Induced Interactions for Ultracold Fermi Gases in Optical Lattices

D.-H. Kim,[1] P. Törmä,[1] and J.-P. Martikainen[2]

[1]*Department of Applied Physics, Helsinki University of Technology, P.O. Box 5100, 02015 HUT, Finland*

[2]*NORDITA, 106 91 Stockholm, Sweden*

(Received 29 January 2009; revised manuscript received 21 May 2009; published 16 June 2009)

We investigate the effect of optical lattices on the BCS superfluidity by using the Gorkov–Melik-Barkhudarov (GMB) correction for a two-component Fermi gas. We find that the suppression of the order parameter is strongly enhanced by the lattice effects. The predictions made by the GMB corrections are in qualitative and, for the cases studied, quantitative agreement with previous quantum Monte Carlo results. We discuss how the GMB correction extends the validity of the mean-field theory to a wider range of tunable optical lattice systems in different dimensions.

DOI: 10.1103/PhysRevLett.102.245301 PACS numbers: 67.85.−d, 03.75.Ss, 05.30.Fk, 37.10.Jk

Bardeen, Cooper, and Schrieffer (BCS) explained superconductivity by the condensation of fermion pairs in the presence of arbitrarily attractive interaction [1]. Based on the idea of the BCS pairing, in dilute Fermi gases, the critical temperature was derived in terms of scattering length [2,3]. Gorkov and Melik-Barkhudarov (GMB) extended this calculation by incorporating many-body effects, which turned out to reduce the critical temperature by a factor $(4e)^{1/4} \approx 2.22$ [4]. Fermionic superfluidity has recently attracted renewed attention in connection with the realization of ultracold atomic gases that allow direct observation of quantum many-body phenomena in highly controllable environments [5–7]. In particular, optical lattices are a perfect platform for emulating crystalline structures of superconductors. While indirect evidence of superfluidity in a system with an optical lattice has recently been reported [8], the full characterization of fermionic superfluidity and strongly correlated quantum states in optical lattices is still under active study, both theoretical and experimental [9,10]. In this Letter we focus on how the lattice potential influences the BCS-type superfluid transition by employing the GMB correction.

We calculate the mean-field BCS order parameters at zero temperature in three- and two-dimensional (3D and 2D) lattices with various settings including the crossover from 3D to 1D. In all the ranges of lattice parameters examined, we find that the induced interaction introduced by the correction leads to remarkable reduction in the order parameter from the usual BCS result. This deviation turns out to be much more pronounced in the lattices than in homogeneous gases and becomes increasingly significant at higher fillings. In particular, in 2D, we find quantitative agreement with previous quantum Monte Carlo (QMC) calculations for the cases studied. Furthermore, near half filling in 2D, the rapid decreasing behavior of the order parameter is in qualitative agreement with the QMC predictions. At half filling in 2D, the induced interaction diverges because of Fermi surface nesting. This divergence is connected to the signature of the charge density waves, known to coexist with superfluidity at half filling in 2D.

We consider a system composed of two different fermionic species denoted by $\uparrow$ and $\downarrow$. Each component is in a lattice with adjustable tunneling strengths $t_{\downarrow\alpha}$ and $t_{\uparrow\alpha}$ in direction $\alpha \in \{x, y, z\}$. When the lattice potential is sufficiently deep so that we can consider only nearest-neighbor tunnelings and on-site interactions, the system is described by the Hubbard Hamiltonian $\mathcal{H} = -\sum_{\sigma,\alpha}\sum_{i_\alpha} t_{\sigma\alpha}\mathcal{K}_{\sigma i_\alpha} + U_0\sum_{\mathbf{i}}\hat{n}_{\uparrow\mathbf{i}}\hat{n}_{\downarrow\mathbf{i}} - \mu\sum_{\sigma,\mathbf{i}}\hat{n}_{\sigma\mathbf{i}}$, where $\mathcal{K}_{\sigma i} \equiv \hat{\psi}^\dagger_{\sigma i+1}\hat{\psi}_{\sigma i} + \hat{\psi}^\dagger_{\sigma i}\hat{\psi}_{\sigma i+1}$, and $\hat{\psi}_{\sigma,\mathbf{i}}(\hat{\psi}^\dagger_{\sigma,\mathbf{i}})$ is the annihilation (creation) operator for atoms of type σ at a site $\mathbf{i} \equiv (i_x, i_y, i_z)$. The chemical potential and density operator are denoted by μ and $\hat{n}_{\sigma,\mathbf{i}}$, respectively. We consider negative interaction strengths U_0. For noninteracting gases, the above Hamiltonian is diagonalized with dispersion $\xi_\sigma(\mathbf{k}) = 2\sum_\alpha t_{\sigma\alpha}[1 - \cos(k_\alpha)] - \mu$, where the lattice spacing is chosen to be unity. In the weak coupling regime, using the standard BCS theory with this dispersion and the interaction U_0, without many-body corrections, one recovers the usual BCS prediction for the critical temperature in the long wavelength limit. However, because the scattering length a gives exponential contribution to the critical temperature as $T_c \propto \exp(-\pi/k_F|a|)$, where k_F is the Fermi momentum, a small correction to the interaction term $k_F a$ can considerably change T_c even in the weak coupling regime. For instance, a second-order correction δ in $k_F|a| \to k_F|a|(1 + \delta k_F|a|)$ leads to $T_c \to e^\delta T_c$.

