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Exact diagonalization of many-fermion Hamiltonian with wave-function renormalization

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We propose a method of determining states for correlated fermions in Fock space, which we supplement with the Lagrange-Euler equation for the single-particle wave functions $\{w_i(\mathbf{r})\}$ contained in the microscopic parameters. The equation is derived by treating the ground state energy of the interacting system as a functional of $\{w_i(\mathbf{r})\}$. The method is applied to a linear chain up to $N=10$ atoms with all pair interactions and all hopping integrals included. Renormalized Wannier functions, the parameters, the distribution function, and the dimerization energy, are all discussed as a function of the lattice parameter.

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In the description of interacting fermions, the second-quantized form of Hamiltonian[1] (or Lagrangian[2]) is often used, which is diagonalized subsequently, and the ground state energy and other characteristics are expressed as a function of the interaction parameters $V_{ijkl}=\langle w_i w_j|V_{12}|w_k w_l\rangle$, where V_{12} is the interaction for a single pair, and $\{w_i \equiv w_i(\mathbf{r})\}$ is an arbitrary (but complete) single-particle basis, with the help of which we define the field operator $\hat{\Psi}_\sigma(\mathbf{r})=\Sigma_{i\sigma} w_i(\mathbf{r})\chi_\sigma a_{i\sigma}$ for the spin state $\sigma=\pm 1$. In effect, the Hamiltonian takes the usual form $H=\Sigma t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + \Sigma V_{ijkl} a^\dagger_{i\sigma} a^\dagger_{j\sigma'} a_{l\sigma'} a_{k\sigma}$, where $t_{ij}=\langle w_i|T|w_j\rangle$ is the hopping matrix element and *T* is the corresponding one-particle energy operator. In this paper we propose the method of optimizing the wave functions $\{w_i(\mathbf{r})\}$ in the Hilbert space, which is performed only after the diagonalization in Fock space has been carried out first.

Such a method has a few advantages. First, as the Fock and Hilbert spaces are separate, the optimization leads to the *renormalized wave equation* for the single-particle wave function in an interacting environment defined in special cases in Ref. 3. Within the existing insightful approach,[4] the single-particle wave function is defined first and then the corresponding electronic correlations are incorporated in an approximate manner. Therefore, the present two-step procedure in a reverse order is strictly speaking possible only in the situation when the exact solution of the many-particle model is available[5] or the numerical diagonalization executable.[6] Secondly, the proposed method is of fundamental importance when the interaction introduces a nonperturbative aspect to the solution (e.g., for the one-dimensional Hubbard model, where the insulating state sets in for an arbitrarily small interaction *U*,[7] or for small systems such as correlated quantum dots). Thirdly, the present method represents the second step in solving models of interacting particles, as it removes the arbitrariness in selecting the basis $\{w_i(\mathbf{r})\}$ when defining $\hat{\Psi}_\sigma(\mathbf{r})$ and *H*, and thus connects the first- and second-quantization aspects of the system analysis. Finally, and probably most importantly, the determination of the basis $\{w_i(\mathbf{r})\}$ allows for an analysis of the system properties as a function of interatomic distance, not only as a function of the microscopic parameters, which are also calculated explicitly. In addition, a number of factors (e.g., the atomic part of the energy) vary with the distance and thus the analysis in terms of model parameters may turn out to be insufficient.

We consider electrons with the Coulomb interaction $V_{12}=e^2/|\mathbf{r}_1-\mathbf{r}_2|$. Then the ground state energy for the system can be written as

$$E_G \equiv \langle H\rangle = \sum_{ij} t_{ij} C_{ij} + \frac{1}{2}\sum_{ijkl} V_{ijkl} C_{ijkl}, \tag{1}$$

where

$$C_{ij}=\sum_\sigma \langle a^\dagger_{i\sigma} a_{j\sigma}\rangle,$$

$$C_{ijkl}=\sum_\sigma \langle a^\dagger_{i\sigma} a^\dagger_{j\sigma} a_{l\sigma} a_{k\sigma} + a^\dagger_{i\sigma} a^\dagger_{j\bar{\sigma}} a_{l\bar{\sigma}} a_{k\sigma}\rangle,$$

