Scaling and nonlinear field studies of the jellium model for Wigner electron systems in *d* dimensions

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A jellium model of interacting electrons has been investigated using scaling arguments on the kinetic and potential energy (KE and PE, respectively) in *d* spatial dimensions. We find that the model exhibits no natural length scale in one dimension (1D), but in 2D and 3D, finite lengths appear indicating a tendency to form periodic structures. This confirms qualitatively the ideas of Wigner, who many years ago [E. P. Wigner, Phys. Rev. **46**, 1002 (1934)] realized the possibility, in three dimensions, below a certain critical electron density, ρ_c, that the effects of the PE due to Coulomb interactions would outweigh those of the KE and that the PE would be minimized by electrons localizing about sites on a body-centered-cubic lattice. In 4D we find a critical length for periodicity that is infinite, indicating the impossibility of a stable periodic structure. We have also cast the model into Landau-Ginzburg functional form with an appropriate order parameter. A minimization procedure is shown to lead to criteria for lattice formation in terms of electron density and screening length. In the continuum limit, the problem has been mapped into two coupled nonlinear field equations whose 1D versions are found to be exactly integrable. A perturbative treatment of these field equations in 2D, at absolute zero temperature, reveals the emergence of a stable triangular lattice structure. [S1063-651X(98)09807-9]

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I. INTRODUCTION

Many years ago, Wigner [1] realized that, at sufficiently low densities and temperatures, a plasma of electrons immersed in a uniform neutralizing background of positive charge would crystallize into a solid—the so-called Wigner solid (WS). This was despite the fact that there appears to be a conflict between a system of classical particles at zero temperature and the quantum case. Classically, one would expect the system to go into a state that minimizes the potential energy and to be accomplished by putting the electrons on a lattice. Quantum mechanically, the electrons would be generally expected to form a uniform density electron gas, at zero temperature, because of the kinetic-energy cost of localizing electrons onto lattice sites required by the uncertainty principle. From this same principle it is expected that the kinetic energy will scale as the inverse square of a typical interelectronic separation (L) and will only become small relative to the potential energy, which scales inversely with L, at low densities. Thus one might expect a quantum phase transition in the state of the system from a fluid at high densities to a solid at low densities. The crystalline state is expected to exist not only in the ground state but also at finite temperatures. For short-range potentials there exist theorems that eliminate the possibility of long-range order of the crystalline variety at finite temperatures and in the ground state, but for the long-range Coulomb interaction they afford no guidance. Quantum effects will become important when the temperature falls below the degeneracy temperature of the electron gas. Furthermore, in such systems the anticipated crystallization is an example of a strong-correlation effect in which electron-electron interactions cannot be treated as weak perturbations since they qualitatively alter the associated physical properties, and hence nonlinear effects, via the Coulomb interaction, become very important.

As a starting point for treating the interacting system of N electrons in a d-dimensional lattice, the so-called jellium model [2,3] will be adopted, where the Hamiltonian is given by

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \frac{e^2}{2}\sum_{i\neq j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|^{d-2}} \quad \text{for } d\neq 2,$$
$$= -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \frac{e^2}{2}\sum_{i\neq j}\ln|\mathbf{r}_i-\mathbf{r}_j| \quad \text{for } d=2. \tag{1}$$

The above Hamiltonian incorporates the individual kinetic energies for the electrons and their mutual repulsion. The positive ions are smeared out into a uniform jellium, which leads to a system with overall charge neutrality. The approach presented below will be based on the jellium Hamiltonian and we shall seek conditions for the formation of periodic charge distributions in a d-dimensional space.

II. SPATIAL SCALING: NEUTRALIZING BACKGROUND

We proceed by scaling the spatial variable so that

$$r \rightarrow r' = r/s. \tag{2}$$

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As a consequence, the Hamiltonian becomes

$$H' = s^2\left[-\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \frac{e^2}{2}\, s^{-\varepsilon}\sum_{i\neq j}\ \frac{1}{|\mathbf{r}_i-\mathbf{r}_j|^{d-2}}\right] \quad \text{for} \quad d\neq 2, \tag{3}$$

where $\varepsilon = 4-d$. To extract information about a natural length scale in the model, we investigate the energy functional based on Eq. (3), which can be represented schematically as

$$E = \alpha s^2 + \beta s^{d-2} \quad \text{for } d\neq 2 \tag{4}$$

and when $d=2$, from Eq. (1) we have

$$E = \alpha s^2 + \beta \ln s,$$

where α and β are constants that are scale independent. Naturally E is to be understood as the expectation value of H' within a multielectron wave function ϕ. Our next step is to minimize the energy functional with respect to the scaling factor in order to find out whether a finite spacing exists at an energy minimum. Thus we require

$$\frac{\partial E}{\partial s} = 0 \quad \text{at} \quad s = s_0 \tag{5}$$

and obtain

$$s_0 = \begin{cases} (\beta/2\alpha)^{1/3} & \text{for } d=1, \\ (-\beta/2\alpha)^{1/2} & \text{for } d=2, \\ -(\beta/2\alpha) & \text{for } d=3, \\ 0 \ \text{ unless } \ \alpha=-\beta & \text{for } d=4. \end{cases} \tag{6}$$

Based on this simple analysis we conclude that for α and β positive, a finitely spaced lattice is expected to arise in 1D while in 2D and 3D cases the signs of α and β coefficients must differ. In 4D the scaling factor required for minimization vanishes, which indicates a preference for an infinitely spaced lattice of charges. This is somewhat surprisingly accurate considering the crudity of the approach presented above because these general qualitative results are borne out by earlier thermodynamic approaches [4]. However, in order to refine the method of investigation, we now intend to reintroduce the screening background and account for the spatial dependence of the KE term. These improvements will be especially important in the 2D case.

