Luttinger Liquid Instability of the 2D t-J Model: A Variational Study

Roser Valentí[a] and Claudius Gros[b]
Institut für Physik, Universität Dortmund, Postfach 500 500, 4600 Dortmund 50, Germany
(Received 13 December 1991)

We study variationally the possible occurrence of a Luttinger liquid in the normal state of the 2D t-J model. For this, we generalize to 2D a Luttinger-Jastrow-Gutzwiller-type wave function introduced by Hellberg and Mele for the 1D t-J model. We show that this wave function does show also in 2D the characteristic correlations of a Luttinger liquid and that gains in *kinetic energy* stabilize the Luttinger liquid state with respect to Fermi liquid states with short-range correlations only. In addition, we provide rigorous lower bounds to the transition to the fully phase-separated state at larger ratios J/t.

PACS numbers: 71.45.Gm, 71.10.+x, 71.30.+h

Normal-state properties of fermionic systems are of interest. While ordinary metals are well described by the Landau theory of Fermi liquids, certain 1D model systems, like the Hubbard and the t-J model, behave like Tomonaga-Luttinger liquids [1-5]. In a Luttinger liquid the spin and charge correlation functions have a power-law falloff at large distances with nonuniversal exponents and the momentum distribution function develops an algebraic singularity near the Fermi surface of the form

$$n(k)=n(k_F)+C|k-k_F|^{\alpha}\operatorname{sgn}(k-k_F)\,, \tag{1}$$

where C is a constant and the exponent α depends on the model parameters. Typically [3,4], α varies between zero and $\frac{1}{8}$. A Fermi liquid would have a jump in $n(k)$ at $k=k_F$, corresponding to $\alpha=0$.

The Luttinger liquid state realized in the context of the 1D Hubbard model shows [6] separation of charge and spin degrees of freedom. Anderson [7] has hypothesized that the normal state of certain strongly interacting one-band models relevant for the high-T_c superconductors [8] might show generalized [9] Luttinger liquid behavior also in two dimensions. In particular, he suggested that the characteristic separation of charge and spin excitations might be responsible for the experimentally observed temperature dependences of the resistivity [10] and the Hall effect [11]. Alternatively, Varma *et al.* [12] proposed a phenomenological explanation of some experimental properties of the Cu-oxide superconductors in terms of logarithmic singularities at the Fermi surface.

Recently, Hellberg and Mele [13] have proposed a simple variational wave function which incorporates the known properties of a Luttinger liquid, namely, the long-distance falloff of the correlation functions and an algebraic singularity in the momentum distribution function [see Eq. (1)] at the Fermi surface. This wave function is a Jastrow-Gutzwiller-type state and contains only one variational parameter which controls the strength of the long-range, spin-independent interactions in the Jastrow prefactor. The long-ranged nature of the Jastrow-type interactions leads to Luttinger-liquid-type correlations in the state [14]. The phase diagram obtained with this wave function for the 1D t-J model agrees in detail with the one obtained from a combination of exact diagonalization of small systems [15] and scaling relations [3]. In this paper we generalize to two dimensions this remarkable wave function and use it to study variationally the possible occurrence of a Luttinger liquid state in the 2D t-J model.

In the subspace of no double occupancy the 2D t-J model is defined as

$$H_{t\text{-}J}=-t\sum_{\langle i,j\rangle,\sigma}(c^{\dagger}_{j,\sigma}c_{i,\sigma}+c^{\dagger}_{i,\sigma}c_{j,\sigma})+J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{2}$$

where the $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) are the creation (annihilation) operators on site i of electrons with spin $\sigma=\uparrow,\downarrow$, the $\mathbf{S}_i$ are the spin operators on site i, and $\langle i,j\rangle$ denotes pairs of nearest neighbors (nn) on the square lattice.

