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Binding of holes in the Hubbard model

E. Dagotto
Institute for Theoretical Physics, University of California, Santa Barbara, California 93106

A. Moreo and R. L. Sugar
Department of Physics, University of California, Santa Barbara, California 93106

D. Toussaint
Department of Physics, University of Arizona, Tucson, Arizona 85721

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We present a new numerical method for the study of binding energies of particles in fermionic systems. Working with an *imaginary* chemical potential we can obtain results in the *canonical* ensemble by simple modifications of standard numerical techniques. We applied the technique to the two-dimensional Hubbard model observing binding of holes at half-filling on lattices of 4×4 sites. For $U/t=4$ we estimate that the binding energy is $\Delta=-0.10\pm0.02$.

The two-dimensional Hubbard model is being studied extensively in relation to the high-temperature superconductors,[1] and it appears to describe some of the features of these new materials. However, it remains an open question whether this model actually has a superconducting phase. Analytic studies of the Hubbard model are difficult in the intermediate and strong coupling regimes where perturbative and mean-field techniques are questionable. Numerical simulations are difficult at low temperatures for the relevant band fillings because the integrands of the Feynman path integrals are not positive definite. In this Rapid Communication we use a new numerical technique to show that two holes in a half-filled sea do bind for a 4×4 lattice. This result provides evidence that an effective attractive interaction appears in the $U>0$ Hubbard model. Previous numerical simulations in the grand canonical ensemble have also suggested an attractive pairing interaction in the d-wave channel for this model.[2,3] Our results do not constitute a proof that a superconducting phase will appear at finite hole doping, but the existence of a net attractive force between holes makes that scenario more plausible. As the criterion for binding we use the quantity,

$$\Delta=(E_2-E_0)-2(E_1-E_0)=(E_2-E_1)-(E_1-E_0)\,, \tag{1}$$

where E_n denotes the energy of the ground state with n holes (i.e., n less fermions than a half-filled band). If there is a bound state of two holes then $\Delta<0$. A calculation of Δ should be done in the canonical (C) ensemble where the number of fermions is fixed, rather than in the grand canonical (GC) ensemble. The Lanczos method can be used for this purpose, and it has produced interesting results for the t-J and Heisenberg models,[4] and very recently for the Hubbard model.[5] However, it cannot be used for large lattices. Stochastic methods have recently been proposed for calculating ground-state properties with fixed numbers of electrons.[3,6] However, they suffer from the sign problem mentioned above. In addition, they provide a direct calculation of the (extensive) energies E_n. This is a problem in evaluating Δ, which is an intensive quantity, since one must take differences of extensive quantities, which requires high-precision measurements. In this Rapid Communication we present an alternative numerical approach, based on a simple modification of the standard quantum Monte Carlo method used in calculations of the GC ensemble.[3,7] Although below we focus our attention specifically on the Hubbard model, the derivation is valid for a wide variety of Hamiltonians.

Consider a model defined by a Hamiltonian $\hat{H}$. We denote the partition function for the GC ensemble with chemical potential μ by $Z_{\rm GC}(\mu)$ and the partition function for the C ensemble with n electrons above half-filling by $Z_C(n)$. They are related by

$$Z_{\rm GC}(\mu)=\mathrm{tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]=e^{\beta\mu N}\sum_{n=-N}^{n=N}e^{\beta\mu n}Z_C(n)\,, \tag{2}$$

where $\hat{N}$ is the number operator and N the number of spatial lattice points. For the Hubbard model the eigenvalues of $\hat{N}$ ranges from 0 to $2N$. Our approach rests on the continuation of Eq. (2) to imaginary chemical potential $\mu\rightarrow i\lambda$. Since the canonical partition functions are independent of μ,

$$Z_C(n)=\frac{1}{2\pi\beta}\int_0^{2\pi/\beta}d\lambda e^{-i\beta\lambda(n+N)}Z_{\rm GC}(\mu=i\lambda)\,. \tag{3}$$

The advantage of Eq. (3) is that for the Hubbard model, and a variety of other models, $\exp(-i\beta\lambda N)Z_{\rm GC}(\mu=i\lambda)$ can be written as a path integral with a *positive* weight. All the problems associated with fluctuating signs are contained in the explicit phase factor $\exp(-i\beta\lambda n)$ rather than in an involved determinant phase as in previous formulations.