III. MINIMIZATION IN *k* SPACE

In the case when $d=2$, the logarithmic form of the potential term causes serious difficulties. Consequently, an alternative line of attack should be devised to deal with this problem. To this end, we recall that the kth Fourier component of a screened Coulomb interaction takes the form

$$\Phi(k) \simeq \frac{\beta}{\xi^{-2}+k^2}, \tag{7}$$

where ξ is a measure of the screening length, β being a constant introduced earlier. The Fourier transform of the KE (Laplacian) term contributes terms that are proportional to k^2. We now put these terms together following the introduction of an order parameter field $\psi(x)$, which represents the electronic degrees of freedom such that $|\psi(x)|^2$ is the electronic charge density and

$$\int |\psi(x)|^2 d^d x = N \tag{8}$$

establishes the total amount, N, of electronic charge on the lattice with a volume L^d. Following the method of coherent structures (MCS), we cast the jellium Hamiltonian in an effective form using the Fourier transform of the electronic order parameter field [5]

$$\psi(x) = \sum_{\mathbf{k}}\ \psi_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{9}$$

Thus, the energy functional in k space can be written as

$$E = \sum_k \left\{ (\alpha k^2 - \lambda)|\psi_{\mathbf{k}}|^2 + \frac{\beta}{\xi^{-2}+k^2}\,|\psi_{\mathbf{k}}|^4 \right\}, \tag{10}$$

where α parametrizes the KE strength, λ is a Lagrange multiplier to be chosen such as to provide charge conservation given by Eq. (8), and β gives the strength of the screened Coulomb repulsion. The main advantage of this approach is the decoupling of the Fourier modes (or wavelengths) in the description of the electronic degrees of freedom. The procedure we now wish to follow consists of three steps. (i) Minimization with respect to $\psi_{\mathbf{k}}$ in order to obtain an optimal choice of the amplitude of the periodic charge-density distribution. (ii) Minimization with respect to k in order to obtain a most energetically favorable lattice spacing. (iii) Proper normalization of the electronic charge distribution. Utilizing (i), we obtain from the condition

$$\partial E/\partial \psi_{\mathbf{k}} = 0 \tag{11}$$

that

$$|\psi_{\mathbf{k}}|^2 = -\frac{(\alpha k^2-\lambda)}{2\beta}\,(\xi^{-2}+k^2). \tag{12}$$

This leads to an upper bound condition on the wave vector

$$k^2 \leqslant \frac{\lambda}{\alpha} \equiv k_0^2 \tag{13}$$

precluding very short-range interactions. Furthermore, normalization requires that

$$N = \int_0^{k_0} |\psi_k|^2 d^d k = \frac{\pi}{4\beta}\, 2^d \alpha k_0^{d+4}\left[\frac{1}{d+2} - \frac{1}{d+4}\right] \tag{14}$$

assuming that ξ is large. Hence,

$$k_0 = \left[\frac{N\beta(d+2)(d+4)}{\pi 2^{d-1}\alpha}\right]^{1/d+4}. \tag{15}$$

Consequently, we find the value of the Lagrange multiplier to be

$$\lambda=\alpha\left[\frac{N\beta(d+2)(d+4)}{\pi 2^{d-1}\alpha}\right]^{2/(d+4)} \tag{16}$$

and the total amount of charge on the lattice is conserved.

The final step is to minimize with respect to k once Eq. (12) has been substituted into the functional in Eq. (10). This yields

$$E=-\sum_k\left\{\frac{(\alpha k^2-\lambda)^2(\xi^{-2}+k^2)}{4\beta}\right\}. \tag{17}$$

Subsequent minimization with respect to k gives the following extrema (see Fig. 1):

$$k=0,\quad k=k_0\quad\text{or}\quad k_{\max}^2=\frac{k_0^2}{3}-\frac{2\xi^{-2}}{3}, \tag{18}$$

where $k=0$ corresponds to a local maximum, k_0 is simultaneously an upper limit on the physically admissible values of the wave number in Eq. (13) and a local maximum, while $k_{\max}$ gives rise to two local minima. The corresponding energy values are

$$E(k_0)=0,\quad E(k=0)=-\frac{\lambda^2\xi^{-2}N}{4\beta}$$

and

$$E(k_{\max})=-\frac{\alpha^2}{27\beta}(k_0^2+\xi^{-2})^3N, \tag{19}$$

where N is the number of Fourier modes in reciprocal space. Note that in view of Eq. (18) the position of the global energy minima, $\pm k_{\max}$, is determined by the screening length ξ. Thus, when $\xi=\infty$, which corresponds to an infinite screening length, $k_{\max}=k_0/\sqrt{3}$ and the energy minimum falls on the point in k space that is the upper limit [see Fig. 1(a)]. As ξ decreases in magnitude, $k_{\max}$ shifts towards zero [see Fig. 1(b)]. For as long as $k_{\max}\neq 0$, a Wigner crystal is expected to arise whose lattice periodicity is given by $a=2\pi/k_{\max}$. This situation persists until

$$\xi=\xi_c\equiv\sqrt{2}\left[\frac{N\beta(d+2)(d+4)}{\pi 2^{d-1}\alpha}\right]^{-2/(d+4)},$$

at which value $k_{\max}$ becomes 0. Thus, for $\xi<\xi_c$, i.e., for short screening lengths, $k_{\max}=0$ giving rise to a single potential well in the $E(k)$ plot, as shown in Fig. 1(c). This latter case is characteristic of a disordered state of the electronic degrees of freedom. It is worth noting that the above conditions only quantitatively depend on lattice dimensionality d and thus indicate a limitation of the approximations used. The broad features therefore remain the same for each dimension. In fact, the value of the critical screening length ξ_c changes only a little between values of d such that $\xi_c^{1D}=0.1148\xi_c^0$, $\xi_c^{2D}=0.120\xi_c^0$, and $\xi_c^{3D}=0.1310\xi_c^0$, where ξ_c^0 is a constant. We must, however, qualify these statements with a word of caution since the calculations involved in this section were very approximate and the energy minimization conditions may be modified by the requisite corrections. We have therefore tried to arrive at a better estimate of the energy in Eq. (17) by discretizing the wave number according to the formula $k_n=2\pi n/L$. We carried out the requisite summations from $n=1$ to $n=M$ [6]. Simple algebra leads to the following result:

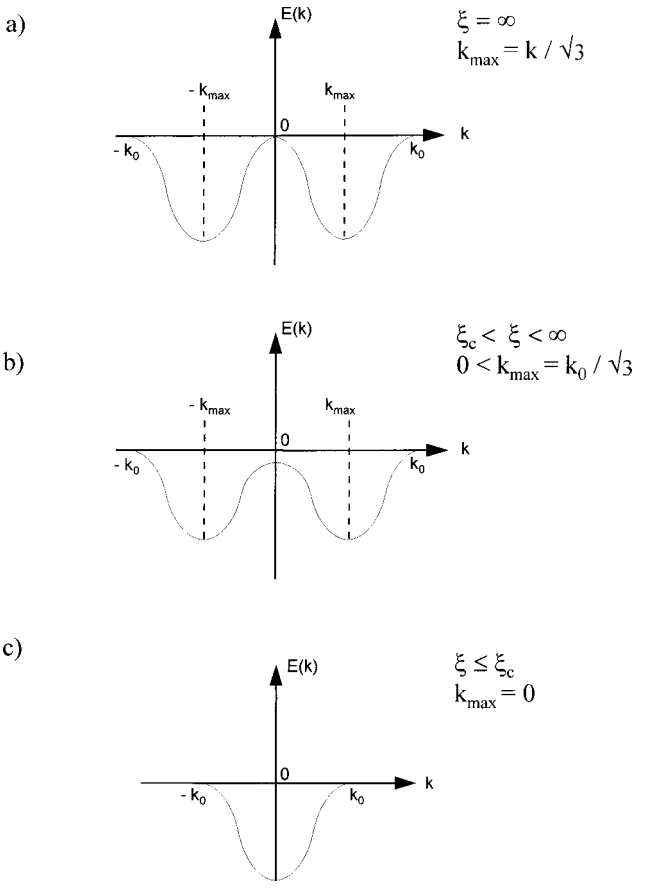

FIG. 1. A schematic illustration of the energy dependence $E(k)$ on the wave number k, following Eq. (17) for (a) $\xi=\infty$, (b) $\xi_c<\xi<\infty$, and (c) $\xi\leqslant\xi_c$. The quantities plotted are in arbitrary units.

$$E=-\frac{1}{4}\left\{\alpha^2\frac{(2\pi)^6}{L^6}\tfrac{1}{42}M(M+1)(2M+1)(3M^4+6M^3-3M+1)+\frac{(2\pi)^4}{L^4}[\alpha^2\xi^{-2}-2\alpha\lambda]\tfrac{1}{30}M(M+1)(2M+1)\right.$$

$$\left.\times(3M^2+3M-1)+\frac{(2\pi)^2}{L^2}[\lambda^2-2\alpha\lambda\xi^{-2}]\tfrac{1}{6}M(M+1)(2M+1)+M\lambda^2\xi^{-2}\right\}. \tag{20}$$

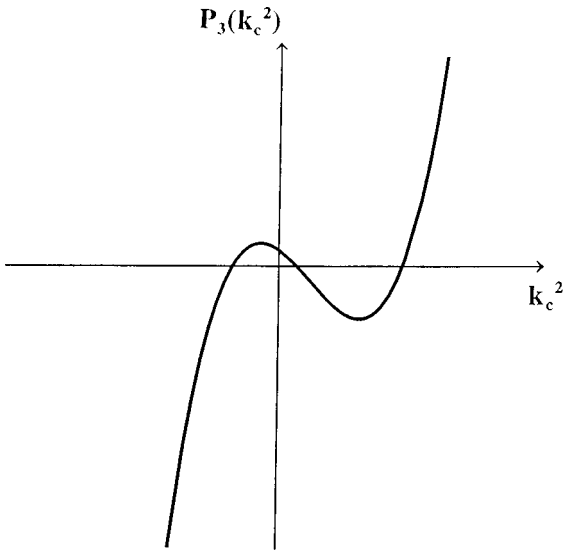

FIG. 2. An illustration of the cubic polynomial $P_3(k_c^2)$ in terms of k_c^2 as given by Eq. (22). The quantities plotted are in arbitrary units.

We then retain only the highest-order terms in each of the polynomials in M and introduce $k_c=2\pi M/L$, which represents the highest-order wave number in the sum, analogous to k_0. This yields

$$E=\tfrac{1}{7}\alpha^2M^7k_c^6+\tfrac{1}{5}(\alpha^2\xi^{-2}-2\alpha\lambda)M^5k_c^5 +\tfrac{1}{3}(\lambda^2-2\alpha\lambda\xi^{-2})M^3k_c^2+\lambda^2\xi^{-2}M. \quad (21)$$

We then differentiate E with respect to M to obtain an equation for the energy extrema in k space. This results in

$$P_3(k_c^2)\equiv a_3k_c^6+a_2k_c^4+a_1k_c^2+a_0=0, \quad (22)$$

where $a_3=\alpha^2$, $a_2=\alpha^2(\xi^{-2}-2k_0^2)$, $a_1=\alpha\lambda(k_0^2-2\xi^{-2})$, and $a_0=(\lambda/\xi)^2$. This, clearly, is a cubic equation in terms of k_c^2. We found approximate values of its roots in two limiting cases: (i) for $\xi\to0$; $k_c=k_0$ is a double root of the associated biquadratic equation. Note that this agrees with our earlier approximation. (ii) When $\xi\to\infty$, $k_c=0$ and $k_c=k_0$ as above. In general, however, for finite and nonzero values of the screening length ξ, the roots will be shifted and the depth of the potential wells around them will also be affected. This is shown in Fig. 2.

This level of approximation has indicated the possibility of Wigner lattice formation at small but finite temperatures in all dimensionalities without singling out the $d=2$ case, which occurred in the mean-field approach. To further refine our analysis we proceed to develop a field-theoretical description.

