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Superconductivity from repulsion: Variational results in the limit of weak interaction

Dionys Baeriswyl
University of Fribourg
and IIP, Natal

Tbilisi, 8 June 2019

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Kakha Berishvili is passionate about his wines and sells some of his wines within Georgia. If planning to visit this small Georgian winery, be sure to contact Kakha in advance.

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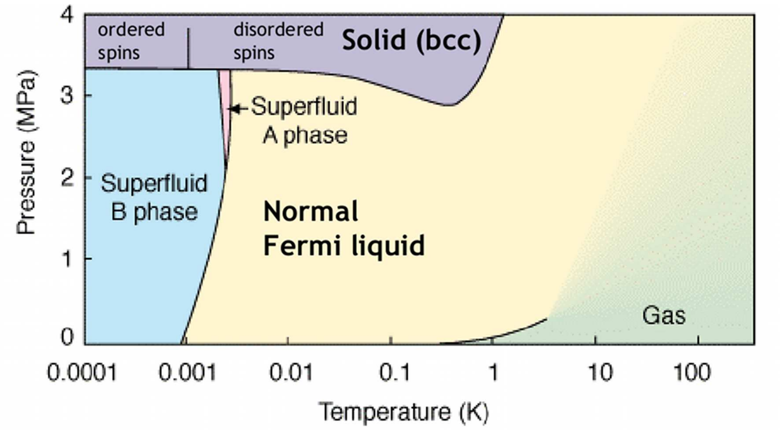
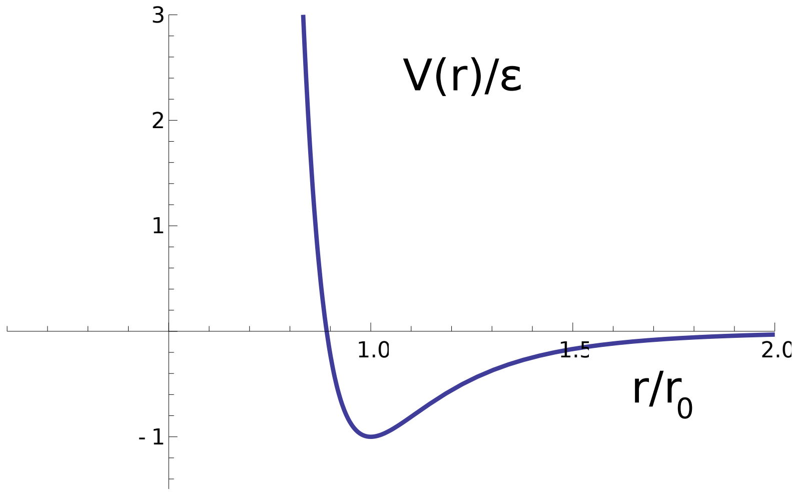
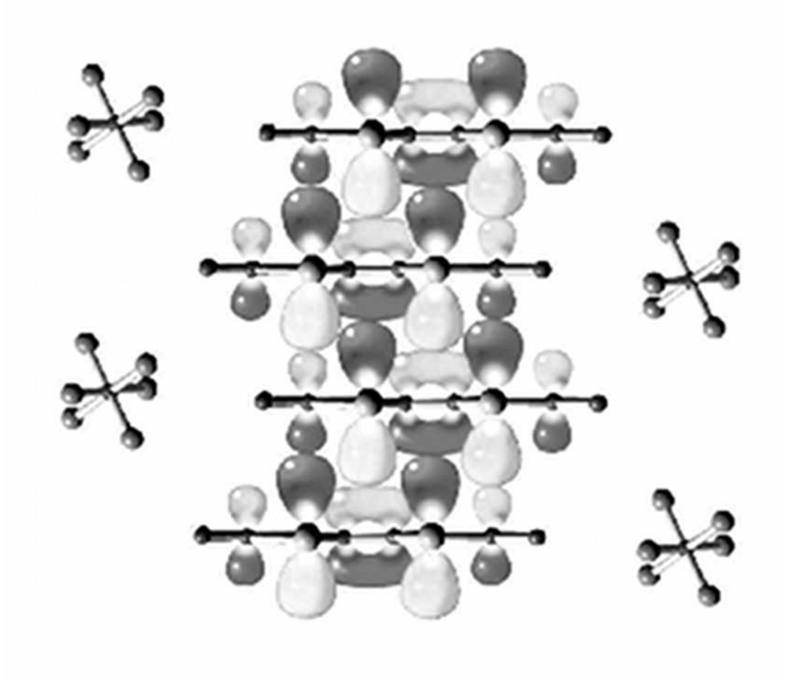
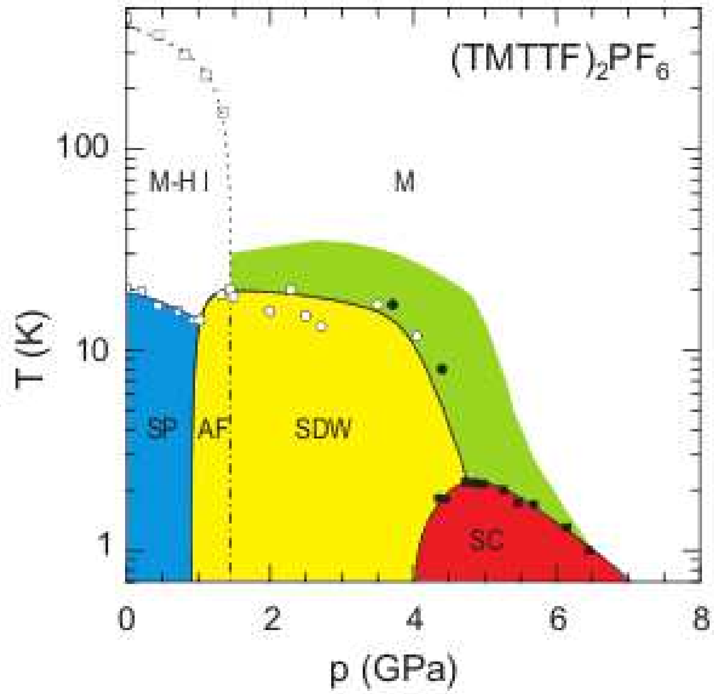
Superfluid ^{3}He