We now specialize to the Hubbard model defined by the Hamiltonian

$$\hat{H}(t,U)=-t\sum_{\langle i,j\rangle,\sigma}(c_{i,\sigma}^{\dagger}c_{j,\sigma}+\mathrm{H.c.})+U\sum_i(n_{i,\uparrow}-\tfrac{1}{2})(n_{i,\downarrow}-\tfrac{1}{2})\,, \tag{4}$$

where the notation is standard. To perform a numerical

calculation we integrate out the fermion degrees of freedom. To this end we use a discrete Hubbard-Stratonovich transformation,[8] introducing an imaginary time-dependent Ising variable $\{s\}$ at each lattice site. The spin-up and spin-down electrons couple to the $\{s\}$ fields in proportion to $n_{i,\sigma}$ with *opposite* signs. Integrating out the fermion degrees of freedom we write the GC ensemble partition function as a sum over configurations, $\{s\}$ (Refs. 3 and 7),

$$Z_{GC}(\mu)=\sum_{\{s\}}\det M(\{s\},\mu)_{\uparrow}\det M(\{s\},\mu)_{\downarrow}, \tag{5}$$

where $M_{\uparrow}$ and $M_{\downarrow}$ are the fermion matrices for spin-up and -down electrons propagating through the configuration $\{s\}$ in a chemical potential μ. We now perform a particle-hole transformation on the spin-down sector given by $c_{i,\downarrow}\rightarrow c_{i,\downarrow}^{\dagger}(-1)^{i_x+i_y}$, $i=(i_x,i_y)$. Under this transformation the coupling of the spin-up and -down electrons to the $\{s\}$ field become identical and

$$\mu(n_{i,\uparrow}+n_{i,\downarrow})\rightarrow\mu(n_{i,\uparrow}-n_{i,\downarrow}+1).$$

Equation (5) can therefore be rewritten as

$$Z_{GC}(\mu)=e^{-\beta\mu N}\sum_{\{s\}}\rho(\{s\})\det M(\{s\},\mu)_{\uparrow}\det M(\{s\},-\mu)_{\uparrow}, \tag{6}$$

where $\rho(\{s\})$ is a positive function of the $\{s\}$ variables.[8] Now each term in the sum Eq. (6) is positive for $\mu=i\lambda$, since each determinant is the complex conjugate of the other.

We are primarily interested in calculating the binding energy Δ and we wish to directly obtain the energy differences on the right-hand side of Eq. (1) to avoid cancellations in subtracting two large quantities. This can be done using the asymptotic result

$$\frac{Z_C(n)}{Z_C(0)}\xrightarrow[\beta\gg 1]{}d_{n,0}e^{-\beta(E_n-E_0)}, \tag{7}$$

where $d_{n,0}$ is the ratio of degeneracies of the ground states with n and 0 holes. A straightforward way to proceed would be to generate a sequence of field configurations $\{s\}$ and complex chemical potential values λ, with a probability distribution $P(\{s\},\lambda)$, proportional to $\rho(\{s\})\,|\det M(\{s\},i\lambda)_{\uparrow}|^2$. $Z_C(n)/Z_C(0)$ is given by the expectation value of $\exp(-i\beta\lambda n)$ in this distribution [particle-hole symmetry implies that $Z_C(n)=Z_C(-n)$, so it is only necessary to measure $\cos(\beta\lambda n)$]. However, because a gap exists in the single-electron density of states, the fermion determinant is nearly λ independent at low temperatures. Then, we can simply generate the field configurations for $\lambda=0$, just as one does in GC ensemble calculations at $\mu=0$. We then have

$$\frac{Z_C(n)}{Z_{GC}(0)}=\sum_{\{s\}}P(\{s\},0)\frac{1}{2\pi\beta}\int_0^{2\pi/\beta}d\lambda e^{-i\beta\lambda n}\frac{|\det M(\{s\},i\lambda)_{\uparrow}|^2}{|\det M(\{s\},0)_{\uparrow}|^2}. \tag{8}$$

