PHYSICAL REVIEW D **80,** 107701 (2009)

Homolumo gap from dynamical energy levels

I. Andrić, L. Jonke, and D. Jurman
Theoretical Physics Division, Rudjer Bošković Institute, P.O. Box 180, 10002 Zagreb, Croatia

H. B. Nielsen
The Niels Bohr Institute, Copenhagen DK 2100, Denmark
(Received 12 September 2009; published 23 November 2009)

We introduce a dynamical matrix model where the matrix is interpreted as a Hamiltonian representing interaction of a bosonic system with a single fermion. We show how a system of second-quantized fermions influences the ground state of the whole system by producing a gap between the highest eigenvalue of the occupied single-fermion states and the lowest eigenvalue of the unoccupied single-fermion states. We describe the development of the gap in both the strong and weak coupling regimes, while for the intermediate coupling strength we expect formation of homolumo kinks.

DOI: 10.1103/PhysRevD.80.107701 PACS numbers: 03.65.−w, 02.10.Yn, 71.70.Ej

In the complex systems composed of fermions interacting with bosons, such as a molecules, nuclei, etc., appearance of the energy gap between the highest energy level occupied by fermions and the lowest unoccupied level, the so-called homolumo gap [1], is a well-known effect which is observed in experiments and determined from the first principles by exact calculations in various specific examples. Some of the most important properties of the system, stability, interaction with another system, size, etc., are determined by the physics in the neighborhood of the gap. In a more general setting, we are interested in the application of the homolumo effect in the project of Random Dynamics [2]. There, one starts from the observation that the energies at our disposal are extremely low, compared to the fundamental energy scale, presumably to be identified with the Planck scale. Consequently, from the fundamental scale point of view, the usual high-energy physics can be described as low-energy excitations in the neighborhood of the gap.

The purpose of this paper is to provide a model which possesses the main features of the interactions involved in the production of the homolumo gap and allows generalizations which incorporate other properties such as the appearance of the single level in the gap or mixing of the densities of the occupied and unoccupied levels. This paper can be viewed as continuation of our previous work [3] which, using a different approach, gives a better insight into the mechanism of production of the gap. In this new approach we would like to confirm that the homolumo gap arises whenever we have a system of fermions and bosons in interaction, provided that bosons are sufficiently soft to yield to the pressure from fermions, while the details of the model itself seem to be unimportant.

The main assumption of the model is dynamics of single-fermion energy levels. This assumption can arise, for example, from the observation that the energies of the single electron levels change as the nucleus of a molecule vibrates. We show that the Hamiltonian describing the system of interacting bosons and fermions can be constructed from very general assumptions and can be written[1] as

$$H = H_B + gH_{FB}, \tag{1}$$

with H_B and H_{FB} given by

$$H_B = \omega(B^\dagger B + BB^\dagger), \qquad H_{FB} = f^\dagger Bf + f^\dagger B^\dagger f. \tag{2}$$

This form of the Hamiltonian appeared in descriptions of black holes [4], mesons and hadrons in QCD [5], and the Jahn-Teller effect [1]. Within our approach, the part of the Hamiltonian which describes fermion-boson interaction is completely determined, while the Hamiltonian describing bosonic degrees of freedom is a matter of choice. Our choice is motivated by possible applications in different branches of physics. As written, the Hamiltonian H_B has been used in descriptions of (a sector within) supersymmetric Yang-Mills theory in four dimensions, two-dimensional quantum gravity and string theory [6], and matrix cosmology [7]. It is also related to integrable models such as the Calogero model [8]. Furthermore, the ground state wave function of H_B corresponds to the Gaussian ensemble from the random matrix theory (RMT) [9] which has been successfully applied in analyses of the spectra of complex molecules and nuclei, transport properties of disordered mesoscopic systems [10].

We start modeling the Hamiltonian by considering a system of the interacting fermions described by the Hamiltonian in which we include appropriate antisymmetrization of fermionic modes in analogy with symmetrization of bosonic modes:

$$H_{FB} = \frac{1}{2}\sum_{l,k}(f_l^\dagger f^k - f^k f_l^\dagger)X_k^l, \tag{3}$$

where matrix X is, for the moment, fixed $N \times N$ Hermitian

[1]The equations should be understood as matrix equations; B's are represented by matrices and f's as rows and columns.

