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Exactly solvable three-dimensional lattice model with attractive and repulsive interactions

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Systems of particles interacting in a lattice are considered; the number of particles at each site is not limited. The model with attraction of particles located at different sites and repulsion of particles, which occupy the same site was discussed in the paper by Belotskii and Lev [Phys. Lett. **147**, 13 (1990)]. In an exactly solved model with repulsion at different sites and attraction at the same site is proposed. In this Rapid Communication, exact expressions for the partition function of the system are derived for both cases; the equation of state is obtained for the continuum limiting case. [S1063-651X(98)50309-1]

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A few model systems of interacting particles are known in statistical physics [1] for which exact solutions have been found for the thermodynamic limit. For the most realistic Ising model, the solution is obtained only for one and two dimensions. To find exact solutions for the three-dimensional models is a more complicated problem, though predictions based on the universality principles are confirmed experimentally [1–3]. For the time being, no exact solution has been found for the three-dimensional models with short-range forces. In [4], a three-dimensional lattice model was proposed, for which the partition function was presented in terms of known functions and an exact solution was found in this sense. This model deals with a system of particles interacting in a lattice with an unlimited number of particles at each site. The partition function was calculated and lattice effect on thermodynamic parameters of the system was considered for the case where particles from different sites attract and particles from the same site repel.

In this paper, another exactly solvable three-dimensional model of a system of particles interacting in a lattice is proposed. As before, the model is based on the assumption that the number of particles at each site is not limited. Particles from different sites are repelled, particles from the same site are attracted. The approach of [4] to the construction of the generating partition function makes it possible to consider the two model systems with opposite interaction mechanisms in a unified manner, and to calculate the partition function. In the continuum limiting case, the equation of state can be derived and phase transition conditions can be discussed.

Let us consider a model system of interacting particles in a lattice with the microstates described by a set of site occupation numbers n_s. The configuration Hamiltonian of a system with the two above-mentioned opposite interaction types can be written in a unique way, i.e.,

$$H(n) = \sum_s \varepsilon_s n_s - \frac{1}{2} \nu^2 \sum_{s,s'} W_{ss'} n_s n_{s'} + \frac{1}{2} \nu^2 \sum_s U_s n_s^2,$$

(1)

where ε_s is the additive part of particle energy at the site s (which plays the role of the external field in the general

approach), and $\nu^2 = \pm 1$. The upper sign corresponds to the model with attraction at different sites and repulsion at the same site, the lower one is associated with the contrary situation—repulsion at different sites and attraction at the same site of the initial lattice. The quantities $W_{ss'}, U_s$ describe the spatial dependences of relevant interaction potentials. It should be noted that the effective Hamiltonian of the Gauss model of spin behavior in fractals [5] can be reduced to the form (1).

The partition function of the system with a fixed number of particles $N = \Sigma_s n_s$ may be described by the expression

$$Z_N = \sum_{\{n_s\}} \exp\{\mu N(n) + H(n)\}\beta$$

$$= \sum_{\{n_s\}} \exp\left\{ \sum_s (\mu - \varepsilon_s)n_s + \frac{1}{2}\nu^2 \sum_{s,s'} W_{ss'} n_s n_{s'} - \frac{1}{2}\nu^2 \sum_s U_s n_s^2 \right\},$$

(2)

where $\Sigma_{\{n_s\}}$ implies summation over all probable distribution configurations of the occupation numbers, n_s is the inverse temperature, and μ is the chemical potential.

In order to calculate the partition function, we employ the known results of the theory of Gauss integrals [6,7], i.e.,

$$\exp\left\{ \frac{1}{2}\nu^2 \sum_{s,s'} W_{ss'} n_s n_{s'} \right\}$$

$$= \int D\varphi \exp\left\{ \nu \sum_s \varphi_s n_s - \frac{\Theta}{2} \sum_{s,s'} W_{ss'}^{-1} \varphi_s \varphi_{s'} \right\},$$

(3)

where $D\varphi = B\Pi d\varphi_s$; the normalization factor B has no effect on the thermodynamic properties; $W_{ss'}^{-1}$ is the inverse of the interaction matrix $\Sigma_{s''} W_{ss''}^{-1} W_{s''s'} = \delta_{ss'}$. Substituting (3) in (2), we reduce the calculation of the partition function to the quantum field theory procedure with respect to the introduced auxiliary field [8,9]. This approach provides a derivation of the partition function even for the case of spatially inhomogeneous particle distribution [8].