We do not need to explicitly evaluate the integral over λ in Eq. (8). The absolute square of the fermion determinant is simply the partition function for electrons in the presence of the $\{s\}$ field, so we can write in analogy with Eq. (2),

$$\frac{|\det M(\{s\},i\lambda)_{\uparrow}|^2}{|\det M(\{s\},0)_{\uparrow}|^2}=c_0(\{s\})+2\sum_{n=1}^{N}\cos(\beta\lambda n)c_n(\{s\}), \tag{9}$$

where we used the fact that the left-hand side of Eq. (9) is even under $\lambda\rightarrow-\lambda$. Clearly $Z_C(n)/Z_{GG}(0)=\langle c_n\rangle$ where the average is over an ensemble of $\{s\}$ configurations generated by the probability $P(\{s\},0)$. To obtain the gaps $\Delta_{nm}=E_n-E_m$ we then need

$$\frac{Z_C(n)}{Z_C(m)}=\frac{\langle c_n\rangle}{\langle c_m\rangle}. \tag{10}$$

Since each $Z_C(m)\propto\exp(-\beta E_m)$ and $Z_{GC}(0)\propto\exp(-\beta E_0)$ for large β, Eq. (10) involves intensive quantities, and no large cancellations occur. To obtain the c_n for a given field configuration, we evaluate the fermion determinant for an arbitrary set of λ_i and invert[9] Eq. (9). Numerical calculations cannot be carried out at arbitrarily low temperatures since the quantities $Z_C(n)/Z_{GC}(0)$ fall off exponentially with β in part because the c_n become small configuration by configuration, and also because of the cancellations between configurations ($c_{n>0}$ can be negative for some configurations of $\{s\}$). The latter effect introduces noise that eventually makes the calculations impractical. For example, for 4×4 lattices we are restricted to $\beta\leq6$. What we have done is to perform calculations for that range of β, and then perform fits to obtain the gaps. Finally we remark that the approach outlined here can be used to calculate the expectation value of any operator in the C ensemble.[10]

We checked our technique on a 2×2 lattice where exact results can be obtained. We used a time step $\Delta\tau=0.075$ and between 2000–5000 iterations after thermalization. Numerically evaluating $-\ln(\langle c_2\rangle/\langle c_2\rangle)$ vs β the agreement with the exact results at each temperature was excellent. The asymptotic regime Eq. (7) is easily reached and from there we obtained $\Delta_{21}=1.16\pm0.01$ (in units of t) while the exact result is 1.1640. For the case $\langle c_1\rangle/\langle c_0\rangle$ special care must be taken. Although the agreement with the exact values at each temperature is also excellent, the asymptotic regime is not easily reachable and important deviations from it can be seen even at relatively low temperatures. The reason is that in the half-filled subspace there is an energy level very close to the ground state (that can be mapped into the spin wave of strong coupling) perturbing the asymptotic result Eq. (7). The remedy to this problem is to fit the data including this "spin-wave" (SW) level, which is threefold degenerate, with its energy (Δ_{SW}) as a free parameter, as

$$\frac{Z_1}{Z_0}=\frac{\langle c_1\rangle}{\langle c_0\rangle}\xrightarrow[\beta\gg1]{}\frac{d_{1,0}e^{-\beta\Delta_{10}}}{1+3e^{-\beta\Delta_{SW}}}. \tag{11}$$

After this improvement the data can be fit very well (Fig. 1) using $d_{1,0}=4$ (see below). The prediction for the gap is $\Delta_{10}=1.24\pm0.01$ while the exact result is 1.2383. The numerical spin-wave gap is $\Delta_{SW}=0.29\pm0.01$ (exact result $\Delta_{SW}=0.2815$).