We shall study the following variational ansatz for the ground state of Eq. (2):

$$|\Psi(T,S)\rangle=\sum_{\{\mathbf{r}_1,\ldots,\mathbf{r}_N\}}\exp\left(-\frac{1}{2T}\sum_{i<j}[(1-S)\ln|\mathbf{r}_i-\mathbf{r}_j|+S\delta_{\langle i,j\rangle}]\right)P_d\det{}_{\uparrow}\det{}_{\downarrow}\prod_{\mathbf{r}_i,\sigma}c^{\dagger}_{\mathbf{r}_i,\sigma}|0\rangle\,. \tag{3}$$

In the limit $T\to\infty$, Eq. (3) reduces to the projected Gutzwiller wave function,

$$\sum_{\{\mathbf{r}_1,\ldots,\mathbf{r}_N\}}P_d\det{}_{\uparrow}\det{}_{\downarrow}\prod_{\mathbf{r}_i,\sigma}c^{\dagger}_{\mathbf{r}_i,\sigma}|0\rangle\,,$$

where $\det_\sigma=\det[e^{i\mathbf{k}_j\cdot\mathbf{r}_{i,\sigma}}]$ are the Slater determinants of a filled Fermi sea of the spin-σ particles, $P_d=\prod_i(1-n_{\mathbf{r}_i,\uparrow}n_{\mathbf{r}_i,\downarrow})$ is the projection operator onto the subspace of no doubly occupied sites, and $\sum_{\{\mathbf{r}_1,\ldots,\mathbf{r}_N\}}$ denotes the sum over all particle configurations (the spin indices are here suppressed). The exponential in front of the Slater determinants in Eq. (3) is the spin-independent Jastrow prefactor corresponding to the partition function of a classical two-component repulsive (attractive) 2D gas at temperature [16] $T>0$ ($T<0$). The interaction has two contributions, a long-ranged Coulomb [17] part of strength $(1-S)$ and a nn interaction of strength S.

In one dimension the logarithmic interaction in the Jastrow prefactor of Eq. (3) has been shown [13,14] to be the correct analytic form which induces Luttinger-liquid-type correlations. Notably, the momentum distribution function acquires an algebraic discontinuity at the Fermi edge with [14] $\alpha=(1/4T')[1/(T'+1)]$ in Eq. (1) [with $T'=T/(1-S)$].

We will show below that also in two dimensions the above defined wave function acquires an algebraic singularity at the Fermi surface, as seen from the momentum distribution function, for $0<T<\infty$ and $0\le S<1$, and that therefore the notion of a Luttinger liquid is well defined even in 2D. In addition, the second variational parameter, S, in Eq. (3) allows us to compare the Luttinger liquid state (which is realized for all $S<1$) to a state with only short-range correlations, realized for $S=1$.

At $T=\infty$, the wave function Eq. (3) reduces to the Gutzwiller wave function which up to now was the best known trial wave function for the 2D t-J model in the limit $J=0$. Lowering the (positive) temperature T, first a Luttinger liquid state is realized and then, for $T\sim\frac{1}{140}$, a transition [18] to a Wigner crystal occurs driven by the repulsive Coulomb interaction. At negative temperatures the interaction is attractive, leading to enhanced pairing fluctuations and phase separation, as in 1D [13].

It is well known [19,20] that the t-J model separates into a hole-rich and a particle-rich phase at large ratios of J/t. Variationally we can obtain the transition to the fully phase-separated region by comparing the best variational energies obtained from Eq. (3) with the energy of the fully phase-separated state, which we can reliably estimate [21] as $2n\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle J\sim-0.6692nJ$, where n is the density of particles per site. Since the variational energies for the homogeneous phase are upper bounds, the transition to the fully phase-separated state in the true ground state therefore has to occur at larger ratios of critical J/t than those obtained by our variational approach presented here.

We have carried out an extensive study of Eq. (3) on finite lattices using the variational Monte Carlo method [22]. At low values of J/t we find the Luttinger state to be energetically stable at all densities $0<n<1$. The optimal variational parameters, $T\sim3.0$ and $S\sim0.4$, vary slightly with particle density, n. We would like to note that it is the *kinetic energy* which stabilizes the Luttinger liquid in the 2D (and the 1D [13]) t-J model, and not the spin-correlation energy. In contrast, the ordered states considered so far variationally [23] lose kinetic energy and are stabilized by gains in spin-correlation energy. The Luttinger liquid state gains about 1% in (projected) kinetic energy with respect to the Gutzwiller state [24,25] and is therefore lower in projected kinetic energy than any other variational wave function proposed [23] so far.