matrix and f^i, $f_i^\dagger$, $i = 1, \ldots, N$ are fermionic operators satisfying the usual anticommutation relations. Using the appropriate unitary matrix U, the matrix X and the fermionic operators can be rewritten as

$$X_k^l = \sum_i U_i^{\dagger k} x_i U_l^i, \quad f_i^\dagger = \sum_k d_k^\dagger U_i^k, \quad f^j = \sum_l U_l^{\dagger j} d^l, \quad (4)$$

where x_i's are eigenvalues of the matrix X. Expressed in the new coordinates the Hamiltonian H_{FB} becomes

$$H_{FB} = \frac{1}{2}\sum_i x_i (d_i^\dagger d^i - d^i d_i^\dagger). \quad (5)$$

As the Hamiltonian H_{FB} does not change the number of fermions, the eigenstates can be chosen with definite number of fermions

$$|\Psi_{i_1,\ldots,i_n}\rangle = d_{i_1}^\dagger \cdots d_{i_n}^\dagger |0\rangle_f, \quad (6)$$

where $|0\rangle_f$ represents a fermionic vacuum with property $d_k|0\rangle_f = 0$. As usual, we interpret operator $d_i^\dagger$ as the creation operator for a fermion at level i with associated energy x_i, and $|\Psi_{i_1,\ldots,i_n}\rangle$ describes the state in which levels $i_1, \ldots, i_n$ are occupied while the rest of the levels are unoccupied. Therefore, the form of H_{FB} is completely determined by the requirement that the eigenvalues x_i are interpreted as the energy levels of a single fermion.

Next, we introduce a model where the matrix elements X_j^i are not fixed, but are random variables, the distribution of which is determined by a probability law $P(X_j^i)$. Then, we can naturally ask the question about densities of occupied and unoccupied levels in a certain state of the system. These are given by the expectation values of the operators

$$\rho^{\text{occ}}(x) = \sum_{i=1}^N \delta(x - x_i) d_i^\dagger d^i, \quad \rho^{\text{unocc}}(x) = \sum_{i=1}^N \delta(x - x_i) d^i d_i^\dagger. \quad (7)$$

For the fixed matrix X, the densities (7) in a generic eigenstate are given by the appropriate sums of the delta functions. Particularly, in the ground state of the system, the interval of nonvanishing density of occupied levels lies below the interval of nonvanishing density of unoccupied levels. The main consequence of introducing the distribution law $P(X_j^i)$ is that the sharp delta-functions' profiles are smeared, thus allowing the penetration of the density of the unoccupied levels into the interval in which density of occupied levels is nonzero and vice versa. In such a situation one expects that the gap between the highest occupied level and the lowest unoccupied level disappears. We explore this question in the setting where matrix X is a dynamical matrix, so that probability law $P(X_j^i)$ is a consequence of the quantization of the dynamical degrees of freedom[2] of the matrix X. In that case the matrix degrees of freedom contribute to the total energy of the system and to be specific, we assume that self-energy of the matrix X is determined by the following Hamiltonian:

$$H_B = \frac{1}{2}\sum_{ij} P_j^i P_i^j + \frac{\omega^2}{2}\sum_{ij} X_j^i X_i^j, \quad (8)$$

where $P_j^i = -i\partial/\partial X_i^j$ is momentum conjugate to X_i^j. After quantization, H_B can be expressed in terms of the appropriate bosonic operators and together with H_{FB}, which we now interpret as the Hamiltonian of fermion-boson interaction, constitute the system governed by the Hamiltonian (1). The parameter g defines fermion-boson interaction strength and can be taken as a positive number without loss of generality, since for negative g we can transform $X \to -X$.

In the following, we are interested in the behavior of densities (7) in the ground state of the system. In the strong coupling limit the dominant behavior of the ground state is determined by H_{FB}. This means that the suitable fermionic coordinates are the coordinates which diagonalize H_{FB}. Accordingly, we rewrite the Hamiltonian (1) in terms of x_i's, U_l^j's, $d_i^\dagger$'s, and d^j's defined by (4), expressing derivatives as [5]

$$\frac{\partial}{\partial X_l^k} = \sum_i U_k^i U_i^{\dagger l} \frac{\partial}{\partial x_i} + \sum_{i,j,m,m\neq i} \frac{U_k^i U_m^{\dagger l} U_j^m}{x_i - x_m} \frac{\partial}{\partial U_j^i} + \sum_{m,n,m\neq n} \frac{U_k^m U_n^{\dagger l}}{x_n - x_m} d_m^\dagger d^n. \quad (9)$$

