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LETTER TO THE EDITOR

Quasi-exact solvability of the one-dimensional Holstein model

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Abstract

The one-dimensional Holstein model of spinless fermions interacting with dispersionless phonons is solved by using a Bethe ansatz in analogue to that for the one-dimensional spinless Fermi–Hubbard model. Excitation energies and the corresponding wavefunctions of the model are determined by a set of partial differential equations. It is shown that the model is, at least, quasi-exactly solvable for the two-site case, when the phonon frequency, the electron–phonon coupling strength and the hopping integral satisfy certain relations. As examples, some quasi-exact solutions of the model for the two-site case are derived.

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The problem of interacting electrons with phonons has been attracting much attention as it is helpful in understanding superconductivity in many aspects, such as in fullerenes, bismuth oxides and the high- T_c superconductors [1]. Unlike conventional metals, these materials are neither necessary in the weak-coupling regime where perturbation theory can be used or the strong-coupling case in which a polaronic treatment is possible, nor necessary in the adiabatic regime in which characteristic phonon energies are much less than characteristic electron energies. This challenge has led to numerical studies of the Holstein model of electrons interacting with phonons in infinite dimensions, two dimensions, one dimension and on just two sites [1, 2]. The one-dimensional case is of importance since a wide range of quasi-one-dimensional materials undergo a Peierls or charge-density-wave (CDW) instability due to the electron–phonon interaction. Most theoretical treatments assume the adiabatic limit and treat the phonons in a mean-field approximation. However, it has been argued that in many CDW materials the quantum lattice fluctuations are important [3]. Up until now, various variational methods [4], renormalization group methods [5], world-line quantum Monte Carlo [6] or Green-function Monte Carlo [2] methods have been used. Other numerical methods including numerical diagonalization [7] and DMRG [8, 9] techniques have also been adopted.

In this letter, we will study the one-dimensional Holstein model of spinless fermions with a Bethe ansatz-like method. This model is particularly interesting because at a finite fermion–phonon coupling, there is a quantum phase transition from a Luttinger liquid (metallic) phase to an insulating phase with CDW long-range order [6, 10].

The Hamiltonian is

$$H = \omega \sum_i b_i^\dagger b_i - t \sum_{i=1}^{p-1} (f_i^\dagger f_{i+1} + f_{i+1}^\dagger f_i) - t(f_1^\dagger f_p + f_p^\dagger f_1)(1 - \delta_{p2}) + g \sum_i f_i^\dagger f_i (b_i^\dagger + b_i), \quad (1)$$

where f_i and f_i^\dagger are fermion annihilation and creation operators on site i , respectively, satisfying anti-commutation relations with $\{f_i, f_j\} = \{f_i^\dagger, f_j^\dagger\} = 0$, $\{f_i, f_j^\dagger\} = \delta_{ij}$, b_i (b_i^\dagger) destroys (creates) a local phonon of frequency ω , which satisfy commutation relations with $[b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0$, $[b_i, b_j^\dagger] = \delta_{ij}$, t is the hopping integral and g is the fermion–phonon coupling, and a periodic chain of p sites is assumed. The phase transition occurs at a critical coupling g_c , separating metallic ($0 \leq g \leq g_c$) and CDW insulating phases ($g > g_c$) [6, 10]. In the strong-coupling limit ($g^2 \gg \omega t$), (1) can be mapped onto the anisotropic, antiferromagnetic Heisenberg (XXZ) model [6] which is exactly solvable. The transition occurs at the spin isotropy point, is of the Kosterlitz–Thouless type and the Luttinger liquid parameters can be found in the metallic phase [2].

In order to diagonalize Hamiltonian (1), let us consider the simpler one-dimensional spinless Fermi–Hubbard model [11] with

$$H = \sum_{i=1}^p h_i f_i^\dagger f_i - t \sum_{i=1}^{p-1} (f_i^\dagger f_{i+1} + f_{i+1}^\dagger f_i) - t(f_1^\dagger f_p + f_p^\dagger f_1)(1 - \delta_{p2}), \quad (2)$$

where $\{h_i\}$ are a set of parameters independent of the number of fermions, and the last term keeps (2) satisfying the periodic condition. It is known that (2) is simply exactly solvable [11]. For k -particle excitation, the eigenstates are

