Monte Carlo study of the energy spectrum of strongly correlated electron systems

D. V. Berkov and S. V. Meshkov
Institute of Solid State Physics, Academy of Sciences of the USSR

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A new method is proposed for reconstructing the density of states of fermion systems on the basis of a Matsubara Green's function derived by quantum-mechanical Monte Carlo methods. This method is distinguished by the absence of adjustable parameters and by the circumstance that the accuracy of the solution can be controlled. The one-particle density of states is studied in the one- and two-dimensional Hubbard models.

Of primary interest in a study of systems of interacting fermions is the energy spectrum of the excitations. Since analytic methods cannot be used here, the best approach seems to be to use quantum-mechanical Monte Carlo methods, which make it possible to determine Matsubara Green's functions for various model Hamiltonians.[1] If reliable information is to be obtained on the energy spectrum, however, one also needs reliable methods for analytically continuing the Green's functions to the real frequency axis. Our purpose in the present study was to develop such methods.

A reconstruction of the density of states $\rho(\epsilon)$ from the Matsubara temperature Green's function $G(\tau,\tau)$ requires solving the integral equation (Ref. 2, for example)

$$G(\tau=0,\tau)=\pi^{-1}\int\frac{\rho(\epsilon)\exp(-\epsilon\tau)d\epsilon}{1+\exp(-\epsilon\beta)}\,. \tag{1}$$

Finding the solution of this equation is an ill-posed problem in the Hadamard sense: Because of an instability with respect to short-wave harmonics, small errors in the initial data $G(\tau)$ lead to arbitrarily large oscillations in the solution $\rho(\epsilon)$. None of the existing methods for solving ill-posed problems leads to reliable results for Eqs. (1) with an exponential kernel. In Refs. 2–5, which were devoted directly to the reconstruction of the density of states of quantum systems, there is no satisfactory condition for choosing the smoothing parameters α, and no method is given for evaluating the error of the result, although it is known that if there is an error in the choice of α, the resulting solution may be greatly different from the actual solution.

We have proposed a new method for solving an ill-posed inverse problem of the type in (1). This method is free of adjustable smoothing parameters and allows one to estimate the accuracy of the result. From the standpoint of processor time, our method is much more economical than those used in Refs. 2–5, since it reduces to a minimization of quadratic functions with linear constraints, for which very efficient algorithms are available.[6]

Method. After a switch to a finite-difference approximation of Eq. (1), $\hat{A}\rho=g$, an *SVD* expansion of the matrix is carried out: $A=USV^T$ (the matrices U and V are

orthogonal, and S is diagonal, with the singular numbers s_i of matrix A on the diagonal). After the substitutions $\rho = \hat{V}y$ and $b = \hat{U}^T g$ and a transformation to a diagonal system $y_i s_i = b_i$, we set $y_i = 0$ for s_i smaller than the computer value ϵ. Two systems of conditions (inequalities) are imposed on the vector y: the condition that $\rho(\epsilon)$ be nonnegative, which is $\hat{V}y \geqslant 0$, and the condition that y_i be close to the exact solution $y_i^0 = b_i/s_i$

$$y_i^0 - \psi\delta_i/s_i \leq y_i \leq y_i^0 + \psi\delta_i/s_i ,$$

where δ_i is the size of the error in b, determined with allowance for the covariance matrix of the errors in the components of g. One then seeks a lower limit $\psi_{\min}$ on the interval width, below which the systems of inequalities become incompatible.

To find a result, one applies this procedure to a series of realizations of the Green's function $G(\tau)$, which are constructed from the experimental function by adding to it a Gaussian noise with the same amplitude as that of the statistical error. The mean value $\bar{\rho}(\epsilon)$ over the resulting set $\rho(\epsilon)$ is then taken to be the solution of the problem, whose accuracy is characterized by the amplitude deviation $\langle[\rho(\epsilon) - \bar{\rho}(\epsilon)]^2\rangle^{1/2}$ of the results for the various realizations. Structural features in the density of states whose height is smaller than the deviation are naturally regarded

