From a Hubbard dimer to a Hubbard model in d dimensions: a path integral solution

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Abstract. A new analytical method is proposed for solving the Hubbard model in d-dimensions. The method permits, in principle, the study of the Hubbard model at any temperature and any band filling. The accuracy of the method is tested against known Bethe *ansatz* results of Lieb and Wu and against known weak- and strong-coupling expansion results. The one-dimensional path integral solution obtained for the ground state (half-filled band case) is in excellent qualitative agreement with Bethe *ansatz* results for all couplings and exactly reproduces weak- and strong-coupling expansion results.

1. Introduction

The model proposed by Hubbard more than two decades ago [1] is still under active investigation. There are many reasons why this model has been studied for so many years. Some reasons are well summarised in a recent theoretical paper [2]; others can be found in a recent review article [3]. The Hubbard model has lately attracted special attention in connection with the phenomenon of high-temperature superconductivity [4]. It is believed to be a likely candidate for the model which describes this phenomenon. In view of great technical difficulties of the rigorous theoretical treatments of the Hubbard model, attempts have been made to study the above model by Monte Carlo methods. In a recent paper [5] the results of Monte Carlo calculations are presented for the three-dimensional half-filled band model at a finite temperature on a simple cubic 4^3 and some 6^3 lattices with periodic boundary conditions. Because of the small size of the lattices, it was difficult to take into account the role of the boundary effects or to study the limit of very low temperatures. Moreover, as was first rigorously established in [6], in the strong-coupling limit, the results for the three-dimensional Hubbard model depend on the lattice structure. In particular, for the slightly less (or slightly more) than half-filled band the ferromagnetic state is the ground state for the simple cubic and body-centred cubic lattices, but not for the face-centred or hexagonal close-packed structures. This result in [6] presents a real challenge for the existing Monte Carlo simulations. Apart from important practical applications of the Hubbard model, there are at least two other reasons for studying this model. The first comes from the fact that the one-dimensional version of the Hubbard model represents an example of an exactly integrable model. This model was solved some time ago by the Bethe *ansatz* methods by Lieb and Wu [7]. This then poses the following problem: if there is an exact many-body result obtained by whatever means *other* than the path integral, what could be said

about the exact path integral solution of the same problem? Evidently, the answer to this question is directly related to the question of how accurately, in principle, the Monte Carlo calculations could be done for the exactly integrable models. The second reason can be formulated as follows: if there is a way to obtain an exact path integral solution for the exactly integrable model, how might it be modified in those cases when the model is no longer exactly integrable? Here I would like to provide some answers to the questions posed above.

This paper is organised as follows. In § 2 the microscopic Hubbard and extended Hubbard models are defined together with the necessary general type of results to be discussed in the subsequent sections. In § 3 a finite-temperature strong-coupling expansion for the Hubbard model is provided. The technical results of this section are then used in § 4. This section provides the path integral solution for the Hubbard dimer problem. The new technical elements introduced here permit the generalisation of the Hubbard dimer problem to the case of the Hubbard model in an arbitrary number of dimensions which is accomplished in § 5. The results of such a generalisation for the case of one dimension are then compared against the exact Bethe *ansatz* results of Lieb and Wu [7] and presented in figure 1. These results coincide exactly with known weak- and strong-coupling expansion results and are in excellent qualitative agreement with Bethe *ansatz* results for all couplings. Section 6 is devoted to a brief conclusion and outlook.
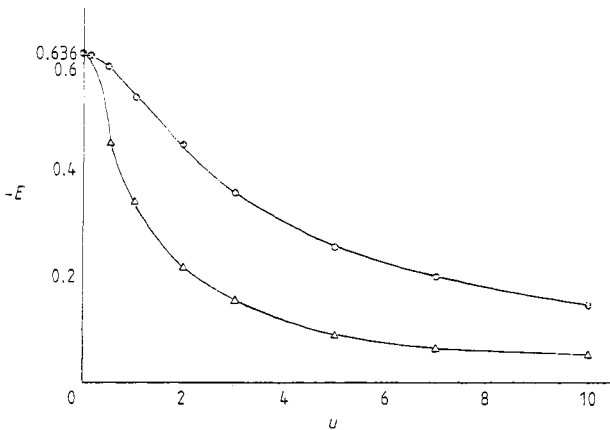

Figure 1. Ground-state energy (per site and per spin) as a function of the coupling constant U: $\bigcirc$, the solution of Lieb and Wu (equation (2.3)); $\triangle$, equation (5.5).

2. The microscopic model: general results

The Hubbard Hamiltonian H_H is well described in the literature [3]. For the purposes of comparison, I would like to present here only the one-dimensional version of H_H. In one dimension, one has

$$H_H = -t \sum_{\substack{i=1 \\ \sigma}}^{N} (c_{i,\sigma}^+ c_{i+1,\sigma} + c_{i+1,\sigma}^+ c_{i,\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}. \tag{2.1}$$

I shall also consider briefly the so-called extended Hubbard model given by the Hamiltonian H_{HE} as [8]

$$H_{HE} = H_H + V \sum_{i=1}^{N} n_i n_{i+1}. \tag{2.2}$$

Here $c_{i,\sigma}^+$ and $c_{i,\sigma}$ are the usual Fermi creation and annihilation operators, respectively, for an electron with spin σ ($\uparrow$ or $\downarrow$) at site i, $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$, $n_i = n_{i\uparrow} + n_{i\downarrow}$, t is the transfer integral and the coupling constants U and V represent the parts of Coulombic-type electron–electron interaction. The sign of t is actually unimportant as was already noted in [7]. In addition, one can, in principle, formally consider the cases when U or V are negative, thus extending the model beyond its original limits. Because of particle–hole duality, in the case of H_H there is no need to consider separately the cases of negative and positive U as was already demonstrated in [7]. Application of the same idea to the extended Hubbard model (2.2) shows that the particle–hole symmetry is broken so that one should consider cases of positive and negative couplings separately.