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In this paper, however, we obtain the partition function in a somewhat different way. We introduce the generating functional which, within the context of (3), is given by

$$\Xi(\mu) = \frac{Z_N(\mu, \varepsilon_s)}{Z(\varepsilon_s)} = \frac{\int D\varphi \, \exp\left\{-\frac{1}{2\beta} \Sigma_{s,s'} W_{ss'}^{-1} \varphi_s \varphi_{s'}\right\} \Sigma_{\{n_s\}} \exp\left\{\Sigma_s(\mu - \varepsilon_s + \nu\varphi_s)n_s - \frac{1}{2}\nu^2 \Sigma_s U_s n_s^2\right\}}{\int D\varphi \, \exp\left\{-\frac{1}{2\beta} \Sigma_{s,s'} W_{ss'}^{-1} \varphi_s \varphi_{s'}\right\} \Sigma_{\{n_s\}} \exp\left\{\Sigma_s(\nu\varphi_s - \beta\varepsilon_s)n_s - \frac{1}{2}\nu^2 \Sigma_s U_s n_s^2\right\}}. \qquad (4)$$

The physical meaning of the generating functional is obvious from the definition, since it is described by the ratio of the partition function with a fixed number of particles to the partition function of the grand canonical ensemble. Now we substitute $\varphi_s \Rightarrow \psi_s + \varphi_s^0$ and $n_s \Rightarrow m_s + \nu^2[(\varphi_s^0 + \beta\mu)/\beta U_s]$ in the denominator of (4), then the generating functional reduces to

$$\Xi(\mu) = \exp \sum_s (\mu - 2\varepsilon_s) \frac{\varphi_s^0 + \nu^2 \beta\mu}{2U_s} \qquad (5)$$

under the condition that φ_s^0 satisfies the equation

$$\varphi_s^0 - U_s \sum_s W_{ss'}^{-1} \varphi_{s'}^0 + \nu^2 \beta\mu = 0. \qquad (6)$$

The shift of the field variable and the equation obtained serve to select the states that bring the dominant contribution in the partition function of the system. Having found the solution of Eq. (6), we can write the generating functional and thus obtain all relevant thermodynamic characteristics of the system. The chemical potential is determined by the equation

$$N = \langle N \rangle = \frac{1}{\beta} \frac{\partial \ln Z_N(\mu, \varepsilon_s)}{\partial\mu} = \frac{1}{\beta} \frac{\partial \ln \Xi(\mu)}{\partial\mu}, \qquad (7)$$

and the compressibility of the system is given by

$$k_T = \frac{N^2}{\beta V^2} \left(\frac{\partial V}{\partial P}\right) = \langle N \rangle^2 - \langle N^2 \rangle$$

$$= -\frac{1}{\beta} \frac{\partial \langle N \rangle}{\partial\mu} = -\frac{1}{\beta} \frac{\partial^2 \ln \Xi(\mu)}{\partial\mu^2}, \qquad (8)$$

where P is the pressure and V is the volume of the system. This becomes possible after the first step of the change of variables, which reduces the partition function $Z_N(\mu, \varepsilon_s) = \Xi(\mu)Z(\varepsilon_s)$ to the product of two factors in which the grand partition function $Z(\varepsilon_s)$ may be written in the form

$$Z(\varepsilon_s) = \int D\psi \, \exp\left\{-\frac{1}{2\beta} \sum_{s,s'} W_{ss'}^{-1} \psi_s \psi_{s'}\right\} \sum_{\{m_s\}}$$

$$\times \exp\left\{\sum_s (\nu_s \psi_s - \beta\varepsilon_s)m_s - \frac{1}{2}\nu^2 \sum_s U_s m_s^2\right\}. \qquad (9)$$

Now we again shift the variables, $\psi_s \Rightarrow \sigma_s + \nu\xi_s^0$ and $m_s \Rightarrow k_s + \nu^2[(\xi_s^0 + \beta\varepsilon_s)/\beta U_s]$, and require that ξ_s^0 must be a solution to the equation

$$\xi_s^0 - U_s \sum_{s'} W_{ss'}^{-1} \xi_s^0 - \beta\varepsilon_s = 0. \qquad (10)$$

