Nonperturbative results for few electrons in the two-dimensional Hubbard model

M. Fabrizio, A. Parola^{*}, and E. Tosatti[†]

International School for Advanced Studies, Via Beirut 4, 34014 Trieste, Italy

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Based on a generalization of the equation which solves exactly the two-electron problem, we have found a method which allows the nonperturbative, asymptotically exact solution for the ground state of any finite number n of electrons in the low-density limit $(n/N \rightarrow 0)$ of the N-site two-dimensional Hubbard model. The three-electron case is checked against the exact numerical diagonalization and the total energy is shown by finite-size scaling to agree well, to leading order of an expansion in powers of $1/\ln N$, with the asymptotic solution. We then indicate how to solve for an arbitrary electron number, including both closed and open shells. The case of four electrons is explicitly presented as an application. More generally, the closed-shell d=2 ground state is a nondegenerate singlet with zero total momentum. Similar to d=1, all observables differ from their U=0 value by a correction which is U independent. Unlike d=1 and similar to d=3, however, the ground state is a linear combination of the unperturbed U=0 Fermi sea with the set of two-particle excitations. Moreover, the momentum distribution $n(\mathbf{k})$ can be evaluated explicitly, and shows a finite Fermi jump $Z = 1 - 4 \ln 2 / \ln^2(n/N)$. This result appears to argue in favor of a Fermi-liquid-like behavior for d=2 in the zero-density limit $n/N \to 0$. The open-shell ground states display an interesting degeneracy between a nondegenerate singlet and high-spin states.

I. INTRODUCTION

A large effort is currently being devoted towards understanding the physics of two-dimensional (2D) strongly correlated electron Hamiltonians, some of which may be related to high-temperature superconductivity.¹ In particular, there has been wide discussion of the possibility that the 2D Hubbard model

$$\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$
(1)

could exhibit non-Fermi-liquid behavior, i.e., a vanishing "Fermi jump" even away from half filling

$$Z = \lim_{\mathbf{q} \to 0} (n_{k_f + \mathbf{q}} - n_{k_f - \mathbf{q}}) = 0 , \qquad (2)$$

where $n_{\mathbf{k}} = \langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \rangle$ is the momentum distribution function. In that case, the implication is that the system has different quasiparticles from electrons and holes, and the very interesting possibility of charge-spin separation, well established for d=1, might arise for d=2.

While most of the ongoing effort is being concentrated on the general case of large electron density, there is less work in the low-density regime. Yet, there are several reasons why the low-density limit is interesting. Firstly, there is more hope for a solution. Secondly, low-density is effectively the same as taking the continuum limit $(a \rightarrow 0)$ at finite density, therefore all understanding obtained will apply to that case, too. Thirdly, the recent understanding obtained in d=1 (Refs. 2-6) implies a surprising behavior in that limit. In essence, in the low-density limit there is a competition between weak coupling—which should prevail for a short-range dilute system according to standard Fermi-liquid methods⁷ and strong coupling, which is, for example, suggested by the form of the two-electron problem.⁸ For d=1, strong coupling actually prevails, and the effective interaction renormalizes to infinity for all values of U in the lowdensity limit. The question is then whether anything like that could take place for d=2 too, or if instead a Galitskiitype Fermi-liquid theory, as proposed earlier by Bloom⁹ and very recently by Engelbrecht and Randeria¹⁰ and by Fukuyama, Narikiyo, and Hasegawa,¹¹ will prevail in the end.

One intriguing suggestion in this context came from solving⁸ the two-electron problem in d=2. The answer in that case was mixed. There is, as in 1D, a change of all ground-state properties which is U independent, so long as U is nonzero. This points to strong coupling. However, the magnitude of these corrections is only logarithmic with size, instead of power law as in d=1 dimension. This suggests that corrections might in the end be insufficient to wash out Fermi-liquid behavior at low densities.

The motivation for this work comes from the need to further clarify this issue. We must develop a nonperturbative method, which should cope with a strong-coupling situation, and be capable of calculating Z and detecting whether it does or does not vanish in the low-density limit. At the same time, we need a small parameter in the theory, or else the many-electron problem is insoluble. As it turns out, the relevant small parameter does exist, and it is $1/\ln L$ for d=2 (L is the linear size, $L^2 = N$ the number of sites, hence $L \to \infty$ in the low-density limit). In the $L \to \infty$ asymptotic limit the ground state can be solved exactly for any number of electrons, with very interesting consequences.

The detailed plan of this paper is as follows. First, in Sec. II, we shall reexamine the two-electron problem. It will be shown how, by introducing the scattering amplitude, the problem can be solved in a way which is asymptotically exact for $L \to \infty$. In Sec. III we demonstrate the use of the asymptotic method by direct application to the three-electron problem. Three electrons in the Hubbard model were considered earlier by Mattis,¹² who discussed in detail the negative-U case. In order to provide a direct visual check of the asymptotic results, we have solved numerically the U > 0 three-electron problem, and shown by finite-size scaling that the two agree well. In Sec. IV we generalize the asymptotic method to any even number n of electrons (the generalization to odd n, although straightforward, is not presented). Separate descriptions are then provided for electron numbers such that the noninteracting Fermi system is nondegenerate (i.e., closed shells in \mathbf{k} space) in the same section, and for the degenerate case (open shells), in Sec. V. In that section the n = 4 case is presented as an exemplification. Finally, a general discussion, including connections with Galitskii's low-density theory, is presented in Sec. VI.

II. TWO ELECTRONS IN THE HUBBARD MODEL: ASYMPTOTIC VERSUS EXACT SOLUTION

Let us consider two electrons in a *d*-dimensional hypercube of L^d sites. The Hubbard Hamiltonian in momentum space is

$$\hat{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{U}{L^{d}} \sum_{\mathbf{p},\mathbf{p}',\mathbf{q}} c_{\mathbf{p}+\mathbf{q}\uparrow}^{\dagger} \dot{c}_{\mathbf{p}'-\mathbf{q}\downarrow}^{\dagger} c_{\mathbf{p}'\downarrow} c_{\mathbf{p}\uparrow} , \qquad (3)$$

where

$$\varepsilon_{\mathbf{k}} = -2t \sum_{i=1}^{d} \cos(\mathbf{k}_i a)$$

and a is the lattice spacing. Since this Hamiltonian conserves the total momentum \mathbf{P} , we limit ourselves in a subspace in which \mathbf{P} is fixed. A generic wave function is

$$|\Psi\rangle = \sum_{\mathbf{q}} L(\mathbf{q}) c^{\dagger}_{\mathbf{q}\uparrow} c^{\dagger}_{\mathbf{P}-\mathbf{q}\downarrow} |0\rangle . \qquad (4)$$

This function is the eigenvector of eigenvalue E if the coefficients $L(\mathbf{q})$ satisfy the Schrödinger equation

$$(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}})L(\mathbf{q}) = \frac{U}{L^d} \sum_{\mathbf{p}} L(\mathbf{p}) \;.$$

We call J the right-hand side of this equation, so that

$$L(\mathbf{q}) = \frac{J}{\left(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}}\right)} \ . \tag{5}$$

By substituting this expression in that for J it is easy to obtain a self-consistent equation of the usual type for the energy, i.e.,^{12,8}

$$1 = \frac{U}{L^d} \sum_{\mathbf{q}} \frac{1}{\left(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}}\right)} \,. \tag{6}$$

The solution to this equation can be found analytically in 1D and asymptotically (large L) or numerically in $d \ge 2$. A possible approach to this problem was presented earlier in Ref. 8. Our strategy in this paper will be to reconsider the asymptotic solution in a form which emphasizes (a) applicability to all space dimensions, (b) the crucial importance of the scattering amplitude, and (c) transferability to more than two electrons.