For a two-component Fermi gas with an s-wave interaction between components, the relevant second-order correction to the effective interaction is represented by the diagram in Fig. 1(a), which describes the exchange of density and spin fluctuations [11,12]. The diagram leads to the induced interaction term, which can be derived for an infinite-size system in D dimensions as

$$U_{\mathrm{ind}}(\mathbf{p}, \mathbf{k}) = -U_0^2 \int \frac{d\mathbf{q}}{(2\pi)^D} \frac{f_{\uparrow,\mathbf{p}+\mathbf{k}+\mathbf{q}} - f_{\downarrow,\mathbf{q}}}{\xi_\uparrow(\mathbf{p}+\mathbf{k}+\mathbf{q}) - \xi_\downarrow(\mathbf{q})}, \quad (1)$$

where the Fermi distribution $f_{\sigma,\mathbf{k}} = 1/[1 + \exp(\beta\xi_\sigma(\mathbf{k}))]$, with $\beta = 1/k_B T$. There are two noticeable properties in Eq. (1). First, U_{ind} is always positive. Thus,

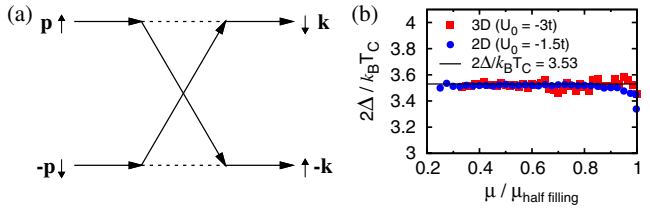

FIG. 1 (color online). (a) The diagram representing the induced interaction $U_{\mathrm{ind}}(\mathbf{p}, \mathbf{k})$. Arrowed lines and dashed lines describe fermionic propagators and the coupling U_0 between the atoms. (b) Equivalence between the zero-temperature order parameter Δ and the critical temperature T_c in the weak coupling regime.

this correction screens the negative interatomic potential, which consequently reduces the critical temperature. Second, the static Lindhard function, representing the spin or density susceptibility χ_0 of a noninteracting gas, is found in U_{ind} if there is no difference in the energy dispersion between the components, or simply $t_{\downarrow\alpha} = t_{\uparrow\alpha}$, which is the case that we mainly consider here.

In the weak coupling regime, the induced interaction correction near the Fermi surface dominantly contributes to the calculations of the BCS order parameter and the critical temperature [11,12], and then the effective interaction is approximately given by only the Fermi surface momenta. Averaging $U_{\mathrm{ind}}(\mathbf{p}, \mathbf{k})$ over the Fermi surface, the induced interaction becomes $\langle U_{\mathrm{ind}}\rangle = \frac{1}{|S_\uparrow||S_\downarrow|} \times \int_{S_\uparrow} dS_{\mathbf{p}} \int_{S_\downarrow} dS_{\mathbf{k}} U_{\mathrm{ind}}(\mathbf{p}, \mathbf{k})$, where S_σ denotes the Fermi surface of the component σ and $|S_\sigma| = \int_{S_\sigma} dS$ is the area. Finally, the effective interaction is written as $U_{\mathrm{eff}} = U_0 + \langle U_{\mathrm{ind}}\rangle$. This effective interaction replaces the interatomic interaction in calculations. Having other parameters fixed, U_{eff} becomes zero when U_0 equals $U_c \equiv -U_0^2/\langle U_{\mathrm{ind}}\rangle$. The susceptibility of an interacting gas is given as $\chi_0/(1 + U_0\chi_0)$ within the random phase approximation, where χ_0 is the susceptibility of the noninteracting gas. At $U_0 = U_c$, this quantity diverges, often indicating a possibility of charge ordered phase. Our approach is formally valid below U_c, and with the GMB correction, the criterion for the weak coupling regime can be established by $U_c \ll U_0 < 0$.