Then the partition function of the grand canonical distribution of the system reduces to the form

$$Z(\varepsilon_s) = \Xi(\varepsilon_s)Z(0), \qquad (11)$$

where

$$\Xi(\varepsilon_s) = \exp\left\{\sum_s \frac{\varepsilon_s}{2U_s}(\beta\varepsilon_s - \xi_s^0)\right\}, \qquad (12)$$

and

$$Z(0) = \int D\sigma \, \exp\left\{-\frac{1}{2\beta} \sum_{s,s'} W_{ss'}^{-1} \sigma_s \sigma_{s'}\right\} \sum_{\{k_s\}}$$

$$\times \exp\left(i\sigma_s k_s + \frac{1}{2}\nu^2 \beta U_s k_s^2\right) \qquad (13)$$

describes the configuration partition function of the system with the external field not taken into account. It is not difficult to see that the last term in formula (13) is the Riemann Θ function doubly periodic with respect to the variables $-i\sigma_s/2\pi$ and $(i\nu^2 \beta U_s)/2\pi$. This function is tabulated for the whole range of change of arguments [10]. Thus the configuration partition function

$$Z(0) = \int D\sigma \, \exp\left\{-\frac{1}{2\beta} \sum_{s,s'} W_{ss'}^{-1} \sigma_s \sigma_{s'}\right\}$$

$$\times \Theta\left(-\frac{i\sigma_s}{2\pi}, \frac{i\nu^2 \beta U_s}{2\pi}\right) \qquad (14)$$

is written in terms of the well known Θ functions. Thus, the partition function of the system is completely determined for the solutions of Eqs. (6) and (10). In this sense we can say that this procedure provides an exact statistical solution for a system of interacting particles described by the Hamiltonian (1). For a system with unfixed number of particles, formula (11) and explicit expressions (12) and (14) yield the thermodynamic characteristics of the system, i.e., the correlation function and the susceptibility. We have

$$g_{ss'} = \frac{\partial^2 \ln \Xi(\varepsilon_s)}{\partial\varepsilon_s \partial\varepsilon_{s'}}, \quad \chi = \frac{1}{N\beta} \sum_{s,s'} g_{ss'}. \qquad (15)$$

Thus we have a complete statistical description of the system in terms of the known Θ functions and solutions of

the relevant equations for φ_s^0 and ξ_s^0. Solutions of Eqs. (6) and (10) select the configuration states that bring the dominant contribution to the partition function. To obtain the final result requires specifying the interaction $W_{ss'}$ and U_s. We rewrite the generating functional (5) in a modified form given by

$$\Xi(\mu) = \exp\left\{\nu^2 \sum_s (\mu - 2\varepsilon_s)\beta\mu f_s\right\}, \qquad (16)$$

where

$$f_s = \frac{1}{U_s}\left(1 - \sum_{s'} G_{ss'}\right) \qquad (17)$$

is written in terms of the Green function $G_{ss'}$ of Eq. (5), i.e.,

$$G_{ss'} - U_s \sum_{s''} W_{ss''}^{-1} G_{s''s'} = \delta_{ss'}. \qquad (18)$$

This presentation reduces Eq. (7) for the chemical potential to

$$N = \sum_s (\mu - \varepsilon_s) f_s. \qquad (19)$$

The compressibility of the system is described by the expression

$$k_T = \frac{N^2}{\beta V^2}\left(\frac{\partial V}{\partial P}\right) = \frac{\nu^2}{\beta}\sum_s f_s. \qquad (20)$$

So, in order to find the thermodynamic characteristics of the system one just has to find the solution of Eq. (18) for the Green function $G_{ss'}$.

The above treatment is based on the initial lattice model and has an exact solution for this case. It is not difficult to extend the approach to the continuum case. To do this, we cannot avoid calculating the inverse operator $W_{ss'}^{-1}$. If the interaction energy is given by $W_{ss'} = W(\vec{R}_s - \vec{R}_{s'})$ (the values of subscript s form a continuous set within the volume V of the system), then the inverse matrix $W_{ss'}^{-1}$ should be interpreted in the operator sense [6,7], i.e.,

$$W^{-1}(\vec{R}_s - \vec{R}_{s'}) = \delta_{RR'}L_{R'}, \qquad (21)$$

where $L_{R'}$ is the operator; for each the interaction potential is the Green function. For the shielded Coulomb or Newton interaction with

$$W_{ss'} = \frac{q^2}{R_s - R_{s'}}\exp\{-\kappa(\vec{R}_s - \vec{R}_{s'})\}, \qquad (22)$$

where q is the interaction constant and κ^{-1} the interaction radius

$$L_R = -\frac{1}{4\pi q^2}(\Delta_R - \kappa^2), \qquad (23)$$

where Δ_R is the Laplace operator.