The difference in energy between the best overall state, $T\sim3.0$, $S\sim0.4$, and the best state with short-range correlations only, $T\sim4.5$ and $S=1$, is about [26,27] 0.2%. Note that for a gain in *kinetic energy* this gain might be considered substantial and should survive the introduction of additional variational parameters. Unfortunately no reliable estimates of the ground-state energy for the 2D t-J model are yet known for general fillings, e.g., the quality of rigorous lower bounds [28] obtained so far for the ground-state energy of the 2D t-J model at $J=0$ is not yet good enough to define a fine scale for comparison of our variational data. On the other hand we might take the case of 1D as a guide. Here we know [29] that the difference in energy (at $J=2t$) between the exact ground state and the Gutzwiller wave function is less than 1%, setting a very small scale as significant.

In Fig. 1 we present our results for the phase diagram of the 2D t-J model as a function of particle density n and ratio J/t determined by evaluating the wave function Eq. (3) on a series of finite clusters with periodic (P) or antiperiodic (AP) boundary conditions (BC). The clusters are such that they tile the square lattice via translations by $\mathbf{L}_1=(L_x,L_y)$ and $\mathbf{L}_2=(-L_y,L_x)$, with a total number of sites $L=L_x^2+L_y^2$. Specifically, we considered the following (n,L,L_x,L_y,BC, symbols in Fig. 1) systems: ($\frac{1}{4}$,32,4,4,AP,circles), ($\frac{1}{2}$,68,8,2,AP,triangles), ($\frac{3}{4}$,32,4,4,AP,circles), ($\frac{3}{4}$,64,8,0,AP,crosses), ($\frac{74}{82}$,82,8,1, P,squares). We observe that the Luttinger state is stable up to $J\sim1.2$ for large $n\sim0.9$ and up to $J\sim4.0$ for $n\sim0.25$. The data, which are obtained from lattices of very different geometry and sizes, show a remarkable consistency. (Note, in particular, the two data points for $n=\frac{3}{4}$.)

The optimal values of the variational parameters change with increasing J/t. The optimal temperature increases monotonically while the admixture of explicit nn correlations, S, remains quite unchanged. For small den-

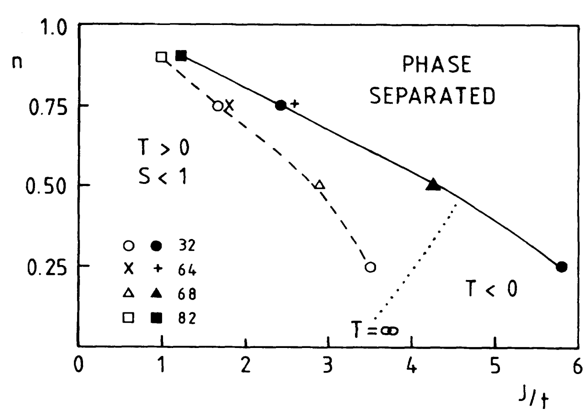

FIG. 1. Phase diagram of the 2D t-J model obtained with the Luttinger-Jastrow-Gutzwiller wave function Eq. (3). For small t/J, a Luttinger liquid state ($0<T<\infty$, $S<1$) is found. The transition to the fully phase-separated state is indicated by the solid symbols (solid line). Only for low densities n does the optimal (variational) temperature pass through ∞ (dotted line), the Gutzwiller state, before phase separation sets in. The open symbols (dashed line) indicate the line of phase separation obtained when the usual density-density attraction term, $-(J/4)n_in_j$, is added to the t-J Hamiltonian Eq. (2). The lines are guides to the eye.

sities, $n \sim \frac{1}{4}$, a Fermi liquid state ($T=\infty$) becomes stable (as in 1D [13]) for $J \sim 4t$ and a region of enhanced pairing fluctuations ($T<0$) occurs before the system phase separates. But at intermediate to large particle densities no region of enhanced pairing fluctuations occurs (in contrast to 1D) and the system phase separates directly out of the Luttinger liquid state.

We have also drawn in Fig. 1 the line of phase separation obtained when we include the term $-(J/4) \times \sum_{\langle i,j \rangle} n_i n_j$ to the t-J Hamiltonian as defined by Eq. (2). This phase-separation line compares very well with results obtained from a high-temperature expansion [20] but differs at larger particle densities n and small ratios J/t from the results obtained from a small-cluster study [19]. Note, in particular, that the region of interest for the high-T_c superconductors ($n \sim 0.8$-0.9 and $J/t \sim 0.2$-0.3) is far away from the region of phase separation. Clearly, in the region of large $n>0.8$ substantial spin-correlation energy can be gained considering phase-condensed states [23] which will push the phase-separation line to still larger J/t. In this study we did not consider these ordered states since we wanted to concentrate on the question whether the (projected) kinetic energy would favor Luttinger-liquid-type correlation in the normal state. In addition, these ordered states might generally coexist [25] with Luttinger-liquid-type correlations.