Let us write the difference ΔE between a generic eigenvalue E of Eq. (6) and the U=0 ground-state energy $2\varepsilon_0$ as

$$\Delta E = E - 2\varepsilon_{0} = \frac{\alpha(L)}{L^{2}} .$$
⁽⁷⁾

We may distinguish two classes of eigenvalues. In the first class we include all the eigenvalues whose $\alpha(L)$ goes to zero when $L \to \infty$, while the second class contains all the other eigenvalues. If the first class is not empty, then it obviously includes the ground state, since $\alpha(L) > 0$ for the repulsive Hubbard model. We note that, by construction, the interaction corrections to the eigenvalues ΔE in the first class go to zero faster than the U = 0excitation energies (which go like $1/L^2$). Let us assume that the first class is indeed not empty, and let us solve Eq. (6) for a generic eigenvalue belonging to it. This assumption will be justified a posteriori. We also assume $\mathbf{P} = \mathbf{0}$, as we want to find the ground state. In order to solve the self-consistent equation let us extract from the sum the term with q = 0, which is the most divergent for $L \to \infty$. In this way Eq. (6) becomes

$$1 \simeq \frac{U}{\alpha(L)L^{d-2}} + \frac{U}{L^d} \sum_{\mathbf{q} \ (\neq 0)} \frac{1}{(\Delta E + 2\varepsilon_0 - 2\varepsilon_{\mathbf{q}})} \ . \tag{8}$$

In the second term of the right-hand side, we can neglect the interaction correction ΔE (we will show later that this is asymptotically correct for $d \geq 2$) with respect to $\varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{0}}$ when taking the limit $L \to \infty$, thus obtaining

$$\frac{U}{L^d} \sum_{\mathbf{q} \ (\neq 0)} \frac{1}{(\Delta E + 2\varepsilon_0 - 2\varepsilon_{\mathbf{q}})} \simeq -Ua^d \int_{\frac{2\pi}{L^a}}^{k_0} \frac{d^d q}{(2\pi)^d} \frac{1}{(2\varepsilon_{\mathbf{q}} - 2\varepsilon_0)} \simeq -Ua^{d-2} \frac{1}{2tf_0} , \tag{9}$$

where $k_0 \sim \pi/a$ is an upper cutoff and f_0 is the lowenergy scattering amplitude, that is,

$$f_{0} = \begin{cases} 4\pi a & \text{in 3D} \\ -\frac{2\pi}{\ln(ka)} \sim \frac{2\pi}{\ln L} & \text{in 2D} \\ \frac{(2\pi)^{2}}{La} & \text{in 1D} . \end{cases}$$
(10)

Equation (6) at last reduces to

$$1 = \frac{U}{\alpha(L)L^{d-2}} - \frac{Ua^{d-2}}{2tf_0} , \qquad (11)$$

whose solution is unique (i.e., the first class for P = 0 contains only the ground state) and yields simply

$$\alpha(L) = \frac{1}{L^{d-2}} \frac{U}{1 + \frac{Ua^{d-2}}{2tf_0}} = \begin{cases} \frac{L^{-1} \frac{U}{1 + U/(8\pi t)} \text{ in } 3D}{\frac{4\pi t}{\ln L}} & \text{in } 2D\\ 8\pi^2 t & \text{in } 1D \end{cases}$$

(12)

This general expression of $\alpha(L)$ shows that, when $f_0 \to 0$ in the large size limit, i.e., in $d \leq 2$, the asymptotic limit $L \to \infty$ drives the system towards strong coupling (i.e., $U \to \infty$) and $\alpha(L)$ tends to a limiting value independent of U, as long as U is not zero.⁸

These results are consistent with the initial assumption $\lim_{L\to\infty} \alpha(L) = 0$ only in $d \ge 2$. In 1D (more generally in d < 2) $\alpha(L)$ is instead finite for $L \to \infty$. Therefore the result (9) does not apply and the first class of eigenvalues is empty. The exact solution of Eq. (6) in 1D is⁸ (for large size and for the ground state) $\Delta E \simeq 2t(\pi/L)^2$ and indeed does not belong to the first class, as the previous simple calculation predicts. We can now address the error made in neglecting ΔE in Eq. (9). For d=2, for example, inserting $\Delta E = 4\pi t/L^2 \ln L$ yields a further correction of order $1/L^2 \ln^3 L$ to ΔE . Therefore, neglect of ΔE in (9) is asymptotically exact to order $1/L^2 \ln^2 L$ (in general f_0^2/L^2).

Besides the ground-state energy given by (7)-(12), we also obtain an explicit form for the ground-state wave function. By using Eq. (7), it follows that, for any dimension d, the "envelope function" L is

$$L(\mathbf{q}) = \begin{cases} \frac{JL^2}{\alpha(L)} & \text{if } \mathbf{q} = \mathbf{0} \\ \frac{J}{2\varepsilon_0 + \alpha(L)L^{-2} - 2\varepsilon_q} & \text{otherwise} \end{cases}$$
(13)

Finally, the momentum distribution $n(\mathbf{p})$ is given by

$$n(\mathbf{p}) = \frac{L^2(\mathbf{p})}{L^2(\mathbf{0}) + \sum_{\mathbf{q} \ (\neq \mathbf{0})} L^2(\mathbf{q})} \ . \tag{14}$$

In the limit $L \to \infty$ the second term in the denominator behaves as L^4 , so that if $\alpha(L) \to 0$ (which is the case in $d \ge 2$), the behavior of the denominator is dominated by $L^2(\mathbf{0}) \simeq L^4/\alpha(L)$. This implies that, inside the U = 0 Fermi surface (i.e., just for the wave vector **0**), the momentum distribution is

$$n(0) \simeq 1 - u\alpha^2(L) \tag{15}$$

while, just outside it is

$$n(2\pi/La, 0, 0, \ldots) = v\alpha^2(L)$$
, (16)

that is,

$$Z = 1 - (u + v)\alpha^{2}(L) , \qquad (17)$$

where u and v are positive coefficients. Inserting (12) we get

$$1 - Z \sim \begin{cases} L^{-2} & \text{in 3D} \\ \ln^{-2} N & \text{in 2D} \end{cases}.$$
 (18)

This result shows that the $U \neq 0$ momentum distribution for $L \to \infty$ reaches the U=0 value in $d \ge 2$. In 1D this is not the case. Exact solution of the Schrödinger equation yields $\alpha(L) = 2t\pi^2$, which inserted into (13) and (20) gives the known result⁸

$$n\left(p = \frac{2\pi l}{La}\right) = \frac{8}{\pi^2} \frac{1}{(4l^2 - 1)^2} , \qquad (19)$$

which is characterized by a jump across the Fermi surface strictly smaller than 1. The main results of this section can be summarized as follows.

(i) The two-electron problem is particularly simplified by working in the asymptotic limit $L \to \infty$, and by focusing on the asymptotic behavior of the ground-state energy shift ΔE . The asymptotic shift is a simple function of the scattering amplitude, and so are all other groundstate properties.

(ii) There is a similarity between d=1 and d=2, in that (for $L \to \infty$) all properties of two electrons are modified by the presence of the interaction U by U-independent terms. In other words, both cases are in the strongcoupling limit.⁸

(iii) By contrast, there is a similarity between d=3 and d=2 in that the energy correction $\Delta E = L^{-2}\alpha(L)$ vanishes for large L faster than the noninteracting energy level spacing. A remarkable consequence of this fact is that the Fermi jump $Z \to 1$ in the asymptotic limit, for $d \geq 2$, but not for d < 2.

III. THREE ELECTRONS

Having solved the two-electron problem, the next question which arises is to what extent the behavior just described is stable or instead radically modified by the presence of a third electron. Mattis considered this problem long ago, in his study of the pair stability for attractive Hubbard $U.^{12}$

Let us consider three electrons in the subspace of total momentum $\mathbf{P} = (\frac{2\pi}{L_a}, 0, 0, ...)$ (in *d* dimension). A generic wave function is

$$|\Psi\rangle = \sum_{\mathbf{q}\mathbf{k}} L(\mathbf{q}, \mathbf{P} - \mathbf{q} - \mathbf{k}, \mathbf{k}) c^{\dagger}_{\mathbf{q}\uparrow} c^{\dagger}_{\mathbf{P}-\mathbf{k}-\mathbf{q}\downarrow} c^{\dagger}_{\mathbf{k}\uparrow} |0\rangle .$$
(20)

The coefficients L must be antisymmetric in the first and third variable. The Schrödinger equation for the L's is