This representation provides a possibility to obtain the equation of state for the continuum case, when interaction at different sites is Newton attraction or Coulomb repulsion and interaction at the same site is constant, $U_s = U = $ const. The passage to the continuum limiting case is carried out by replacing $\Sigma_s \Rightarrow N/V \int dV$ and rewriting the equations in the differential form. The equation for the Green function in the continuous case is given by

$$\rho G(r) + \frac{U}{4\pi q^2}(\Delta_R - \kappa^2)G(r) = \delta(r), \qquad (24)$$

where $\rho = N/V$ is the density.

For $\kappa^2 > (4\pi q^2)/U\rho$, the solution of this equation is given by

$$G(r) = -\frac{q^2}{Ur}\exp(-\lambda r), \qquad (25)$$

where $\lambda^2 = \kappa^2 - [(4\pi q^2)/U]\rho$. If the reversed inequality holds, then

$$G(r) = -\frac{q^2}{Ur}\cos(-\lambda r). \qquad (26)$$

Substituting the Green function in the definition (17) and making use of the continuum analogue of Eq. (20),

$$\int d\vec{R} f(\vec{R}) = -\frac{N}{V}\left(\frac{\partial V}{\partial P}\right), \qquad (27)$$

we find that for the first case,

$$\left(\frac{\partial \rho}{\partial P}\right)_T = \frac{\nu^2}{U}\left\{1 + \frac{\rho^2}{\rho_0^2}\right\}, \qquad (28)$$

where $\rho_0^2 = (\lambda^5 U N^2)/(4\pi q^2)$. The pressure increase over the lattice gas pressure $P_0 = kT\rho$ is described, for $\kappa^2 > (4\pi q^2)/U\rho$, by a simple expression

$$\Delta P = P - P_0 = \frac{U}{\nu^2}\rho_0 \arctan\left(\frac{\rho}{\rho_0}\right), \qquad (29)$$

which for $\rho/\rho_0 \ll 1$ reduces to

$$\Delta P = \frac{U}{\nu^2}\rho\left\{1 - \frac{1}{3}\left(\frac{\rho}{\rho_0}\right)^2\right\}. \qquad (30)$$

If the reversed inequality $\kappa^2 < [(4\pi q^2)/U]\rho$ is satisfied, then the pressure increase may be obtained in the integral form. If the interaction at different lattice sites is constant too, $W_{ss'} = W = $ const., we have

$$\Delta P = \nu^2(U - W)\rho, \qquad (31)$$

which provides a complete physical picture of the situation under consideration. Equation of state (29) is not of van der Waals form; nevertheless, it allows a phase transition for

$kT_c = -U/\kappa^2$ in the case $\nu^2 = -1$. The phase transition in the system with constant interaction energies occurs for $kT_c = \nu^2(U-W)$.

In conclusion, we reduced the partition function of the three-dimensional lattice system, with long range interaction (22) and the short range interaction on sites, to the form that can be calculated by conventional numerical methods. For instance, the distribution function of the particles can be obtained as a result of such calculations. However, the conventional thermodynamic characteristics (pressure, compressibility, and so on) and equation of state, which do not imply knowing the distribution function, can be obtained even without such calculations, due to the factorization of the partition function. We emphasize that our choice of the interaction and dimension 3 is dictated by the fact that the inverse operator has the form (23) that is essential to our approach in just three dimensions. However, since the potentials $\frac{1}{2}|\vec{R} - \vec{R}'|$, $-1/2\pi \ln|\vec{R} - \vec{R}'|$, and $-1/[(n-2)|\vec{R} - \vec{R}'|^{n-2}]$ have the same inverse operator (23) with $\kappa = 0$, respectively, in $1,2,n \geq 3$ dimensions, the method can also be applied to the corresponding systems in dimensions different from $n = 3$.

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