This transformation of coordinates induces a nontrivial measure in the definition of the scalar product of the states. After performing similarity transformation and defining a new Hamiltonian $\tilde{H} = SHS^{-1}$ with S being $S = \prod_{i\neq j}(x_i - x_j)^{1/2}$, the scalar product of new states $|\tilde{\Psi}\rangle = S|\Psi\rangle$ is defined with respect to the desirable trivial measure. Finally, the Hamiltonian (1) can be recast into the following form:

$$\tilde{H} = -\frac{1}{2}\sum_k \frac{\partial^2}{\partial x_k^2} + \frac{\omega^2}{2}\sum_k x_k^2 + \frac{g}{2}\sum_k x_k (d_k^\dagger d^k - d^k d_k^\dagger) + \frac{1}{2}\sum_{m,n,m\neq n} \frac{L_m^n L_n^m}{(x_m - x_n)^2}, \quad (10)$$

where we defined for $n \neq m$

$$L_m^n = U_l^n \frac{\partial}{\partial U_l^m} - \frac{i}{2}(d_m^\dagger d^n - d^n d_m^\dagger). \quad (11)$$

The operators $L_m^n = U_m^{k\dagger} J_k^l U_l^n$ are transformed "angular momentum" generators J_k^l which commute with the Hamiltonian (1) and generate the unitary group. Assuming that the last term in the Hamiltonian (10) may be ignored, an assumption to be justified later on, the

[2]One might say that we approximate fundamentally random physics by more tractable Hamiltonian dynamics. The other point of view would be to attribute the success of RMT to the underlying Hamiltonian dynamics.

eigenstates of the Hamiltonian (10) can be written as[3]:

$$|\tilde{\Psi}\rangle = \tilde{\phi}(x_1, \ldots, x_n, y_1, \ldots, y_{N-n}) d_1^\dagger \cdots d_n^\dagger |0\rangle_f, \quad (12)$$

where coordinates x_i, $i = 1, \ldots, n$ correspond to occupied levels, while coordinates $y_j = x_{n+j}$, $j = 1, \ldots, N-n$ correspond to unoccupied levels. In the following, we require that function $\tilde{\phi}$ is antisymmetric under the exchange of two indices of the occupied levels and separately under the exchange of two indices of the unoccupied levels. Therefore, the proper state of the system is obtained by antisymmetrising the state (12) with respect to exchange of indices of occupied and unoccupied levels. The action of the Hamiltonian (10), without the last term, on the state (12) reduces to the action of the Hamiltonian $\tilde{H}_{\text{red}}$ on the wave function $\tilde{\phi}$, with $\tilde{H}_{\text{red}}$ given as

$$\tilde{H}_{\text{red}} = -\frac{1}{2}\sum_k \frac{\partial^2}{\partial \tilde{x}_k^2} + \frac{\omega^2}{2}\sum_k \tilde{x}_k^2 - \frac{1}{2}\sum_k \frac{\partial^2}{\partial \tilde{y}_k^2} + \frac{\omega^2}{2}\sum_k \tilde{y}_k^2, \quad (13)$$

where $\tilde{x}_i = x_i + g/2\omega^2$, $\tilde{y}_i = y_i - g/2\omega^2$. The properly symmetrized ground state of the Hamiltonian $\tilde{H}_{\text{red}}$ is

$$\tilde{\phi}_{\text{gs}} \sim \prod_{i\neq j}(\tilde{x}_i - \tilde{x}_j)^{1/2} \prod_{i\neq j}(\tilde{y}_i - \tilde{y}_j)^{1/2} \times e^{-(\omega/2)\sum_i \tilde{x}_i^2} e^{-(\omega/2)\sum_j \tilde{y}_j^2}. \quad (14)$$

Suppose now that we have exact ground state $|\Psi_{\text{exact}}\rangle$. Because of singularity for $x_i \approx y_j$ of the last term in the Hamiltonian (10), the exact ground state contains the prefactor $\prod_{i,j}(x_i - y_j)$ with the suitable power, as is usual in the Calogero-like models [8]. In the leading order in g the introduction of this prefactor into the state (14) results in multiplication of the state by a constant, and formally the appearance of this prefactor is out of the scope of present approximation. However, the important effect of this prefactor is that the contribution to the expectation value of the last term in the Hamiltonian (10) in the exact ground state reduces to the principal value integral avoiding singularity. Using the principal value prescription we can expand the integrand into powers of g, showing that this contribution in the state (14) is of order g^{-2} relative to the other terms in the Hamiltonian. This justifies our assumption that the last term of the Hamiltonian (10) may be ignored and the bosonic part of the ground state separates into the product of the part depending solely on the occupied levels and the part depending on the unoccupied levels. Using the usual methods from random matrix theory [9], evaluation of the densities (7) in approximate ground state gives

$$\langle \rho^{\text{occ}}(x)\rangle = e^{-\omega(x+g/2\omega^2)^2} \sum_{i=1}^{n} \frac{H_i^2(\sqrt{\omega}(x + \frac{g}{2\omega^2}))}{2^i i!\sqrt{\pi}},$$
$$\langle \rho^{\text{unocc}}(x)\rangle = e^{-\omega(x-g/2\omega^2)^2} \sum_{i=1}^{N-n} \frac{H_i^2(\sqrt{\omega}(x - \frac{g}{2\omega^2}))}{2^i i!\sqrt{\pi}}, \quad (15)$$

where $H_n(x)$ is the Hermite polynomial of order n.