and $\bar{\sigma}=-\sigma$. The correlation functions have the form of functionals $C_{ij}(t_{ij},V_{ijkl})$ and $C_{ijkl}(t_{ij},V_{ijkl})$ defined for the basis functions $\{w_i(\mathbf{r})\}$. Therefore, the diagonalization in Fock space should be supplemented by minimization of the functional

$$\mathcal{F}\{w_i\} = E_G\{w_i\} - \sum_{i\leqslant j} \lambda_{ij}\left(\int d^3r\, w_i^*(\mathbf{r}) w_j(\mathbf{r}) - \delta_{ij}\right), \tag{2}$$

where the Lagrange multipliers λ_{ij} express the fact that the basis $\{w_i(\mathbf{r})\}$ should be orthonormal. Hence, the Lagrange-Euler equations can be symbolically written as

$$\sum_{ij} \frac{\partial E_G}{\partial t_{ij}} \frac{\delta t_{ij}}{\delta w_n^*(\mathbf{r})} + \sum_{ijkl} \frac{\partial E_G}{\partial V_{ijkl}} \frac{\delta V_{ijkl}}{\delta w_n^*(\mathbf{r})} - \sum_{i\leqslant n} \lambda_{in} w_i(\mathbf{r}) = 0. \tag{3}$$

This equation can be called the renormalized wave equation for the wave functions $\{w_i(\mathbf{r})\}$ in the interacting environment.

To specify the basis on the lattice we construct the exact Wannier functions (for a single band) with the help of atomic functions $\{\psi_i(\mathbf{r}) \equiv \psi(\mathbf{r}-\mathbf{R}_i)\}$ in the following way:

$$w_i(\mathbf{r}) = \sum_{j=1}^{N} \beta_{i-j}\psi_j(\mathbf{r}), \tag{4}$$

with

$$\beta_p = N^{-1}\sum_{\mathbf{k}} \left\{ \sum_{p'} S_{p'}\cos(\mathbf{k}\cdot\mathbf{R}_{p'}) \right\}^{-1/2} \cos(\mathbf{k}\cdot\mathbf{R}_p),$$

where $S_p \equiv \langle \psi_i | \psi_{i+p} \rangle$ is the overlap integral for pth neighbors and $\mathbf{R}_p$ is the lattice site position. In that situation, the orthonormality is built in automatically and then Eq. (3) reduces to the form

$$\sum_{iji'j'} \frac{\partial E_G}{\partial t_{ij}} \frac{\partial t_{ij}}{\partial t'_{ij}} \frac{\delta t'_{ij}}{\delta \psi(\mathbf{r})} + \sum_{ijkli'j'k'l'} \frac{\partial E_G}{\partial V_{ijkl}} \frac{\partial V_{ijkl}}{\partial V'_{i'j'k'l'}} \times \frac{\delta V'_{i'j'k'l'}}{\delta \psi(\mathbf{r})} = 0, \tag{5}$$

where $t'_{ij} \equiv \langle \psi_i | T | \psi_j \rangle$ and $V'_{ijkl} = \langle \psi_i \psi_j | V_{12} | \psi_k \psi_l \rangle$ are the matrix elements in the atomic (nonorthogonal) basis. The variational derivative is defined in a slightly nonstandard manner.[8] Noting that $t_{ij} = \Sigma_{i'j'} \beta_{ii'} \beta_{jj'} \langle \psi_i | T | \psi_j \rangle = \Sigma_{i'j'} \beta_{ii'} \beta_{jj'} t'_{i'j'}$ and $V_{ijkl} = \Sigma_{i'j'k'l'} \beta_{ii'} \beta_{jj'} \beta_{kk'} \beta_{ll'} V'_{i'j'k'l'}$, we easily obtain the derivatives $\partial t_{ij} / \partial t'_{ij}$ and $\partial V_{ijkl} / \partial V'_{i'j'k'l'}$. The variational derivatives can also be obtained explicitly; for example,