IV. FIELD-THEORETIC INVESTIGATIONS

A. Spinless particles

The starting point in the present analysis is to consider the second quantized form of the multielectron Hamiltonian in a plane-wave basis formulation. This takes the form [5]

$$H_1=\sum_{\mathbf{k}}\omega_{\mathbf{k}}q_{\mathbf{k}}^\dagger q_{\mathbf{k}}+\sum_{\mathbf{k},l,\mathbf{m}}\Delta_{\mathbf{k},l,\mathbf{m}}q_{\mathbf{k}}^\dagger q_l^\dagger q_{\mathbf{m}}q_{\mathbf{k}+l-\mathbf{m}}, \quad (23)$$

where

$$\omega_{\mathbf{k}}=\frac{\hbar^2k^2}{2m}-|e|U \quad (24)$$

and

$$\Delta_{\mathbf{k},l,\mathbf{m}}=\langle\mathbf{k}(1),l(2)|e^2/2r_{12}|(\mathbf{k}+l-\mathbf{m})(1),\mathbf{m}(2)\rangle. \quad (25)$$

In the above, each plane-wave state $|\mathbf{k}\rangle$ is normalized over a volume, Ω, so that

$$|\mathbf{k}\rangle\to\exp(i\mathbf{k}\cdot\mathbf{r})/\sqrt{\Omega} \quad (26)$$

and U is fixing the zero level of energy, involving the jellium background. The Hamiltonian in Eq. (23) is now utilized to obtain the Heisenberg equation of motion for a particular annihilator q_η so that

$$i\hbar\partial_tq_\eta=-[H_1,q_\eta]_-. \quad (27)$$

Calculating the various commutators in Eq. (27) gives

$$i\hbar\partial_tq_\eta=\omega_\eta+2\sum_{\mathbf{k},\mathbf{m}}\Delta_{\eta,\mathbf{k},\mathbf{m}}q_{\mathbf{k}}^\dagger q_{\mathbf{m}}q_{\mathbf{k}+\eta-\mathbf{m}}. \quad (28)$$

To translate Eq. (28) into the language of fields, we follow the prescription that has been termed the method of coherent structures (MCS) [5]. This has been fully described in a series of papers [7–9] and a research monograph [5]. The procedure employs a standard definition of a field variable,

$$\psi(\mathbf{r})=\frac{1}{\sqrt{\Omega}}\sum_{\mathbf{k}}\exp(-i\mathbf{k}\cdot\mathbf{r})q_{\mathbf{k}}, \quad (29)$$

with its Hermitian conjugate counterpart. Both sides of Eq. (28) can now be multiplied by $\exp(-i\boldsymbol{\eta}\cdot\mathbf{r})/\sqrt{\Omega}$ and summed over η.

Assuming that the volume Ω over which our plane waves are normalized has a radius R, we find that

$$2\Delta_{\eta,\mathbf{k},\mathbf{m}}=\frac{e^2\pi}{2\Omega|\mathbf{k}-\mathbf{m}|^2}\{1-\cos(|\mathbf{k}-\mathbf{m}|R)\} \quad (30)$$

and

$$\omega_\eta=\frac{\hbar^2\eta^2}{2m}-|e|U. \quad (31)$$

Each of these expressions is now expanded about a particular point, $\mathbf{k}_0$, in reciprocal space in deviations in $\mathbf{k}$ from this point when the wave vector $\mathbf{k}$ becomes close to $\mathbf{m}$ in magnitude. Retaining only zero-order terms from $\Delta_{\eta,\mathbf{k},\mathbf{m}}$ and up to quadratic contributions from ω_η we obtain the nonlinear Schrödinger equation with a potential U for the field ψ,

$$i\hbar\partial_t\psi=\left(\frac{\hbar^2k_0^2}{2m}-|e|U\right)\psi+\frac{i\hbar^2\mathbf{k}_0}{m}\nabla\psi-\frac{\hbar^2}{2m}\nabla^2\psi +\psi^\dagger\psi\psi\left(\frac{3e^2}{16R}\right). \quad (32)$$

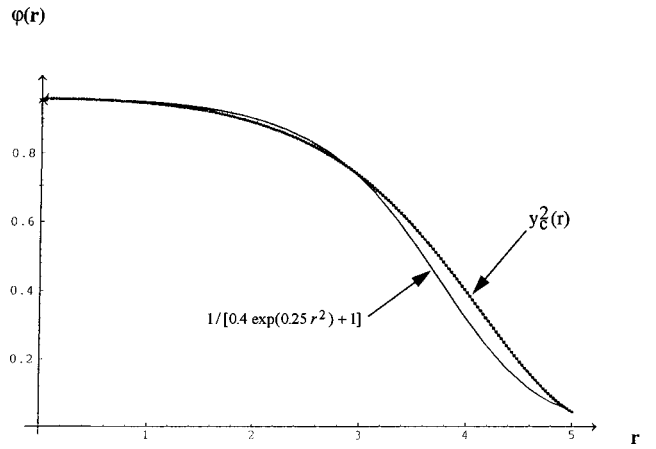

FIG. 3. Comparison of the numerical nodeless solution of Eq. (34) with its estimate given in Eq. (37). The quantities plotted are in arbitrary units.

The central gradient term on the right of Eq. (32) may now be eliminated by transforming to a moving reference frame so that new independent coordinates become

$$t' = t, \qquad x' = x - vt, \tag{33}$$

where v is chosen so that $-\hbar v = |\hbar^2 \mathbf{k}_0/m|$.