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$$(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}-\mathbf{k}} - \varepsilon_{\mathbf{k}})L(\mathbf{q}, \mathbf{P} - \mathbf{q} - \mathbf{k}, \mathbf{k}) = \frac{U}{L^d} \sum_{\mathbf{p}} [L(\mathbf{p}, \mathbf{P} - \mathbf{p} - \mathbf{k}, \mathbf{k}) - L(\mathbf{p}, \mathbf{P} - \mathbf{p} - \mathbf{q}, \mathbf{q})], \qquad (21)$$

whose solution is

$$L(\mathbf{q}, \mathbf{P} - \mathbf{q} - \mathbf{k}, \mathbf{k}) = \frac{J(\mathbf{k}) - J(\mathbf{q})}{(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P} - \mathbf{q} - \mathbf{k}} - \varepsilon_{\mathbf{k}})}, \quad (22)$$

where

$$J(\mathbf{k}) = \frac{U}{L^d} \sum_{\mathbf{q}} L(\mathbf{q}, \mathbf{P} - \mathbf{q} - \mathbf{k}, \mathbf{k}) .$$
 (23)

Substituting the expression of L in that of J we obtain a homogeneous set of equations¹² (instead of a simple self-consistent equation as for two electrons),

$$J(\mathbf{k}) = J(\mathbf{k}) \frac{U}{L^d} \sum_{q} \frac{1}{(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}-\mathbf{k}} - \varepsilon_{\mathbf{k}})} - \frac{U}{L^d} \sum_{q} \frac{J(\mathbf{q})}{(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}-\mathbf{k}} - \varepsilon_{\mathbf{k}})}, \quad (24)$$

which can be formally written in matrix form

$$\vec{J} = U\hat{T}(E) \cdot \vec{J} \tag{25}$$

Together with (24), this equation defines the operator $\hat{T}(E)$. The rows and columns of this matrix are labeled

by the k vector of the third particle only. The third particle is a "spectator," while the other two are getting virtually excited. The final ground state is, if $\alpha(L) \to 0$, a linear superposition of the unperturbed Fermi sea (FS) plus all these doubly excited states [which would not be the case if $\alpha(L) \neq 0$ for $L \to \infty$]. The crucial point which will make the asymptotic solution very easy, is, as it will turn out, that the spectator particle belongs to the unperturbed Fermi sea with probability one, as $L \to \infty$. This makes the (otherwise infinite) matrix $\hat{T}(E)$ finite and very small, as we now show.

The self-consistent set of equations (25) will only find solution when E corresponds to an eigenvalue of Schrödinger equation (21). We now show how the asymptotic procedure of Sec. II can be applied to the groundstate problem. Let us define as usual $\alpha(L) = (E - E_0)L^2$, where $E_0 = 2\varepsilon_0 + \varepsilon_P \simeq t[-6d + (2\pi)^2/L^2]$ is the U=0ground-state energy of three electrons. If we assume that the ground state satisfies the asymptotic condition $\lim_{L\to\infty} \alpha(L) = 0$, then it is possible to show, using Eq. (24), that the matrix $\hat{T}(E)$ has a part $\hat{T}^{(s)}$ which dominates for $L \to \infty$. Let us consider first the off-diagonal elements of the full $\hat{T}(E)$, which are of the form

$$\frac{1}{L^{d}(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}-\mathbf{k}} - \varepsilon_{\mathbf{k}})} \sim \begin{cases} L^{(2-d)}/\alpha(L) & \text{if } (\mathbf{k}, \mathbf{q}) = (\mathbf{0}, \mathbf{0}) , (\mathbf{0}, \mathbf{P}), \text{ or } (\mathbf{P}, \mathbf{0}) \\ L^{(2-d)} & \text{otherwise.} \end{cases}$$
(26)

Hence, if $\alpha(L) \to 0$, the upper case, when all momenta belong to the unperturbed Fermi sea (FS) (which consists only of the two wave vectors **0** and **P**), dominates the second. If we extract from the diagonal elements the dominant terms in the sense of Eq. (26), the remaining terms may be used to define a function $I(\mathbf{k})$

$$I(\mathbf{k}) = -L^{-d} \sum_{\mathbf{q} \notin \mathrm{FS}} \frac{1}{(E - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}-\mathbf{k}} - \varepsilon_{\mathbf{k}})} \simeq \frac{a^{d-2}}{2tf_0} \ ,$$

the last equality holding only for small k. For small wave vectors this function is of the same order in L as the leading terms of Eq. (26). Asymptotically we obtain the dominant part of $\hat{T}(E)$, which is

where some ordering of the k's is implicit in order to change a matrix of dimension $(L \times L \times L \times L)$ in one $(L^2 \times L^2)$. In Eq. (27), the first 2×2 block represents the two states where $\mathbf{k} = 0$, \mathbf{P} , that is, precisely that where the spectator particle belongs to the unperturbed Fermi sea. As one can see, all couplings to other spectator states $I(\mathbf{k}_i)$ are exactly zero in the asymptotic limit. Equation (24) now becomes $\vec{J} = U\hat{T}^{(s)} \cdot \vec{J}$ in d > 2 and $\hat{T}^{(s)} \cdot \vec{J} = 0$ in $d \leq 2$. The solution of these equations (in d = 3 we take $U \to \infty$ for simplicity) is

$$J(\mathbf{0}) = -J(\mathbf{P})$$
, $J(\mathbf{k}) = 0$ if $\mathbf{k} \neq \mathbf{0}, \mathbf{P}$, (28)

$$\alpha(L) \simeq \frac{4tf_0}{(aL)^{d-2}} . \tag{29}$$

In $d \ge 2$ Eq. (29) is compatible with the initial assumption $\lim_{L\to\infty} \alpha(L) = 0$. On the contrary, in d < 2, the result does not satisfy that assumption, exactly as we found for two electrons.

The d = 2 three-electron ground-state energy is thus predicted to be, according to Eq. (29)

$$E \simeq -12t + \frac{t(2\pi)^2}{L^2} + \frac{16\pi t}{L^2 \ln L^2} + \cdots$$
 (30)

The persistence of the logarithmic term already found for two electrons (however, a factor 2 larger), suggests that the essential physics of that case is stable against addition of a third electron. From Eq. (20) it is easy to derive the expression of the momentum distribution in terms of the function $J(\mathbf{k})$, i.e.,

$$n_{\mathbf{k}\uparrow} = 4 \sum_{\mathbf{q}} \left(\frac{J(\mathbf{q}) - J(\mathbf{k})}{E - \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{q}-\mathbf{k}}} \right)^2 , \qquad (31)$$

$$n_{\mathbf{k}\downarrow} = 2 \sum_{\mathbf{q}} \left(\frac{J(\mathbf{q}) - J(\mathbf{P} - \mathbf{q} - \mathbf{k})}{E - \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P} - \mathbf{q} - \mathbf{k}}} \right)^2 .$$
(32)

We calculate the momentum distribution simply substituting Eqs. (28), (29), and (30) into Eqs. (31) and (32). Again the result does not differ substantially from the two-electron problem. In fact it is easy to convince ourselves (although we will not show in detail here) that the momentum distribution again differs by terms of order $\alpha^2(L)$ from the unperturbed $n(\mathbf{q}) = 1$ only when $\mathbf{q} = \mathbf{0}, \mathbf{P}$, while $n(\mathbf{q}) = 0$ otherwise.

The three-electron Schrödinger equation (24) has also been solved numerically in order to provide an independent check of the asymptotic solution given above. The numerical solution is obtained by exact diagonalization of (24) for square lattices of size 8×8 , 9×9 ,..., 23×23 , 24×24 . In Fig. 1 we have plotted the asymptotic ground-state energy of Eq. (30) versus linear size L, together with the numerical solution of (24) for U = 10t(black squares), U = 100t (open squares), and U = 1000t(starred points). The agreement at larger sizes appears to be quite good. In order to get to a more quantitative



FIG. 1. Ground-state energy of three electrons on a 2D $L \times L$ square lattice vs L. The points are the exact numerical result for U = 10t (black squares), U = 100t (open squares), and U = 1000t (starred points). The solid curve is the asymptotic solution Eq. (28), while the dashed curve is the U = 0 ground-state energy.

level we have also performed a finite-size scaling of the numerical results. Let us notice that, according to our asymptotic solution, the quantity

$$\alpha(L)\ln L = (E - E_0)L^2\ln L$$
(33)

is predicted to be equal to $8\pi t + O(1/\ln L)$. In Fig. 2 we have plotted the right hand side of Eq. (33) versus $1/\ln L$ for the exact numerical results. The solid lines



FIG. 2. Finite-size scaling of the asymptotic solution Eq. (28). We have plotted the quantity $(E - E_0)L^2 \ln L$ vs $1/\ln L$. The points are the numerical results. The curves are fittings by using a three-parameter function $(E - E_0)L^2 \ln L = A + B/\ln L + C/\ln^2 L$. The isolated point at $1/\ln L = 0$ is the asymptotic result $A_{\infty} = 8\pi$, to be compared with the zero intercepts of the three curves.

