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RIGOROUS BOUNDS ON THE FREE ENERGY OF ELECTRON–PHONON MODELS

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We present a collection of rigorous upper and lower bounds to the free energy of electron–phonon models with linear electron–phonon interaction. These bounds are used to compare different variational approaches. It is shown rigorously that the ground states corresponding to the sharpest bounds do not exhibit Off-Diagonal Long-Range Order in the two-particle density matrix.

1. Introduction

The Hamiltonian of a model describing the interaction of electrons and lattice deformations can be written as

$$H = \sum_{i,j} \sum_{\sigma=\uparrow,\downarrow} c^+_{i,\sigma} T_{i,j}(\{x_k\},\mu) c_{j,\sigma} + \sum_i \frac{p_i^2}{2M} + \sum_{i,j} \frac{x_i K_{i,j} x_j}{2}\,, \tag{1}$$

where $c^+_{i,\sigma}$ and $c_{i,\sigma}$ are the fermion creation and annihilation operators, respectively, for an electron with spin $\sigma = \uparrow, \downarrow$ at the generalized site index i, $T_{i,j}(\{x_k\},\mu)$ specifies the free-electron energy for a fixed lattice deformation (e.g. the hopping matrix elements (if $i \neq j$) as well as the local potential (if $i = j$)), and is assumed to be a linear function of the phonon coordinates $\{x_i\}$. Occasionally we will use the linear character of the electron–phonon interaction explicitly by writing

$$T_{i,j}(\{x_k\},\mu) = T^{(0)}_{i,j}(\mu) + T^{(1)}_{i,j}(\{x_k\})\,. \tag{2}$$

As we will work with the grand canonical ensemble throughout, it is convenient to absorb in $T_{i,j}$ the term proportional to the chemical potential μ. As usual p_i denotes the momentum operator of the oscillator with index i. The mass of the oscillators is denoted by M and $K_{i,j}$ is the matrix of oscillator spring constants. As usual T and K are hermitian matrices. As most of the results presented below do not depend on the dimensionality and connectivity of the lattice we will not specify the matrix

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T any further. The form of (2) is sufficiently general to encompass all standard electron–phonon (EP) models such as the Holstein model, the Su–Schrieffer–Heeger (SSH) model, the Fröhlich polaron model, etc.

For brevity we will write (2) in the more compact form

$$H = c^+ T(x,\mu) c + \frac{p^2}{2M} + \frac{x^+ K x}{2}\,, \tag{3}$$

where $c^+ = (c^+_{1,\uparrow}, \ldots, c^+_{L,\uparrow}, c^+_{1,\downarrow}, \ldots, c^+_{L,\downarrow})$, $c = (c^+)^\dagger$, etc. The number of lattice sites is denoted by L. As model (3) is block-diagonal with respect to the spin label we have

$$T = \begin{pmatrix} (T_{i,j}) & 0 \\ 0 & (T_{i,j}) \end{pmatrix}\,, \tag{4}$$

and we will implicitly assume that any matrix X that appears in expressions such as $c^+ X c$ will have an identical structure.

The purpose of this paper is to present a number of rigorous bounds on the free energy and ground state energy of (1). These bounds are relatively easy to compute (numerically) and are used to assess the range of applicability of the Quantum Molecular Dynamics (QMD) simulation technique recently introduced by two of us.[1,2] The basic idea of this approach is to decompose the propagator of (1) in such a way that it becomes possible to compute, from first-principles, the static and dynamic properties of (1) with high precision. An advantage of this approach over conventional Quantum Monte Carlo techniques[3] is the absence of numerical instabilities, minus-sign problems, and the analytical continuation or MaxEnt procedures. The upper and lower bounds presented below also suggest various ways of extending the range of the QMD technique with little extra computational effort. We also prove that the states of the system, corresponding to the sharpest bounds derived in this paper, do not exhibit Off-Diagonal Long-Range-Order (ODLRO) in the two-particle density matrix.[4]

The outline of the paper is as follows. An overview of the tools needed is given in Sec. 2. In Sec. 3, we derive some upper bounds to the partition function. In Sec. 4 we construct two lower bounds and we combine the results of Secs. 3 and 4 to obtain upper and lower bounds to the ground state energy of the EP-model (1). We illustrate the use of these bounds by applying it to the SSH model. In Sec. 5 we specialize to the Holstein model, derive upper and lower bounds to the free energy and relate some of these bounds to the free energy of the Hubbard model and the Bardeen–Cooper–Schrieffer (BCS) trial Hamiltonian. Some rigorous results on the existence of ODLRO are given in Sec. 6.