In Fig. 2 we present the momentum distribution function $n(k)$ for the Gutzwiller wave function ($T=\infty$, squares), the Luttinger liquid state ($T=3.0$, $S=0.4$, circles), and the correlated Fermi liquid state ($T=4.5$, $S=1$, triangles). We did evaluate these three states for two lattices [30], ($\frac{3}{4}$,64,8,0,AP, open symbols) and ($\frac{3}{4}$,256,16,0,AP, solid symbols) along the (1,0) direction (Γ-X) and the (1,1) direction (Γ-M). Inside the Fermi surface the $n(k)$ for the Luttinger state deviates qualitatively from the $n(k)$ of the Gutzwiller state, which is strictly constant. In Fig. 3 the same data for the $n(k)$ inside the Fermi surface are plotted as $\ln|n(\mathbf{k})-\frac{1}{2}|$ vs $\ln|\mathbf{k}-\mathbf{k}_F|$, where $\mathbf{k}_F=(0.7543,0)\pi$ and $\mathbf{k}_F=(0.4545, 0.4545)\pi$ are the respective Fermi wave vectors for $n=\frac{3}{4}$ in the thermodynamic limit. The curves for both Fermi liquid states are flat, indicating a jump at the Fermi surface for the momentum distribution function. In contrast, the data for the Luttinger liquid state has a finite slope, indicating an algebraic singularity, as in 1D [13,14] with exponents [31] $\alpha_{(1,0)} \sim \frac{1}{30}$ and $\alpha_{(1,1)} \sim \frac{1}{60}$ in the (1,0) and the (1,1) direction, respectively [see Eq. (1)]. The data for $n(k)$ for the Luttinger liquid state deviates quantitatively only by a small amount from those of the Gutzwiller state (note the scale in Fig. 2), due to the high effective temperature, $T'=T/(1-S) \sim 5.7$. In 1D the optimal temperature is $\sim \frac{2}{3}$ for $J=0$ and the resulting effects in the momentum distribution function are much larger. To check that this is true also in 2D, we calculated $n(k)$ for parameters $T=0.7$, $S=0$ and found strongly enhanced Luttinger liquid effects with [31] $\alpha_{(1,0)} \sim \frac{8}{10}$ and $\alpha_{(1,1)} \sim \frac{1}{4}$. In Fig. 2 no upturn is observed in the momentum distribution function for the Luttinger liquid state for values of $\mathbf{k}$ outside the Fermi surface [as expected from Eq. (1)] since the systems evaluated do not contain $\mathbf{k}$'s considered close enough to the Fermi surface at the high effective temperature $T'=T/(1-S) \sim 5.7$. But for the wave function with $T=0.7$, $S=0$ the Luttinger liquid exponents α are large enough to observe such an upturn in the momentum dis-

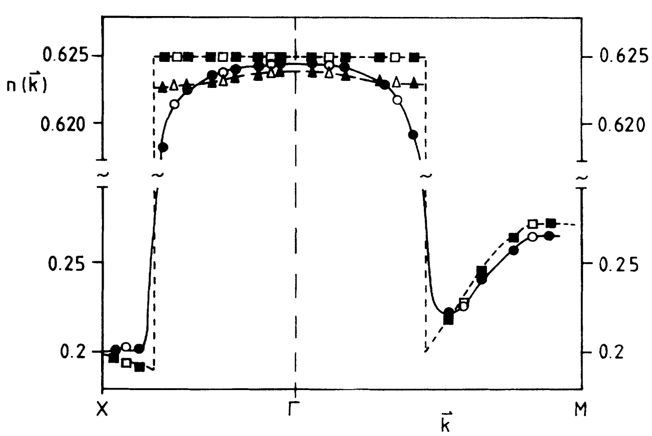

FIG. 2. Momentum distribution function $n(\mathbf{k})$ for the Gutzwiller state (squares), the Luttinger liquid state (circles), and the Fermi liquid state with nn correlations (triangles) along the (1,0) direction (Γ-X) and the (1,1) direction (Γ-M). The open (solid) symbols denote data obtained from lattices with 64 (256) sites. Note the different scales for $n(k)$ inside and outside the Fermi surface. The statistical errors are (1-2)% (about the symbol size). The lines are guides to the eye.