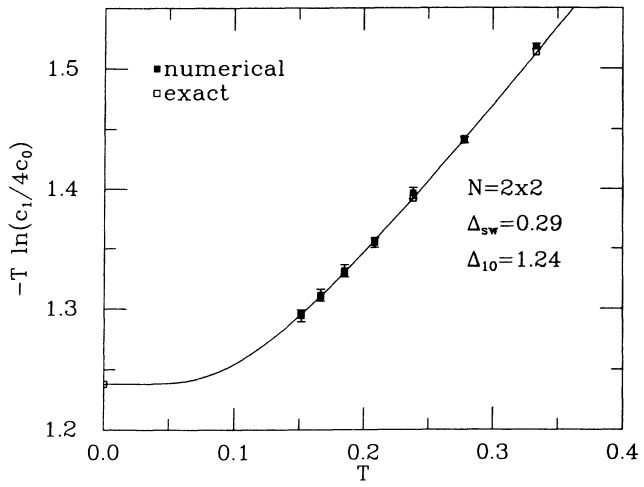

FIG. 1. $-T\ln(\langle c_1\rangle/d_{1,0}\langle c_0\rangle)$ vs T for the 2×2 lattice with $U/t=4$. The solid line is our extrapolation using Eq. (11) with $d_{1,0}=4$.

Is the factor $d_{1,0}$ relevant in the fits? Suppose we incorrectly guess its value using a degeneracy $\tilde{d}_{1,0}$. The correct gap at $T=0$ will still be obtained but with a finite temperature correction $\sim T\ln(d_{1,0}/\tilde{d}_{1,0})$ in a $-T\ln(\langle c_1\rangle/\tilde{d}_{1,0}\langle c_0\rangle)$ vs T plot. Then, minimizing the slope of this linear term in T we can also *predict* the relative degeneracy of the states under study. Following these ideas we found for the 2×2 lattice that $d_{1,0}\approx 4$ in agreement with the exact result. $d_{2,1}$ can also be deduced numerically following the same procedure. For the 2×2 lattice we correctly found that the ground state with two holes is not degenerate. For a 4×4 lattice it is known[11] that the one-hole ground state has a degeneracy 12 since it can have total spin $\pm\frac{1}{2}$ and momentum $\mathbf{k}=(\pm\frac{1}{2}\pi,\pm\frac{1}{2}\pi)$ or $(\pi,0),(0,\pi)$. On the other hand, the ground state in the zero-hole subspace is not degenerate. So we expect that $d_{1,0}=12$ will produce the best fit in Eq. (11) for a 4×4 lattice.

Now we present results for the 4×4 lattice. For the gap Δ_{10} we follow the same technique used for the 2×2 lattice. In Fig. 2(a), we show

$$Y=-T\ln\left[\frac{\langle c_1\rangle(1+3e^{-\beta\Delta_{SW}})}{d_{1,0}\langle c_0\rangle}\right]$$

vs T at $U/t=4$ for different degeneracies. If the fit is reasonable and if d_{10} is correctly selected then Y should be approximately constant as effectively happens for $d_{1,0}\approx 12$ in agreement with our expectations. Our numerical results are $\Delta_{10}=0.98\pm0.02$ and $\Delta_{SW}=0.47\pm0.03$. In Fig. 2(b) we show $-\ln(\langle c_2\rangle/\langle c_1\rangle)$ vs β at $U/t=4$. A good straight-line behavior is observed obtaining a gap $\Delta_{21}=0.88\pm0.02$. The optimal value of $d_{2,1}$ is ≈ 1.5 implying that the two-hole ground state is highly degenerate or that many other levels are very close to it. Combining these results we predict $\Delta=-0.10\pm0.02$ at $U/t=4$.

We have repeated this procedure for many values of U/t with results for Δ shown in Fig. 3. We can safely conclude that Δ is negative for $U\leq 7$ on[2] 4×4 lattice. Our technique works better at intermediate values of U/t since