We calculate zero-temperature order parameters by using this effective interaction U_{eff} in the mean-field formalism [13,14]. The diagram in Fig. 1(a) representing the induced interaction is relevant in normal states, and thus the critical temperature T_c has been of interest in previous studies. However, in the weak coupling limit, the validity of the induced interaction can be readily extended for the calculation of the zero-temperature order parameter Δ because the contribution of the broken symmetry phase is expected to be of higher order in Δ that becomes very small. Moreover, with $U \equiv U_{\mathrm{eff}}$, we confirm that a general relation $2\Delta/k_B T_c \sim 3.53$ [15,16] still holds in lattices, as shown in Fig. 1(b), in the weak coupling regime. The calculation of Δ is computationally less demanding than T_c but gives a concise picture of the transition. At very low filling factors (small μ), one recovers the well-known prefactor 2.22 in comparison between the usual BCS result and our calculation with the correction in U_{eff}. In contrast, as the filling factor increases, the reduction of the order parameter with the correction becomes much more subtle in a lattice than indicated by the prefactor in continuum.

Figure 2 shows the effect of the induced interaction in isotropic 3D lattices. We find that the order parameter Δ with the correction shows a dramatic deviation from the usual BCS result $\Delta^{(0)}$ without the correction. The ratio $\Delta^{(0)}/\Delta$ turns out to be nearly 25 at half filling, which implies that the usual BCS prediction largely overestimates the order parameter and critical temperature. While the order parameter Δ with the correction is maximized around $\mu = 4t$ where the Fermi surface reaches the Brillouin zone boundaries, it decreases substantially at higher filling factors because of increasing contributions of states with $\mathbf{p} + \mathbf{k} + \mathbf{q}$ in Eq. (1) outside the first Brillouin zone. This deviation from the usual BCS result that we find here is qualitatively consistent with the previous study of the $1/D$ correction in high dimensions [17], where the order-of-unity reduction of the order parameter was estimated at half filling. However, our calculations in 3D lattices reveal much more significant suppression in Δ with the GMB correction. In all the figures, the curve for $|U_c|$ provides a simple estimate of the area in the parameter space (U_0, μ) where the GMB correction can extend the validity of the BCS mean-field theory. The range of U_0 in this space decreases as μ increases towards half filling in 3D and 2D lattices, which may affect the accuracy. Particularly in 2D, half filling is not included in this space because of divergent $\langle U_{\mathrm{ind}}\rangle$.

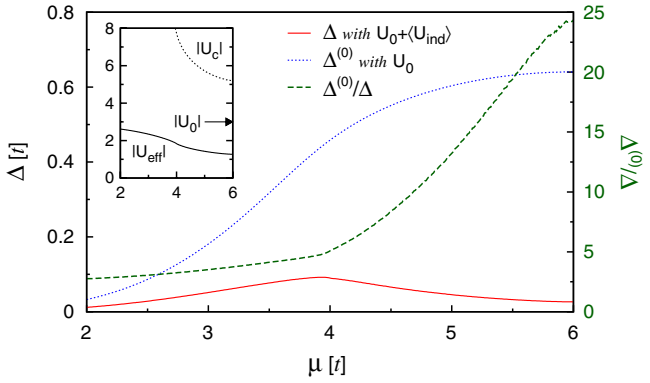

FIG. 2 (color online). Three-dimensional lattices. The order parameters Δ (with the GMB correction) and $\Delta^{(0)}$ (the usual BCS result) are calculated with $U_0 = -3t$ as a function of chemical potential μ. The comparison between Δ and $\Delta^{(0)}$ shows an increasing deviation as μ increases. The ratio $\Delta^{(0)}/\Delta$ becomes $\sim$25 at half filling ($\mu = 6t$). The inset shows comparison between the magnitude of the interactions. Here and in the other figures, the critical coupling $|U_c|$ (see text) allows one to estimate the ranges of $|U_0|$ and μ where the BCS mean-field theory with the GMB correction is applicable.