Charge transfer salts, the example of $(TMTTF)_2PF_6$

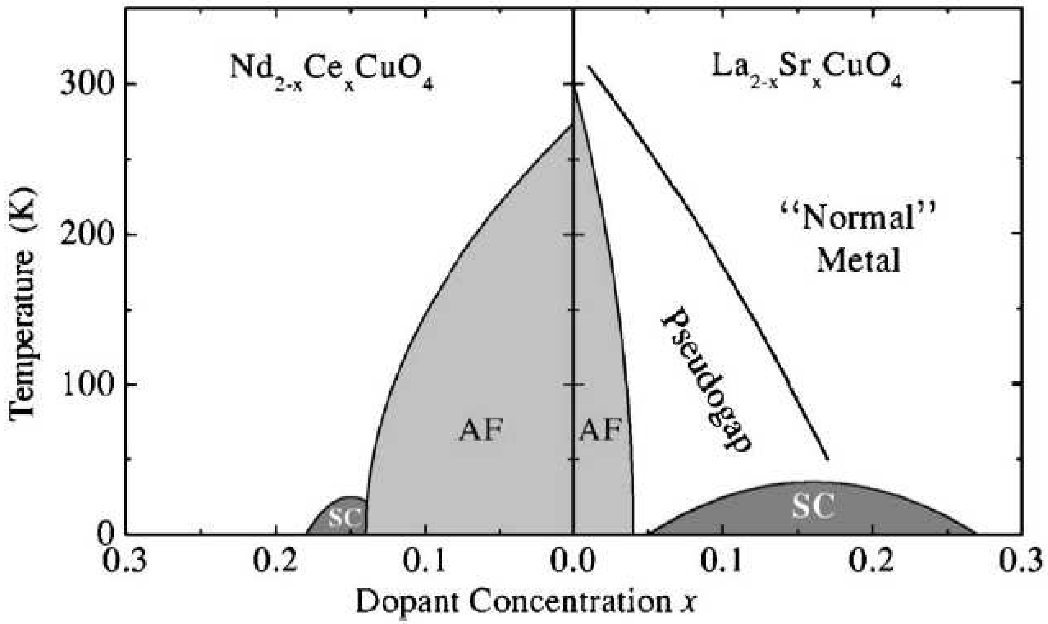




Superconductivity: Triplet p-wave, singlet d-wave or singlet f-wave?[a]

[a] J. C. Nickel *et al.*, Phys. Rev. B **73**, 165126 (2006)

Cuprate superconductors



Hubbard model on a square lattice

$$H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_0 + H_{\text{int}}$$

$n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$

$L \times L$ square lattice with $N_s = L^2$ sites

$t_{ij} = -t$ for nearest neighbors (and 0 otherwise)

$t = 1$ (unit of energy)

Cuprates: $U \approx 8$, hopping between second neighbors

Superconductivity in the $2D$ Hubbard model: Variational ansatz

Starting point: Mean-field BCS state $|\Psi_m\rangle$ with gap parameter

$$\Delta(\mathbf{k}) = \Delta_0(\cos k_x - \cos k_y)\,.$$

Refined Gutzwiller ansatz: $|\Psi\rangle = e^{-\tau H_0} e^{-\eta D} |\Psi_m\rangle\,.$

Variational parameters: η, τ and Δ_0, as well as the parameter μ, which fixes the average number of electrons (but is not identical to the true chemical potential).[a]

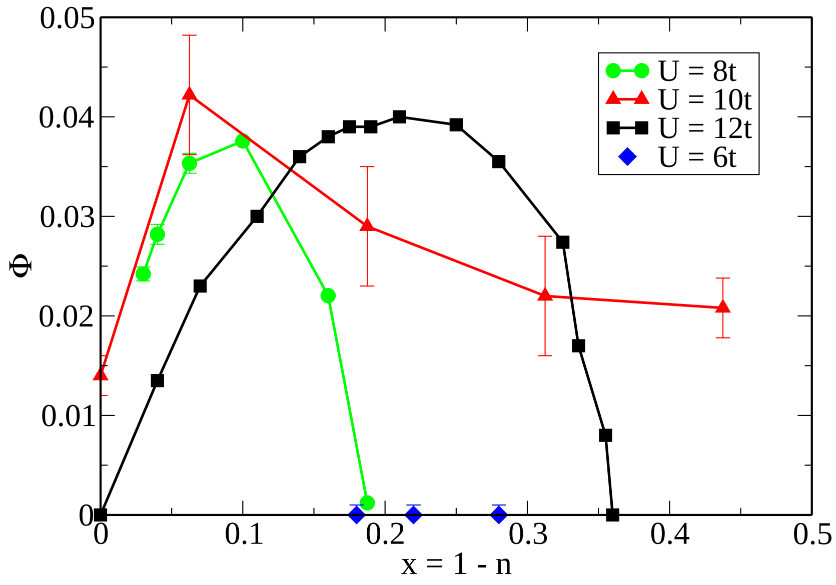
Order parameter: $\Phi = \langle\Psi|c_{\mathbf{R}\downarrow} c_{\mathbf{R}+\hat{\mathbf{x}}\uparrow}|\Psi\rangle / \langle\Psi|\Psi\rangle$.