Stationary solutions are then easily found by setting $\psi = \phi \exp(-iE_0 t/\hbar)$, where ϕ is spatially dependent only. We find that the equation for the field's amplitude ϕ is

$$\frac{d^2\phi}{dr^2} + \frac{\kappa}{r}\frac{d\phi}{dr} = A\phi + B\phi^3. \tag{34}$$

In Eq. (34) it has been assumed that ϕ is real, $\kappa = 1$ in two dimensions, $\kappa = 2$ in three dimensions ($\kappa = d-1$ in general), and A and B are constants defined by

$$A = \frac{2m}{\hbar^2}\left(\frac{\hbar^2 k_0^2}{2m} - |e|U - E_0\right) \tag{35}$$

and

$$B = \frac{2m}{\hbar^2}\frac{3e^2}{16R}. \tag{36}$$

We comment that we expect A to be small relative to B since E_0 represents the total energy of the system. In this limit, Eq. (34) reduces to the familiar Emden equation [10]. However, only a very limited set of solutions is available in 2D for this case. Equation (34), when $A<0$ and $B>0$, has been analyzed by Alfimov *et al.* [11], who found two classes of physically meaningful solutions: (a) radially symmetric and localized ''bumplike'' solutions and (b) solutions that are localized in one independent variable and periodic in the other. Another recent paper [12] found an approximate analytical nodeless bump solution in 3D when the equation's coefficients are scaled to $A=-1$ and $B=+1$, in which case (see Fig. 3)

$$\phi(r) \cong [0.04\exp(0.25r^2)+1]^{-1/2}. \tag{37}$$

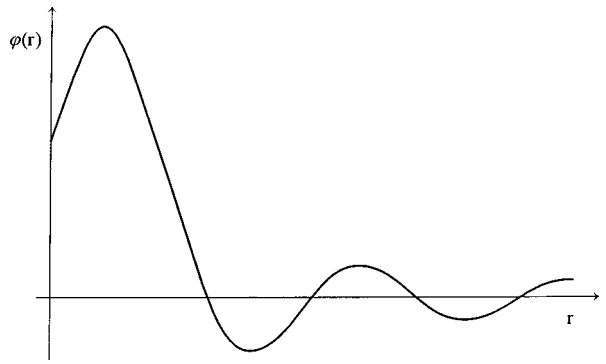

FIG. 4. Plot of the damped oscillatory solution of Eq. (34) as given in Eq. (39). The quantities plotted are in arbitrary units.

Unfortunately, the version of the Emden equation corresponding to Eq. (34) does not satisfy the Painlevé property except in four dimensions and hence one should not expect to find an exact solution to this problem. We have analyzed a class of damped oscillatory solutions through numerical means, which, asymptotically behave as

$$\phi(r) \sim \phi_0 r^{-1} e^{-r} \quad \text{for } r \to \infty \tag{38}$$

and in the vicinity of the origin they can be approximated by (see Fig. 4)

$$\phi(r) \cong \phi_0 \frac{\mathrm{sn}(r-r',k)}{r-r'}, \tag{39}$$

where ϕ_0 and r' are parameters to be fitted and $0 \leqslant k \leqslant 1$ is the Jacobi elliptic modulus for the elliptic sn function above. The problem with these solutions in the present context, however, is that they cannot be properly normalized in 3D as our extensive numerical efforts demonstrated. Without arbitrary joining procedures they do not result in solutions that would represent a periodic lattice in 2D or 3D. Although localization and quasiperiodicity properties can be clearly seen through these solutions, Wigner lattice formation by a single scalar field equation remains elusive. In order to remedy this deficiency, we now propose to consider a field-theoretical model involving two spin projection fields for electronic degrees of freedom.

B. Fields with spin

Our starting point is similar to that in Sec. IV A with the Hamiltonian given by [13]

$$H_2 = \sum_{\mathbf{k}\sigma} \omega_{\mathbf{k}} q^\dagger_{\mathbf{k}\sigma} q_{\mathbf{k}\sigma} + \sum_{\substack{\mathbf{k},l,\mathbf{m} \\ \sigma,\sigma'}} \Delta_{\mathbf{k},l,\mathbf{m}} q^\dagger_{\mathbf{k}\sigma} q^\dagger_{l\sigma'} q_{\mathbf{m}\sigma'} q_{(\mathbf{k}+l-\mathbf{m})\sigma}, \tag{40}$$

where $\sigma, \sigma' = \mp \frac{1}{2}$ denote the components of spin, which will be identified with the corresponding $\mp$ indices. Again we use Heisenberg's equation of motion for the spin-up and spin-down annihilator, respectively. The commutators are straightforward to evaluate and we find that

$$i\hbar\partial_t q_{\eta+} = \omega_\eta q_{\mathbf{k}+} + \sum_{\mathbf{k},\mathbf{m}} [\Delta_{\eta,\mathbf{k},\mathbf{m}} q^\dagger_{\mathbf{k}+} q_{\mathbf{m}+} q_{(\eta+\mathbf{k}-\mathbf{m})+} - \Delta_{\mathbf{k},\eta,\mathbf{m}} q^\dagger_{\mathbf{k}+} q_{\mathbf{m}+} q_{(\mathbf{k}+\eta-\mathbf{m})+} + \Delta_{\eta,\mathbf{k},\mathbf{m}} q^\dagger_{\mathbf{k}-} q_{\mathbf{m}-} q_{(\eta+\mathbf{k}-\mathbf{m})+} - \Delta_{\mathbf{k},\eta,\mathbf{m}} q^\dagger_{\mathbf{k}-} q_{\mathbf{m}+} q_{(\mathbf{k}+\eta-\mathbf{m})-}] \tag{41}$$

and

$$i\hbar\partial_t q_{\eta-} = \omega_\eta q_{\mathbf{k}-} + \sum_{\mathbf{k},\mathbf{m}} [\Delta_{\eta,\mathbf{k},\mathbf{m}} q^\dagger_{\mathbf{k}-} q_{\mathbf{m}-} q_{(\eta+\mathbf{k}-\mathbf{m})-} - \Delta_{\mathbf{k},\eta,\mathbf{m}} q^\dagger_{\mathbf{k}-} q_{\mathbf{m}-} q_{(\mathbf{k}+\eta-\mathbf{m})-} + \Delta_{\eta,\mathbf{k},\mathbf{m}} q^\dagger_{\mathbf{k}+} q_{\mathbf{m}+} q_{(\eta+\mathbf{k}-\mathbf{m})-} - \Delta_{\mathbf{k},\eta,\mathbf{m}} q^\dagger_{\mathbf{k}+} q_{\mathbf{m}-} q_{(\mathbf{k}+\eta-\mathbf{m})+}]. \tag{42}$$