2. Tools

Our main tools to derive upper and lower bounds are the Golden–Symanzik–Thompson (GTS) inequality[5–7]

$$\mathrm{Tr}\, e^{A+B} \leq \mathrm{Tr}\, e^A e^B = \mathrm{Tr}\, e^{A/2} e^B e^{A/2}\,, \tag{5}$$

a generalized form of Jensen's inequality,[8]

$$\operatorname{Tr} e^{A+B} \geq \exp\left(\frac{\operatorname{Tr} e^{A} B}{\operatorname{Tr} e^{A}}\right) \operatorname{Tr} e^{A}, \tag{6}$$

the Lie–Trotter formula[9–12]

$$e^{A+B} = \lim_{m\to\infty} (e^{A/m} e^{B/m})^{m}, \tag{7}$$

and some of its generalizations.[13–15]

We also need identity[3]

$$\operatorname{tr} e^{c^{+}X_1 c} \cdots e^{c^{+}X_n c} = \det(1 + e^{X_1} \cdots e^{X_n})^{2}, \tag{8}$$

where tr denotes the trace over all possible electron states, and the X_i's are arbitrary $L \times L$ matrices. The proof of (8) relies on the fact that each of the exponentials at the l.h.s. is a quadratic form in the fermion operators. Equations (5) and (8) imply

$$\det(1 + e^{A+B}) \leq \det(1 + e^{A} e^{B}) = \det(1 + e^{A/2} e^{B} e^{A/2}). \tag{9}$$

From (8) it follows that[3]

$$\frac{\operatorname{tr} e^{c^{+}X_1 c} \cdots e^{c^{+}X_n c} c^{+} Y c}{\operatorname{tr} e^{c^{+}X_1 c} \cdots e^{c^{+}X_n c}} = 2 \operatorname{Sp} Y (1 + e^{-X_n} \cdots e^{-X_1})^{-1}, \tag{10}$$

where $\operatorname{Sp} X \equiv \sum_{i=1}^{L} X_{i,i}$ denotes the trace of the $L \times L$ matrix X. The factor of two in front of Sp is due to the fact that the electrons have spin.

3. Upper Bounds to the Partition Function

Application of the above inequalities to the EP model requires a choice of the decomposition of the Hamiltonian (3). Of particular interest are decompositons that lead to upper and lower bounds that are easy to compute. Decomposing (3) as

$$\begin{gathered} H = H_1 + H_2, \\ H_1 = \frac{p^2}{2M}, \qquad H_2 = c^{+} T(x,\mu) c + \frac{x^{+} K x}{2}, \end{gathered} \tag{11}$$

and application of the GTS inequality yields for the partition function

$$Z \equiv \operatorname{Tr} e^{-\beta H} \leq Z_1 \equiv \operatorname{Tr} e^{-\beta H_1} e^{-\beta H_2}, \tag{12a}$$

$$= \int dx \langle x | e^{-\beta p^2/2M} | x \rangle \rho_1(x) \operatorname{tr} e^{-\beta c^{+} T(x,\mu) c}, \tag{12b}$$

$$= \left(\frac{M}{2\pi\beta\hbar^2}\right)^{L/2} \int dx\ \rho_1(x) \operatorname{tr} e^{-\beta c^{+} T(x,\mu) c}, \tag{12c}$$

$$= \left(\frac{M}{2\pi\beta\hbar^2}\right)^{L/2} \int dx\ \rho_1(x)\ \det(1 + e^{-\beta T(x,\mu)})^{2}, \tag{12d}$$

where $\rho_1(x) \equiv e^{-\beta x^{+} K x/2}$.

In deriving upperbound (12b) use has been made of the fact that H_2 is diagonal with respect to the oscillator coordinates. The standard result[16]

$$\langle x_i|e^{-\beta p_i^2/2M}|x_i'\rangle = \sqrt{\frac{M}{2\pi\beta\hbar^2}}e^{-M(x_i-x_i')/2\beta\hbar^2}\,, \tag{13}$$

was used to go from (12b) to (12c). The multiple integrals appearing in (12) (as well as in the other bounds presented below) are readily calculated by standard numerical simulation methods.[17] Accordingly, for any specific EP model of the type (1) it is possible to actually compute these bounds.