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are a fitting of Eq. (33) with a three-parameter function

$$(E - E_0)L^2 \ln L = A + B/\ln L + C/\ln^2 L$$
(34)

suggested by the asymptotic expansion. Even if the exact results are not in the asymptotic regime $(1/\ln L \rightarrow 0)$, the fitted parameter A, as shown by the zero intercept of Fig. 2, is not far from the predicted asymptotic value 8π (the isolated black point). In conclusion, we believe the remaining error to be due to slow convergence of the expansion (34), and 8π to be asymptotically exact.

IV. GENERALIZATION TO ANY FINITE (EVEN) NUMBER OF ELECTRONS

We have shown that also the three-electron problem can be solved using as an asymptotic assumption that $\alpha(L) = (E_{U\neq 0} - E_{U=0})L^2 \rightarrow 0$, at least in $d \geq 2$. The result is compatible with the initial hypothesis if the size of the system is very large, and it agrees quite well with the exact solution. In this section we generalize the method to any number of electrons n and solve approximately the problem when the U=0 Fermi surface is not degenerate. Let us suppose to have n electrons in a subspace of **P** total momentum (for simplicity n is taken even). A generic wave function can be written as

$$|\Psi_n\rangle = \sum_{\mathbf{k}_1\mathbf{k}_2\cdots} L(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n) c^{\dagger}_{\mathbf{k}_1\uparrow} c^{\dagger}_{\mathbf{k}_2\downarrow} \cdots c^{\dagger}_{\mathbf{k}_n\downarrow} |0\rangle .$$
(35)

The coefficients L are odd functions with respect to the interchange of two odd (even) momenta. Notice that L depends only on n-1 momenta because of the conservation of the total momentum. The eigenvalue equation is

$$(E - \varepsilon_{\mathbf{k}_1} - \dots - \varepsilon_{\mathbf{k}_n})L(\mathbf{k}_1, \dots, \mathbf{k}_n) = \frac{U}{L^d} \sum_{\mathbf{q}} L(\mathbf{k}_1 + \mathbf{q}, \mathbf{k}_2 - \mathbf{q}, \mathbf{k}_3, \dots, \mathbf{k}_n) + L(\mathbf{k}_1 + \mathbf{q}, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4 - \mathbf{q}, \dots, \mathbf{k}_n) + \dots ,$$
(36)

where the dots correspond to all the possible pairings of momenta of one spin-up and one spin-down electron. Analogously to the three electron problem we define a function of n-2 momenta

$$(\mathbf{k}_3, \dots, \mathbf{k}_n) = \frac{U}{L^d} \sum_{\mathbf{q}} L\left(\mathbf{q}, \mathbf{P} - \mathbf{q} - \sum_{i=3}^n \mathbf{k}_i, \mathbf{k}_3, \dots, \mathbf{k}_n\right) ,$$
(37)

which allows rewriting the coefficients L as

$$L(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \dots, \mathbf{k}_n) = \frac{J(\mathbf{k}_3, \mathbf{k}_4, \dots, \mathbf{k}_n) - J(\mathbf{k}_3, \mathbf{k}_2, \dots, \mathbf{k}_n) + \cdots}{(E - \varepsilon_{\mathbf{k}_1} - \dots - \varepsilon_{\mathbf{k}_n})} .$$
(38)

The self-consistent set of equations that the J's have to

satisfy, turns out again to be of the general form

$$\vec{J} = U\hat{T}(E) \cdot \vec{J} . \tag{39}$$

The main advantage in working with the J rather than the L, is that the asymptotic expansion for large system size $L \to \infty$ is far more straightforward. To solve the set of equations we assume again that

$$E = E_0 + \frac{\alpha(L)}{L^2}$$
, where $\lim_{L \to \infty} \alpha(L) = 0$. (40)

This condition is fully compatible with zero density (n/L^d) for $L \to \infty$ (if the density were finite in the thermodynamic limit, the interaction correction to the total energy would instead be finite and proportional to the number of electrons). As in the case of three electrons, the matrix $\hat{T}(E)$ has a singular part $\hat{T}(E)^{(s)}$ which includes terms like

$$\frac{1}{(E-\varepsilon_{\mathbf{k}_1}-\cdots-\varepsilon_{\mathbf{k}_n})}\sim\frac{L^2}{\alpha(L)}$$

and

$$\frac{1}{L^{d}}\sum_{\mathbf{q},\mathbf{q}'\notin\mathbf{FS}}\delta\left(\mathbf{q}'+\mathbf{q}+\sum_{i=3}^{n}\mathbf{k}_{i}-\mathbf{P}\right)\frac{1}{\left(E-\varepsilon_{\mathbf{q}}-\varepsilon_{\mathbf{q}'}-\varepsilon_{\mathbf{k}_{3}}-\cdots-\varepsilon_{\mathbf{k}_{n}}\right)}\sim-\frac{a^{d-2}}{2t\,f_{0}}$$

where all the k's belong to the U=0 FS. As a first approximation we just solve the equation $\hat{T}(E)^{(s)} \cdot \vec{J} = 0$ (as before, that implies $U \to \infty$ in 3D, but not in 2D). This again requires that the only J different from zero are those whose arguments k are part of the Fermi sphere of the unperturbed n electrons. [Their number N_j is $(n/2)^2$ for nondegenerate closed shells, counting the possible pairings of different spin states in the Fermi sphere. In the case of open shells this number is bigger, because the pairings involve all the degenerate possibilities which can be realized at the outer shell of the Fermi sea.] In general, the equations these J must satisfy look like an eigenvalue problem of the type seen earlier,

$$\hat{M} \cdot \vec{J} = \lambda \vec{J} , \qquad (41)$$

where λ determines the unknown $\alpha(L)$ through

$$\lambda = \left(\frac{\alpha(L)a^{d-2}L^{d-2}}{2tf_0}\right) \tag{42}$$

and the ground-state energy expressed as a function of λ is

$$E = E_0 + \frac{\lambda^{2t} f_0}{a^{d-2} L^d} .$$
 (43)

In (41) the matrix \hat{M} is independent of E and has dimension N_j . The method for constructing \hat{M} is very simple and can be deduced by inspection of (36) and by using the symmetry properties of the L's.

For the sake of physical clarity, we recall again the significance of the rows and columns. In this matrix \hat{M} , each vector represents a given configuration of the n-2 spectator electrons, while the remaining two are getting into a doubly excited state. Similar to what happened for three electrons, it turns out that, if $\alpha(L) \to 0$ for $L \to \infty$ (i.e., first class not empty), then in the limit no spectators are allowed to lie outside of the unperturbed FS. Since the number of ways N_j in which the spectator electrons can be assigned inside the FS is finite and small, the matrix \hat{M} is always very simple, and can be diagonalized exactly.

First, suppose the U=0 Fermi surface to be nondegenerate (closed shell). Then \hat{M} is the matrix

$$\hat{M} = \begin{pmatrix} 1 & -1 & 1 & -1 & 1 & -1 & \cdots \\ -1 & 1 & -1 & 1 & -1 & 1 & \cdots \\ 1 & -1 & 1 & -1 & 1 & -1 & \cdots \\ \vdots & \vdots \\ \end{pmatrix}$$
(44)

of dimension $(n/2)^2 \times (n/2)^2$. The case in which the Fermi surface is degenerate (open shell) is a little bit more complicated. Let us suppose that it is *m*-fold degenerate. First we construct a block matrix made up of *m* boxes like (44) each of which is defined in a particular degenerate

TABLE I. Values of λ and of the total spin for the degenerate ground state of 4, 6, and 8 electrons.

No. of electrons	λ	Total spin
4	3	0,1,1
6	7	0,2
8	15	0,1,1

Fermi surface. However, some rows (columns) of different boxes correspond to the same J component. For this reason we move these rows (columns) in order to let them coincide with just one. The final matrix will look much more complicated than (44), and it will generally be more difficult to diagonalize. In this case we expect that the interaction partially removes the degeneracy. In Table I we show the value of λ and the possible (degenerate) values of the total spin of the ground states of 4, 6, and 8 electrons.