At zero temperature the model (2.1) was solved in [7] by means of the Bethe *ansatz* method. For the case of the half-filled band (one electron with spin up or down per lattice site), the following result ($t = 1$) for the ground-state energy (per site) was obtained in [7]:

$$E_0 = -4 \int_0^{\infty} \frac{J_0(\omega)J_1(\omega)\, \mathrm{d}\,\omega}{\omega[1 + \exp(\tfrac{1}{2}\omega\, U)]} \tag{2.3}$$

where $J_0(\omega)$ and $J_1(\omega)$ are the Bessel functions. In the limit $U \to \infty$, this produces (with t restored)

$$E_0(U \to \infty) = -4t^2(\ln 2)/U \tag{2.4a}$$

while in the opposite limit one obtains

$$E_0(U = 0) = -4/\pi. \tag{2.4b}$$

The last result requires some comments. In the limit $U = 0$, the model (2.1) becomes effectively spinless. Such a spinless model was considered some time ago in [9] in connection with calculation of the energy spectrum for the antiferromagnetic chain. To understand the result (2.4b), it is sufficient to consider the Hamiltonian in equation (2.11) of [9] with appropriately rescaled value of the hopping integral (note in our case that $t = 1$). This then immediately produces

$$E_0(U = 0) = -2/\pi \equiv -0.6366. \tag{2.5}$$

In the subsequent sections, in view of (2.4) and (2.5), I shall consider energies per site and per spin.

Using the general results of Lieb and Wu, E_0 was obtained in [10] for arbitrary band fillings. Later the results of Lieb and Wu were extended in [11] to the case of finite temperatures using the finite-temperature version of the Bethe *ansatz* as formulated in [12]. The solution obtained turns out to be so complicated that it was possible to check explicitly rather trivial limiting cases such as $U \to 0$, $U \to \infty$, $T \to 0$ (Lieb and Wu) and $T \to \infty$. In the subsequent paper [11], only the low-temperature specific heat for the half-filled band Hubbard model was calculated and other results are rather inconclusive as was acknowledged. The main achievement is the computation of the limiting value of the specific heat C:

$$\lim_{H \to 0} \left[\lim_{T \to 0} (C/T) \right] = (\pi/6)\, I_0(\pi/2U)/I_1(\pi/2U) \tag{2.6}$$

where H is the magnetic field, and I_0 and I_1 are the Bessel functions of imaginary argument. I have recently used the result (2.6) for the computation of the central charge c, which for the half-filled band Hubbard model, turns out to be unity [13]. The central charge plays an important role in calculations of the finite-size corrections to the ground-state energy as is demonstrated in [14]. For completeness, I would like to present here the expression of Lieb and Wu for the gap. For the half-filled band case, they obtain $(t = 1)$

$$\Delta(U) = U - 2(2 + I) \tag{2.7a}$$

where

$$I = -4 \int_0^\infty \frac{J_1(x)\,dx}{x(1 + \exp(\tfrac{1}{2}xU))}. \tag{2.7b}$$

Recently I have recomputed [15] the gap energy (2.7) using the formalism developed in [12] in order to investigate what happens to the gap at finite temperatures. As a result of such recomputation with the help of the formalism in [12], I found that the result (2.7a) is actually valid only for rather strong couplings ($U > 1$) and, in addition, equation (2.7a) should be replaced by

$$\Delta(u) = U - 2(2 + \tilde{I}) \tag{2.8}$$

where $\tilde{I}$ is obtained from I, given by equation (2.7b), by obvious rescaling $U \to U/2$ in (2.7b). In [2], it was demonstrated that for the half-filled band the gap Δ exists for all dimensions.

Finally, modification of the Hubbard model given by equation (2.2) makes this model non-integrable so that there are no exact results available for this model.

To proceed, I would like to consider briefly a single-site approximation for the Hubbard model. In spite of the fact that this approximation is rather trivial, it contains all the technical features needed for the subsequent development. Moreover, it is of some practical value as can be seen from the recent review article [16] devoted to the solid state applications of the above truncated model. Here I would like to emphasise only the technical side of the problem for reasons which were described in § 1.

The single-site Hubbard Hamiltonian is given by

$$\mathcal{H} \equiv H_{\text{H.ss}} = U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_{i\sigma} \mu_\sigma n_{i\sigma} \tag{2.9}$$

with μ_σ being a chemical potential. The Hamiltonian (2.9) can easily be diagonalised in the single-site basis spanned by the vectors $|0\rangle$, $|\uparrow\rangle = c_\uparrow^+ |0\rangle$, $|\downarrow\rangle = c_\downarrow^+ |0\rangle$, $|\uparrow\downarrow\rangle = c_\uparrow^+ c_\downarrow^+ |0\rangle$ with the eigenvalues 0, $-\mu_\uparrow$, $-\mu_\downarrow$ and $U - \mu_\uparrow - \mu_\downarrow$, respectively. This permits one immediately to write the expression for the partition function:

$$Z_{\text{ss}} = \{1 + \exp(\beta\mu_\uparrow) + \exp(\beta\mu_\downarrow) + \exp[\beta(\mu_\uparrow + \mu_\downarrow - U)]\}^N. \tag{2.10}$$

In terms of Grassmann path integral, one can write the partition function as [17]

$$Z_{\text{ss}} = \int \prod_{tn\sigma} d\bar{\eta}_{tn\sigma}\, d\eta_{tn\sigma}\, \exp(-S_{\text{H}}[\bar{\eta}, \eta]) \tag{2.11a}$$

where

$$S_{\text{H}}[\bar{\eta}, \eta] = \sum_{tn\sigma} \bar{\eta}_{tn\sigma}(\eta_{t+1,n,\sigma} - \eta_{tn\sigma}) - \sum_{tn\sigma} \tau\mu_\sigma n_{tn\sigma} + \hat{U}\sum_{tn} n_{tn\uparrow} n_{tn\downarrow}. \tag{2.11b}$$