$$\frac{\delta t'_{ij}}{\delta \psi(\mathbf{r})} = T(\mathbf{R}_i - \mathbf{r})\,\psi(\mathbf{R}_i - \mathbf{R}_j + \mathbf{r}) + T(\mathbf{R}_j - \mathbf{r})\,\psi(\mathbf{R}_j - \mathbf{R}_i + \mathbf{r}), \tag{6}$$

and analogously for $\delta V'_{ijkl} / \delta \psi(\mathbf{r})$. As a result, the system of equations is closed provided we know the expression for the ground state energy of the interacting system. Here we apply the procedure to a short chain and discuss physical results as a function of $R \equiv |\mathbf{R}_{ij}|$.

The Hamiltonian containing N sites with all two-center interactions and for the linear chain with periodic boundary conditions can be written as

$$H = \sum_{i=0}^{N-1} (\epsilon_a n_i + U n_{i\uparrow} n_{i\downarrow}) + \sum_{j=0}^{i-1} \Bigg\{ \left(K_{ij} - \frac{1}{2} J_{ij} \right) n_i n_j - 2 J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\sigma} [t_{ij} + V_{ij}(n_{i\bar{\sigma}} + n_{j\bar{\sigma}})](a^{\dagger}_{i\sigma} a_{j\sigma} + a^{\dagger}_{j\sigma} a_{i\sigma}) + J_{ij}(a^{\dagger}_{i\uparrow} a^{\dagger}_{i\downarrow} a_{j\downarrow} a_{j\uparrow} + \mathrm{H.c.}) \Bigg\}, \tag{7}$$

where the first three terms represent, respectively, the atomic energy and intra- and intersite Coulomb interactions, the fourth describes Heisenberg exchange, the fifth is composed of the hopping term (together with the so-called correlated hopping $\sim V_{ij}$), and the last expresses pair hopping processes. The intersite parameters are: $K_{ij} = \langle w_i w_j | V_{12} | w_j w_i \rangle$, etc.

As established above, the parameters ϵ_a, U, t_p, K_p, J_p, and V_p (for $p = |i-j|$) can be transformed to the atomic basis, where they can be explicitly calculated (the Slater integrals) for the $1s$-type trial wave function $\psi_i(\mathbf{r}) = (\alpha^3/\pi)^{1/2} \exp(-\alpha|\mathbf{r} - \mathbf{R}_i|)$, where α is the variational parameter. For example,

$$\epsilon_a = \sum_q \beta_q^2 \epsilon'_a + 2 \sum_{qr(q>r)} \beta_q \beta_r t'_{q-r},$$

$$t_p = \sum_q \beta_q \beta_{p-q} \epsilon'_a + 2 \sum_{qr(q>r)} \beta_q \beta_{p-r} t'_{q-r},$$

$$U = \sum_q \beta_q^4 U' + 2 \sum_{qr(q>r)} [\beta_q^2 \beta_r^2 (K'_{q-r} + 2 J'_{q-r}) + 8 \beta_q^3 \beta_r V'_{q-r}],$$

$$K_p = \sum_q \beta_q^2 \beta_{p-q}^2 U' + 2 \sum_{qr(q>r)} \beta_q^2 \beta_{p-r}^2 K'_{p-r} + 4 \sum_{qr(q>r)} \beta_q \beta_{p-q} \beta_r \beta_{p-r} J'_{q-r} + 4 \sum_{qr(q>r)} (\beta_q^2 \beta_{p-q} \beta_{p-r} + \beta_q \beta_{p-q}^2 \beta_r) V'_{q-r}, \quad \text{etc.} \tag{8}$$