For the nondegenerate case, however, the solution is very simple. In fact the matrix (44) has only one physical solution, i.e., $\lambda \neq 0$, which is $\lambda = (n/2)^2$. For this solution the ground-state energy is

$$E = E_0 + \frac{n^2 t f_0}{2a^{d-2}L^d} \tag{45}$$

and

$$\vec{J} = \begin{pmatrix} 1\\ -1\\ 1\\ -1\\ \vdots\\ 0\\ 0\\ 0\\ \vdots \end{pmatrix} , \qquad (46)$$

where, as was said before, the components different from zero correspond to the spectator electrons belonging to the unperturbed FS.

The expression of the momentum distribution can be easily derived from (35) and (38). Apart from a normalization factor, it is

$$n_{\mathbf{k}\uparrow} = \sum_{(\mathbf{k}_3,\dots,\mathbf{k}_n)} L^2 \left(\mathbf{k}, \mathbf{P} - \mathbf{k} - \sum_{i=3}^n \mathbf{k}_i, \, \mathbf{k}_3, \dots, \mathbf{k}_n \right)$$
(47)

for spin-up electrons, and analogously for spin-down ones. The asymptotic solution of Eqs. (45) and (46) implies that the only L's different from zero are

$$L^{2}({\rm FS}) \simeq V^{2}/f_{0}^{2} = \Delta$$
, (48)

$$L^{2}(\{\mathrm{FS}-\mathbf{k}_{i}-\mathbf{k}_{i}'+\mathbf{k}_{o}+\mathbf{k}_{o}'\}) \simeq \frac{1}{(E-\varepsilon_{k_{i}}-\varepsilon_{k_{i}'}+\varepsilon_{k_{o}}+\varepsilon_{k_{o}'})^{2}} = \Lambda(\mathbf{k}_{i},\mathbf{k}_{i}',\mathbf{k}_{o},\mathbf{k}_{o}') , \qquad (49)$$

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where {FS} means the set of k vectors defining the Fermi sea, the \mathbf{k}_i are wave vectors inside the FS while \mathbf{k}_o are outside, and the prime refers to down-spin electrons. Notice that $\mathbf{k}_i + \mathbf{k}'_i = \mathbf{k}_o + \mathbf{k}'_o$. As was said before, the asymptotic ground state is a linear combination of the unperturbed Fermi sea with the entire set of two-particle excitations. Let us consider first the case $\mathbf{k} \in FS$. Then

$$n_{\mathbf{k}\uparrow} = L^{2}(\{\mathrm{FS}\}) + \sum_{\mathbf{k}_{o},\mathbf{k}_{o}'\notin\mathrm{FS}}^{\mathbf{k}_{i},\mathbf{k}_{o}'\in\mathrm{FS},\mathbf{k}_{i}\neq\mathbf{k}} L^{2}(\{\mathrm{FS}-\mathbf{k}_{i}-\mathbf{k}_{o}'+\mathbf{k}_{o}'+\mathbf{k}_{o}'\})\delta(\mathbf{k}_{i}+\mathbf{k}_{i}'-\mathbf{k}_{o}-\mathbf{k}_{o}')$$

$$= \Delta + \sum_{\mathbf{k}_{o},\mathbf{k}_{o}'\notin\mathrm{FS}}^{\mathbf{k}_{i},\mathbf{k}_{o}'\in\mathrm{FS}} \Lambda(\mathbf{k}_{i},\mathbf{k}_{i}',\mathbf{k}_{o},\mathbf{k}_{o}')\delta(\mathbf{k}_{i}+\mathbf{k}_{i}'-\mathbf{k}_{o}-\mathbf{k}_{o}')$$

$$- \sum_{\mathbf{k}_{o},\mathbf{k}_{o}'\notin\mathrm{FS}}^{\mathbf{k}_{i}'\in\mathrm{FS}} \Lambda(\mathbf{k},\mathbf{k}_{i}',\mathbf{k}_{o},\mathbf{k}_{o}')\delta(\mathbf{k}+\mathbf{k}_{i}'-\mathbf{k}_{o}-\mathbf{k}_{o}') = \Delta + \Omega - \Xi(\mathbf{k})^{-} , \qquad (50)$$

which also serves as a definition for Ω and $\Xi(\mathbf{k})^-$. When $\mathbf{k} \notin FS$ then

$$n_{\mathbf{k}\uparrow} = \sum_{\mathbf{k}'_o \notin FS}^{\mathbf{k}_i, \mathbf{k}'_i \in FS} L^2(\{FS + \mathbf{k} + \mathbf{k}'_o - \mathbf{k}_i - \mathbf{k}'_i\})\delta(\mathbf{k}_i + \mathbf{k}'_i - \mathbf{k} - \mathbf{k}'_o) = \Xi(\mathbf{k})^+ , \qquad (51)$$

where the + or - refers to $\mathbf{k} \notin FS$ or $\mathbf{k} \in FS$, respectively. It is easy to see that

$$\sum_{\mathbf{k}\in\mathrm{FS}}n_{\mathbf{k}\uparrow} = \frac{n}{2}(\Delta+\Omega) - \Omega \tag{52}$$

and

$$\sum_{\mathbf{k}\notin \mathrm{FS}} n_{\mathbf{k}\uparrow} = \Omega \ . \tag{53}$$

If we properly normalize the momentum distribution, i.e., we divide by

$$\frac{2\sum_{\mathbf{k}} n_{\mathbf{k}\uparrow}}{n} = \Delta + \Omega , \qquad (54)$$

then we find

$$n_{\mathbf{k}} = \frac{\Delta + \Omega - \Xi(\mathbf{k})^{-}}{\Delta + \Omega} \simeq 1 - \frac{\Xi(\mathbf{k})^{-}}{\Delta}$$
(55)

for $k \in FS$. Outside the Fermi surface, instead

$$n_{\mathbf{k}} = \frac{\Xi(\mathbf{k})^{+}}{\Delta + \Omega} \simeq \frac{\Xi(\mathbf{k})^{+}}{\Delta} .$$
 (56)

To obtain (55)-(56) we have assumed $\Delta \gg \Omega$. This is actually true in our approximation (i.e., $L \to \infty$ while *n* is finite), because $\Omega \simeq n \cdot \Xi^{-}(\mathbf{k})$, where, as we are going to show, $\Xi^{-}(\mathbf{k}) \sim L^{4}$, so that $\Omega \sim L^{4} \ll \Delta$ ($\sim L^{4} \ln^{2} L$ in d = 2 and $\sim L^{6}$ in d = 3). It is possible to evaluate the asymptotic behavior of $n_{\mathbf{k}}$ close to the Fermi surface. In this case, orders of magnitude are

$$\Xi(\mathbf{k})^{-} \sim \Xi(\mathbf{k})^{+} \sim \frac{n}{2} \sum_{\mathbf{q} \notin FS} \frac{1}{(2\varepsilon_{\mathbf{q}} - 2\varepsilon_{f})^{2}} \sim L^{d} n k_{f}^{d-4}$$
(57)

(the factor n/2 counts the down-spin electrons, i.e., \mathbf{k}'_i , inside the FS). This means that

$$\frac{\Xi(\mathbf{k})^{-}}{\Delta} \sim k_f^{2(d-2)} f_0^2 \tag{58}$$

and that the jump Z in the momentum distribution scales to one when $k_f \sim n^{1/d}/L \rightarrow 0$ as

$$1 - Z = 1 - (n_{k_f - 0\uparrow} - n_{k_f + 0\uparrow}) \sim k_f^{2(d-2)} f_0^2 \sim \begin{cases} (k_f a)^2 \text{ in } 3D \\ \ln^{-2} L \text{ in } 2D \end{cases}.$$
(59)

V. FOUR ELECTRONS, AND OTHER OPEN SHELLS

In this section we solve the asymptotic set of equations (41) for an open shell, in particular two extra electrons added to an otherwise closed shell. As an exemplification we consider first the case of n = 4 electrons. A generic $S_z = 0$ wave function of four electrons is

$$|\Psi\rangle = \sum L(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) c^{\dagger}_{\mathbf{k}_1\uparrow} c^{\dagger}_{\mathbf{k}_2\downarrow} c^{\dagger}_{\mathbf{k}_3\uparrow} c^{\dagger}_{\mathbf{k}_4\downarrow} |0\rangle , \qquad (60)$$

where $L(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) = -L(\mathbf{k}_3, \mathbf{k}_2, \mathbf{k}_1, \mathbf{k}_4) = -L(\mathbf{k}_1, \mathbf{k}_4, \mathbf{k}_3, \mathbf{k}_2)$. The Schrödinger equation for the coefficients is