Here $\bar{U} = U\tau/\hbar$, $t = 0, 1, 2, \ldots, \mathcal{N} - 1$, $\mathcal{N}\tau = \beta\hbar$, $\beta = (kT)^{-1}$, with T being a temperature, $n_{tn\sigma} \equiv \bar{\eta}_{tn\sigma}\eta_{tn\sigma}$, $\eta_{\mathcal{N},n\sigma} = -\eta_{0,n,\sigma}$. Let us put constants $\hbar$ and k equal to unity below. To obtain the result (2.10), one should use the Hubbard–Stratonovich transformation in computing (2.11). One has (for fixed t and n)

$$\exp(-\bar{U}n_{tn\uparrow}n_{tn\downarrow}) = N \int d\bar{x}\, dx \exp[-(\tau\bar{x}x + \lambda_\uparrow \bar{x}n_{tn\uparrow} + \lambda_\downarrow xn_{tn\downarrow})] \tag{2.12}$$

where $\bar{x}(x)$ is a pair of complex Bose fields given at each point t, n; N is the normalisation factor and $\lambda_\uparrow \lambda_\downarrow = -\bar{U}$. Use of equation (2.12) permits one to rewrite (2.11) as

$$Z_{ss} = \text{constant} \times \left[\int \prod_t d\bar{x}_t\, dx_t \exp\left(-\int_0^\beta d\tau(x) + a_\uparrow + a_\downarrow\right)\right]^N \tag{2.13}$$

where

$$a_\uparrow = \ln(\det_\uparrow) = \ln\left\{\text{Tr}_\uparrow\left[\exp\left(-\int_0^\beta d\tau(\bar{\eta}_\uparrow \dot{\eta}_\uparrow + \lambda_\uparrow \bar{x}n_\uparrow - \mu_\uparrow n_\uparrow)\right)\right]\right\} \tag{2.13a}$$

$$\text{Tr}_\uparrow \ldots = \int d\bar{\eta}_\uparrow\, d\eta_\uparrow \ldots \qquad \dot{\eta}_\uparrow = (d/d\tau)n_\uparrow \qquad n_\uparrow = \bar{\eta}_\uparrow\eta_\uparrow.$$

Similar expressions hold for $a_\downarrow$ with the obvious change of $\uparrow$ to $\downarrow$ and of $\bar{x}$ to x. Following [18] the determinant (2.13a) can be easily computed, thus providing the final result

$$\det_\uparrow = 1 + \exp\left(\beta\mu_\uparrow - \lambda_\uparrow \int_0^\beta d\tau\, \bar{x}\right) \equiv D_\uparrow. \tag{2.14}$$

Use of (2.14) together with a similar $\det_\downarrow$ expression in (2.13) permits one to integrate out Bose fields, thus giving the result (2.10) again. The above results are essentially used in the subsequent sections.

3. Finite-temperature strong-coupling expansion for the Hubbard model

The results in § 2 permit me now to consider the strong-coupling expansion for the Hubbard model. The first leading term in such expansion was obtained some time ago in [19] (which contains some obvious misprints). The second-order results require considerable computational efforts if the conventional operator formalism is used, as was acknowledged in [20]. Although the results of these computations are in excellent agreement with the results obtained by the direct diagonalisation of the corresponding short-chain Hamiltonian [21], the technical difficulties made the conventional operator approach impractical for the computation of the higher-order terms in the above strong-coupling expansions. I would like to demonstrate here that use of the path integral method makes the calculations almost as easy as calculations with the conventional (momentum space) Feynman diagrams. To proceed with the actual calculations, I need now to introduce some additional notations. Use of the results in [17] and [18] permits one to write for the single-site fermionic Green function the following expressions:

$$G_\uparrow(\tau, \tau') = -e_1^\uparrow/D_\uparrow \qquad \text{for } \tau > \tau' \tag{3.1}$$

and

$$G_\uparrow(\tau, \tau') = e_2^\uparrow / D_\uparrow \qquad \text{for } \tau < \tau'. \tag{3.2}$$

Here $D_\uparrow$ was defined in equation (2.14) and

$$e_1^\uparrow \exp\left((\tau - \tau')\mu_\uparrow - \int_{\tau'}^\tau d\tau\, \lambda_\uparrow \bar{x}\right) \tag{3.3a}$$

$$e_2^\uparrow = \exp\left(\beta\mu_\uparrow - \mu_\uparrow(\tau' - \tau) + \int_\tau^{\tau'} d\tau\, \lambda_\uparrow \bar{x} - \int_0^\beta d\tau\, \lambda_\uparrow \bar{x}\right). \tag{3.3b}$$

Similar expressions for $G_\downarrow$ are obtained with evident redefinitions of $\uparrow$ onto $\downarrow$ and $\bar{x}$ onto x. Now let

$$H_1^\uparrow = \bar{\eta}_{ln\uparrow}(\eta_{l+1,n\uparrow} - \eta_{ln\uparrow}) - \mu_\uparrow n_{ln\uparrow} + \lambda_\uparrow \bar{x}_{ln} n_{ln\uparrow} \tag{3.4a}$$

$$H_2^\uparrow = \tilde{T}(\bar{\eta}_{ln\uparrow}\eta_{l,n+1,\uparrow} + \bar{\eta}_{l,n+1,\uparrow}\eta_{ln\uparrow}) \tag{3.4b}$$

where $\tilde{T} = t\tau$. Using the notations in § 2, I have now

$$a_\uparrow = \ln\left\langle \exp\left(-\sum_{ln} H_2^\uparrow\right)\right\rangle + \ln\left\{\text{Tr}_\uparrow\left[\exp\left(-\sum_{ln} H_1^\uparrow\right)\right]\right\} \tag{3.5}$$

where

$$\langle\ldots\rangle = \text{Tr}_\uparrow\left[\exp\left(-\sum_{ln} H_1^\uparrow\right)\ldots\right]\bigg/\text{Tr}_\uparrow\left[\exp\left(-\sum_{ln} H_1^\uparrow\right)\right]. \tag{3.6}$$