In 2D lattices, the order parameter Δ decreases very rapidly near half filling as the screening by the induced interaction dominates (see Fig. 3). This rapid decrease of Δ near half filling is in agreement with the previous QMC results on the critical temperatures [18,19]. In contrast, the usual BCS mean-field calculation without the correction suggests a monotonically increasing order parameter $\Delta^{(0)}$ when approaching half filling. At lower filling factors, the order parameter with the GMB correction turns out to be around 5 times smaller than the one without the correction, which is consistent with other previous estimations of many-body effects [15,20,21]. At higher μ close to half filling, the deviation from the usual BCS theory becomes even more substantial and leads to highly suppressed order parameter near half filling.

At half filling, it is known that the 2D attractive Hubbard model has the charge-density-wave order and the pairing order coexisting in the ground state, and the critical temperature of the superfluid transition goes to zero. Our calculations show that the induced interaction logarithmically diverges because of the Fermi surface nesting, making the denominator in Eq. (1) infinitesimally small with the nesting vector $\mathbf{p} + \mathbf{k} = (\pm\pi, \pm\pi)$, for *all* $\mathbf{q}$ at the Fermi surface, by mapping one side of the Fermi surface onto the other side [see Fig. 3(d)]. Despite the tendency for the order parameter Δ to vanish when approaching half filling, the order parameter is not well defined with the large correction in our perturbative approach. However, this divergence of the induced interaction means that, for arbitrary small U_0, the susceptibility diverges. It thus provides the connection to a different type of phase that cannot be anticipated by the usual BCS mean-field theory. The divergent Lindhard function appearing in the correction term can be interpreted as the signature of the charge density waves [22].

For direct comparison with the QMC values of T_c in 2D lattices, we have used $U_0 = -4t$. With the GMB corrections, we obtained $\Delta\ (T_c) \sim 0.07t\ (0.04t)$, $0.03t\ (0.02t)$, $0.008t\ (0.005t)$ at the filling factors ($|U_c|$'s) of 0.2 ($7.3t$), 0.25 ($6.2t$), 0.3 ($5.4t$). The farther away U_c is from U_0, the more accurate Δ is expected. The QMC result $k_B T_c \sim 0.05t$ at quarter filling [18,19] is remarkably close to our value of Δ, and the results in [23] are of the same order of magnitude as ours. Note that the usual BCS mean-field calculations for these parameters would give results that are about 10–35 times larger than the QMC and our GMB corrected mean-field results.

Motivated by the fact that anisotropy is easily controllable in optical lattices, we now explore dimensional crossover from 3D to 1D by introducing directional difference in the tunneling strengths t_α. For this purpose, we define the lattice anisotropy as a ratio of the tunneling strengths, $\tilde{t} \equiv t_y/t_x = t_z/t_x$, with which one can change the dimensionality from 3D ($\tilde{t} = 1$) to 1D ($\tilde{t} = 0$). Figure 4 shows the effect of the lattice anisotropy on the induced interaction and the order parameter. As the anisotropy evolves with $\tilde{t}$, the screening by the induced interaction becomes stronger and finally diverges in the limit of 1D because of Fermi surface nesting.

Similar to isotropic 3D cases, the order parameter Δ in the anisotropic lattice also shows highly suppressed values compared with the usual BCS result $\Delta^{(0)}$. While the transition from 3D to 1D appears continuous in the induced interaction $\langle U_{\rm ind}\rangle$, we identify two special points of $\tilde{t}$ indicating structural changes of the Fermi surface. First,