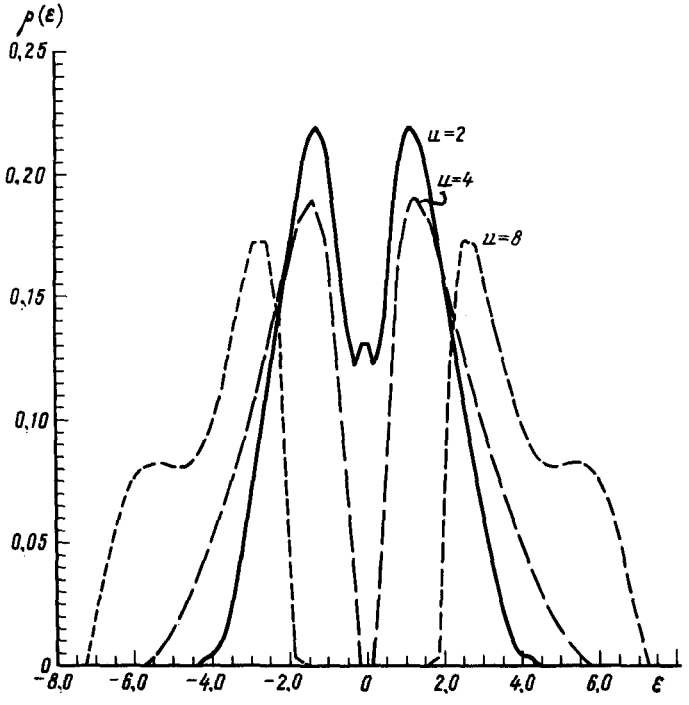

FIG. 1. Normalized density of states of a one-dimensional Hubbard model with a 50% occupation for various values of U.

as nonphysical. A direct test shows that the solution is smooth, and no additional regularization is required.

Results. We studied the Hubbard model

$$H = -\sum(c_{i\sigma}^{+}c_{j\sigma} + c_{j\sigma}^{+}c_{i\sigma}) + U\sum n_{i\uparrow}n_{i\downarrow} - \mu\sum(n_{i\uparrow} + n_{i\downarrow})$$

for various occupations in the one-dimensional case and for a 50% occupation in two dimensions (a 50% occupation, $\bar{n} = 0.5$, corresponds to a chemical potential $\mu = U/2$) with $N = 16$ sites. To find the one-particle temperature Green's function, we used the standard version of the "determinant" algorithm[1] with $M = 64$ "time" intervals, separated by a distance $\Delta\tau = 0.25/U$. The number of "measurements" of the Green's function was chosen large enough that the error in the results of the simulation did not exceed 0.002.

Lieb and Wu[7] have demonstrated that with $\bar{n} = 0.5$ and $U > 0$ in the one-dimensional model ($d = 1$) the spectrum of one-particle excitations splits up into two subbands, separated by a gap which grows with increasing U. It is also known that in the limit $U \to \infty$ the shape of $\rho(\epsilon)$ in each subband is the same as that of the density of states with $U = 0$ (Ref. 8).

Our results on $\rho(\epsilon)$ for $d = 1$ and $\bar{n} = 0.5$ are summarized in Fig. 1. With $U = 2$,

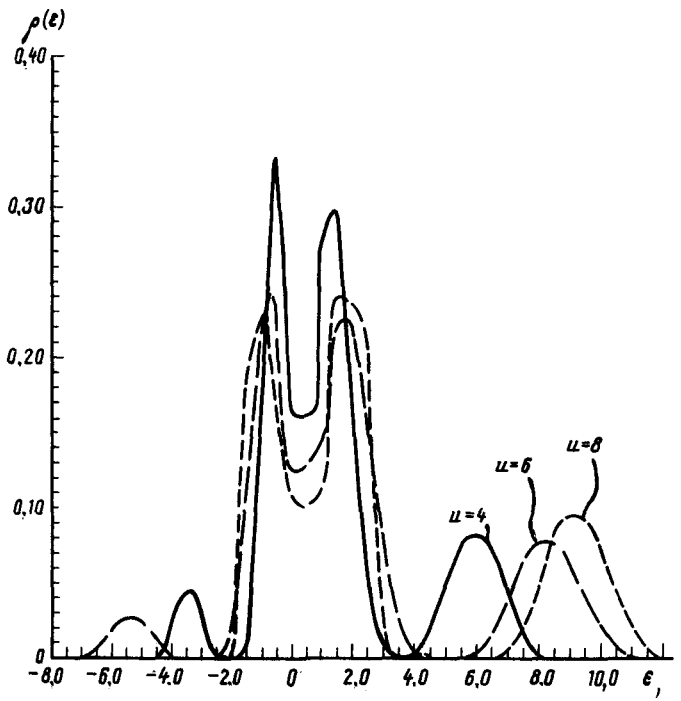

FIG. 2. Normalized density of states of a one-dimensional Hubbard model with a non-50% occupation ($\mu = 0$) for various values of U.