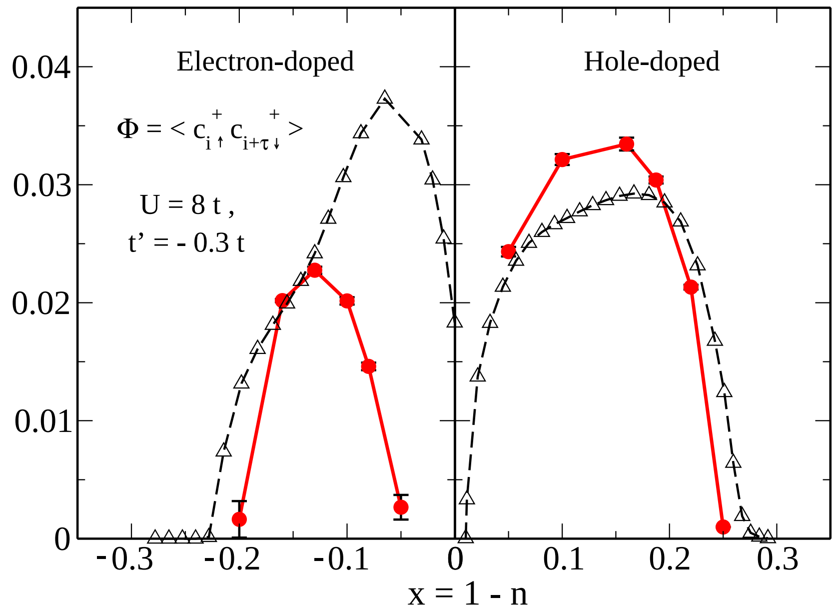
This ansatz tends to the "plain vanilla RVB theory" for $U \to \infty$.

[a] D. Eichenberger and D. B., Phys. Rev. B **76**, 180504 (2007), *ibidem* **79**, 100510 (2009), D. B., D. Eichenberger and M. Menteshashvili, New J. Phys. **11**, 075010 (2009).

Results for the order parameter

Variational schemes, QMC[a] ... and cluster DMFT[b]





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[a] Paramekanti *et al.* (2004, black squares), Giamarchi and Lhuillier (1991, red triangles), our work (2009, green dots), Aimi and Imada (2007, blue diamonds)

[b] Our results (red) compared with cluster DMFT by Kancharla et al. (2008)

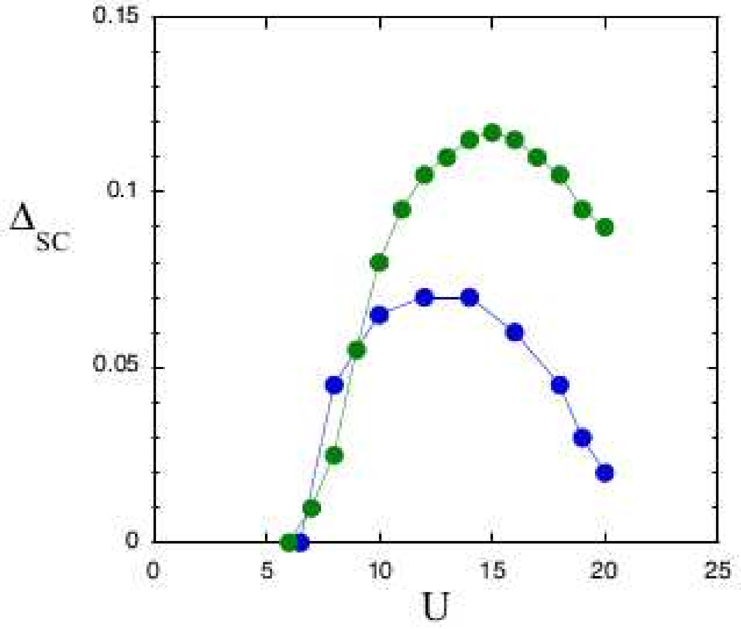
Is there a threshold value of U?

"Asymptotically exact" solution for $U \to 0$[a]:

$$\Delta_0 \sim e^{-\alpha/U^2}$$

[a] S. Raghu, S. A. Kivelson and D. J. Scalapino, Phys. Rev. B **81**, 224505 (2010)

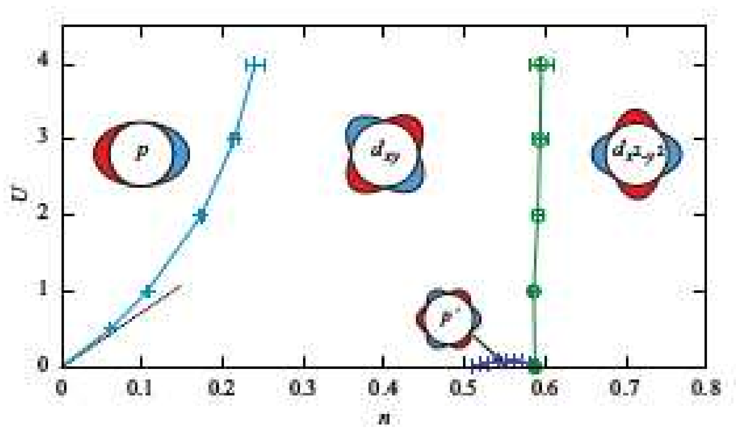
Variational: n=0.88, 10x10 lattice[a]:



[a] T. Yanagisawa, J. Phys. Soc. Jpn. **88**, 054702 (2019)

Hubbard model on a square lattice for small U

Phase diagram (far) away from half filling, from perturbation theory[a] [b]:



[a] R. Hlubina, Phys. Rev. B **59**, 9600 (1990).