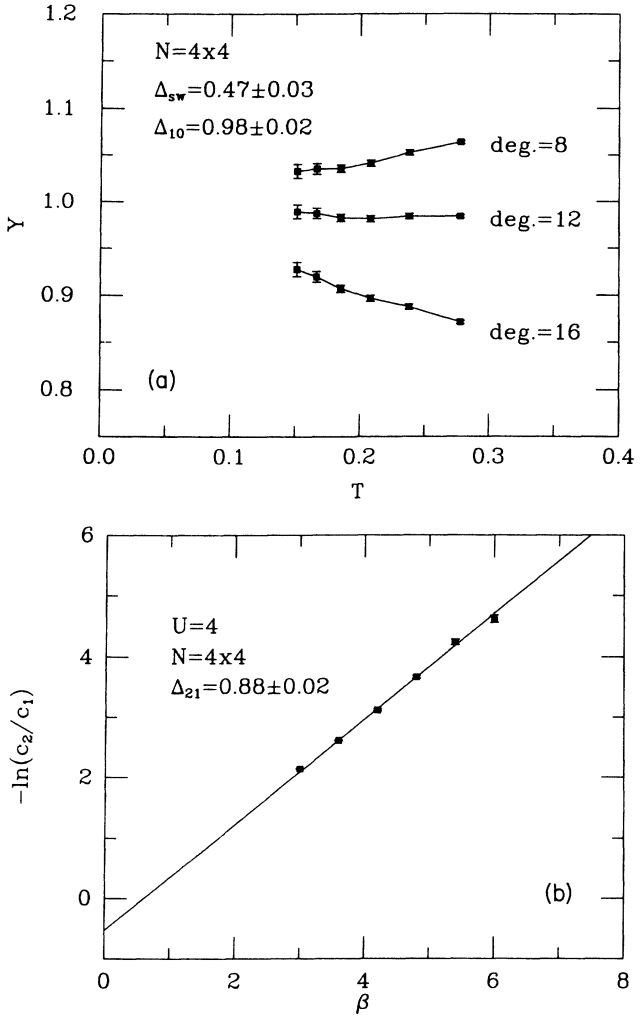

FIG. 2. (a) $Y=-T\ln[\langle c_1\rangle(1+3e^{-\beta\Delta_{SW}})/d_{1,0}\langle c_0\rangle]$ as a function of T for the 4×4 lattice with $U/t=4$. (b) $-\ln(\langle c_2\rangle/\langle c_1\rangle)$ as a function of β for the 4×4 lattice with $U/t=4$.

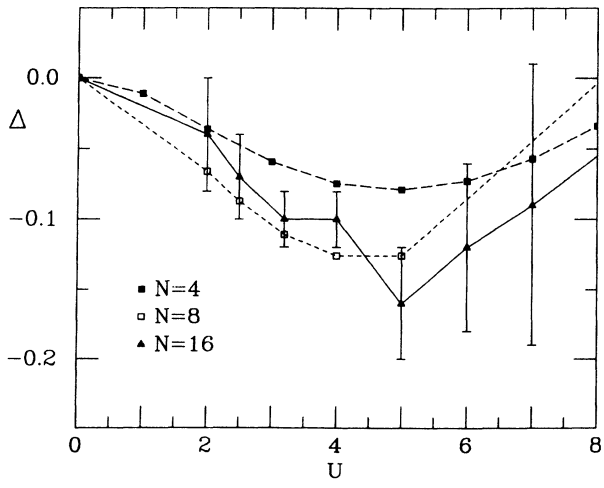

FIG. 3. Δ as a function of U/T for the 2×2 (long-dashed line), $\sqrt{8}\times\sqrt{8}$ (short-dashed line), and 4×4 (continuous line) lattices.

for $U/t \ll 1$, Δ_{SW}, and the energies of other levels are very small affecting the extrapolation to $T=0$ while for $U/t \gg 1$ the fluctuations are very strong. For comparison, in Fig. 3 we also show exact results for a 2×2 lattice and Lanczos results for a $\sqrt{8}\times\sqrt{8}$ lattice.[12] Both are very close to the new results on a 4×4 lattice suggesting that we may be already near the bulk limit.[13] However, note that at least for $U/t=4$, Δ seems to be smaller for the sixteen-site lattice than for the eight-site lattice. Then our result $|\Delta|=0.10\pm0.02$ is perhaps an upper bound for the bound-state energy. For large U/t, Δ is positive meaning that the holes prefer to be separate as much as possible in the small lattice we studied (in the bulk limit Δ cannot be positive). That roughly happens for values of $U/t \geq 8$ where the holes may prefer to form independent ferromagnetic polarons. So the interesting regime in this model appears to be $U/t \approx 4-5$ rather than larger values.