Expanding now the exponent in the first term in equation (3.5) and averaging with the single-site Hamiltonian produces in the lowest order in $\tilde{T}$

$$\tilde{a}_\uparrow = \ln\left\langle\exp\left(-\sum_{ln} H_2^\uparrow\right)\right\rangle = \ln\left(1 + \tfrac{1}{2}\sum_n\sum_{l,l'}\langle H_2^\uparrow H_2^\uparrow\rangle + \text{O}(\tilde{T}^4)\right) \tag{3.7}$$

where $\tilde{a}_\uparrow$ corresponds to the first term in equation (3.5). Combining the $\uparrow$ part with the $\downarrow$ part analogously to equation (2.13), one obtains

$$Z = \text{constant} \times \left[\int\prod_l d\bar{x}_l\, dx_l \exp\left(-\int_0^\beta d\tau(\bar{x}x)\right)\det_\uparrow(\det_\downarrow x)\right.$$

$$\left.\times\left(1 + \tfrac{1}{2}\sum_\sigma\int_0^\beta d\tau\int_0^\beta d\tau'\,\langle H_2^\sigma H_2^\sigma\rangle + \text{O}(\tilde{T}^4)\right)\right]^N \tag{3.8}$$

where $\det_\uparrow$ is given by (2.14), etc. Let $\langle\ldots\rangle_x$ denote the operation of averaging with respect to fields $\bar{x}(x)$. Then if the thermodynamic potential Ω (per site) is defined as

$$\beta\Omega = -(1/N)\ln Z \tag{3.9}$$

one obtains, using (3.8), the following result:

$$\beta\Omega = -\ln Z_{ss} - \tfrac{1}{2}\sum_\sigma\int_0^\beta d\tau\int_0^\beta d\tau'\,\langle\!\langle H_2^\sigma H_2^\sigma\rangle\!\rangle_x. \tag{3.10}$$

Use of Wick's theorem and definitions (3.1)–(3.3) produces now the following result:

$$\tfrac{1}{2} \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' \langle\!\langle H_0^\sigma H_2^\sigma \rangle\!\rangle_x$$

$$= \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' \left\langle \left[\left(\frac{e_1^\sigma}{d_\sigma}\right)_{n+1} \left(\frac{e_2^\sigma}{d_\sigma}\right)_n + \left(\frac{e_1^\sigma}{D_\sigma}\right)_n \left(\frac{e_2^\sigma}{D_\sigma}\right)_{n+1} \right] \right\rangle_x. \tag{3.11}$$

Use of equations (3.1)–(3.3) and straightforward averaging over the field x permits one to obtain without delay the following result ($\mu_\uparrow = \mu_\downarrow = \mu$):

$$\tfrac{1}{2} \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' \langle\!\langle H_2^\sigma H_2^\sigma \rangle\!\rangle_x$$

$$= \frac{4t^2}{Z_{ss}^2} \int_0^\beta d\tau \int_0^\tau d\tau' \exp(\beta\mu)\{1 + \exp[\beta\mu - (\tau - \tau')U]\}$$

$$\times \{1 + \exp[\beta\mu - \beta U + (\tau - \tau')U]\}$$

$$= \frac{2\exp(\beta\mu)}{Z_{ss}^2} (\beta t)^2 \{1 + \exp(2\beta\mu - \beta U)$$

$$+ \frac{2}{\beta U}[1 - \exp(-\beta U)]\exp(\beta\mu)\}. \tag{3.12}$$

This then, when combined with equation (3.10), produces the result which coincides with that obtained in [19] (in the limit when the magnetic field (in [19]) is zero). It is interesting here to compare the results (3.10) and (3.12) with the result of the exact Bethe *ansatz* calculations at zero temperature (equation (2.4a)). To do so, it is useful to recall a couple of well known formulae. First, using the notation in § 2, one has for the occupation number α_σ per site the standard result

$$\alpha_\sigma = (1/\beta N)\, \partial (\ln Z)/\partial \mu_\sigma. \tag{3.13}$$

The ground-state energy (per site) E_0 can be defined now as ($\beta \to \infty$)

$$E_0 = \sum_\sigma \alpha_\sigma \mu_\sigma - \frac{1}{N}\frac{d}{\partial\beta}(\ln Z). \tag{3.14}$$

For the half-filled band $\alpha_\uparrow = \alpha_\downarrow = \tfrac{1}{2}$. Use of equation (2.10) together with (3.13) shows that the consistency is achieved (for $\alpha_\uparrow = \alpha_\downarrow = \tfrac{1}{2}$) if $\mu_\uparrow = \mu_\downarrow = U/2$. Use of equation (3.14) then produces for the single-site model $E_0 = 0$. Consider now equation (3.12) for the case $\mu = U/2$ and $\beta \to \infty$. It is not difficult to see that, in this limit, one obtains just $\beta t^2/U$. Taking into account equations (3.10) and (3.14) together with the limiting result for (3.12), one arrives at the final result

$$E_0 = -t^2/U \tag{3.15}$$

to be compared with the exact Bethe *ansatz* result (2.4a). The discrepancy (because of the factor of 4 ln 2) can be explained, perhaps, on the basis of the fact that in the course of Bethe *ansatz* calculations some sums are replaced by integrals [7, 15] which inevitably introduce factors such as ln 2. This feature is known from other statistical mechanics calculations [22]. Having obtained the result in the lowest order in t^2/U, one can, in principle, easily obtain the higher-order terms using the diagrammatic methods

developed in [23]. Instead, I would like to choose another route and to investigate the possibility of obtaining the closed-form results.