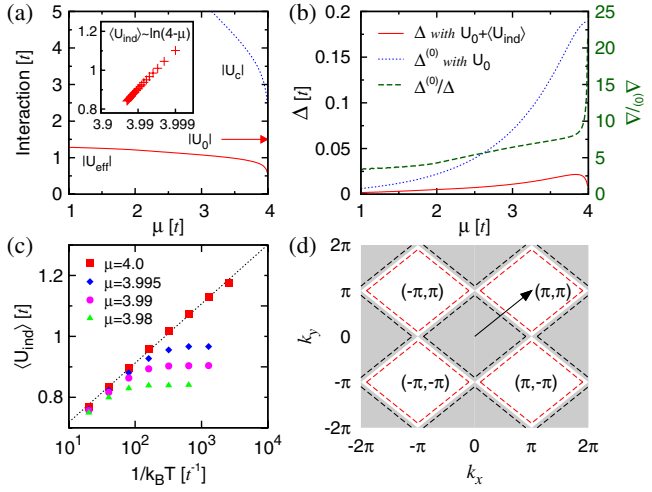

FIG. 3 (color online). Two-dimensional lattices. (a) The effective interaction $U_{\rm eff}$ and (b) the order parameter Δ are calculated with $U_0 = -1.5t$. The usual BCS mean-field result $\Delta^{(0)}$ shows very large deviation from Δ with the GMB correction, exhibiting $\Delta^{(0)}/\Delta \approx 10$ near half filling $\mu = 4t$. (c) Logarithmic divergence of the GMB correction and (d) Fermi seas (shaded area) at half filling indicating the nesting of Fermi surfaces (dashed lines) with momentum transfers $\mathbf{p} + \mathbf{k} = (\pm\pi, \pm\pi)$.

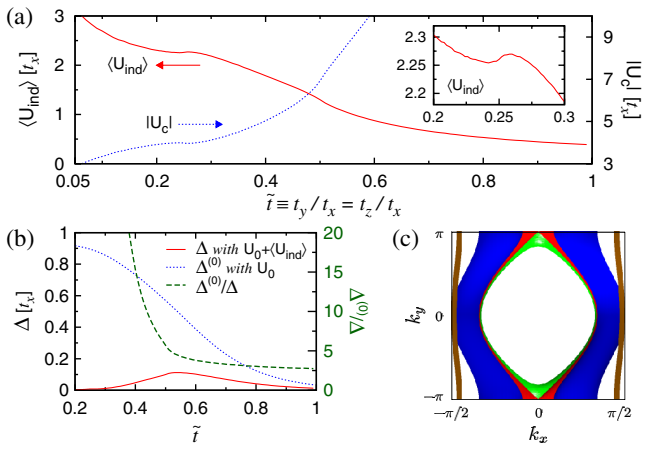

FIG. 4 (color online). Crossover from 3D to 1D. (a) The induced interaction $\langle U_{\rm ind}\rangle$ and (b) the order parameter Δ as a function of the lattice anisotropy $\tilde{t} \equiv t_y/t_x = t_z/t_x$ in anisotropic three-dimensional lattices. In (b), the usual BCS mean-field results $\Delta^{(0)}$ without the correction is given for comparison. (c) Fermi surfaces projected to $k_x - k_y$ space at $\tilde{t} = 0.26, 0.25, 0.24, 0.05$ (from center). The chemical potential is fixed at $\mu = 2t_x$, and $U_0 = -3t_x$ is used in the calculations.

$\langle U_{\mathrm{ind}} \rangle$ has a kink around $\tilde{t} = 0.5$ at which Δ begins to decrease. The Fermi surface is closed originally in the 3D lattice with the given chemical potential $\mu = 2t_x$. With decreasing $\tilde{t}$, the Fermi surface becomes deformed, and then at $\tilde{t} = 0.5$, the Fermi surface becomes open. The second is a bump of $\langle U_{\mathrm{ind}} \rangle$ near $\tilde{t} = 0.25$ at which a dimensional change of the Fermi surface occurs and the nesting effect develops to escalate $\langle U_{\mathrm{ind}} \rangle$. As plotted in Fig. 4(c), finally at $\tilde{t} = 0.25$, the surface completely opens in the k_y and k_z directions and splits into two disconnected sheets causing the nesting effect.

However, in the quasi-1D regime, it turns out that the parameter space given by U_c does not cover the low $\tilde{t}$ region, and our calculation predicts a vanishing order parameter at low $\tilde{t}$, which deviates from previous rigorous studies of the Hubbard model. In the attractive Hubbard model in quasi-1D, the spin gap and the critical temperature are finite [24]. In the limit of 1D, the gap is still finite though the critical temperature goes to zero [25]. Singlet superfluidity dominates in the ground state, but there is no true long-range order in the 1D Hubbard model [26].

We have also considered the problem of the fermions in component-dependent lattice potentials [27] where each component experiences a different tunneling strength in a lattice. This difference in tunneling in a lattice is analogous to unequal effective masses of Fermi gases in continuum. In 3D lattices, we have found that the screening effect of the induced interaction becomes stronger as the difference between the tunneling strengths increases, which agrees well with the results for homogeneous gases [12,28] where similarly the stronger screening effect at the larger mass imbalance was found.