$$|k; \eta\rangle = \sum_{i_1 < i_2 < \dots < i_k} C_{i_1 i_2 \dots i_k}^{(\eta)} f_{i_1}^\dagger f_{i_2}^\dagger \dots f_{i_k}^\dagger |0\rangle, \quad (3)$$

where

$$C_{i_1 i_2 \dots i_k}^{(\eta)} = \begin{pmatrix} g_{i_1}^{(\eta_1)} & g_{i_2}^{(\eta_1)} & \dots & g_{i_k}^{(\eta_1)} \\ g_{i_1}^{(\eta_2)} & g_{i_2}^{(\eta_2)} & \dots & g_{i_k}^{(\eta_2)} \\ \vdots & \dots & \dots & \vdots \\ g_{i_1}^{(\eta_k)} & g_{i_2}^{(\eta_k)} & \dots & g_{i_k}^{(\eta_k)} \end{pmatrix}, \quad (4)$$

in which $\{g_i^{(\eta_\mu)}\}$ should satisfy the following eigenequation for a $p \times p$ matrix T with

$$\sum_j T_{ij}(p) g_j^{(\eta_\mu)} = E^\eta g_i^{(\eta_\mu)}, \quad (5)$$

where $\{T_{ij}(p)\}$ are elements of the matrix

$$T(2) = \begin{pmatrix} h_1 & -t \\ -t & h_2 \end{pmatrix}, \quad T(p) = \begin{pmatrix} h_1 & -t & 0 & \dots & -t \\ -t & h_2 & -t & 0 & \dots \\ 0 & \ddots & \ddots & \ddots & \ddots \\ \vdots & \dots & -t & h_{p-1} & -t \\ -t & 0 & \dots & -t & h_p \end{pmatrix} \quad \text{for } p \geq 3, \quad (6)$$

which is tridiagonal except the elements $T_{1p} = T_{p1} = -t$ for $p \geq 3$ originating from the last term in (2) which are needed in order to satisfy the periodic condition.

Let us introduce the differential realization for the boson operators with

$$b_i^\dagger \Rightarrow y_i, \quad b_i \Rightarrow \frac{\partial}{\partial y_i} \quad (7)$$

for $i = 1, 2, \dots, p$. Then, Hamiltonian (1) is mapped into the following form:

$$H = \omega \sum_{i=1}^p y_i \frac{\partial}{\partial y_i} - t \sum_{i=1}^{p-1} (f_i^\dagger f_{i+1} + f_{i+1}^\dagger f_i) - t (f_1^\dagger f_p + f_p^\dagger f_1) (1 - \delta_{p2}) + g \sum_{i=1}^p f_i^\dagger f_i \left(y_i + \frac{\partial}{\partial y_i} \right). \quad (8)$$

According to the diagonalization procedure used to solve the eigenvalue problem (2), the one-fermion excitation states can be assumed to be of the following ansatz form:

$$|k = 1; \eta\rangle = \sum_{\mu=1}^p q_\mu^{(\eta)}(y_1, y_2, \dots, y_p) e^{-\frac{g}{\omega} y_\mu} f_\mu^\dagger |0\rangle, \quad (9)$$

where $|0\rangle$ is the fermion vacuum state and η is used to label different energy eigenstates.

By using expressions (8) and (9), the energy eigenequation becomes

$$\begin{aligned} & \sum_{\mu} \left(\sum_i \omega y_i \frac{\partial q_\mu^{(\eta)}}{\partial y_i} e^{-\frac{g}{\omega} y_\mu} + g \frac{\partial q_\mu^{(\eta)}}{\partial y_\mu} e^{-\frac{g}{\omega} y_\mu} \right) f_\mu^\dagger |0\rangle \\ & - t \left(\sum_{i=1}^{p-1} (f_i^\dagger f_{i+1} + f_{i+1}^\dagger f_i) + (f_1^\dagger f_p + f_p^\dagger f_1) (1 - \delta_{p2}) \right) \sum_{\mu} q_\mu^{(\eta)} e^{-\frac{g}{\omega} y_\mu} f_\mu^\dagger |0\rangle \\ & = \left(E^{(\eta)} + \frac{g^2}{\omega} \right) \sum_{\mu} q_\mu^{(\eta)} e^{-\frac{g}{\omega} y_\mu} f_\mu^\dagger |0\rangle, \end{aligned} \quad (10)$$