The inequality (12) becomes an equality if the mass of the oscillators tends to infinity, i.e.

$$\lim_{M\to\infty} M^{-L/2}Z = \lim_{M\to\infty} M^{-L/2}Z_1\,. \tag{14}$$

At zero temperature, taking this limit is tantamount to making the adiabatic approximation in which the phonon coordinates are determined by minimizing the expectation value of H_2.

Upperbound (12) can be improved by decomposing the EP-Hamiltonian as $H = H_3 + H_4$ where

$$H_3 = \frac{p^2}{2M} + \frac{gx^+Kx}{2}, \qquad H_4 = c^+T(x,\mu)c + \frac{(1-g)x^+Kx}{2}\,, \tag{15}$$

and repeating the steps that led to (12). The parameter $0 \le g < 1$ has been introduced to assure that H_4 is bounded from below, a property that will prove useful to obtain lower bounds on the ground state energy. It is convenient to bring H_3 into diagonal form

$$H_3 = \frac{\tilde{p}^2}{2M} + \frac{gM\tilde{x}^+\omega^2\tilde{x}}{2}\,, \tag{16}$$

where $\tilde{x}_k = \sum_j U_{k,j}x_j$, $\tilde{p}_k = \sum_j U_{k,j}p_j$ and U is the unitary transformation that diagonalizes K. The matrix $\omega = \delta_{k,k'}\omega_k$ is, by construction, diagonal. Using the exact expression for the propagator of the harmonic oscillator[16]

$$\langle\tilde{x}_k|e^{-\beta(p_k^2/2M+M\omega_k^2x_k^2/2)}|\tilde{x}_k'\rangle$$

$$= \sqrt{\frac{M\omega_k}{2\pi\hbar\,\sinh\,\beta\hbar\omega_k}}\exp\left\{-\frac{M\omega_k[(\tilde{x}_k^2+\tilde{x}_k'^2)\cosh\,\beta\hbar\omega_k - 2\tilde{x}_k\tilde{x}_k']}{2\hbar\,\sinh\,\beta\hbar\omega_k}\right\}\,, \tag{17}$$

we obtain the upperbound

$$Z \le Z_2(g) \equiv \left(\frac{M\omega_k\sqrt{g}}{2\pi\hbar\,\sinh\,\beta\hbar\omega_k\sqrt{g}}\right)^{L/2}\int d\tilde{x}\;\rho_2(\tilde{x},g)\;\det(1+e^{-\beta T(\tilde{x},\mu)})^2\,, \tag{18a}$$

with

$$\rho_2(\tilde{x},g) \equiv e^{-\beta(1-g)M\tilde{x}^+\omega^2\tilde{x}/2}\exp\left[-\frac{\beta gM}{2}\tilde{x}^+\omega^2\frac{\tanh\,\beta\hbar\omega\sqrt{g}/2}{\beta\hbar\omega\sqrt{g}/2}\tilde{x}\right]\,. \tag{18b}$$

From decomposition (15) it follows immediately that inequality (18) becomes an equality for zero EP-coupling.

Upperbound (18) is as easy to compute as upperbound (12) as can be seen by rewriting (18b) as

$$\rho_2(x, g) = e^{-\beta x^+ \tilde{K}(\beta\hbar)x/2}, \tag{19}$$

where

$$\tilde{K} \equiv \tilde{K}(\beta\hbar)_{j,j'} = (1-g)K_{j,j'} + \frac{2\sqrt{g}M}{\beta\hbar}\sum_k U^\dagger_{j,k}\omega_k \tanh\frac{\beta\hbar\omega_k\sqrt{g}}{2}U_{k,j'}, \tag{20}$$

is the matrix of "renormalized" spring constants. From (20) it follows that

$$\lim_{\beta\hbar\ \max_k(\omega_k)\to 0} \tilde{K} = K. \tag{21}$$

Furthermore it is easy to convince oneself that

$$Z \le Z_2(g) \le Z_1. \tag{22}$$

At zero temperature (22) yields, for the ground state energy E_0, the lower bounds

$$E_0^{(A)}(1) \le \sqrt{g}E_0^{(p)} + E_0^{(A)}(1-g) \le E_0, \tag{23}$$

where $E_0^{(p)}$ is the ground-state energy of the phonon system and

$$E_0^{(A)}(\gamma) = \min_{\{x\}}\left[\frac{\gamma x^+ Kx}{2} - 2\lim_{\beta\to\infty}\beta^{-1}\,\mathrm{Sp}\,\ln(1+e^{-\beta T(x,\mu)})\right], \tag{24}$$

is the ground-state energy of model (with modified couplings γK) in the adiabatic limit.