4. The Hubbard dimer problem

Recently the two-site Hubbard model in which atoms of the dimer are not frozen was considered [24]. This model can be described by the following Hubbard–Frölich Hamiltonian:

$$H = H_{\mathrm{H}} + H_{\mathrm{eL}} + H_{\mathrm{L}} \tag{4.1}$$

where H_{H} was given in (2.1), and H_{eL} and H_{L}, respectively, are given as

$$H_{\mathrm{L}} = \sum_i \tfrac{1}{2}(\omega^2 P_i^2 + Q_i^2) \tag{4.2}$$

$$H_{\mathrm{eL}} = -\sqrt{S} \sum_{i\sigma} n_{i\sigma} Q_i \tag{4.3}$$

with $i = 1, 2, \ldots$. In [24], it was shown that in the limit $S = 0$ the model can be solved exactly and when $S \neq 0$ it can be solved within certain limits ($S \to 0$, $\omega \to 0(\infty)$, etc). In the limit $S = 0$ by analogy with the single-site *ansatz* in § 2, it is convenient to introduce the following set of states:

$$|0\rangle, |i\rangle = c_{i\uparrow}^+ c_{i\downarrow}^+ |0\rangle \qquad (i = 1, 2)$$

and

$$|h\rangle = (1/\sqrt{2})(c_{1\uparrow}^+ c_{2\downarrow}^+ - c_{1\downarrow}^+ c_{2\uparrow}^+)|0\rangle.$$

Now introduce $|\Psi\rangle = \sum_j a_j |j\rangle$ with $j = 0, 1, 2, h$ and a_j being some constant coefficients. This then permits one to diagonalise the Hubbard dimer with the following result for the spectrum (half-filled band) [24, 25]:

$$E = (U/2)[1 \mp \sqrt{1 + 16(t/U)^2}]. \tag{4.4}$$

In the limit $t/U \to 0$, one obtains evidently

$$E \simeq \mp 4t^2/U \tag{4.5}$$

to be compared with (2.4a) and (3.15). I shall return to this comparison later in the text. It is interesting to note at this point that, if the higher orders in the t/U expansion of (4.4) are kept, the resulting series expansion would be of the same functional form as can be obtained by the direct integration of (2.3), namely one would have in *both* cases the following expansion:

$$E = U \sum_{i=1}^{\infty} (-1)^i b_i \left(\frac{t}{U}\right)^{2i} \tag{4.6}$$

with b_i being some known coefficients. This observation together with the relative ease of obtaining the result (4.4) naturally poses the following question: can the Hubbard dimer problem be solved exactly by the path integral method? I shall demonstrate here that this is indeed possible to a large extent. Moreover, the simplicity in obtaining the result (4.4) imposes an additional requirement: if there is a path integral method of

solution of the dimer problem, to be practical it should be rather simple. With this in mind, consider now the partition function for the dimer. One has

$$Z = \int \prod_{tn\sigma} d\bar{\eta}_{tn\sigma} \, d\eta_{tn\sigma} \, \exp(-S_{H_d}[\bar{\eta}, \eta]) \tag{4.7}$$

where $n = 1, 2$, and

$$S_{H_d} = -\hat{t} \sum_{t\sigma} (\bar{\eta}_{t1\sigma}\eta_{t2\sigma} + \bar{\eta}_{t2\sigma}\eta_{t1\sigma}) + S_H[\bar{\eta}, \eta] \tag{4.8}$$

with S_H defined by the equation (2.11b). As in the single-site case, introduce now two sets of the auxiliary Bose fields $\bar{x}_1(x_1)$ and $\bar{x}_2(x_2)$ associated with each site via Hubbard–Stratonovich transformation (2.12). In addition, it is convenient to introduce two auxiliary sets of *Fermi* fields (two for a given spin ($\uparrow$ or $\downarrow$)) via the relation

$$\exp\left(-\hat{t}\int_0^\beta d\tau \, \bar{\eta}_2\eta_1\right) = N \int D[\bar{\varphi}_1, \varphi_1] \exp\left(-\int_0^\beta d\tau \, \bar{\varphi}_1\varphi_1\right)$$

$$\times \exp\left(-\alpha \int_0^\beta d\tau \, \bar{\varphi}_1\eta_1 - \alpha \int_0^\beta d\tau \, \varphi_1\bar{\eta}_2\right) \tag{4.9}$$

and similar for the combination $\bar{\eta}_1\eta_2$. Here the spin indices are temporarily suppressed and $\alpha^2 = -\hat{t}$. Use of equations (2.12) and (4.7)–(4.9) permits one to rewrite the partition function (4.7) in the following form:

$$Z = \left\langle \prod_\sigma (\det x_1^\sigma) \exp\left(-\hat{t}\int_0^\beta d\tau \int_0^\beta d\tau' \, \bar{\varphi}_1^\sigma G_{x_1}^\sigma \varphi_2^\sigma\right)\right.$$

$$\left. \times (\det x_2^\sigma) \exp\left(-\hat{t}\int_0^\beta d\tau \int_0^\beta d\tau' \, \bar{\varphi}_2^\sigma G_{x_2}^\sigma \varphi_1^\sigma\right)\right\rangle_{x,\varphi}. \tag{4.10}$$

Here $\langle \ldots \rangle_{x,\varphi}$ denotes an obvious integration over φ and x fields, $\det x_1^\sigma$ and $\det x_2^\sigma$ correspond to the single-site determinants as was defined in § 2, and $G_{x_1}^\sigma$ and $G_{x_2}^\sigma$ correspond to the fermionic Green functions defined by (3.1)–(3.3). Using the same technique as in § 3, it is convenient now to perform a cumulant average of the exponents in (4.10) with respect to fields x_1 and x_2, respectively. I shall use only the first cumulant average result. It will become evident subsequently that such accuracy is sufficient to reproduce the result (4.4) qualitatively. Using the results in § 3 (in particular, equations (3.1)–(3.3), (3.5) and (3.12)), one has for the averaged fermionic Green function the following result

$$G_>(\tau) = [-\theta(\tau)/Z_{ss}] \exp(\tau\mu)[1 + \exp(\beta\mu - \tau U)] \tag{4.11a}$$

$$G_<(\tau) = [\theta(-\tau)/Z_{ss}) \exp(\beta\mu) \exp(\tau\mu)[1 + \exp(\beta\mu - \beta U - \tau U)] \tag{4.11b}$$

where $\theta(t)$ is the usual step function and Z_{ss} is given by (2.10) (for $N = 1$). I shall concentrate (only for comparison) on the half-filled band case $\mu = U/2$. When $\beta \to \infty$, one obtains, according to (2.10),

$$Z_{ss}(\beta \to \infty) = 2 \exp(\beta U/2). \tag{4.12}$$

Combining (4.12) with (4.11), one obtains in the limit $\beta \to \infty$ the following result for $G_{>(<)}$:

$$G_>(\tau) = [-\theta(\tau)/2] \exp(-\tau U/2) \qquad G_<(\tau) = [\theta(-\tau)/2] \exp(-\tau U/2). \tag{4.13}$$

Using (4.13) and standard definition of Fourier transform for Green function [26], one also obtains

$$G(\tau) = \frac{1}{\beta} \sum_n \exp(-i\omega_n \tau)\, G(\omega_n) \tag{4.14}$$

where $(\beta \to \infty)$

$$2G(\omega_n) = 1/(i\omega_n - U/2) + 1/(i\omega_n + U/2) \tag{4.14a}$$

and ω_n is the usual Fermi frequency: $\omega_n = (2n + 1)\pi/\beta$.