which results in the following set of the extended Bethe ansatz equations:

$$\sum_{i=1}^p \omega y_i \frac{\partial q_\mu^{(\eta)}}{\partial y_i} + g \frac{\partial q_\mu^{(\eta)}}{\partial y_\mu} - \frac{t}{1 + \delta_{2p}} q_{\mu-1}^{(\eta)} e^{-\frac{g}{\omega} x_{\mu-1}} - \frac{t}{1 + \delta_{2p}} q_{\mu+1}^{(\eta)} e^{\frac{g}{\omega} x_\mu} = \left(E^{(\eta)} + \frac{g^2}{\omega} \right) q_\mu^{(\eta)} \quad (11)$$

for $\mu = 1, 2, \dots, p$, which is a set of coupled rank-1 nonlinear partial differential equations (PDEs), where the periodic conditions with $q_0^{(\eta)} = q_p^{(\eta)}$, $q_{p+1}^{(\eta)} = q_1^{(\eta)}$ are assumed, and

$$x_1 = y_1 - y_2, \dots, x_{k-1} = y_{k-1} - y_k, x_k = y_k - y_{k+1}, \dots, x_{p-1} = y_{p-1} - y_p, x_p = y_p - y_1. \quad (12)$$

Equation (11) completely determines the eigenenergies and the corresponding coefficients $\{q_\mu^{(\eta)} \equiv q_\mu^{(\eta)}(y_1, y_2, \dots, y_p)\}$. Once the above PDEs are solved for one-fermion excitations, according to the procedure used for solving the one-dimensional spinless Fermi–Hubbard model, the k -fermion excitation wavefunction can be organized into the following form:

$$|n_f = k; \eta\rangle = \sum_{1 \leq i_1 < i_2 < \dots < i_k \leq p} C_{i_1 i_2 \dots i_k}^{(\eta)} e^{-\frac{g}{\omega} \sum_{\mu=1}^k y_{i_\mu}} f_{i_1}^\dagger f_{i_2}^\dagger \dots f_{i_k}^\dagger |0\rangle \quad (13)$$

with

$$C_{i_1 i_2 \dots i_k}^{(\eta)} = \begin{vmatrix} q_{i_1}^{(\eta_1)} & q_{i_2}^{(\eta_1)} & \dots & q_{i_k}^{(\eta_1)} \\ q_{i_1}^{(\eta_2)} & q_{i_2}^{(\eta_2)} & \dots & q_{i_k}^{(\eta_2)} \\ \vdots & \dots & \dots & \vdots \\ q_{i_1}^{(\eta_k)} & q_{i_2}^{(\eta_k)} & \dots & q_{i_k}^{(\eta_k)} \end{vmatrix}. \quad (14)$$

The corresponding k -fermion excitation energy is given by

$$E_k^{(\eta)} = \sum_{\nu=1}^k E^{(\eta_\nu)}, \quad (15)$$

in which $E^{(\eta_\nu)}$ is the ν th eigenvalue of equation (11).

In order to get quasi-exact solutions of (11), we make use of the coordinate transformation (12) with new variables $\{x_1, x_2, \dots, x_{p-1}\}$ and $X = \sum_{i=1}^p y_i$, and assume that $q_\mu^{(\eta)}$ can be expressed as

$$\begin{aligned} q_1^{(\eta)}(x_1, x_2, \dots, x_{p-1}, X) &= e^{\frac{g}{\omega}x_1} (\omega X + g)^n f_1(x_1, x_2, \dots, x_{p-1}), \\ q_2^{(\eta)}(x_1, x_2, \dots, x_{p-1}, X) &= (\omega X + g)^n f_2(x_1, x_2, \dots, x_{p-1}), \\ q_i^{(\eta)}(x_1, x_2, \dots, x_{p-1}, X) &= e^{-\frac{g}{\omega} \sum_{\mu=2}^{i-1} x_\mu} (\omega X + g)^n f_i(x_1, x_2, \dots, x_{p-1}) \end{aligned} \quad (16)$$

for $3 \leq i \leq p$ and $n = 0, 1, 2, \dots$. Then, equation (11) can be simplified as