4. Lower Bounds to the Partition Function

As we have assumed that the EP interaction is linear in the phonon coordinates a first, rather trivial, lower bound follows from the decomposition $H = H_\mathrm{p} + H_\mathrm{e} + H_\mathrm{ep}$ where

$$H_\mathrm{p} = \frac{p^2}{2M} + \frac{x^+Kx}{2}; \qquad H_\mathrm{e} = c^+T^{(0)}(\mu)c; \qquad H_\mathrm{ep} = c^+T^{(1)}(x)c. \tag{25}$$

Using inequality (6) we find

$$Z \ge \mathrm{Tr}\, e^{-\beta(H_\mathrm{e}+H_\mathrm{p})}\exp(-\beta\langle H_\mathrm{ep}\rangle_{\mathrm{e+p}}), \tag{26a}$$

$$\ge \mathrm{Tr}\, e^{-\beta(H_\mathrm{e}+H_\mathrm{p})} = Z_\mathrm{p}Z_\mathrm{e}, \tag{26b}$$

where $\langle X\rangle_{\mathrm{e+p}} = \mathrm{Tr}\, e^{-\beta(H_\mathrm{e}+H_\mathrm{p})}X/\mathrm{Tr}\, e^{-\beta(H_\mathrm{e}+H_\mathrm{p})}$, and Z_p and Z_e are the partition functions of the free oscillators and electrons respectively. To obtain (26b) we made

use of $[H_{\rm p}, H_{\rm e}] = 0$ and $\langle H_{\rm ep}\rangle_{\rm e+p} = 0$. Lower bound (26) does not dependent on the EP interaction strength and is, in this respect, not very useful.

Writing

$$H = \frac{p^2}{2M} + \frac{(x^+ - \bar{x}^+)K(x-\bar{x})}{2} + \frac{\bar{x}^+ K\bar{x}}{2} + c^+ T(x,\mu)c + \frac{(x^+ - \bar{x}^+)K\bar{x} + \bar{x}^+ K(x-\bar{x})}{2}, \tag{27}$$

application of inequality (6) with

$$A = \frac{p^2}{2M} + \frac{(x^+ - \bar{x}^+)K(x-\bar{x})}{2} + \frac{\bar{x}^+ K\bar{x}}{2} + c^+ T(\bar{x},\mu)c, \tag{28a}$$

and

$$B = \frac{(x^+ - \bar{x}^+)K\bar{x} + \bar{x}^+ K(x-\bar{x})}{2} + c^+ T(x-\bar{x},\mu)c, \tag{28b}$$

gives

$$Z \geq Z_p \max_{\bar{x}} e^{-\beta \bar{x}^+ K\bar{x}/2} \det(1 + e^{-\beta T(\bar{x},\mu)})^2 . \tag{29}$$

Collecting all results, the upper and lower bounds to the ground-state energy read

$$E_0^{(A)}(1) \leq \sqrt{g} E_0^{(p)} + E_0^{(A)}(1-g) \leq E_0 \leq E_0^{(p)} + E_0^{(A)}(1). \tag{30}$$

As already pointed out above, both bounds are readily computed by standard simulation techniques, for any EP-model of the type (1). From (30) it also follows that if $E_0^{(p)} \ll |E_0^{(A)}(1)|$, treating the phonon degrees of freedom as classical variables will be a good approximation.

4.1. *Application to the SSH model*

For the SSH model at half filling one has[18,19]

$$\frac{E_0^{(A)}(\gamma)}{L} = \min_z \left(-\frac{4t}{\pi}\mathcal{E}(1-z^2) + \frac{\gamma K t^2 z^2}{2\alpha^2} \right), \tag{31a}$$

and

$$\frac{E_0^{(p)}}{L} = \frac{1}{\pi}\sqrt{\frac{4K}{M}}, \tag{31b}$$

where $\mathcal{E}(x)$ denotes the complete elliptic integral of the second kind. For polyacetylene representative values of the model parameters are $t \approx 2.5$ eV (the nearest neighbor hopping matrix element), $K \approx 21$ eV/Å^2 (the spring constant), $M\hbar^2 = 3145$ eV^{-1}/Å^2 (the mass of the oscillators) and $\alpha \approx 4.1$ eV/Å. For these parameters one has[18,19]

$$\frac{E_0^{(A)}(\gamma)}{L} = -3.18(1 - e^{-2-4.88\gamma}) \text{ eV}, \tag{32a}$$