After completing Fig. 3 we received a paper by Parola *et al.*[5] in which Lanczos and stochastic results for the 4×4 lattice are presented for two and zero holes at $U/t=4$. The Lanczos result for this gap is $\Delta_{20}=1.8784$ while our prediction is $\Delta_{20}=\Delta_{21}+\Delta_{10}=1.87\pm0.02$ in excellent agreement within statistical errors. The stochastic result of Parola *et al.* is[14] $\Delta_{20}=1.76\pm0.08$, which was obtained by directly measuring the extensive energies rather than energy differences.[15]

Summarizing, in this Rapid Communication we presented a new numerical method to study binding of holes in fermionic systems. In particular we have shown that on a 4×4 there is a bound state of two holes in the two-dimensional Hubbard model at half-filling. Although from the existence of a bound state of two holes at half-filling we cannot show the existence of a superconducting phase at low temperatures,[16] nevertheless, it is gratifying to observe an effective attractive force coming out of the repulsive Hubbard model. An analysis of the symmetry of the state as well as extensions to larger lattices and other models[17] are in progress.

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[9] The c_n fall off rapidly with n at low temperatures, so the sum can be truncated, and the fermion determinant need only be evaluated for a limited number of λ_i (on the 4×4 lattice we needed only five terms).

[10] If $A(\{s\})$ denotes the value of the operator $\hat{A}$ in the field configuration $\{s\}$, then in analogy to Eq. (9) one can write

$$A(\{s\})\frac{|\det M(\{s\},i\lambda)_\uparrow|^2}{|\det M(\{s\},0)_\uparrow|^2}=a_0(\{s\})+2\sum_{n=1}^{N}\cos(\beta\lambda n)a_n(\{s\}).$$

The expectation value of $\hat{A}$ in the C ensemble is then given by $\langle\hat{A}\rangle_n=\langle a_n\rangle/\langle c_n\rangle$ where the expectation values on the right-hand side are taken with the probability $P(\{s\},0)$.

[11] E. Dagotto, A. Moreo, and T. Barnes, Phys. Rev. B **40**, 6721 (1989), and references therein. This result was obtained in the $t-J$ model (strong coupling limit of the Hubbard model) and is supposed to persist for any value of U/t smoothly connected to the strong coupling region.

[12] J. Riera and A. P. Young, Phys. Rev. B **39**, 9697 (1989).

[13] We do not expect phase separation in this model based on the results for an eight-site lattice of Ref. 12.

[14] We follow the convention that the error bars of a sum of energies is the biggest of the two error bars.

[15] In this model Δ is very small compared with the energies themselves and high accuracy ($<10\%$) is necessary. Then the 2D Hubbard model is a particularly rigorous test of our technique. For the t-J, multiband Hubbard, or $U<0$ Hubbard models where Δ is expected to be larger, our technique should work very well.

[16] The two-body potential producing this bound state may be screened by a finite density of holes, although for large U/t the bound states are expected to be small in size and that effect may not be relevant. But even neglecting that effect it is not clear how to relate Δ and T_c since the pairs may exist even for $T>T_c$ at large U/t [see, for example, A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter,* edited by A. Pekalski and J. Przystawa (Springer-Verlag, Berlin, 1980), p. 14].

[17] We reiterate that the present method can be applied to a wide range of Hamiltonians, like those appearing in lattice gauge theory, where the fermionic determinant is complex at finite density [I. Barbour *et al.*, Nucl. Phys. **275**, 296 (1986)]. In fact, in the context of particle physics, Eq. (3) has been previously derived [N. Weiss, Phys. Rev. D **35**, 2495 (1987)] and a method similar to ours has been applied to the study of phase transitions at finite quark density in the C ensemble [see I. Barbour, C. Davies, and Z. Sabeur, Phys. Lett. B **215**, 567 (1988)]. Considering sectors with different quark numbers one could hope to calculate hadronic masses, at least in strong coupling.