Use of Fourier representation of the fields φ_1 and φ_2 and the orthogonality condition for frequencies gives the partition function (4.10) in the following form:

$$Z = \text{constant} \times Z_{\text{ss}}^2 \left(\int \prod_{i=1}^{2} D[\bar{\varphi}_i, \varphi_i] \exp(-S[\bar{\varphi}, \varphi]) \right)^2 \tag{4.15}$$

where the quadratic form $S[\bar{\varphi}, \varphi]$ is given by

$$S[\bar{\varphi}, \varphi] = \sum_n (\bar{\varphi}_1 \varphi_1 + \bar{\varphi}_2 \varphi_2 - t\bar{\varphi}_1 G \varphi_2 - t\bar{\varphi}_2 G \varphi_1) \tag{4.16}$$

with frequency arguments being suppressed for abbreviation and where the summation is over the Matsubara frequencies.

The functional integral (4.15) is squared because of the presence of two spin components. To compute the functional integral (4.15), one needs to diagonalise the quadratic form (4.16) for *each fixed n*. It is very instructive at this point to note that the structure of the off-diagonal terms in (4.16) is *exactly that* of the first term in (4.8) which naturally permits one to generalise the dimer problem. This will be discussed in detail in § 5. In the meantime, I choose here the conventional diagonalisation procedure which produces (for fixed n) the following eigenvalues:

$$E_{1,2}(n) = 1 \pm B_n \tag{4.17}$$

where

$$B_n = t i\omega_n / [\omega_n^2 + (U/2)^2]. \tag{4.18}$$

With this result, and remembering that φ_i ($\bar{\varphi}_i$) are Fermi fields, one can without delay write the following expression for the partition function (4.1):

$$Z = \text{constant} \times Z_{\text{ss}}^2 \left(\prod_{n=-\infty}^{\infty} \prod_{i=1}^{2} E_i(n) \right)^2. \tag{4.19}$$

Before taking logarithms of both sides of (4.19), it is convenient to rearrange somehow the infinite products in (4.21) to make the result look explicitly real. One has therefore

$$Z = \text{constant} \times Z_{\text{ss}}^2 \left[\prod_{n=0}^{\infty} \left(1 + \frac{t^2 \omega_n^2}{[\omega_n^2 + (U/2)^2]^2} \right) \right]^4. \tag{4.20}$$

Using (3.9), one obtains now the thermodynamic potential Ω (per site and per spin) as

$$\beta\Omega = -\tfrac{1}{2} \ln Z_{\text{ss}} - \sum_{n=0}^{\infty} \ln(1 + \cdots). \tag{4.21}$$

Finally, one needs to replace the summation by the integration in (4.21). To do so, it is convenient to introduce a new variable $x = 4\tilde{\omega}\pi/\beta U$ where $\tilde{\omega} = n + \frac{1}{2} \simeq n$. In terms of this variable, one can rewrite (4.21) as

$$\beta\Omega = -\tfrac{1}{2}\ln Z_{\text{ss}} - \frac{\beta U}{4\pi}\int_0^x dx \ln\left[1 + 4\left(\frac{t}{U}\right)^2\frac{x^2}{(x^2+1)^2}\right]. \tag{4.22}$$

The integral in (4.22) can now be calculated exactly. The calculation, although straightforward, contains all elements needed for the subsequent generalisation. Because of that, the sketch of the calculation is presented in the Appendix. Here I provide only the final result for the energy (per site and per spin)

$$E = (U/2)[1 - \sqrt{1 + (t/U)^2}] \tag{4.23}$$

to be compared with the result (4.4). This comparison yields exact agreement if t is rescaled to $4t$. Such a procedure, although permissible, is not desirable in the light of subsequent generalisations to be presented in § 5.

   If necessary, one can easily find a justification for the above rescaling of t. Recall that the result (4.11) was obtained as a first cumulant average approximation. Because of this average, the normalising factor of Z_{ss} has emerged in (4.11). Note also that the result (4.12) is valid only for the half-filled band case which I am considering only for comparison with (4.4). Because of the half-filled band condition the factor of 2 emerged in (4.12). If I *first* extracted this factor from Z_{ss}, included it in the normalisation constant in (4.15) and *then* performed the cumulant average, this would be equivalent to rescaling of t to $2t$. The appearance of yet another factor of 2 will be discussed in § 5. As already mentioned, such artificial rescaling is actually *unnecessary* when the dimer problem is generalised to the infinite chain and to higher dimensions.

5. From Hubbard dimer to Hubbard model

The results of § 4 permit rather a natural extension. This extension is possible in view of the structure of the partition function (4.15). The straightforward generalisation to finite chains of size N and to higher dimensions of the result (4.15) can be written now as

$$Z = \text{constant} \times Z_{\text{ss}}^N\left(\sum_{i=1}^N D[\bar{\varphi}, \varphi_i]\exp[-S[\bar{\varphi}, \varphi]]\right)^2 \tag{5.1}$$

where $S[\bar{\varphi}, \varphi]$ is given by

$$S[\bar{\varphi}, \varphi] = \sum_i \sum_n [\bar{\varphi}_i\varphi_i - t\sum_l (\bar{\varphi}_i G\varphi_{i+l} + \bar{\varphi}_{i+l}G\varphi_i)]. \tag{5.2}$$