We now introduce spin-dependent fields by analogy with the spin-independent case. Thus

$$\psi_+(\mathbf{r}) = \Omega^{-1/2} \sum_{\mathbf{k}} \exp(-i\mathbf{k}\cdot\mathbf{r}) q_{\mathbf{k}+}, \qquad \psi_-(\mathbf{r}) = \Omega^{-1/2} \sum_{\mathbf{k}} \exp(-i\mathbf{k}\cdot\mathbf{r}) q_{\mathbf{k}-}. \tag{43}$$

The single gradient is again transformed away by using a moving frame of reference, ''E_0'' being assumed to have different values, E_+ and E_-, for each field. The net result of this whole procedure is that the two fields, ψ_+ and ψ_-, written as

$$\psi_+ = \phi_+ e^{-iE_+ t/\hbar} \quad \text{and} \quad \psi_- = \phi_- e^{-iE_- t/\hbar} \tag{44}$$

satisfy the following equations of motion:

$$\omega_2 \nabla^2 \phi_+ = \lambda_+ \phi_+ + \lambda_2 [|\phi_+|^2 \phi_+ + |\phi_-|^2 \phi_+] \tag{45}$$

and

$$\omega_2 \nabla^2 \phi_- = \lambda_- \phi_- + \lambda_2 [|\phi_-|^2 \phi_- + |\phi_+|^2 \phi_-], \tag{46}$$

where ω_2, λ_+, λ_-, and λ_2 are constants.

We shall assume for simplicity that both ϕ_+ and ϕ_- are real—a fuller analysis [13] writing each field in modulus-argument form makes this a possibility. Interestingly, an identical set of differential equations has been investigated in connection with self-localized states in molecular chains [14]. These authors point out that the above equations are completely integrable in one dimension. The solutions are listed as

$$\phi_1 = \left(\frac{(\lambda_- - \lambda_+)\lambda_+}{\lambda_2 \omega_2}\right)^{1/2} \frac{\cosh \xi_2}{\Delta}, \qquad \phi_2 = \left(\frac{(\lambda_- - \lambda_+)\lambda_-}{\lambda_2 \omega_2}\right)^{1/2} \frac{\sinh \xi_2}{\Delta}, \tag{47}$$

where

$$\xi_1 = \left(\frac{\lambda_+}{\omega_2}\right)^{1/2} (x + x_0), \quad \xi_2 = \left(\frac{\lambda_-}{\omega_2}\right)^{1/2} (x - x_0) \tag{48}$$

$$\Delta = \left(\frac{\lambda_+}{\omega_2}\right)^{1/2} \cosh \xi_1 \cosh \xi_2 - \left(\frac{\lambda_-}{\omega_2}\right)^{1/2} \sinh \xi_1 \sinh \xi_2. \tag{49}$$

These solutions correspond to two coupled sech-like bump solitons. The reader is referred to the paper by Brizhik *et al.* [14] for graphical illustration and asymptotic analysis. The above authors also found coupled two-soliton solutions. Furthermore, a class of elliptic solutions can be found following Clarkson and Mansfield [15]. In order to bring Eqs. (45) and (46) into a suitable form (provided $\lambda_+ = \lambda_- = \lambda$) for comparison with this latter paper, we first set the dependent variables into a linear combination form

$$\phi_+ + i\phi_- = u_1 \tag{50}$$

and

$$\phi_+ - i\phi_- = u_2 \tag{51}$$

so that the equations of motion become

$$\omega_2 \nabla^2 u_1 = \lambda u_1 + \lambda_2 u_1^2 u_2 \tag{52}$$

and

$$\omega_2 \nabla^2 u_2 = \lambda u_2 + \lambda_2 u_2^2 u_1. \tag{53}$$

For $\lambda = 0$, which can always be arranged by the choice of E_+ and E_- and scaling the dependent variables, this system of equations results in two coupled ordinary differential equations

$$U'' + 2U^2 V = 0, \qquad V'' + 2UV^2 = 0. \tag{54}$$

The equations are solved by setting $W = -UV$ giving a Weierstrass elliptic function equation

$$W'' = 6W^2 - g_2, \tag{55}$$

where g_2 is an arbitrary constant. Thus both U and V satisfy Lamé equations of the form

$$\omega'' - 2\wp(z)\omega = 0, \tag{56}$$

where $\wp$ is the Weierstrass elliptic function $W(z) = \wp(z; g_2, g_3)$, where g_3 is an arbitrary constant. Finally, an exact solution may be found in the form