In the limit $N - n$, $n \to \infty$, densities (15) reduce to Wigner's semicircle laws, as indicated in Fig. 1, with centers separated by g/ω^2 in accordance with the two-cut solution previously found [3]. This result shows that in the strong coupling limit we still have well-separated densities of occupied and unoccupied levels, although the probability nature of the levels dynamics allows mixing of levels. Furthermore, Eq. (15) shows that in the case of finite number of levels and finite number of fermions there exist states in the previously found homolumo gap [3]. Note that in precisely this regime, i.e., in the limit of strong interaction, the model defined by (1) was used as a toy model for QCD in the analysis of the spectrum of mesons and baryons [5].

In the case of weak interaction, up to first order in g we can write the Hamiltonian (1) as

$$H = e^{iH_{fb}} H_B e^{-iH_{fb}}, \quad (16)$$

where

$$H_{fb} = \frac{g}{2\omega^2}\sum_{l,k}(f_l^\dagger f^k - f^k f_l^\dagger) P_k^l. \quad (17)$$

The eigenstate of the Hamiltonian (16) is $|\Psi\rangle = e^{iH_{fb}}|\Phi\rangle$, where $|\Phi\rangle$ is an eigenstate of H_B. The density of occupied eigenvalues in this state is

$$\langle \rho^{\text{occ}}(x)\rangle = \langle \Psi | \sum_i d_i^\dagger d^i \delta(x - x_i) |\Psi\rangle = \sum_i \langle \Phi | e^{-iH_{fb}} d_i^\dagger d^i \delta(x - x_i) e^{iH_{fb}} |\Phi\rangle. \quad (18)$$

Expanding in g up to first order we obtain

$$\langle \rho^{\text{occ}}(x)\rangle = \langle \rho_0^{\text{occ}}(x)\rangle + \frac{g}{2\omega^2}\partial_x \langle \rho_0^{\text{occ}}(x)\rangle, \quad (19)$$

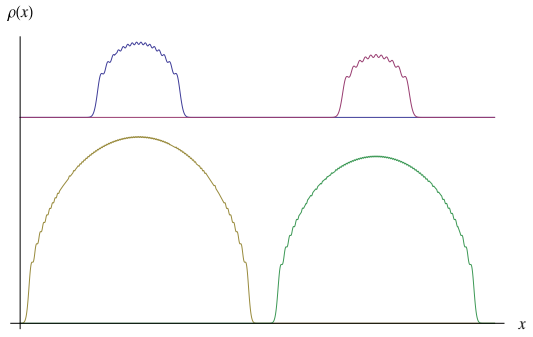

FIG. 1 (color online). Smoothing out the densities (15); on the upper graph is plotted $\rho^{\text{occ}}(n = 20)$ and $\rho^{\text{unocc}}(N - n = 15)$, and on the lower graph is plotted $\rho^{\text{occ}}(n = 100)$ and $\rho^{\text{unocc}}(N - n = 80)$, with $g/2\omega^2 = 15$.

[3]The condition that the eigenstate of the Hamiltonian H is antisymmetric with respect to exchange of two fermions implies that state transformed by aforementioned similarity transformation is symmetric with respect to this exchange. By this transformation the matrix degrees of freedom are effectively described as fermions.

where $\langle \rho_0^{\mathrm{occ}}(x)\rangle$ is the density of occupied levels for $g = 0$. Analogously we find

$$\langle \rho^{\mathrm{unocc}}(x)\rangle = \langle \rho_0^{\mathrm{unocc}}(x)\rangle - \frac{g}{2\omega^2}\,\partial_x\langle \rho_0^{\mathrm{unocc}}(x)\rangle. \qquad (20)$$

The case of weak interaction shows that starting with the system of bosons determined by the Hamiltonian H_B, introduction of boson-fermion interaction results in the displacement of the occupied levels by $-g/2\omega^2$ and unoccupied levels by $g/2\omega^2$, whatever these densities are in the case $g = 0$.