The index i runs over each lattice site in d-dimensional space while l is a unit vector in positive directions of d-dimensional lattice. The spatial Fourier transform of the fields φ_i now can be done in the usual way, thus providing one with the following result for $S[\bar{\varphi}, \varphi]$:

$$S[\bar{\varphi}, \varphi] = \sum_k \sum_n \bar{\varphi}_{kn}\varphi_{kn}\left(1 - t\frac{i\omega_n}{\omega_n^2 + (U/2)^2}2\sum_l \cos k_l\right). \tag{5.3}$$

Here it should be noted that the technique of Fourier transforms automatically imposes the periodic conditions. For a dimer, this would lead to the incorrect result by effectively reducing the problem to the single-site monomer, but for long chains the imposition of the periodic boundary conditions should not cause any problem. The Fourier transform technique introduces an extra factor of 2 for the eigenvalues B_n given by (4.18) which, in turn, brings the result (4.23) into agreement with the 'exact' result (4.4) if in addition the factor of 2 is extracted from Z_{ss} prior to the operation of cumulant averaging. It is possible to treat the case of finite open chains in one dimension without imposing the periodic boundary condition by noting that the matrix of the quadratic form (5.2) is tridiagonal. The determinant of the tridiagonal matrix can easily be calculated [27]. For higher than one dimension, it is also possible to treat the open volumes but, in the thermodynamic limit, boundary conditions should not play any role. Finally, the Bethe *ansatz* calculations of Lieb and Wu [7], like many other calculations of this type, assume the periodic boundary conditions. Thus, one is left with the following options:

(i) to use the periodic boundary conditions and, therefore, to use the result (5.3) or
(ii) to remove the factor of 2 in (5.3) to achieve a formal agreement with the dimer problem.

With these options there are still questions as to what to do with the rescaling of Z_{ss}. I choose here option (i). I shall avoid the rescaling of Z_{ss} as well. For comparison only, the one-dimensional case will be treated in full detail. Extension to higher dimensions will then be only sketched. Use of results (4.19) and (5.1)–(5.3) permits one to write for the thermodynamic potential (per site and per spin) the following result (compare with (4.24)):

$$\beta\Omega = -\tfrac{1}{2}\ln Z_{ss} - \frac{\beta U}{4\pi}\int_0^{\pi/2}\frac{2}{\pi}\,dk\int_0^\infty dx \ln\left[1 + 16\left(\frac{t}{U}\right)^2\frac{x^2\cos^2 k}{(x^2+1)^2}\right]. \tag{5.4}$$

The integral over the variable x is of the same nature as that discussed in the Appendix. Therefore, use of the results of the Appendix together with equation (3.14) permits one to write the expression for the energy per site and per spin in the following way:

$$E = \frac{U}{2}\left[1 - \frac{2}{\pi}\int_0^{\pi/2} dk\sqrt{1 + 4\left(\frac{t}{U}\right)^2\cos^2 k}\right]$$

$$= \frac{U}{2}\left\{1 - \frac{2}{\pi}\left[\sqrt{1 + 4\left(\frac{t}{U}\right)^2}\right]E(\mathcal{R}^2)\right\} \tag{5.5}$$

where $E(\mathcal{R}^2)$ is the complete elliptic integral of the second kind and $\mathcal{R}^2 = \gamma^2/(1+\gamma^2)$, $\gamma^2 = (2t/U)^2$.

Consider now the expression (5.5). First, let $U \to 0$ and $t = 1$. Using the fact that $E(1) = 1$, one arrives at the result

$$E(U = 0) = -2/\pi \tag{5.6}$$

which coincides with (2.5). Now let $U \to \infty$; then, taking into account that in this limit $E(x^2) \simeq (\pi/2)(1 - \tfrac{1}{4}x^2)$, one arrives at the following result ($t = 1$):

$$E(U \to \infty) = -1/2U \tag{5.7}$$

which *exactly* coincides with the result (3.15) (recall that (5.7) is the energy per site and per spin while, in (3.15), E_0 is the energy per site only). I have already discussed after

equation (3.15) the difference between the Bethe *ansatz* result (2.4*a*) and that given by (3.15) (or (5.7)). To understand this difference better, I have performed a numerical integration of the result (2.3) of Lieb and Wu and the results of this integration are presented in figure 1 together with the solution (5.5). As one can see from this figure, the solution obtained (equation (5.5)) is in qualitative agreement with that given by Bethe *ansatz* method for all couplings. The quantitative difference between these solutions *may or may not* be caused by the approximate nature of our calculations. To obtain better insight into the nature of this discrepancy, it is desirable in the future to compare the results obtained with those from the weak- and strong-coupling expansions which contain a sufficient number of terms. The asymptotic result (5.7) (or (3.15)) suggests, however, that one should expect the discrepancy to persist, at least for the large-coupling-constant regime. It is essential also to understand better why the first cumulant average in x fields (see the discussion after equation (4.10)) is sufficient to reproduce the exact results for dimer and for the one-dimensional chain.

The generalisation of the results obtained to the multi-dimensional case is rather straightforward now. Taking into account the results (5.3) and (5.4), one obtains for the thermodynamic potential (per site and per spin) in d-dimensions the following result:

$$\beta\Omega = -\tfrac{1}{2}\ln Z_{ss} - \frac{\beta U}{4\pi}\int_0^{\pi/2}\frac{\mathrm{d}^d k}{(\pi/2)^d}$$
$$\times \int_0^\infty \mathrm{d}x \ln\left[1 + 16\left(\frac{t}{U}\right)^2 \frac{x^2}{(x^2+1)^2}\left(\sum_l \cos k_l\right)^2\right]. \tag{5.8}$$

The structure of the integral over the x variable is the same as in the one-dimensional case (equation (5.4)). This immediately permits one to use the results of the Appendix in order to write, instead of equation (5.3), its d-dimensional analogue

$$E = \frac{U}{2}\left[1 - \int_0^{\pi/2}\frac{\mathrm{d}^d k}{(\pi/2)^d}\sqrt{1 + 4\left(\frac{t}{U}\right)^2\left(\sum_l \cos k_l\right)^2}\right]. \tag{5.9}$$

The subsequent analysis then proceeds in exactly the same way as before.