[b] F. Šimkovic *et al.*, Phys. Rev. B **94**, 085106 (2016).

Variational study of d-wave superconductivity for $U \approx 1$ and large lattices (L of the order of 1000) [a]

1. Formalism
2. Superconductivity
3. Finite-size effects

[a] D. Baeriswyl, to be published in Phys. Rev. B.

1. Formalism

Ansatz: $$|\Psi\rangle := e^{-\tau H_m} e^{-\eta D} \; |\Psi_m\rangle = e^{-\tau E_m} e^{-\eta D(\tau)} \; |\Psi_m\rangle \,,$$

where $|\Psi_m\rangle$ is the BCS mean-field Hamiltonian, with a d-wave gap parameter, and $\mathcal{O}(\tau) := e^{-\tau H_m} \mathcal{O} e^{\tau H_m}$.

Linked-cluster theorem:

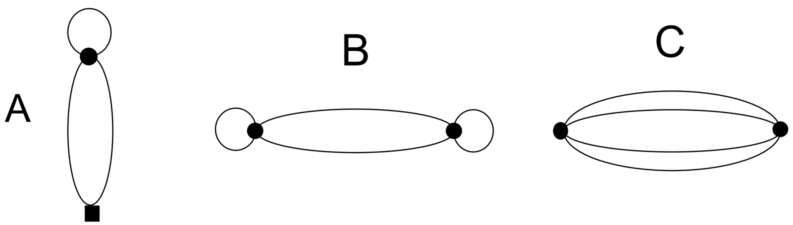
$$\bar{E} = \frac{\langle \Psi_m | e^{-\eta D(-\tau)} H e^{-\eta D(\tau)} | \Psi_m \rangle}{\langle \Psi_m | e^{-\eta D(-\tau)} e^{-\eta D(\tau)} | \Psi_m \rangle} = \langle \Psi_m | e^{-\eta D(-\tau)} H e^{-\eta D(\tau)} | \Psi_m \rangle_c \,.$$

Expansion to second order in U (one uses the fact that the optimized value of η is linear in U for small values of U),

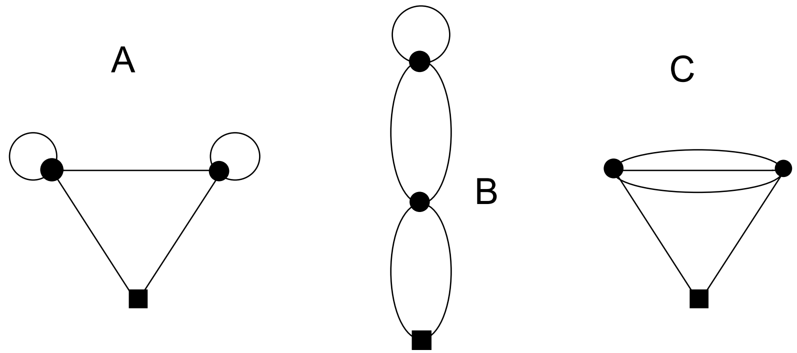
$$E^{(2)} = \langle H \rangle - 2\eta \langle H D(\tau) \rangle_c + \eta^2 \left[\langle H_0 D^2(\tau) \rangle_c + \langle D(-\tau) H_0 D(\tau) \rangle_c \right] \,.$$

where $\langle \mathcal{O} \rangle := \langle \Psi_m | \mathcal{O} | \Psi_m \rangle$. Similar relations hold for the average number of particles.

1st order diagrams



2nd order diagrams



Here the lines can represent distribution functions for particles or holes or also pair amplitudes. There are 63 different second-order diagrams. Nevertheless they lead to relatively compact expressions, which involve only simple sums, both in k-space and in R-space.

Variational parameter τ

The relations

$$c_{\mathbf{k}\sigma}(\tau)|\Psi_m\rangle = e^{-\tau E_k} c_{\mathbf{k}\sigma}|\Psi_m\rangle, \qquad c^\dagger_{\mathbf{k}\sigma}(\tau)|\Psi_m\rangle = e^{-\tau E_k} c^\dagger_{\mathbf{k}\sigma}|\Psi_m\rangle\,,$$

where $E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta^2_{\mathbf{k}}}$ is the excitation spectrum of the mean-field Hamiltonian H_m, show that τ plays the role of a soft cut-off away from the Fermi surface.

A small gap parameter affects mostly the region of the Fermi surface where τ has a negligible effect. Therefore the parameters τ and Δ_0 interfere only very weakly and we determine the optimal value of τ initially, i.e., for $\Delta_0 = 0$. We have checked that a full variational treatment of all parameters would only slightly increase the stability of the superconducting state.