$$\begin{aligned} \omega \sum_{i=1}^{p-1} x_i \frac{\partial f_1}{\partial x_i} + g x_1 f_1^{(\eta)} + g \frac{\partial f_1}{\partial x_1} - \frac{t}{1 + \delta_{p2}} f_p - \frac{t}{1 + \delta_{p2}} f_2 &= (E^{(\eta)} - n\omega) f_1, \\ \omega \sum_{i=1}^{p-1} x_i \frac{\partial f_2}{\partial x_i} + g \left(\frac{\partial f_2}{\partial x_2} - \frac{\partial f_2}{\partial x_1} \right) - \frac{t}{1 + \delta_{p2}} f_1 - \frac{t}{1 + \delta_{p2}} f_3 &= (E^{(\eta)} + g^2/\omega - n\omega) f_2, \\ \omega \sum_{i=1}^{p-1} x_i \frac{\partial f_\mu}{\partial x_i} - g \sum_{\rho=2}^{\mu-1} x_\rho f_\mu + g \left(\frac{\partial f_\mu}{\partial x_\mu} - \frac{\partial f_\mu}{\partial x_{\mu-1}} \right) - \frac{t}{1 + \delta_{p2}} f_{\mu-1} - \frac{t}{1 + \delta_{p2}} f_{\mu+1} \\ &= (E^{(\eta)} - n\omega) f_\mu \quad \text{for } 3 \leq \mu \leq p-1, \\ \omega \sum_{i=1}^{p-1} x_i \frac{\partial f_p}{\partial x_i} - g \sum_{\rho=2}^{p-1} x_\rho f_p - g \frac{\partial f_p}{\partial x_{p-1}} - \frac{t}{1 + \delta_{p2}} f_{p-1} - \frac{t}{1 + \delta_{p2}} f_1 \\ &= \left(E^{(\eta)} + \frac{g^2}{\omega} - \frac{g^2}{\omega} \delta_{p2} - n\omega \right) f_p. \end{aligned} \quad (17)$$

It can be verified that (17) has finite-rank polynomial solutions with

$$f_i(x_1, x_2, \dots, x_{p-1}) \equiv f_i^{(m_1^i, m_2^i, \dots, m_{p-1}^i)} = \sum_{v_1 v_2 \dots v_{p-1}} C_{v_1 v_2 \dots v_{p-1}}^{m_1^i m_2^i \dots m_{p-1}^i} x_1^{v_1} x_2^{v_2} \dots x_{p-1}^{v_{p-1}}, \quad (18)$$

for $i = 1, 2, \dots, p$ when the phonon frequency ω , the electron–phonon coupling strength g and the hopping integral t satisfy certain relations, where $\{m_1^i, m_2^i, \dots, m_{p-1}^i\}$ is a set of integers, and $C_{v_1 v_2 \dots v_{p-1}}^{m_1^i m_2^i \dots m_{p-1}^i}$ is the expansion coefficient depending on the parameters ω , g and t . In such cases, a set of highly nonlinear equations is involved, which cannot be solved analytically in general. Therefore, as a simple example, only a few simple solutions for $p = 2$ case will be shown.

In the two-site case, equation (17) becomes

$$\begin{aligned} (\omega x + g) f_1'(x) + x g f_1(x) - t f_2(x) &= \left(E^{(\eta)} - \omega n - \frac{g^2}{\omega} \right) f_1(x), \\ (\omega x - g) f_2'(x) - t f_1(x) &= \left(E^{(\eta)} + \frac{g^2}{\omega} - \omega n \right) f_2(x), \end{aligned} \quad (19)$$

where $x \equiv x_1$ and $n = 0, 1, 2, \dots$. We seek finite-rank polynomial solutions for $f_1(x)$ and $f_2(x)$ in the form shown in (18), and the corresponding relations among the phonon frequency