In conclusion, we have found that the presence of the optical lattices substantially strengthens the effect of the GMB correction on the BCS superfluidity. The consequent suppression of the order parameter is found to be much beyond the ratio 2.22 predicted in homogeneous gases, which agrees with the estimations of other previous many-body correction studies at low filling factors. As the filling factor becomes higher, the inclusion of the correction becomes increasingly important. For instance, the order parameter turns out to be almost 25 times smaller with the correction than the usual BCS mean-field results at half filing in 3D lattices. Moreover, the behavior of the order parameter in 2D lattices shows excellent agreement with the previous QMC values. Naturally, when the correction becomes very large, our perturbative approach breaks. The divergence of the correction is related to the phase at half filling in 2D where superfluid order and charge-density-wave order coexist.

One of the general shortcomings of a mean-field theory is that it gives a valid approximation only in high dimensions. Particularly for BCS superfluidity, our findings suggest that the effective theory with the many-body correction to the interatomic interaction can significantly extend the applicability of the mean-field calculations in the lower dimensions, namely, 3D and 2D, and in the crossover from 3D to 1D lattices, in spite of the obvious failure in the strict 1D limit. With the GMB correction, the simple mean-field calculation can also provide quantitatively reliable values in a wider range of the coupling strength, without sophisticated QMC calculations. The unanticipated large suppression of the order parameter at high filling factors highlights the practical importance of our results, which may provide a new insight to the issue of the critical temperature in future realizations of fermionic superfluids in optical lattices.

The authors thank Dr. T. K. Koponen for fruitful discussions. This work was supported by Academy of Finland and EuroQUAM/FerMix (Projects No. 213362, No. 217041, No. 217043, and No. 210953) and conducted as a part of a EURYI scheme grant [29].

[1] J. Bardeen *et al.*, Phys. Rev. **108**, 1175 (1957).
[2] C. A. R. Sá de Melo *et al.*, Phys. Rev. Lett. **71**, 3202 (1993).
[3] H. T. C. Stoof *et al.*, Phys. Rev. Lett. **76**, 10 (1996).
[4] L. P. Gorkov and T. K. Melik-Barkhudarov, Sov. Phys. JETP **13**, 1018 (1961).
[5] M. Lewenstein *et al.*, Adv. Phys. **56**, 243 (2007).
[6] I. Bloch *et al.*, Rev. Mod. Phys. **80**, 885 (2008).
[7] S. Giorgini *et al.*, Rev. Mod. Phys. **80**, 1215 (2008).
[8] J. K. Chin *et al.*, Nature (London) **443**, 961 (2006).
[9] R. Jördens *et al.*, Nature (London) **455**, 204 (2008).
[10] U. Schneider *et al.*, Science **322**, 1520 (2008).
[11] H. Heiselberg *et al.*, Phys. Rev. Lett. **85**, 2418 (2000).
[12] M. A. Baranov *et al.*, Phys. Rev. A **78**, 033620 (2008).
[13] T. K. Koponen *et al.*, Phys. Rev. Lett. **99**, 120403 (2007).
[14] T. K. Koponen *et al.*, New J. Phys. **10**, 045014 (2008).
[15] A. Martín-Rodero and F. Flores, Phys. Rev. B **45**, 13 008 (1992).
[16] See, e.g., for homogeneous gases, C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, England, 2008), p. 505.
[17] P. G. J. van Dongen, Phys. Rev. Lett. **67**, 757 (1991).
[18] R. T. Scalettar *et al.*, Phys. Rev. Lett. **62**, 1407 (1989).
[19] A. Moreo and D. J. Scalapino, Phys. Rev. Lett. **66**, 946 (1991).
[20] J. J. Deisz *et al.*, Phys. Rev. B **66**, 014539 (2002).
[21] P. Strack *et al.*, Phys. Rev. B **78**, 014522 (2008).
[22] G. Grüner, Rev. Mod. Phys. **60**, 1129 (1988).
[23] T. Paiva *et al.*, Phys. Rev. B **69**, 184501 (2004).
[24] A. I. Larkin and J. Sak, Phys. Rev. B **18**, 6053 (1978).
[25] T. Giamarchi, *Quantum Physics in One Dimension* (Clarendon, Oxford, 2004).
[26] F. H. L. Essler *et al.*, *The One-Dimensional Hubbard Model* (Cambridge University Press, Cambridge, England, 2005).
[27] M. A. Cazalilla *et al.*, Phys. Rev. Lett. **95**, 226402 (2005).
[28] T. Paananen *et al.*, Phys. Rev. A **75**, 023622 (2007).
[29] www.esf.org/euryi.