Technicalities

- We put $t = 1$. The possible values of U are limited to $U \approx 1$, because for $U > 1.2$ the parameter η is too large (> 0.6) and for $U < 0.3$ the parameter Δ_0 is too small (for the system sizes we have considered).
- A square lattice is chosen with $N_s = L \times L$ sites and L typically 1000.
- Periodic-antiperiodic boundary conditions are applied to reduce degeneracies, at the same time they break the fourfold rotational symmetry.
- The number of particles $\bar{N}$ is chosen in such a way that for $\Delta_0 = 0$ all levels are either completely occupied or empty.
- The condensation energy per site is at most of the order of 10^{-5}. Therefore the constraint of a fixed particle number has to be satisfied extremely accurately (to about 10^{-14}).

Correlation energy for $\Delta_0 = 0$

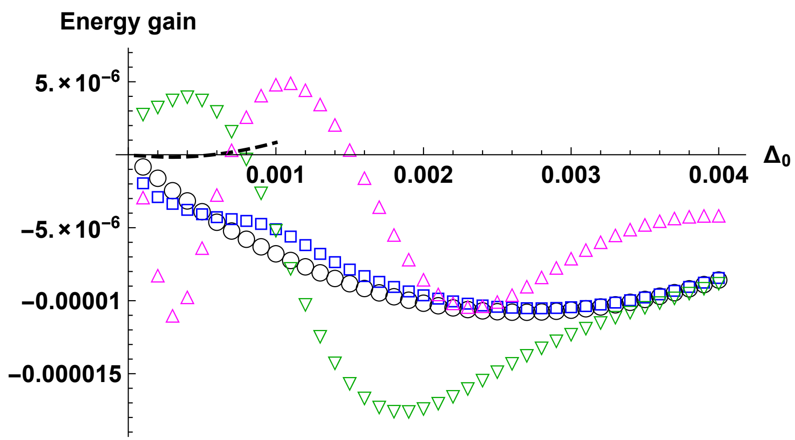
n	η	τ	E_{corr}/L	$E^{(\mathrm{ex})}_{\mathrm{corr}}/L$
1.0	0.59633	0.19805	-0.012169	-0.012562
0.9	0.57690	0.19286	-0.011774	-0.012072
0.8	0.54594	0.18435	-0.010787	-0.010995
0.7	0.5175	0.17618	-0.009406	-0.009553
0.6	0.49427	0.16917	-0.007774	-0.007880
0.5	0.47666	0.16349	-0.006014	-0.006092

Variational parameters η, τ and correlation energy per site for $U = 1$, $L_x = 1000$ and various densities ρ. E_{corr} is the variational result, $E^{(\mathrm{ex})}_{\mathrm{corr}}$ is the exact second-order term.[a]

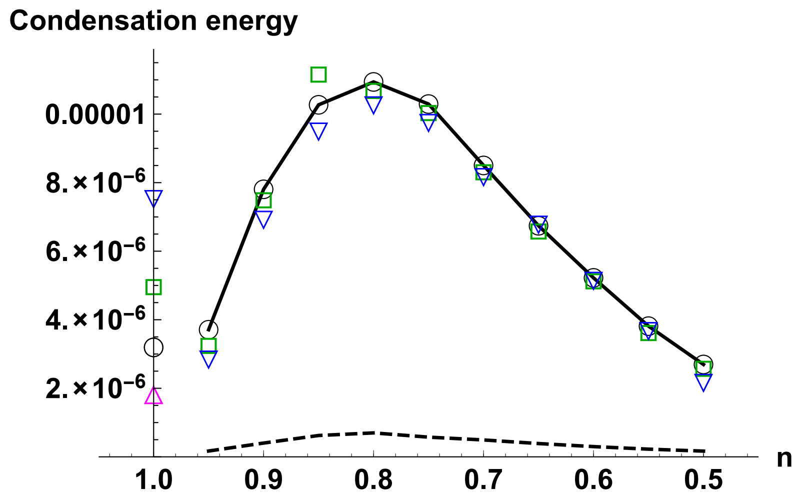
[a] W. Metzner and D. Vollhardt, Phys. Rev. B **39**, 4462 (1989)

2. Superconductivity

Energetics

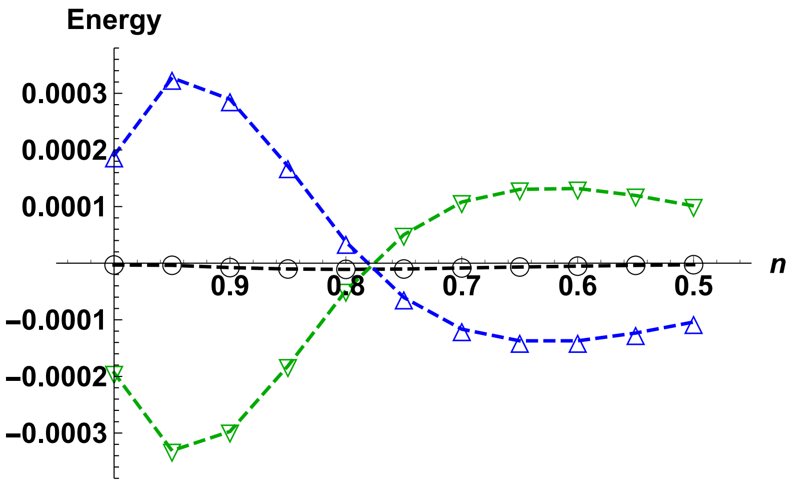


Energy gain due to superconductivity as a function of the gap parameter Δ_0 for $n = 0.8$ and $U = 1$. Symbols correspond to different system sizes, $L = 1000$ (circles), $L = 500$ (squares), $L = 200$ (down-pointing triangles) and $L = 100$ (up-pointing triangles). The dashed line represents results obtained with the Gutzwiller ansatz (for $L = 1000$.)