no gap appears in $\rho(\epsilon)$, since even at $T=0$ the gap width, $\Delta(U=2)\approx 0.17$, is very small, comparable to the temperature ($T=0.125$) at which the simulation was carried out for $U=2$. At $U=4$, we see a gap which is close to the exact result, $\Delta(U=4)\approx 1.29$ at $T=0$. At $U=8$, the gap becomes quite prominent, and when the possible temperature tails ($\approx 2T$) are taken into account, this gap agrees satisfactorily with Lieb and Wu's result $\Delta(U=8)\approx 4.68$. Note also the nucleation of a second peak in each subband at $U=8$, which demonstrates that $\rho(\epsilon)$ is tending toward the asymptotic behavior as $U\to\infty$, which was described above.

In studying the one-dimensional model for $n\neq 0.5$ we restricted the analysis to a fixed value of the chemical potential, namely, $\mu=0$. As U increases, the occupation falls from $\bar{n}=0.5$ at $U=0$ to $\bar{n}=0.25$ at $U=\infty$. It is known[1] that at $\bar{n}\neq 0.5$ the system is a paramagnetic metal, so we have $\rho(\mu)>0$. Furthermore, at $U=\infty$ the model is equivalent to the problem of free spinless fermions with the same total particle density at a site.

Figure 2 shows our reconstruction of $\rho(\epsilon)$ for $\mu=0$ and for $U=4$, 6, and 8. The density $\rho(\epsilon)$ is dominated by the zone near $\epsilon=0$, whose shape does indeed tend toward the density of states of noninteracting fermions with increasing U. The peak at $\epsilon\approx U$ corresponds to the arrival of an added electron at an occupied site. For values of U which are not too large, there is a significant probability for finding two electrons in

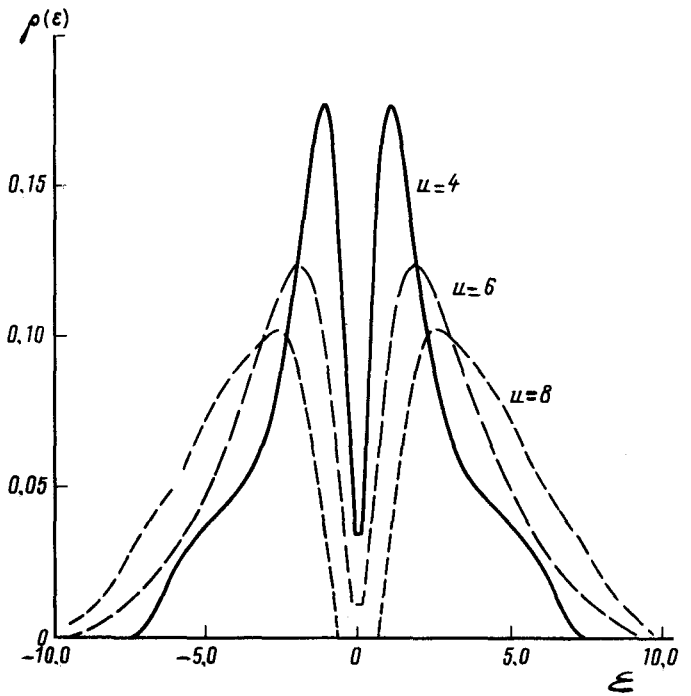

FIG. 3. Normalized density of states of the two-dimensional Hubbard model with a 50% occupation for various values of U.

one site. The removal of one of these electrons should lower the energy of the system by an amount $\approx U$. The peak at $\epsilon \approx -U$ for $U = 4$ and (with a smaller area) for $U = 6$ is indeed observed.

For the two-dimensional Hubbard model, the exact form of $\rho(\epsilon)$ is not known even in the limit $U \to \infty$. The interaction of electrons at a site should lead to the appearance of a gap in $\rho(\epsilon)$ near $\epsilon = 0$ at a certain $U > 0$, as in the one-dimensional case. The state densities $\rho(\epsilon)$ which we reconstructed for $U = 6$ and $U = 8$ are shown in Fig. 3. In the density of states for $U = 8$ we do indeed see a gap, whose size agrees with the results of Ref. 2.

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