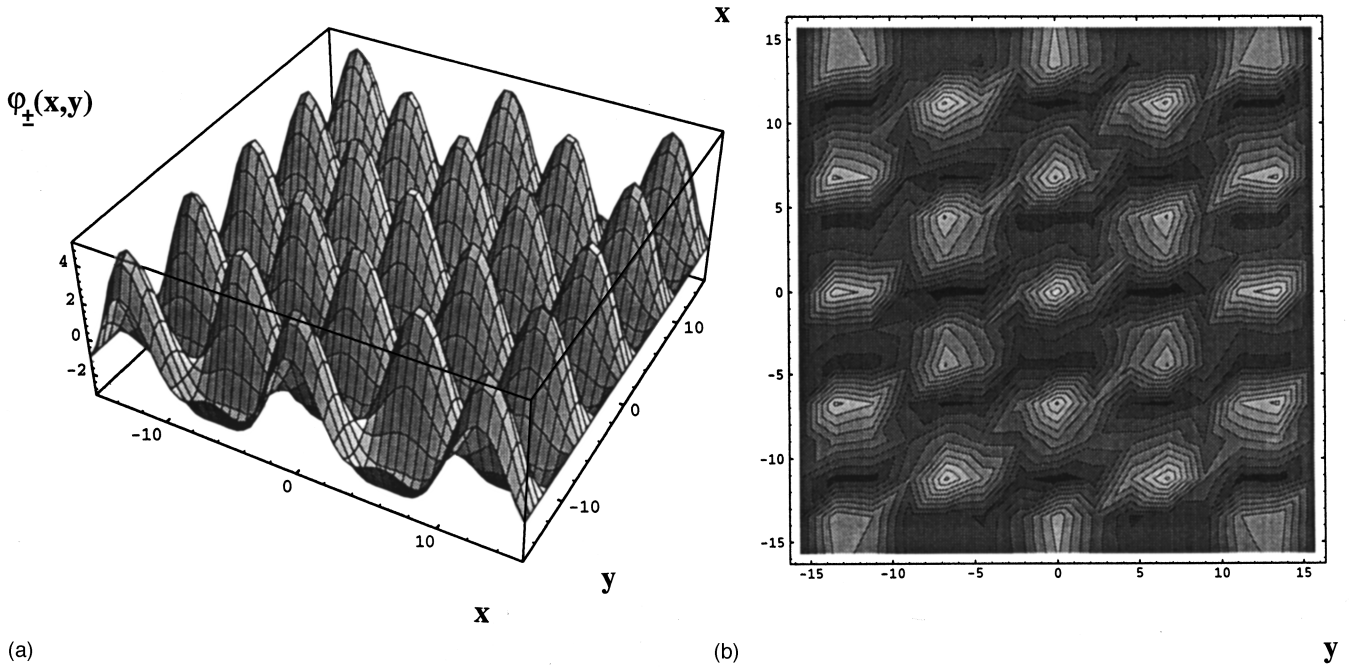

FIG. 5. A 3D plot (a) and a contour plot (b) of the solution given in Eq. (67). The quantities plotted are in arbitrary units.

$$\omega(z)=c_1\exp\{-z\zeta(a)\}\,\frac{\sigma(z+a)}{\sigma(z)}+c_2\exp\{z\zeta(a)\}\,\frac{\sigma(z-a)}{\sigma(z)}, \tag{57}$$

where $\zeta(z)$ and $\sigma(z)$ are the Weierstrass zeta and sigma functions, respectively, and a is any solution of $\wp(a)=0$. Alternatively, we may multiply both sides of Eq. (55) by W' and integrate once to give

$$(W')^2=2W^3-g_2W+c, \tag{58}$$

where c is an integration constant. Equation (58) is easily integrated to give Jacobi elliptic functions so that

$$W=\mathrm{sn}\left(\frac{(x-x_0)}{\sqrt{2}g_2},k\right), \tag{59}$$

where the elliptic modulus k is given by

$$k^2=\frac{W_2-W_1}{W_3-W_1} \tag{60}$$

and W_1, W_2, and W_3 are the roots of the polynomial on the right-hand side of Eq. (58).

We observe that elliptic functions are periodic, indicating the possibility of crystal lattice formation in this one-dimensional case, which encourages us to examine the two-dimensional case in the next section for latticelike structures.

V. LATTICE FORMATION IN TWO DIMENSIONS

Earlier analysis in this paper has clearly demonstrated the possibility of localization of electronic charges in one-, two-, and higher-dimensional spaces. At the same time, it appears highly improbable that exact analytical solutions exist beyond the one-dimensional case for these fields as shown above. We therefore turn our attention to perturbative methods to study pattern formation in nonlinear systems—see, for example, Shtilman and Sivashinsky [16] and Pismen and Nepomnyashchy [17]. Following these methods, we write Eqs. (45) and (46) as

$$\nabla^2\phi_+=-\gamma_+\phi_++\varepsilon\,\delta[\,\phi_+^3+\phi_-^2\,\phi_+] \tag{61}$$

and

$$\nabla^2\phi_-=-\gamma_-\phi_-+\varepsilon\,\delta[\,\phi_-^3+\phi_+^2\,\phi_-], \tag{62}$$

where we assume for convenience that both γ_+ and γ_- are negative, $\delta>0$, and ε is a small parameter in which we expand. To begin our procedure we set the field variables as

$$\phi_+=\phi_{+0}+\varepsilon\,\phi_{+1}+\cdots, \tag{63}$$

$$\phi_-=\phi_{-0}+\varepsilon\,\phi_{-1}+\cdots, \tag{64}$$

where ''0'' and ''1'' denote zeroth and first order, respectively. Clearly, in zero order we obtain

$$\nabla^2\phi_{+0}+\gamma_+\phi_{+0}=0 \tag{65}$$

and

$$\nabla^2\phi_{-0}+\gamma_-\phi_{-0}=0. \tag{66}$$

It is clear that the independent variable in each case may be scaled so that γ_+ or $\gamma_-=+1$. We follow Shtilman and Sivashinsky [17] and observe that one particularly important solution of these two equations with $\gamma_+=\gamma_-=1$ is

$$\phi_{+0}=\phi_{-0}=A\,\cos x+2B\,\cos\left(\frac{x}{2}\right)\cos\left(\frac{\sqrt{3}}{2}\right)y. \tag{67}$$

It should be emphasized that only when $B=2A$ does this describe a triangular pattern in two dimensions. We have displayed this for $A=1$ in Fig. 5. In an obvious way it is seen that to first order in ε we obtain

$$\nabla^2\phi_{+1}+\phi_{+1}=\delta[\phi_{+0}^3+\phi_{-0}^2\phi_{+0}] \tag{68}$$

and

$$\nabla^2\phi_{-1}+\phi_{-1}=\delta[\phi_{-0}^3+\phi_{+0}^2\phi_{-0}]. \tag{69}$$

The solution of each of these equations will be given by a complementary function, when the left-hand side is zero, plus any particular integral when the right-hand side is included. If we take Eq. (68) as an example, setting temporarily $\delta=0$, we may solve this using a separation of variables technique setting $\phi_{+1}=S(x)T(y)$. Denoting the separation constant by K we then have

$$S''=-KS \tag{70}$$

and

$$T''=(K-1)T. \tag{71}$$

When $K=1$, the solutions of Eq. (70) are oscillatory whereas T takes a form linear in y. If $K>1$, S is again periodic and T is represented by a decaying or exponentially increasing function. Obviously for $0<K<1$, T is oscillatory as is S but for $K<0$, T is periodic whereas S becomes hyperbolic. As regards stability, as only the decreasing exponentials may be chosen, the contribution from T with $K=1$ may cause problems because of a possible function of y increasing beyond limit. This may be avoided either by assuming $K\neq 1$ or else that the ''arbitrary'' constant premultiplying y in T for $K=1$ may be set to zero.