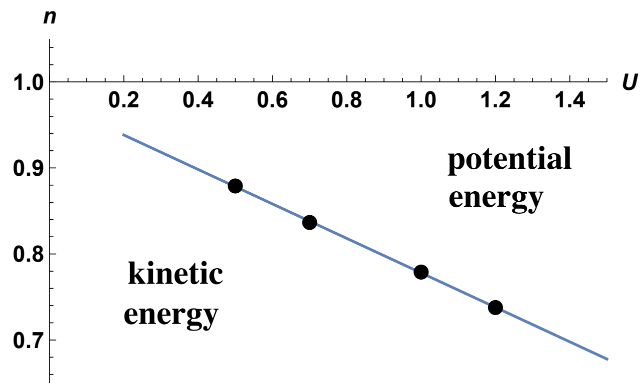


Condensation energy for $U = 1$ and different system sizes. Down-pointing triangles: $L = 500$, squares: $L = 1000$, circles and solid line: $L = 2000$, up-pointing triangle: $L = 4000$. The dashed line represents the BCS prediction.

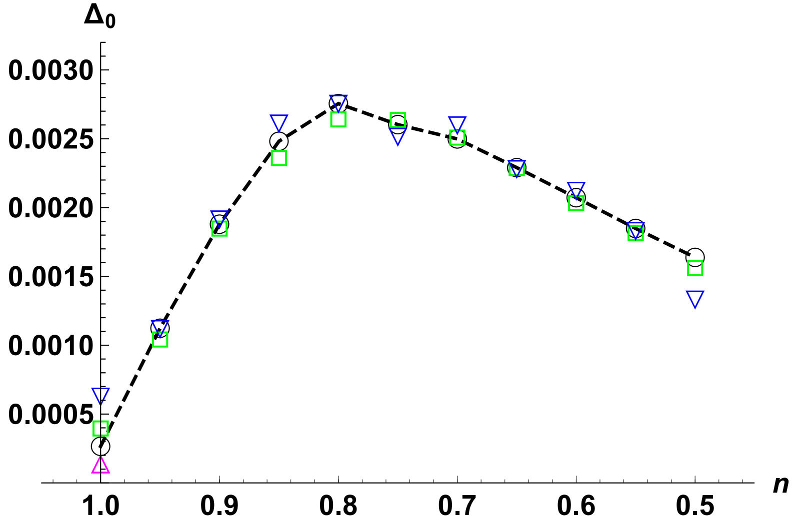
Conventional or unconventional?



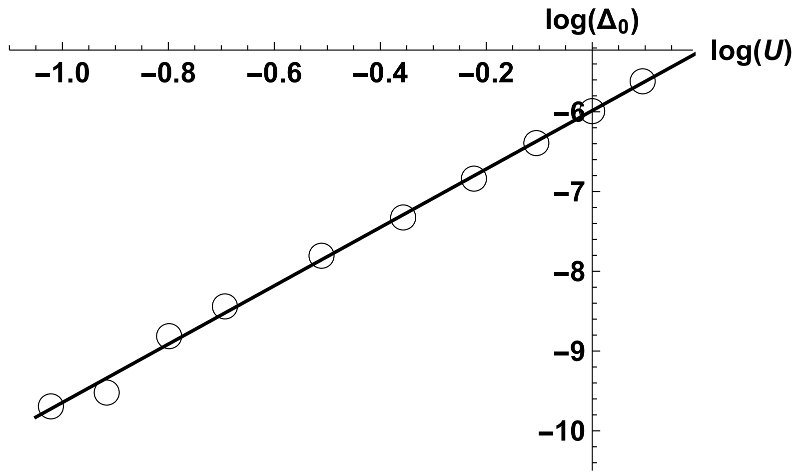
Changes in kinetic (up-pointing triangles), potential (down-pointing triangles) and total energies (circles) for $U = 1$ and $L = 2000$.



Gap parameter



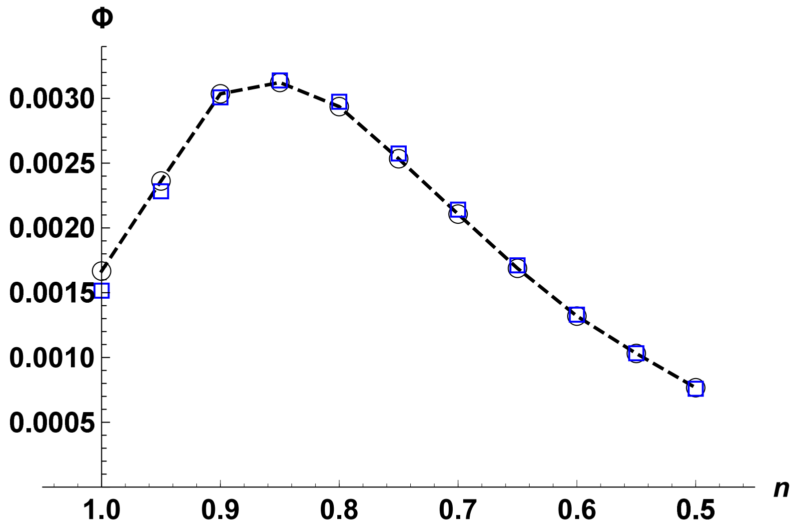
Gap parameter as a function of electron density for $U = 1$ and different system sizes. Down-pointing triangles: $L = 500$, squares: $L = 1000$, circles and dashed line: $L = 2000$, up-pointing triangle: $L = 4000$.