Additionally, as we include also all hopping terms for chains up to $N \leqslant 10$ atoms, it is necessary to calculate the hopping integrals between the sites i and j containing the potential of the kth atom, which in atomic units takes the form

$$t'_{ij} = \langle \psi_i | -\nabla^2 - \sum_k \frac{2}{r_k} | \psi_j \rangle \equiv \tau_0 - 2 \sum_k \tau_{ikj}, \tag{9}$$

where $\tau_0 = \langle \psi_i | -\nabla^2 | \psi_j \rangle = \alpha^2 e^{-\alpha a}(1 + \alpha a - \frac{1}{2}\alpha^2 a^2)$, $a = |\mathbf{R}_i - \mathbf{R}_j|$, $i < k < j$, and

$$\tau_{ikj} = \left(\frac{\alpha^3}{\pi} \right) \int d^3 r \, \frac{\exp[-\alpha(|\mathbf{r} - \mathbf{R}_i| + |\mathbf{r} - \mathbf{R}_j|)]}{|\mathbf{r} - \mathbf{R}_k|}, \tag{10}$$

which is calculated in spheroidal coordinates.

The bare and renormalized Wannier functions obtained for an exactly diagonalized chain of $N = 8$ atoms are depicted in Fig. 1 for the interatomic distance $R = 2a_0$ (a_0 is the Bohr radius). The repulsive interaction shrinks the Wannier function remarkably, even though all hopping terms have been included. The renormalized values of the microscopic parameters for different R values are presented in Table I. We note two essential features of these results: (i) the atomic energy ϵ_a depends relatively strongly on the distance, and (ii) the intersite Coulomb interaction falls off slowly and has the asymptotic form $K_{ij} \approx 2/R_{ij}$ (in Ry). The exchange integral (J_1) and the correlated hopping (V_{ij}) have amplitudes at least two orders of magnitude smaller than U or K_1. The renormalized hopping t_1 is almost an order of magnitude larger than either t_2 or t_3, making the tight-binding approximation realistic.

The momentum distribution function $n_{k\sigma} = \langle 0 | a^{\dagger}_{k\sigma} a_{k\sigma} | 0 \rangle$ for different lattice parameters R is presented for $N = 10$ in Fig. 2. For a small lattice constant ($R = 2a_0$) a clear sign of

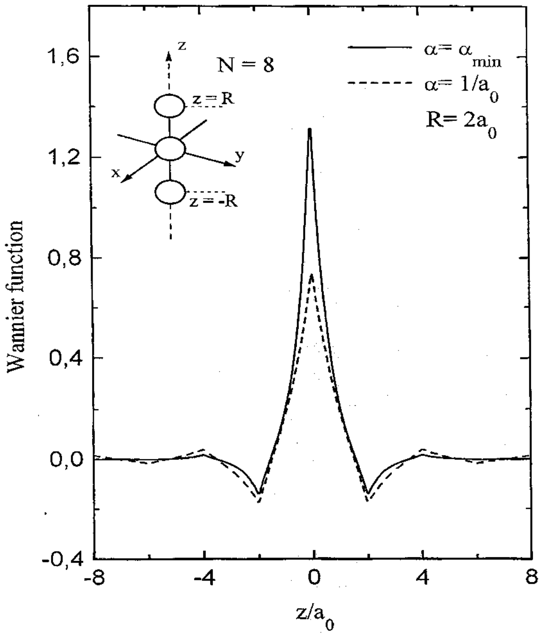

FIG. 1. Renormalized (solid line) and bare (dashed line) Wannier functions for the chain of $N=8$ atoms. All overlap integrals S_{ij} have been taken into account for the interatomic distance $R=2a_0$ $(a_0 \simeq 0.53 rA)$.