If we define the function

$$J(\mathbf{k}_1, \mathbf{k}_2) = \frac{U}{L^d} \sum_{\mathbf{q}} L(\mathbf{q}, \mathbf{P} - \mathbf{q}, \mathbf{k}_1, \mathbf{k}_2) , \qquad (62)$$

then the coefficients L are

$$L(\mathbf{k}_{1}, \mathbf{k}_{2}, \mathbf{k}_{3}, \mathbf{k}_{4}) = \frac{J(\mathbf{k}_{3}, \mathbf{k}_{4}) - J(\mathbf{k}_{3}, \mathbf{k}_{2}) - J(\mathbf{k}_{1}, \mathbf{k}_{4}) + J(\mathbf{k}_{1}, \mathbf{k}_{2})}{E - \varepsilon_{\mathbf{k}_{1}} - \varepsilon_{\mathbf{k}_{2}} - \varepsilon_{\mathbf{k}_{3}} - \varepsilon_{\mathbf{k}_{4}}}$$
(63)

The self-consistent set of equations the J's have to satisfy is

$$J(\mathbf{k}_{1},\mathbf{k}_{2}) = J(\mathbf{k}_{1},\mathbf{k}_{2}) \frac{U}{L^{d}} \sum_{\mathbf{q}} \frac{1}{E - \varepsilon_{\mathbf{k}_{1}} - \varepsilon_{\mathbf{k}_{2}} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{k}_{1}-\mathbf{k}_{2}-\mathbf{q}}} - \frac{U}{L^{d}} \sum_{\mathbf{q}} \frac{J(\mathbf{k}_{1},\mathbf{q}) + J(\mathbf{q},\mathbf{k}_{2})}{E - \varepsilon_{\mathbf{k}_{1}} - \varepsilon_{\mathbf{k}_{2}} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{k}_{1}-\mathbf{k}_{2}-\mathbf{q}}} + \frac{U}{L^{d}} \sum_{\mathbf{q}} \frac{J(\mathbf{q},\mathbf{P}-\mathbf{q}-\mathbf{k}_{1}-\mathbf{k}_{2})}{E - \varepsilon_{\mathbf{k}_{1}} - \varepsilon_{\mathbf{k}_{2}} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P}-\mathbf{k}_{1}-\mathbf{k}_{2}-\mathbf{q}}}$$
(64)

Let us define the functions

$$A(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) = \frac{U}{L^d} \frac{1}{E - \varepsilon_{\mathbf{k}_1} - \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}_3} - \varepsilon_{\mathbf{k}_4}} , \qquad (65)$$

$$I(\mathbf{k}_1, \mathbf{k}_2) = -\frac{U}{L^d} \sum_{\mathbf{q}} \frac{1}{E - \varepsilon_{\mathbf{k}_1} - \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{P} - \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{q}}} \simeq \frac{Ua^{d-2}}{2tf_0}$$
(66)

and the wave vectors (for simplicity we work in 2D)

$$\mathbf{0} = (0,0) , \quad \mathbf{1} = \left(0, \frac{2\pi}{La}\right) , \quad \mathbf{2} = \left(0, -\frac{2\pi}{La}\right) , \quad \mathbf{3} = \left(\frac{2\pi}{La}, 0\right) , \quad \mathbf{4} = \left(-\frac{2\pi}{La}, 0\right) . \tag{67}$$

Let us look for the $\mathbf{P} = \mathbf{0}$ ground state (for $\mathbf{P} \neq \mathbf{0}$ the problem becomes effectively closed shell, and is solved as in the previous section). The unperturbed Fermi sea for total momentum zero is fourfold degenerate. If we assume the asymptotic condition $\alpha(L) = (E - E_0)L^2 \rightarrow 0$ where, as usual, $E_0 = 2\varepsilon_0 + 2\varepsilon_1$ is the U = 0 ground-state energy, then the value of A is more singular when the arguments belong to one of the possible Fermi surfaces, i.e.,

$$A(0,0,1,2) = A(0,0,2,1) = A(0,0,3,4) = A(0,0,4,3) = \dots = \frac{U}{\alpha(L)} ,$$
(68)

while in the other cases A does not diverge when $L \to \infty$. As it happened for closed shells, just the J whose arguments (the two spectator electron momenta for this n = 4 problem) belong to the degenerate Fermi surfaces are nonzero, to leading order. The number of spectator configurations is 13. The peculiarity of the general case $n = n_0$ (closed shell)+2 (of which n = 4 is an example), is that the spectator configuration of the electrons which belong to the n_0 Fermi surface mixes with all the others. Let us show how this happens for n = 4. We can write explicitly the set of Eq. (64) as

$$\begin{aligned} J(0,0) &= J(0,0)[-I + A(0,0,1,2) + A(0,0,2,1) + A(0,0,3,4) + A(0,0,4,3)] \\ &- A(0,0,1,2)[J(0,2) + J(1,2)] - A(0,0,2,1)[J(0,1) + J(2,0)] \\ &+ A(0,0,1,2)J(1,2) + A(0,0,2,1)J(2,1) + A(0,0,3,4)J(3,4) + A(0,0,4,3)J(4,3) , \end{aligned}$$

$$J(0,1) = J(0,1)[-I + A(0,1,0,2) + A(0,1,2,0)] - A(0,1,0,2)[J(0,2) + J(0,1)] - A(0,1,2,0)[J(0,0) + J(2,1)] + A(0,1,2,0)J(2,0) + A(0,1,0,2)J(0,2) ,$$
(69)

J(1,2) = J(1,2)[-I + A(1,2,0,0)] - A(1,2,0,0)[J(1,0) + J(0,2)] + A(1,2,0,0)J(0,0) .

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All the other ten equations can be easily obtained by these ones. Again, since both A and I are logarithmically divergent we can set the left-hand-side terms equal to zero. Then we can divide the equations by the term $U/\alpha(L)$ of Eq. (68), so that the resulting set of equations look like an eigenvalue problem, where the eigenvalue is

$$\lambda = \frac{I}{A} \simeq \frac{\alpha(L)}{2tf_0}$$

and the 13×13 matrix \hat{M} is

-1 $\hat{M} = \begin{bmatrix} -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & -1 & 1 & 0 \\ 1 & 0 & 0 & 0 & -1 & 1 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ -1-1-1-1-1-1

The first row (column) corresponds to J(0,0), while the others in order to J(0,1), J(2,1), J(2,0), J(0,2), J(1,2), J(1,0), J(0,3), J(4,3), J(4,0), J(0,4), J(3,4), and J(3,0). We see that matrix has the form we anticipated in Sec. IV. However, in the present open-shell case, the (0,0) spectator configuration mixes with all others. The matrix can be easily diagonalized to find two physical (i.e., nonzero) eigenvalues, $\lambda = 3$ (threefold degenerate), and $\lambda = 7$ (nondegenerate), and nine unphysical $\lambda = 0$ eigenvalues [unphysical eigenvalues of \hat{M} are generally caused by the transformation from Eq. (61) to Eq. (63), which is singular for $\lambda = 0$]. The $\lambda = 3$ eigenvectors are

 $\vec{J_1}$ and $\vec{J_2}$ correspond to triplet states, while $\vec{J_3}$ is a singlet, as is seen by direct inspection of the relative sign of, e.g., J(0,1) [second from top in (72)], and J(1,0) [seventh from top in (72)]. The eigenvector corresponding to $\lambda = 7$ is



and is a singlet.

We note that the lowest singlet J_3 has a rotational d symmetry, while the highest J_4 , s symmetry.

We further note that for the lowest eigenvalues, J_1 , J_2 , J_3 , the component J(0,0) is zero. This result, inserted in Eq. (63) for the coefficients L, implies that in the lowest-energy states, it is not possible to excite a pair of electrons keeping the "core" of the Fermi sea frozen. In other words, the coefficient of the states with two spectator electrons at $\mathbf{k} = \mathbf{0}$ and the other two excited out of the FS are rigorously zero in the four-electron ground state.