Gap parameter as a function of U for $n = 0.7$ and $L = 2000$. The solid line is a linear fit through the data points.

Order parameter

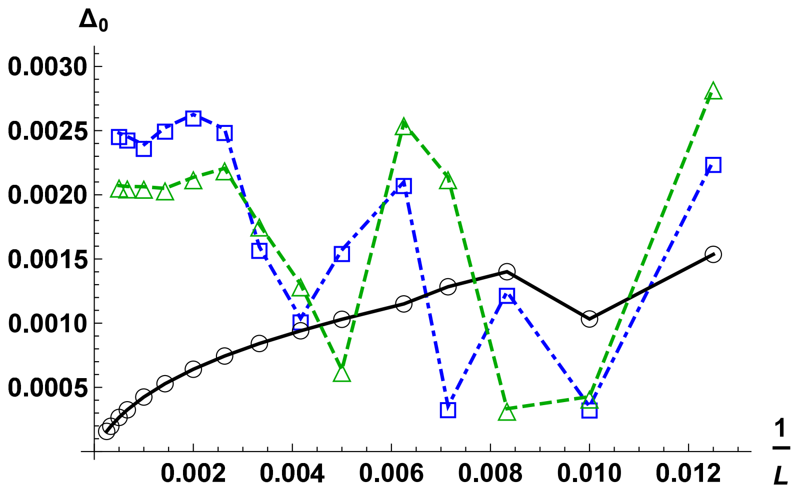
The calculation of the order parameter Φ proceeds in the same way as that of the kinetic energy, as an expansion in the correlation parameter η. The zeroth order term is just the Gor'kov function, which determines the order parameter in BCS theory.



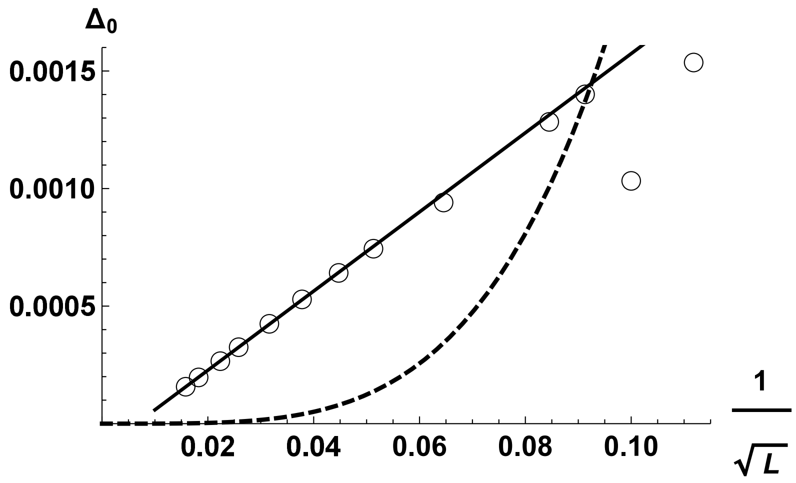
Order parameter for $U = 1$ and $L = 1000$ as a function of the density n. Circles and the dashed line represent the second-order expansion, squares the zeroth-order contribution.

3. Finite-size effects

Size-dependence of the gap parameter

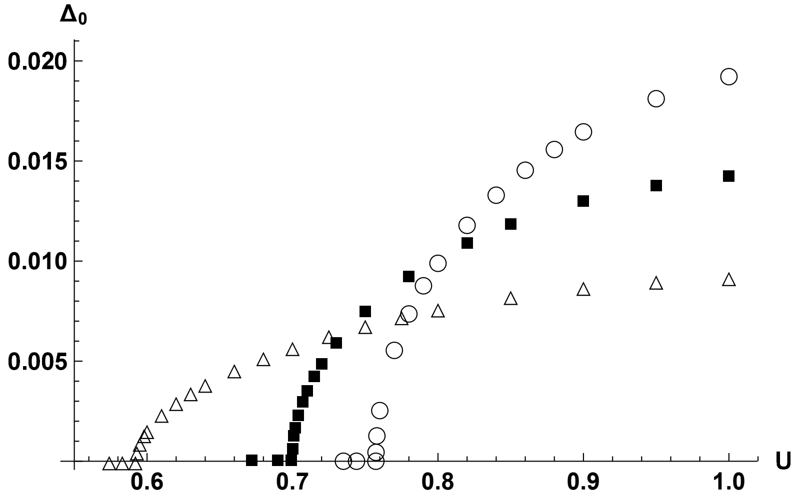


Variation of the gap parameter with system size ($U = 1$). Circles and solid line: $n = 1$, squares: $n = 0.85$, triangles: $n = 0.6$.