6. Conclusions and outlook

In § 1, I posed two problems of which I would like now to remind the reader. First, if the quantum many-body model is exactly integrable, what could be said about the exact path integral solution of the same model? Secondly, how is this solution modified in those cases when the model is no longer integrable?

In §§ 4 and 5 a serious step towards resolution of the first problem is provided. The key idea of the analysis is to look for the exact solution of the simplest many-body problem, e.g. a dimer, which already contains all the technical difficulties of the original problem, and to try to reproduce this solution by means of the path integral methods. If the solution of this simple problem can be found, then it might be possible to generalise it to the larger system. The exact integrability of the Hubbard model is possible owing to the locality of the self-interaction term in equation (2.1). Because of this locality, it has been possible to find a path integral solution which, unlike the conventional Bethe *ansatz* method, is not restricted to the one-dimensional case. For the extended Hubbard model (equation (2.2)) the locality is lost; therefore the integrability is lost as well. The

presented method of calculation permits one, in principle, to perform various types of perturbational calculation around the 'exactly solvable' local Hubbard model. As this model is technically rather simple, it permits the consideration of a variety of Hubbard-related models. Such models could occur, for example, in disordered systems, when the quenched type of average is performed with use of the replica-trick method, or if one wants to consider the disordered Ising model written in terms of Grassmann path integrals.

Finally, the Hubbard model has recently attracted special interest in connection with the phenomenon of high-temperature superconductivity [4]. It is believed to be a very likely candidate for a model which explains this phenomenon.

Appendix

To calculate the integral (4.22), three known formulae are used:

$$\int dx \ln(x^2 + A^2) = x \ln(x^2 + A^2) - 2x + 2A \tan^{-1}\left(\frac{x}{A}\right) \tag{A1}$$

$$\tan^{-1} x = \pi/2 - 1/x + 1/3x^2 - \cdots \qquad x > 1 \tag{A2}$$

$$\tan^{-1} x = x - x^3/3 + \cdots \qquad x^2 < 1. \tag{A3}$$

It is convenient actually to consider a more general integral than that given by (4.22) for the purposes of its further use in § 5. One has

$$I = \int_0^\infty dx \ln\left(1 + \frac{\alpha^2 x^2}{(1 + x^2)^2}\right)$$

$$= 2 \int_0^\infty dx \ln\left(\frac{x^2 + a^2}{1 + x^2}\right) + \int_0^\infty dx \ln\left(1 - \frac{\alpha^2(1 + \alpha^2/4)}{(x^2 + a^2)^2}\right) \tag{A4}$$

where

$$a^2 = 1 + \alpha^2/2. \tag{A5}$$

The first integral in (A4) can now be directly calculated with the use of (A1)–(A3). The second integral in (A4) can be further rearranged as follows:

$$I_1 = \int_0^\infty dx \ln\left(1 + \frac{\alpha^2(1 + \alpha^2/4)}{(x^2 + a^2)^2}\right)$$

$$= \int_0^\infty dx \ln\left(x^2 + a^2 - \alpha\sqrt{1 + \frac{\alpha^2}{4}}\right) + \int_0^\infty dx \ln\left(x^2 + a^2 + \alpha\sqrt{1 + \frac{\alpha^2}{4}}\right)$$

$$- 2\int_0^\infty dx \ln(x^2 + a^2). \tag{A6}$$

Now one can use (A1)–(A3) in order to obtain the final answer for I:

$$I = -2\pi(1 - I_1) \tag{A7}$$

where I_1 is given by

$$I_1 = \sqrt{1 + \alpha^2/2} \left[\tfrac{1}{2}(\sqrt{1 + f(\alpha)} + \sqrt{1 - f(\alpha)})\right] \tag{A8}$$

and

$$f(\alpha) \simeq \alpha\sqrt{1 + \alpha^2/4}/(1 + \alpha^2/2). \tag{A9}$$

The function $f(\alpha)$ for *any* non-negative α is bounded between 0 and 1. This observation permits one to expand the corresponding square roots in (A8) in convergent power series as follows:

$$\tfrac{1}{2}[\sqrt{1 + f(\alpha)} + \sqrt{1 - f(\alpha)}] = 1 - \tfrac{1}{8}f^2(\alpha) - \tfrac{15}{384}f^4(\alpha) - \cdots \simeq 1 - \tfrac{1}{8}f^2(\alpha). \tag{A10}$$

Consider more accurately the limits $\alpha \to 0$ $(U \to \infty)$ and $\alpha \to \infty$ $(U \to 0)$. In the first case, one obtains $f(\alpha) = \alpha$ while, in the second case, $f(\alpha) \simeq 1 + 2/\alpha^2$. These estimates permit one to write, instead of (A10), the following expressions in the above limits:

$$1 - \tfrac{1}{8}f^2(\alpha) = 1 - \alpha^2/8 \simeq \sqrt{1 - \alpha^2/4} \qquad (\alpha \to 0) \tag{A11}$$

and

$$1 - \tfrac{1}{8}f^2(\alpha) = 2^{-1/2} \qquad (\alpha \to \infty) \tag{A12}$$

Combining (A11) and (A12) with (A8), one obtains

$$I_1 = \sqrt{1 + \alpha^2/4} \qquad (\alpha \to 0) \tag{A13}$$

and

$$I_1 = \alpha/2 \qquad (\alpha \to \infty). \tag{A14}$$

Comparison between (A13) and (A14) suggests that, in fact, (A13) correctly reproduces both $\alpha \to 0$ and $\alpha \to \infty$ limits and therefore can be used instead of equation (A8) as an interpolating *ansatz* for all α. This *ansatz* is used in the main text.

Acknowledgments

Note added in proof. After this paper had already been completed, I received two papers on small Hubbard clusters from Professor Callaway. The references on exact results obtained by his group and some other important results could be found in a recent paper [28] devoted to the small-cluster approach to the extended Hubbard model. An exact solution for the four-site cluster with periodic boundary conditions was obtained. It would be interesting to reproduce their results by the path integral formalism.

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