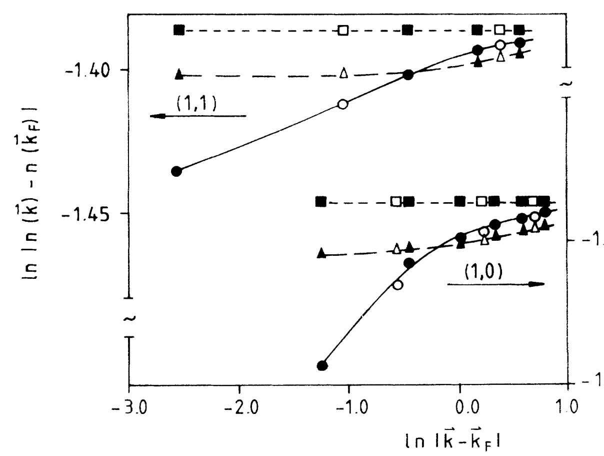

FIG. 3. A log-log plot of the momentum distribution function $n(\mathbf{k})$ inside the Fermi surface for the Gutzwiller state (squares), the Luttinger liquid state (circles), and the Fermi liquid state with nn correlations (triangles) along the (1,0) direction (Γ-X, scale to the right) and the (1,1) direction (Γ-M, scale to the left). The open (solid) symbols denote data obtained from lattices with 64 (256) sites. Note the finite slope of the data for the Luttinger liquid state, indicating an algebraic singularity at the Fermi edge. The statistical errors are (1-2)% (about the symbol size). The lines are guides to the eye.

tribution function when approaching the Fermi surface from outside.

In conclusion, we have shown that a Luttinger liquid state can be defined in two dimensions. For this we have generalized a Jastrow-Luttinger-Gutzwiller-type wave function proposed by Hellberg and Mele [13] for the 1D t-J model to two dimensions. We have shown that this wave function does indeed contain the typical correlations of a Luttinger liquid, notably an algebraic singularity in the momentum distribution function at the Fermi edge. We found that this Luttinger-liquid-type state is stabilized by gains in (projected) *kinetic energy* even in the presence of some additional variational parameters. We calculated the phase diagram and obtained rigorous variational bounds for the transition to the fully phase-separated region at large J/t which agree quantitatively very well with results [20] from a high-temperature expansion. In particular, we found that the region of interest for the high-T_c superconductors is far away from the phase-separated region.

This work was initiated from discussion with E. J. Mele and C. S. Hellberg during a visit at the University of Pennsylvania. In addition we would like to thank N. Kawakami, H. Schulz, P. Wölfle, and P. Hirschfeld for useful discussions. This work was supported by the Deutsche Forschungsgemeinschaft, by the Minister für Wissenschaft und Forschung des Landes Nordrhein-Westfalen, and by the European Community European Strategic Program for Research in Information Technology, Project No. 3041-MESH. Part of the numerical calculations were done at the Hochleistungs Rechenzentrum Jülich.

(a)Electronic address (bitnet): uph084@ddohrz11.
(b)Electronic address (bitnet): uph031@ddohrz11.