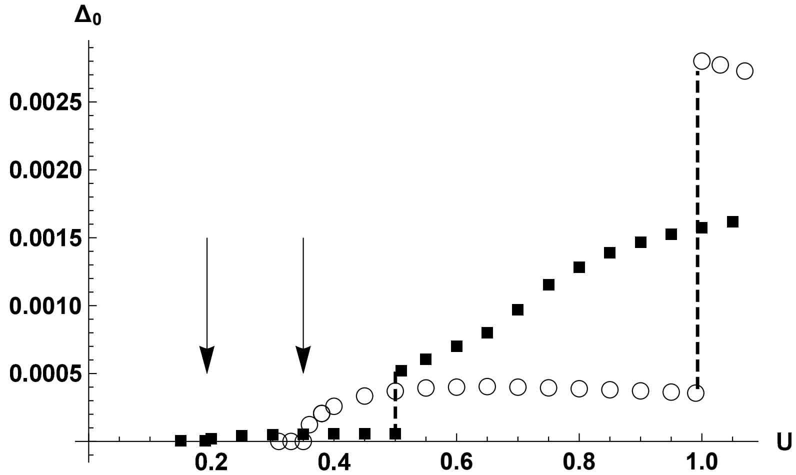


Size dependence of the gap parameter for $U = 1$ at half filling ($n = 1$). The dashed line corresponds to the HOMO-LUMO gap.

Onset of superconductivity



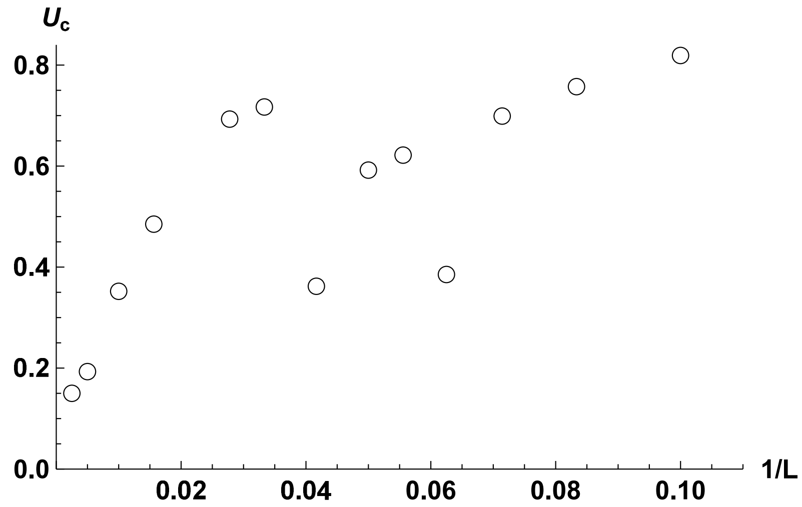
U-dependence of the gap parameter for $n =$ 0.85 and small system sizes, $L = 12$ (circles), $L = 14$ (squares) and $L = 20$ (triangles).



U-dependence of the gap parameter for $n =$ 0.85 and intermediate system sizes, $L = 100$ (circles) and $L = 200$ (squares).

Asymptotic limit

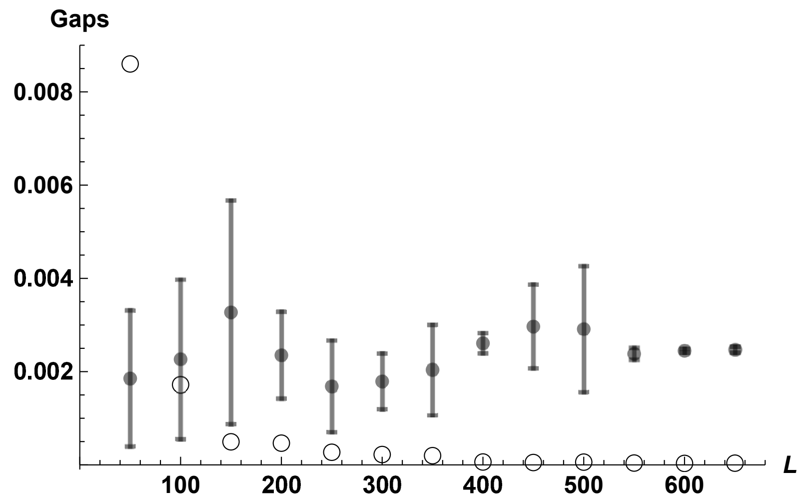
The critical value U_c decreases with system size, although the detailed size dependence is irregular. The overall behavior is consistent with a vanishing of U_c for $L \to \infty$, i.e. for an infinite system there is superconductivity for arbitrarily small U.



Critical values U_c for various system sizes and a density $n = 0.85$.

Fluctuations due to level statistics

Fluctuations appear in a large region about Anderson's critical size (defined by $\Delta_0(\infty) = \Delta_{\mathrm{HL}}(L)$). They only disappear if $\Delta_0(\infty)$ spans several level spacings.



Average gap parameter Δ_0 (dots) and standard deviation (error bars) for $n = 0.85$, $U = 1$ and various (average) system sizes. The circles indicate the average HOMO-LUMO gap Δ_{HL}. Its standard deviation is of the order of the average value.

Summary

1. Superconductivity with d-wave symmetry exists away from half filling $(0.5 \leq n < 1)$ for $U \approx 1$.

2. The discrepancy between fRG and VMC (or QMC) is due to the limited sizes used in numerical approaches.

3. Finite size effects: Two characteristic values of U, U_1 for the onset of pairing, U_2 for the disappearance of statistical fluctuations due to level statistics.

4. New problems:
   - $\Phi(U)$, $\Delta_0(U)$ for $U \to 0$.
   - Possible non-Fermi liquid phase away from half filling.