4)$. In this limit, the density is a very sharply peaked periodic function with amplitude $\sim \Delta a_0^2/8$ and the width of each peak is $O(1/\Delta)$, and all the valence-band eigenvalues are degenerate, $E_n \sim \Delta - (\Delta a_0/4)^2 + O(\Delta^2 e^{-C\Delta})$. This agrees with Ref. 7. (5) The form of the solution agrees with that of LL for $N = 1$ and 2. (6) The present solution, Eq. (8), is complex in general (except for $p = 0$ and $p = K'$ which are real). How-

ever, in keeping with result (c) of LL, we can choose the orbitals to be real for any N in view of $\psi_p{}^* = \psi_{-p}$, and the fact that the occupied orbitals have labels $[0, \pm p_1, \dots, \pm p_{N/2-1/2}]$ for N odd and $[0, \pm p_1, \dots, \pm p_{N/2-1}, K']$ for N even. (7) Although the general solution obtained here is valid for any N, I have concentrated on the thermodynamic limit (i.e., $L \to \infty$, $N \to \infty$, $L/N \to \text{const}$). The present solution exists for any $\Delta (\geq 0)$ and evolves continuously from the weak-coupling to the strong-coupling limit. The states may thus be viewed as undergoing a smooth transition from an extended to a localized character. This behavior is in contrast with that before taking the thermodynamic limit, where, following LL, one may expect for odd N bifurcations for Δ of $O(1/L^2)$.

I have not succeeded in proving that the solution presented here is minimal, but conjecture that it is so.

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[11]I follow the usual notation for Jacobian elliptic functions (as in Ref. 8) but indicate the parameter rather than the modulus, thus $sn(u|m) \equiv sn(u, \sqrt{m})$, etc. Unless otherwise indicated the parameter is m.

[12]This form can be obtained from Ref. 8 or Eq. (13) of Ref. 9 by putting $\alpha_0 = K + iK' + ip$ and using the addition theorem of the zeta function.