ω , the electron–phonon coupling strength g and the hopping integral t . Since a set of highly nonlinear equations is involved, in the following, we only list solutions corresponding to a few lower rank polynomials:

$$f_1(x) = -\frac{t\omega}{g^2 + t^2}, \quad f_2(x) = 1 - \frac{g\omega}{g^2 + t^2}x \quad (20a)$$

with

$$E^{(n,0)} = \omega(n+1) - \frac{g^2}{\omega}, \quad (20b)$$

when

$$\omega^2 = 2g^2 + t^2, \quad (20c)$$

$$f_1(x) = 2t\omega \frac{g\omega x + \omega^2 - t^2 - 3g^2}{2g^4 + 4g^2t^2 + t^4 - t^2\omega^2}, \quad f_2(x) = 1 + 2g\omega \frac{g\omega x^2 - (2g^2 + t^2)x}{2g^4 + 4g^2t^2 + t^4 - t^2\omega^2} \quad (21a)$$

with

$$E^{(n,1)} = \omega(n+2) - \frac{g^2}{\omega} \quad (21b)$$

when

$$\omega^2 = 2g^2 + \frac{5t^2}{8} \pm \frac{1}{8}\sqrt{128g^4 + 64g^2t^2 + 9t^4}; \quad (21c)$$

$$f_1(x) = \frac{-6g^2t\omega^3x^2 + 6tg\omega^2(4g^2 + t^2 - \omega^2)x - 3t\omega(14g^4 + t^4 - 5t^2\omega^2 + 4\omega^4 + 2g^2(4t^2 - 11\omega^2))}{6g^6 + 20g^4t^2 + t^6 - 5t^4\omega^2 + 4t^2\omega^4 + g^2t^2(9t^2 - 23\omega^2)},$$

$$f_2(x) = 1 + \frac{-6g^3\omega^3x^3 + 6g^2\omega^2(3g^2 + t^2)x^2 - 3g\omega(6g^4 + 6g^2t^2 + t^4 - t^2\omega^2)x}{6g^6 + 20g^4t^2 + t^6 - 5t^4\omega^2 + 4t^2\omega^4 + g^2t^2(9t^2 - 23\omega^2)} \quad (22a)$$

with

$$E^{(n,2)} = \omega(n+3) - \frac{g^2}{\omega} \quad (22b)$$

when ω^2 are roots of the equation

$$48g^6 + t^6 - 14t^4\omega^2 + 49t^2\omega^4 - 36\omega^6 + 4g^4(11t^2 - 54\omega^2) + 4g^2(3t^4 - 29t^2\omega^2 + 54\omega^4) = 0, \quad (22c)$$

and so on, which form an infinite quasi-exactly solvable series with $f_1^{(m)}(x) = \sum_{i=0}^m a_i x^i$ and $f_2^{(m+1)}(x) = \sum_{i=0}^{m+1} c_i x^i$ being rank m and rank $m+1$ polynomials of x , respectively, where a_i and c_i are the corresponding expansion coefficients. The corresponding energy eigenvalue is

$$E^{(n,m)} = \omega(n+m+1) - g^2/\omega \quad (23)$$

for $m = 0, 1, 2, \dots$ and $n = 0, 1, 2, \dots$. However, relations in determining the expansion coefficients a_i and c_i and those among ω , g and t will become more and more complicated with increasing m . Since the phonon frequency ω , coupling strength g and hopping integral t must be real parameters, some solutions from the restricted conditions among these parameters must be real. Fortunately, for up to the $m = 2$ cases listed in (20)–(22), solutions for ω^2 from the corresponding relations are greater than zero as long as g and t are real parameters, especially the roots ω^2 of (22c). Once the functions $f_1^{(m)}(x)$ and $f_2^{(m+1)}(x)$ are determined, the

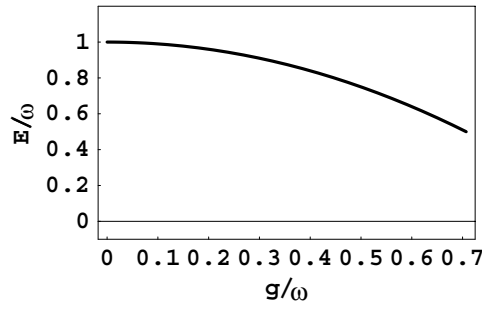


Figure 1. One-electron excitation energy E/ω as a function of g/ω within the quasi-exactly solvable region.

final functions $q_1(X, x)$ and $q_2(X, x)$ needed to construct the corresponding eigenstate (13) can be written as

$$q_1^{(n,m)}(X, x) = (\omega X + g)^n f_1^{(m)}(x) e^{\frac{g}{\omega} x}, \quad q_2^{(n,m)}(X, x) = (\omega X + g)^n f_2^{(m+1)}(x) \quad (24)$$

according to (16). Though only some simple solutions of $p = 2$ case are exemplified, more complicated quasi-exact solutions for any number of site p can be derived similarly based on (18).