The results just found for n = 4 can be immediately generalized to the case $n = n_0$ (closed shell) +2-electrons. Let us suppose that there are 2m degenerate states in the outer k-space shell. The matrix \hat{M} will be similar to the matrix (71), the only differences being that now there are 2m boxes of dimension $[(n/2)^2 - 1] \times [(n/2)^2 - 1]$ instead of $2 \cdot 2 = 4$ boxes of dimension 3×3 , and that

(70)

(71)

the first diagonal element is 2m instead of 4. The first (top left) \hat{M} matrix element corresponds to the J whose arguments belong to the "core," that is to the case where n_o spectator electrons rigidly occupy the (n-2) closed-shell FS. It is easy to show that the lowest eigenvalue is

$$\lambda = \frac{n^2}{4} - 1 \tag{74}$$

and it is 2m-1 times degenerate. Of the lowest eigenvectors, m are triplets and m-1 *d*-like singlets. As before, for all these eigenvectors the component corresponding to the J of the "core," is zero. This again implies that the ground state has exactly no components in which the spectator electrons are in the "core." The other nondegenerate eigenvalue is

$$\lambda = \frac{n^2}{4} + (2m - 1) \tag{75}$$

and corresponds to an s-like singlet (in this case the component corresponding to the J of the core is 2m times bigger than the others).

For the sake of completeness, we report here also the ground-state energy for $P = 2k_f + 4\pi/La$. In that case, we have a singlet with

$$\lambda = \frac{n^2}{4} , \qquad (76)$$

which is higher than the true 2m - 1 degenerate ground state (74).

VI. DISCUSSION, AND CONNECTION WITH FINITE DENSITY

We have presented a solution for the ground state of n electrons in the d=2 and d=3 Hubbard model. The results are simple, analytical, and formally exact. However, they are asymptotic in the sense that only the lowest-order term of an ordered expansion in powers of $1/\ln L$ (for d=2) and 1/L (for d=3) is obtained. In particular, we have not yet shown that the coefficients of the higher orders in this expansion are all finite, for any finite number of particles n. With this only provision, which we hope to be able to clarify in the future, the results presented are exact.

We obtain the ground-state energy, total momentum,

symmetry, wave function, and momentum distribution. For a general closed shell in k space (i.e., n = 2, 10, 18, ...in d=2) the ground state is a $\mathbf{P} = \mathbf{0}$ singlet, with energy given by Eq. (45). The situation is considerably richer for open shells, which display degeneracy. However, the basic physics should converge to that of closed shells for large n, at least to within correction of order $n^{-1/d}$.

The momentum distribution $n(\mathbf{k})$ for the closed-shell case yields a Fermi jump [Eq. (59)] which, modulo *U*independent logarithmic corrections, scales asymptotically to 1 for d=2. This result foreshadows a Fermi-liquid behavior at very small density, which is what Bloom⁹, Engelbrecht and Randeria¹⁰ and Fukuyama, Narikiyo, and Hasegawa¹¹ have claimed.

In fact, if we assume, reasonably but without proof, that our results can be extrapolated to small but finite densities $\rho = n/(aL)^d$, we obtain formally the same ground-state energy and momentum distribution obtainable by T-matrix technique in the low-density limit.^{7,9-11}. The analogy between finite $n, \rho \to 0$ and finite ρ is direct in d=3, where the low-energy limit of the scattering amplitude is a constant. In this case, by substituting $f_0 = 4\pi a$ in Eq. (45), we obtain

$$E = E_0 + n2\pi\rho ta^3 , \qquad (77)$$

which is exactly the first-order correction obtained by Galitskii.⁷ In the same way, it is not difficult to realize that the momentum distribution as given by Eq. (55) and (56), coincides with the general expression obtained, for example, by Belyakov.¹³

In d=2 the extrapolation to finite density is not so straightforward, simply because the low-energy limit of the scattering amplitude Eq. (10) is not a constant. The problem in d=2 is that we have no unique prescription to extrapolate $f_0 \sim 1/\ln L$ to finite density. In order for this question to be answered, we need the corrections to next order in f_0 both for the ground-state energy and the momentum distribution. We show in the Appendix how this can be achieved for the ground-state energy, which has the form

$$E = E_0 + \frac{1}{L^d} \sum_{\mathbf{k}_i, \mathbf{k}'_i \in \text{FS}} \frac{1}{\chi(\mathbf{k}_i, \mathbf{k}'_i; \mathbf{k}_i, \mathbf{k}'_i)} , \qquad (78)$$

where the function $\chi(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_1, \mathbf{k}_2)$ $(\mathbf{k}_1, \mathbf{k}_2 \in FS)$ is defined as

$$\chi(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_1, \mathbf{k}_2) = -\frac{1}{L^d} \sum_{\mathbf{q}, \mathbf{q}' \notin FS} \delta(\mathbf{q} + \mathbf{q}' - \mathbf{k}_1 - \mathbf{k}_2) \frac{1}{\varepsilon_{\mathbf{k}_1} + \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{q}'}}$$
(79)

One can immediately see that Eq. (78) coincides with the ground-state energy obtainable by the *T*-matrix technique. The function $\chi(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_1, \mathbf{k}_2)$ is in fact similar to the low-density limit of the *T* matrix, and at leading order its analytical expression is

$$\chi(\mathbf{P}/2 + \mathbf{k}, \mathbf{P}/2 - \mathbf{k}; \mathbf{P}/2 + \mathbf{k}, \mathbf{P}/2 - \mathbf{k}) = -\frac{1}{4\pi} \left(\ln(k_f a) + \frac{1}{2} \ln \frac{[(k_f + P/2)^2 - k^2]}{k_f^2} \right)$$
(80)

Equation (80) diverges both for $k_f a \to 0$ and for P = 0and $k = k_f$. Hence there is strictly no contribution to $E - E_0$ of Eq. (78) from backward scattering.¹⁴ However, the error made by ignoring this cancellation, i.e., by ignoring the second term in Eq. (80), is small, of order $1/\ln^2(k_f a)$. Therefore, if we are only interested in the first order in $1/\ln(k_f a)$ corrections, then we can consistently take

$$\chi(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_1, \mathbf{k}_2) \simeq -\frac{1}{4\pi} \ln(k_f a)$$
(81)

in Eq. (78) which yields finally

$$E = E_0 - n \frac{2\pi t \rho a^2}{\ln(\rho a^2)} .$$
 (82)

This is the same expression we would have obtained by simply substituting $f_0 = 2\pi/\ln L$ in Eq. (45) with $-2\pi/\ln(k_f a)$. The same consideration holds for the momentum distribution,¹⁵ whose jump at the Fermi level turns out to be¹⁶

$$Z = 1 - \frac{4\ln 2}{\ln^2(\rho a^2)} .$$
 (83)

Therefore, unless some yet undetected change of regime, or phase transition, takes place precisely for $n \to \infty$, there is every reason to believe that the very low-density Fermi-liquid results are correct also in d=2. We stress in particular that the formal coincidence with our extrapolated results for finite electron numbers of Eq. (45) was by no means expected from the start, because our approach is nonperturbative. It is interesting to note, as a side remark, that also in d = 1 the $\rho = 0$ point is nonsingular, so that even there, the finite $n, n/L^d \to 0$ results extrapolate smoothly into the finite-density, small ρ regime.^{4,8}

It is also instructive to discuss how dimensionality affects the low-density behavior of interacting electrons. Our basic assumption (40), that the interaction correction to the ground-state energy is of higher order with respect to the bare kinetic energy level spacing, gives a consistent solution to the Schrödinger equation, only for d > 2. At the same time, the independence of the lowdensity behavior from the strength of the interaction U, occurs only for $d \leq 2$. These two inequalities suggest that d=2 is the marginal dimension separating strong coupling (possibly always non-Fermi-liquid) for d < 2from the conventional perturbative Fermi liquid which applies for d > 2. In other words, the whole region d < 2might be governed by a kind of Luttinger-liquid fixed point while interacting electrons in high dimensionality always belong to the usual Fermi-liquid regime. If such a conjecture is true, it implies that particular care is required in the two-dimensional Hubbard model and that leading order results, as Eqs. (82)-(83), might give only a partial answer to the delicate question of the possible

breakdown of Fermi-liquid theory in such a model.¹⁷

The question of a possible phase transition to a state with totally different properties at finite densities, even quite small, remains of course untouched. These issues are fully open and will require more work.