[1] For a review, see J. Solyom, Adv. Phys. **28**, 201 (1979).
[2] F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980); J. Phys. C **14**, 201 (1981).
[3] H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990).
[4] N. Kawakami and S.-K. Yang, Phys. Rev. Lett. **65**, 2309 (1990).
[5] H. Frahm and V. E. Korepin, Phys. Rev. B **42**, 10553 (1990).
[6] M. Ogata and H. Shiba, Phys. Rev. B **41**, 2326 (1990).
[7] P. W. Anderson, Phys. Rev. Lett. **64**, 1839 (1990); **67**, 2092 (1991).
[8] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988); S. B. Bacci, E. R. Gagliano, R. M. Martin, and J. F. Annett, Phys. Rev. B **44**, 7504 (1991).
[9] A. Luther, Phys. Rev. B **19**, 2094 (1979).
[10] M. Gurvitch and A. T. Fiory, Phys. Rev. Lett. **59**, 1337 (1987).
[11] T. R. Chien, Z. Z. Wang, and N. P. Ong, Phys. Rev. Lett. **67**, 2088 (1991).
[12] C. M. Varma, P. B. Littlewood, S. Schmitt-Rink, E. Abrahams, and A. E. Ruckenstein, Phys. Rev. Lett. **63**, 1996 (1989).
[13] C. S. Hellberg and E. J. Mele, Phys. Rev. Lett. **67**, 2080 (1991).
[14] N. Kawakami and P. Horsch, Comment on "Phase Diagram of the One-Dimensional t-J Model from Variational Theory" (to be published). Their derivation is for the $S=0$ case in Eq. (3).
[15] M. Ogata, M. U. Luchini, S. Sorella, and F. F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).
[16] Note that configuration probabilities, and not the amplitudes, are weighted corresponding to the classical partition function [see Eq. (3)].
[17] For a finite system we generalized the logarithmic interaction in the Jastrow prefactor of Eq. (3) to $\ln(r)$ where $r=(L/\pi)[\sin^2(\pi\mathbf{r}\cdot\mathbf{L}_1/L)+\sin^2(\pi\mathbf{r}\cdot\mathbf{L}_2/L)]^{1/2}$ respects the lattice periodicity given by $\mathbf{L}_1,\mathbf{L}_2$ ($L=\mathbf{L}_1^2=\mathbf{L}_2^2$).
[18] J. M. Caillol, D. Levesque, J. J. Weis, and J. P. Hansen, J. Stat. Phys. **28**, 325 (1982). On a lattice the transition temperature depends strongly on the density of particles and resulting nesting effects.
[19] V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).
[20] W. O. Putikka, M. U. Luchini, and T. M. Rice, Phys. Rev. Lett. **68**, 538 (1992).
[21] N. Trivedi and D. Ceperley, Phys. Rev. B **41**, 4552 (1990).
[22] For an introduction see, e.g., C. Gros, Ann. Phys. (N.Y.) **189**, 53 (1989).
[23] T. Giamarchi and C. Lhuiller, Phys. Rev. B **43**, 12943 (1991); G. J. Chen, R. J. Joynt, F. C. Zhang, and C. Gros, Phys. Rev. B **42**, 2662 (1990); S. Liang and N. Trivedi, Phys. Rev. Lett. **64**, 232 (1990).
[24] We did check for a series of lattices with 20, 68, 148, and 260 sites and $n=0.5$ that this energy gain extrapolates well to the thermodynamic limit.
[25] We have some preliminary results indicating that a Jastrow prefactor of the type in Eq. (3) gains kinetic energy also for other types of projected wave functions [22,23] (and loses spin-correlation energy).
[26] The respective minima are found most easily following the gradients, which can be evaluated analytically [13] for Eq. (3). Up to 500000 (statistically independent) Monte Carlo measurements were necessary to extract the energy differences of 0.2%.
[27] For 64 holes on a lattice with $L=256$ sites the kinetic energies are -0.5814 ± 0.0007, -0.5866 ± 0.0005, and -0.5857 ± 0.0005 in units of t per site, for parameters (T,S) being $(\infty,0)$, $(3.0,0.4)$, and $(4.5,1.0)$, respectively. The corresponding spin correlations energies are -0.2569 ± 0.0006, -0.2570 ± 0.0005, and -0.2571 ± 0.0005 in units of J per site.
[28] R. Valentí, C. Gros, P. J. Hirschfeld, and W. Stephan, Phys. Rev. B **44**, 13203 (1991).
[29] H. Yokoyama and M. Ogata, Phys. Rev. Lett. **67**, 3610 (1991).
[30] The criteria determining the choice of appropriate finite clusters are (i) filled shells for the Fermi sea [22] and (ii) no crossing of the finite-lattice and the infinite-lattice Fermi surfaces. Such a crossing might generally occur due to a geometry mismatch.
[31] This estimate for the exponents is about a factor 2–4 larger than the estimate obtained from Kawakami and Horsch's [14] formula for the 1D wave function which yields $\alpha\sim\frac{1}{150}$ for $T'\sim5.7$ and $\alpha\sim\frac{1}{5}$ for $T=T'=0.7$.