Furthermore, though these quasi-exact solutions are valid only when the phonon frequency ω , the electron–phonon coupling strength g and the hopping integral t satisfy certain relations, the results should be useful in studying the model within the restricted parameter regions and in checking approximation methods. As an example analysis, let us consider the ground state corresponding to one-electron excitation with $E^{(0,0)}/\omega = 1 - (g/\omega)^2$ in the series. In this case, the hopping integral t and the coupling strength g should satisfy the relation given by (20c) and $0 \leq g/\omega \leq 1/\sqrt{2}$. With increasing g/ω within this region, t/ω must decrease from 1 to 0 to keep the quasi-exact solvability according to (20c). One can obtain exact quantities within such a parameter region. One-electron excited ground-state energy of the two-site model and the phonon number expectation value defined by

$$\langle n_f = 1; (0, 0) | \sum_{i=1}^2 b_i^\dagger b_i | n_f = 1; (0, 0) \rangle \quad (25)$$

as a function of g/ω within $[0, 1/\sqrt{2}]$ are shown in figures 1 and 2, respectively. It can be seen that the excitation energy decreases from the hopping energy $E^{(0,0)} = t = \omega$ in the electron–phonon decoupled case $g = 0$ to $E^{(0,0)} = \omega/2$ with $t = 0$ and the electron confined on the second site. While the phonon number expectation value increases from 0 to $7/6$, g/ω increases from 0 to $1/\sqrt{2}$.

As is known, quasi-exact solvability implies a situation where an infinite-dimensional matrix version of an eigenvalue problem can be reduced explicitly into a block diagonal form with one of the blocks being finite [12]. Though we still do not know the exact dynamical symmetry in the quasi-exact cases of the 1-dim Holstein model, it can be inferred from the Hilbert subspace spanned by all Fock states of the model that there may be a kind of symmetry, of which the corresponding dynamical symmetry group may be a subgroup of $GL(m/p)$, where m corresponds to the highest rank of the polynomials $f_i(x_1, x_2, \dots, x_p)$ shown in (18). To reveal exact dynamical symmetry in the quasi-exact solvable cases of the model is a challenge, which should be helpful in solving the model more efficiently.

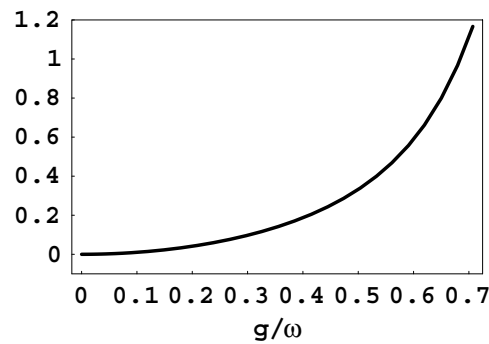


Figure 2. The phonon number expectation value of the one-electron ground state as a function of g/ω within the quasi-exactly solvable region.

In summary, general solutions of the 1-dim Holstein model are derived based on an algebraic approach similar to that used in solving 1-dim spinless Fermi–Hubbard model. A set of the extended Bethe ansatz equations is coupled rank-1 nonlinear partial differential equations (PDEs), which completely determine the eigenenergies and the corresponding wavefunctions of the model. Though we still do not know whether the PDEs are exactly solvable or not, at least, these PDEs are quasi-exactly solvable. In such cases, the phonon frequency ω , the electron–phonon coupling strength g and the hopping integral t must satisfy certain relations. As examples, some quasi-exact solutions of the model for a two-site case are explicitly derived. Though these quasi-exact solutions are valid only when the phonon frequency ω , the electron–phonon coupling strength g and the hopping integral t satisfy certain relations, the results should be helpful in studying the model within the restricted parameter regions and in checking approximation methods. There exist similar quasi-exact solutions for any number of sites p , which will be reported in detail elsewhere in the near future.

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