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APPENDIX

In this appendix we address the question of a possible generalization of our results to small but finite density in the thermodynamic limit. The problem does not arise in d=3 where the low-energy limit of the scattering amplitude is a constant. In fact, in d=3, the ground-state energy as given by Eq. (45) substituting f_0 with $4\pi a$, and the expression of the momentum distribution given by Eqs. (55) and (56) coincide exactly with the result Galitskii obtained in 1958 for a dilute system of electrons interacting through a strong short-range repulsion⁷ (see Ref. 13 for the expression of the momentum distribution). In d=2 the generalization is not straightforward because the low-energy limit of the scattering amplitude does depend on the energy. The consequence is that the simple result (45) cannot be extrapolated at finite density simply because we have no a priori prescription to extend $f_0 = 2\pi / \ln L$ to finite density. This problem can be solved by a little refinement of our calculations, which amounts to evaluating corrections up to second order in $1/\ln L$. The second-order correction to the ground-state energy, which is proportional to $1/\ln^2 L$, can, as usual, be obtained simply through the first-order correction to the eigenvector \vec{J} given by Eq. (46). Unfortunately, the nextorder correction to the momentum distribution (proportional to $1/\ln^3 L$) is more complicated, because it involves the second-order correction to the eigenvector \vec{J} , which is harder to evaluate. For simplicity, let us consider only the next-order correction to the ground-state energy. It is not difficult to show that Eq. (41) is the large size limit of another equation, namely

$$\hat{M} \cdot \vec{J} = L^{d-2} \alpha(L) \hat{\chi} \cdot \vec{J} , \qquad (A1)$$

where \hat{M} and \vec{J} are the same as in Eq. (41), while $\hat{\chi}$ is a diagonal matrix in the "spectator electron" configurations of the unperturbed FS, whose diagonal elements are

$$\chi(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_1, \mathbf{k}_2) = -\frac{1}{L^d} \sum_{\mathbf{q}, \mathbf{q}' \notin \mathrm{FS}} \delta(\mathbf{q} + \mathbf{q}' - \mathbf{k}_1 - \mathbf{k}_2) \frac{1}{\varepsilon_{\mathbf{k}_1} + \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{q}'}} .$$
(A2)

In Eq. (A2) \mathbf{k}_1 and \mathbf{k}_2 are the two states (one for a spin-up electron, the other for a spin-down) which belong to the unperturbed FS and are going to be excited to higher states \mathbf{q}, \mathbf{q}' . In other words, all electrons inside the FS are spectators except \mathbf{k}_1 , \uparrow and \mathbf{k}_2 , \downarrow . In the largesize, zero-density limit $L \to \infty$, $n/L^d \to 0$, the matrix $L^{d-2}\alpha(L)\hat{\chi} \to \lambda \hat{I}$ where \hat{I} is the identity operator and λ has the same meaning as in Eqs. (41) and (42), so that we recover all the results already quoted. It is important, however, to retain the full momentum dependence of $\hat{\chi}$. It is then easy to show that the solution of Eq. (A1) (we restrict to closed shells, because the differences with the open-shell case is expected not to survive in the thermodynamic limit) is now

$$\alpha(L) = L^{2-d} \sum_{\mathbf{k}_1, \mathbf{k}_2 \in \mathrm{FS}} \frac{1}{\chi(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_1, \mathbf{k}_2)} . \tag{A3}$$

From Eq. (A1) it is also possible to calculate the secondorder correction to the components of the eigenvector \vec{J} corresponding to the spectator electron configurations inside the FS. This is, however, not enough, because other spectator configurations are also allowed at that order (in particular those which refer to three- and four-particle correlations), and Eq. (A1) is not sufficient to calculate these corrections, unlike as was the case for the energy. From Eq. (A3) the ground-state energy turns out to be

$$E = E_0 + \frac{1}{L^d} \sum_{\mathbf{k}_i, \mathbf{k}'_i \in FS} \frac{1}{\chi(\mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_1, \mathbf{k}_2)} , \qquad (A4)$$

which, in the limit $L \to \infty$, is just Eq. (45). In order to obtain self-consistent results, the sum in Eq. (A4) must be expanded in powers of $1/\ln L$ up to second order. Hence Eq. (A4) provides the formally correct generalization of the energy shift to small but finite density, in a way which is unique. The next-order correction to the momentum distribution is harder to evaluate. However, one can show that Eq. (55) and (56) give the right result with the same definition of the functions $\Xi^+(\mathbf{k})$ and $\Xi^-(\mathbf{k})$, and with the only provision that the correct function $\Lambda(\mathbf{k}_i, \mathbf{k}'_i; \mathbf{k}_o, \mathbf{k}'_o)$ to be used is

$$\Lambda(\mathbf{k}_{i}, \mathbf{k}_{i}'; \mathbf{k}_{o}, \mathbf{k}_{o}') = \frac{1}{(\varepsilon_{\mathbf{k}_{o}} + \varepsilon_{\mathbf{k}_{o}'} - \varepsilon_{\mathbf{k}_{i}} - \varepsilon_{\mathbf{k}_{i}'})^{2}} \times \left(\chi^{-2}(\mathbf{k}_{i}, \mathbf{k}_{i}'; \mathbf{k}_{i}, \mathbf{k}_{i}') + \frac{2(2tf_{0})^{3}}{L^{2}} \sum_{\mathbf{k} \in \mathrm{FS}} \sum_{\mathbf{q}' \notin \mathrm{FS}} \delta(\mathbf{k}_{o} + \mathbf{q}' - \mathbf{k} - \mathbf{k}_{i}') \frac{1}{\varepsilon_{\mathbf{k}_{o}} + \varepsilon_{\mathbf{q}'} - \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}_{i}'}} + \frac{2(2tf_{0})^{3}}{L^{2}} \sum_{\mathbf{k}' \in \mathrm{FS}} \sum_{\mathbf{q} \notin \mathrm{FS}} \delta(\mathbf{k}_{o}' + \mathbf{q} - \mathbf{k}' - \mathbf{k}_{i}) \frac{1}{\varepsilon_{\mathbf{k}_{o}'} + \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{k}_{i}} - \varepsilon_{\mathbf{k}'}}\right).$$
(A5)

The first term inside the large parentheses corresponds to the spectator configurations of the Fermi sea [it is simply the solution of Eq. (A1)], while the second term derives from the three-particle correlations, which must also be included at this order. These corrections remain of higher order in $1/\ln(k_f a)$, even when we generalize the results to finite density. This is not trivial, and was not a priori evident nor guaranteed. In particular, there might have been terms, e.g., like $n/\ln L$, which are well ordered in $1/\ln L$, but diverge when $n \to \infty$. However, these types of terms turn out to be strictly absent, at least up to third order. Let us see qualitatively, how this happens. The function $\Lambda(\mathbf{k}_i, \mathbf{k}'_i; \mathbf{k}_o, \mathbf{k}'_o)$ which gives the Fermi jump through Eqs. (50)-(56), is just the square of a function L, that is, from Eq. (38)

$$L(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \dots, \mathbf{k}_n) = \frac{J(\mathbf{k}_3, \mathbf{k}_4, \dots, \mathbf{k}_n) - J(\mathbf{k}_3, \mathbf{k}_2, \dots, \mathbf{k}_n) + \cdots}{(E - \varepsilon_{\mathbf{k}_1} - \cdots - \varepsilon_{\mathbf{k}_n})}$$

We see that, in order to obtain consistent results to third order in $1/\ln L$, it is necessary to expand up to first order the energy denominator in $\Delta E = E - E_0$. This expansion, however, yields terms proportional to $\Delta E \sim n\rho/\ln \rho$, which is not well ordered at finite density, as discussed earlier. However, a consistent calculation shows that, at least up to third order in f_0 , each time one of these dangerous terms appears, it is canceled by an identical one coming from the numerator. Thus, in the end, the net result is well ordered in $1/\ln(k_f a)$ as well as in $1/\ln L$.

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- *Present address: Dipartimento di Fisica, Universitá di Milano, via Celoria 16, 20133 Milano, Italy.
- [†]Also at the International Centre for Theoretical Physics, P.O. Box 586, 34014 Trieste, Italy.
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