We now investigate the terms that can arise from any particular integral of Eq. (68) when the right-hand side is expressed as

$$R=2\delta\left[A\,\cos x+2B\,\cos\left(\frac{x}{2}\right)\cos\left(\frac{\sqrt{3}}{2}\,y\right)\right]^3, \tag{72}$$

which may be reexpressed using elementary trigonometric sum rules to give

$$R=\frac{A^3}{2}\{\cos 3x+\cos x\}+3A^2B\left\{\frac{1}{2}\left[\cos\left(\frac{5x}{2}\right)+\cos\left(\frac{3x}{2}\right)\right]+\cos\left(\frac{x}{2}\right)\right\}\cos\left(\frac{\sqrt{3}y}{2}\right)+3B^2A\{\tfrac{1}{2}[\cos 2x+1]+\cos x\}$$
$$\times[\cos(\sqrt{3}y)+1]+4B^3\left\{\frac{1}{2}\left[\cos\left(\frac{3x}{2}\right)+\cos\left(\frac{x}{2}\right)\right]+\cos\left(\frac{x}{2}\right)\right\}\left\{\frac{1}{2}\left[\cos\left(\frac{3\sqrt{3}y}{2}\right)-\cos\left(\frac{\sqrt{3}y}{2}\right)\right]+\cos(\sqrt{3}y)\right\}. \tag{73}$$

To find particular integrals (PI) of the various terms, we concentrate on one particular type, namely $\cos(\gamma_1 x)\cos(\gamma_2 y)$. We simply assume that we may take

$$\phi_{\rm PI}=\mu_1\cos(\gamma_1 x)\cos(\gamma_2 y). \tag{74}$$

For this to be so, we require μ_1 to be given by

$$\mu_1=(1-\gamma_1^2-\gamma_2^2)^{-1}. \tag{75}$$

This prescription will clearly not work for the terms $(A^3/2)\cos x$, $3A^2B\cos(x/2)\cos(\sqrt{3}y/2)$, $3B^2A\cos x$, and $-2B^3\cos(x/2)\cos(\sqrt{3}y/2)$ twice since $\gamma_1^2+\gamma_2^2=1$ and the denominator of Eq. (75) is zero. That is, the sum of ''frequencies'' from x and y components resonates with that from the complementary function. This is easily overcome if, for example, we choose the term in $\cos x$, then a particular integral is $(x/2)\sin x$. Similarly, a particular integral for $\cos(x/2)\cos(\sqrt{3}y/2)$ is $x\sin(x/2)\cos(\sqrt{3}y/2)$. Both of these last examples contain an amplitude varying with x and therefore may lead to instability of ϕ_{+1} or ϕ_{-1}. A particular integral with a y multiplicative factor may also be found in a similar way. In the unperturbed case, represented by Eq. (65), the associated frequencies are $\sqrt{\gamma_+}$ and $\sqrt{\gamma_-}$, where the $\gamma_\mp$ arise from the difference in energy between the total energy (E_0) and the positive background energy divided by the magnitude of the kinetic energy, i.e., the ratio of the repulsive Coulomb energy to kinetic energy. Thus the denominator of Eq. (75) would become (with $\gamma_+,\gamma_-\neq 0$)

$$\gamma_\mp-\gamma_1^2-\gamma_2^2,$$

which is highly unlikely to vanish since we expect $|\gamma_\mp|\sim(e^2/a_0)/(\hbar^2/2ma_0^2)$, where m is the electronic mass and a_0 the first Bohr radius. We therefore conclude that secular terms in x or y multiplied by oscillatory functions are unlikely to arise and that the first-order components ϕ_{+1} and ϕ_{-1} will be stable against large increases in x or y. This then leads to our final conclusion that introducing two coupled spin field variables in the description of the Wigner problem in 2D space results in a fairly robust periodic lattice.

VI. SUMMARY AND FUTURE DIRECTIONS

The present paper lays down some routes by which further analytical work may prove possible in the future relating to Wigner solidification in d spatial dimensions. Our emphasis has consistently been placed on the effects due to nonlinearity, which itself stems from Coulomb interactions between electrons. The scaling arguments that have been presented at the beginning of the paper encouraged us on this path by being consistent with the thermodynamics of Wigner crystallisation [2,18]. Landau-Ginzburg phenomenology has then been presented in this paper, and, again, it makes some rather general predictions that should act as guidelines for future analytical work. Numerical work based on density-functional theory is already available in $d=3$ and $d=2$ dimensions, and agrees well with quantum computer simula-

tion results, as recently reviewed by Senatore and March [19].

Finally, we have presented nonlinear field equations derived from the MCS formalism [5], first of all for spinless particles and, more importantly, for two coupled fields with spin $\frac{1}{2}$. In this context it is relevant to mention earlier work on instabilities of a single Slater determinant ground-state wave function for jellium, where plane waves (which are certainly appropriate in the high-density limit in 3D) are replaced by Bloch waves having the periodicity of the Wigner body-centered-cubic lattice. One is then discussing charge-density waves, as considered in the early work of Young [3] as well as Young and March [2]. Edwards and Hillel [18] later considered more generally instabilities of the Slater determinant of plane waves, following pioneering studies of Overhauser [20]. These instabilities are known to occur in 3D jellium at much higher densities than the phase transition to the Wigner crystal. Turning finally to long-range magnetic order in Wigner solids, the most natural description of the spin arrangement in the 3D bcc lattice is a Néel antiferromagnet in which the up-spins reside on the sites of one of the two interpenetrating simple cubic lattices, with down-spins on the other. However, following the general work of Carr [21], we know that at the very low densities required in 3D for the absolute zero phase transition to a Wigner crystal of localized electrons, wave-function overlaps are so small that the energy difference between the ferromagnetic Wigner crystal and the antiferromagnetic state is extremely small [22].

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