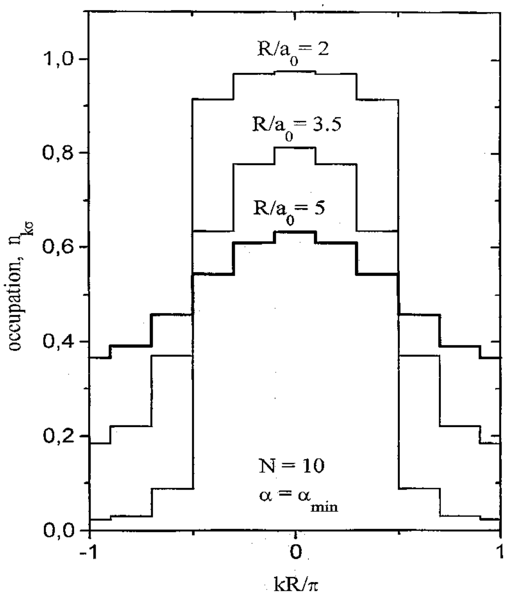

FIG. 2. Momentum distribution $n_{\mathbf{k}\sigma}$ for electrons in the first Brillouin zone for a chain of $N=10$ atoms and the interatomic distances R specified. All pair interactions and hopping integrals are included.

the Fermi wave vector $k_F \sim \pi R/2$ (corresponding to the half-filled band) is present, whereas for $R \geqslant 5a_0$ $n_{k\sigma}$ is smeared out throughout the Brillouin zone, meaning that a metal-insulator transformation is taking place for R in between. Unfortunately, the small size of the system does not allow us to differentiate between the Fermi- and Luttinger-liquid types of behavior.[9] The extension to larger $N \sim 10^2$ with the help of the e.g., DMRG method[10] would be required to clarify this point. The ground state $|0\rangle$ of the system for any N is a true singlet, i.e., with $\langle 0|\Sigma_{i=1}^{N}\mathbf{S}_i|0\rangle = 0$.

As the method determines the evolution of the system with increasing lattice constant, we also calculate the amplitude of the zero-point motion of the nuclei. For the chain with masses m and M of electrons and ions, respectively, we can determine the mean-square amplitude. For $N=10$ and $R/a_0 = 3$–4 it is of the order 0.067 (7%) (for $M=M_H \simeq 1838m$), whereas the corresponding increase of E_G is $\sim 10^{-2}$ Ry (note that $\partial^2 E_G/\partial R^2$ has been obtained numerically). Leaving this interesting feature of the proposed approach to a detailed discussion elsewhere, we mention here the special test, namely, the possibility of lattice dimerization. In Fig. 3 we have repeated all diagonalization procedure in the dimerized state and plotted the change in $E_G(R)$ in that state, with R_1 as the shorter lattice parameter (R is then the average lattice parameter). We observe a clear sign of dimerization $(1-R_1/R \sim 0.15)$ around $R \sim (3$–$5)a_0$. These calculations, while making the computation longer by an order of magnitude, prove that neither the zero-point motion nor the dimerization greatly influences the values of electronic parameters displayed in Table I, as they almost compensate each other.

Two basic aspects of the method should be explained. First, the linear chain with isotropic orbitals is globally stable only in special situations.[3] This means that in order to stabilize such a configuration of a linear chain we have to either put the system in an external binding potential (e.g., make a correlated quantum dot on the substrate) or consider anisotropic orbitals, e.g., sp^3 hybrids. Both these projects are executable, but make the calculations purely numerical and thus unsuitable for the type of discussion presented above. The second aspect concerns the relatively long-range nature of the interaction K_{ij} (cf. Table I) which one can overcome by redefining the atomic level position in the following man-

TABLE I. Microscopic parameters (in Ry) as a function of interatomic distance R for different neighbors $p=1,2,3$.