Moreover, one can show that even to the second order the boson-fermion interaction results only in the displacement of the of occupied levels by $-g/2\omega^2$ and unoccupied levels by $g/2\omega^2$. As this is exactly the result of the strong coupling approximation, one might speculate that this would be also true for the intermediate g. In that case, in the transition region where densities, although displaced, still overlap, as in Fig. 2, the total density of levels in the large N limit (the sum of two semicircle distributions) would display two (ignoring the end points) homolumo ''kinks.''

The appearance of the gap in our picture depends on the frequency ω, the interaction strength g, the number of levels N, and number of fermions n. The control over these parameters effectively controls the size of the gap. A possible disappearance of the gap, observed in reality, can be also interpreted within our picture as a consequence of the existence of the several subsystems whose gaps are arranged in appropriate way. Namely, one could introduce different frequencies ω_i in a bosonic part of the model, which would result in a different gap for each subsystem, and these could be arranged to overlap. This could provide a simple model for exploring the insertion of a single level into the gap.

Furthermore, the Hamiltonian (1) looks exactly as the Hamiltonian used to derive the linear Jahn-Teller effect [1],

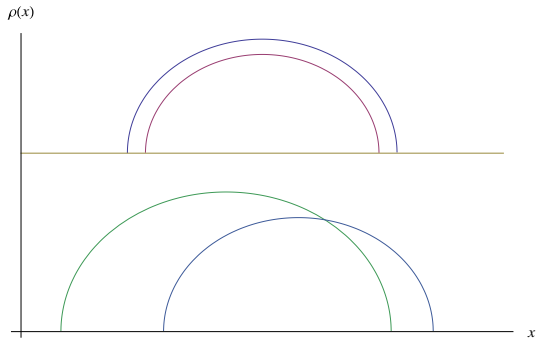

FIG. 2 (color online). We sketched development of the gap in the weak coupling limit for $N - n$, $n \to \infty$.

which says that due to the degeneracy of orbital fermion levels the symmetry of the molecule is broken in the ground state. Although in description of this effect the Hamiltonian (1) is defined in configuration rather than in momentum/energy space, the homolumo gap we observe can be interpreted as a manifestation of breaking of gauge symmetry, representing a generalization of the Jahn-Teller effect.

In our approach, the crucial point was the use of suitable unitary transformation that enabled us to diagonalize the model in both the strong and weak coupling approximations. On the other hand, using the conserved ''angular momentum'' generators and appropriate spectrum generating algebra, one should attempt to construct exact eigenstates of the system. We hope to report on the related results in future publications.

This work was supported by the Ministry of Science, Education and Sports of the Republic of Croatia under Contract No. 098-0982930-2861, and by ESF within the framework of the Research Networking Programme on ''Quantum Geometry and Quantum Gravity.''

[1] H. A. Jahn and E. Teller, Proc. R. Soc. A **161**, 220 (1937); M. Pope and C. E. Swenberg, *Electronic Processes in Organic Crystals and Polymers* (Oxford University Press, NY, 1999), 2nd ed..

[2] H. B. Nielsen, in *Proceedings of the Seventeenth Scottish Universities' Summer School in Physics, St. Andrews, 1976*, edited by I. M. Barbour and A. T. Davies (1977); D. L. Bennett, N. Brene, and H. B. Nielsen, Phys. Scr. **T15**, 158 (1987); C. D. Froggatt and H. B. Nielsen, *Origin of Symmetries* (World Scientific, Singapore, 1991); C. D. Froggatt and H. B. Nielsen, Ann. Phys. (Leipzig) **14**, 115 (2005); see also www.nbi.dk/~kleppe/random/qa/qa.html.

[3] I. Andrić, L. Jonke, D. Jurman, and H. B. Nielsen, Phys. Rev. D **77**, 127701 (2008).

[4] N. Iizuka and J. Polchinski, J. High Energy Phys. 10 (2008) 028.

[5] I. Affleck, Nucl. Phys. **B185**, 346 (1981); J. D. Lykken, Phys. Rev. D **25**, 1653 (1982).

[6] S. Alexandrov, arXiv:hep-th/0311273.

[7] J. L. Karczmarek and A. Strominger, J. High Energy Phys. 04 (2004) 055.

[8] F. Calogero, J. Math. Phys. (N.Y.) **10**, 2197 (1969); M. A. Olshanetsky and A. M. Perelomov, Phys. Rep. **94**, 313 (1983); I. Andrić and D. Jurman, J. High Energy Phys. 01 (2005) 039.

[9] M. L. Mehta, *Random Matrices* (Academic Press, New York, 1991), 2nd ed..

[10] T. Guhr, A. Mueller-Groeling, and H. A. Weidenmueller, Phys. Rep. **299**, 189 (1998).