R/a_0	ϵ_a	t_1	$10^3 t_2$	$10^3 t_3$	U	K_1	K_2	K_3	$10^3 J_1$	$10^3 V_1$	$10^3 V_2$
2.0	−4.043	−0.585	89.6	−98.3	2.301	1.077	0.676	0.450	9.54	−18.07	33.58
2.5	−3.734	−0.331	45.5	−45.0	1.949	0.843	0.499	0.331	7.39	−17.45	19.58
3.0	−3.422	−0.200	24.4	−21.9	1.717	0.692	0.391	0.259	5.59	−16.08	11.95
4.0	−2.916	−0.083	7.4	−5.3	1.452	0.508	0.269	0.179	2.90	−12.92	4.49
5.0	−2.558	−0.037	4.2	−2.7	1.327	0.403	0.206	0.138	1.26	−9.64	1.56

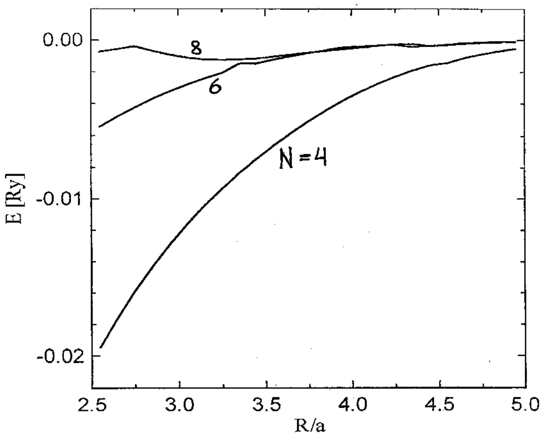

FIG. 3. Ground state energy change in the dimerized state for $N=4$–8 atoms vs average interatomic distance.

ner: $\epsilon_a^{eff} \equiv \epsilon_a + N^{-1}\Sigma_{i<j}(2/R_{ij}+K_{ij})$. In effect, the effective electronic model containing the lattice contribution $(2/R_{ij}$ [Ry]) implicitly in ϵ_a^{eff} is represented by the Hamiltonian

$$H_R = \sum_i (\epsilon_a^{eff} n_i + U n_{i\uparrow} n_{i\downarrow}) + \sum_{ij}{}' t_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + \sum_{i<j} K_{ij}\delta n_i \delta n_j , \qquad (11)$$

where $\delta n_i \equiv n_i - 1$. We have neglected the terms $\sim J_{ij}$ and $\sim V_{ij}$, as they provide much smaller contributions. In Table II we list the intersite correlation function $\langle \delta n_i \delta n_{i+p} \rangle$ and show that indeed the residual intersite interaction [last term in Eq. (11)] decays with increasing p, making the application of a procedure such as DMRG possible. The reason for the decomposition in Eq. (11) is that the attractive potential acting on an electron located on site i from neighboring ions is $(-4/R_{ij})$. This attraction is roughly compensated by the electron repulsions $K_{ij} \sim 2/R_{ij}$ and the ion-ion part $(2/R_{ij})$. Therefore, we are left effectively with the *purely electronic* part, with R dependent parameters.

TABLE II. Intersite discrete density-density correlation functions versus interatomic distance.

R/a_0	$\langle \delta n_i \delta_{n+1} \rangle$	$\langle \delta n_i \delta_{n+2} \rangle$	$\langle \delta n_i \delta_{n+3} \rangle$
2.0	-0.1312	-1.02×10^{-3}	-4.4×10^{-3}
2.5	-0.1022	-5.2×10^{-3}	-2.0×10^{-3}
3.0	-0.0707	-2.4×10^{-3}	-1.4×10^{-3}
4.0	-0.0245	-3.4×10^{-4}	-1.4×10^{-4}
5.0	-0.0068	-3.5×10^{-5}	-8×10^{-6}

In summary, we have devised a method of solving the models of interacting fermions on a lattice, combined with the *a posteriori* optimization of the single-particle wave function contained in their microscopic parameters. The results are obtained as a function of lattice parameter (there are up to ten microscopic parameters we calculate explicitly). We apply this approach to a finite ($N \leq 10$) linear chain, with all hopping elements and all pair interactions included. In this manner, the approach puts on a firm basis the variational optimization of orbitals,[11] since we use, albeit in a model situation, an exact expression for the total energy. The method, nonperturbative in nature, can be applied to *ab initio* description of correlated quantum dots and to two-dimensional cluster systems, both as a function of interatomic distance.

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