and

$$\frac{E_0^{(p)}}{L} = 0.052 \text{ eV}. \tag{32b}$$

From (30) it follows that

$$-3.17 \text{ eV} \leq -3.14 \text{ eV} \leq \frac{E_0}{L} \leq -3.12 \text{ eV}, \tag{33}$$

where the better of the two lower bounds has been obtained by putting $\gamma = 7/8$. Equation (33) suggests that replacing the full quantum mechanical density matrix by the simplest ($m = 1$) Lie-Trotter formula may be a rather good approximation, even down to zero temperature. As inequalities (12) and (29) become equalities as the temperature increases, at temperatures of interest (room temperature in the case of polyacetylene) the $m = 1$ approximation will perform even better than (33) suggests. Further results on the thermodynamic properties, the density of states and the conductivity of the SSH model can be found in Refs. 1 and 2.

5. Holstein Model

In some cases the particular form of T can be exploited to derive additional bounds and to relate the upper and lower bounds to the partition functions of other models. Here we illustrate how this can be done for the case of the Holstein model for which the Hamiltonian (in our notation) reads

$$H = \sum_{i,j} \sum_{\sigma=\uparrow,\downarrow} c_{i,\sigma}^{+} T_{i,j}^{(0)}(\mu) c_{j,\sigma} + \lambda \sum_{i} \sum_{\sigma=\uparrow,\downarrow} n_{i,\sigma} x_i + \sum_{i} \frac{p_i^2}{2M} + \sum_{i} \frac{M\Omega^2 x_i^2}{2}, \tag{34}$$

where $n_{i,\sigma} = c_{i,\sigma}^{+} c_{i,\sigma}$ is the number operator for a fermion with spin σ at site i. From (34) it is clear that the model describes Einstein oscillators with a frequency Ω interacting with the electrons through a linear on-site potential, characterized by a coupling constant λ. The inequalities presented below can be generalized to include the case of phonons with dispersion.

Eliminating the term linear in x by the unitary transformation $S = \exp(i\alpha np)$ with $\alpha = -\lambda/\hbar M\Omega^2$ brings the Hamiltonian into the form

$$SHS^{\dagger} = \sum_{l,j} \sum_{\sigma=\uparrow,\downarrow} c_{l,\sigma}^{+} e^{i\alpha p_l} T_{l,j}^{(0)}(\mu) e^{-i\alpha p_j} c_{j,\sigma} + \frac{U}{2} \sum_{i} \sum_{\sigma,\sigma'=\uparrow,\downarrow} n_{i,\sigma} n_{i,\sigma'}$$

$$+ \sum_{i} \frac{p_i^2}{2M} + \sum_{i} \frac{M\Omega^2 x_i^2}{2}, \tag{35a}$$

or, in shorthand notation,

$$SHS^{\dagger} = c^{+} e^{i\alpha p} T^{(0)}(\mu) e^{-i\alpha p} c + \frac{Un^2}{2} + \frac{p^2}{2M} + \frac{M\Omega^2 x^2}{2}, \tag{35b}$$

where $U = -\lambda^2/M\Omega^2$ determines the strength of an effective, attractive electron-electron interaction mediated by the phonons. Using $n_{i,\sigma}^2 = n_{i,\sigma}$, we can rewrite

(35a) as

$$SHS^{\dagger} = \sum_{i,j} \sum_{\sigma=\uparrow,\downarrow} c^{+}_{i,\sigma} T^{(0)}_{i,j} \left(\mu - \frac{U}{2}\right) c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$
$$+ \sum_{i} \frac{p_i^2}{2M} + \sum_{i} \frac{M\Omega^2 x_i^2}{2}$$
$$+ \sum_{l,j} \sum_{\sigma=\uparrow,\downarrow} c^{+}_{l,\sigma} (e^{i\alpha(p_l - p_j)} - 1) T^{(0)}_{l,j} \left(\mu - \frac{U}{2}\right) c_{j,\sigma} , \tag{36}$$

where we have made explicit that the transformed Hamiltonian is the sum of the Hubbard model Hamiltonian, the free phonon Hamiltonian (H_{p}), and a hopping term that account for the "retarded" EP interactions.

Putting $A = M\Omega^2 x^2/2$ and $B = c^{+} e^{i\alpha p} T^{(0)}(\mu) e^{-i\alpha p} c + Un^2/2 + p^2/2M$, application of the GTS inequality yields

$$Z \leq \mathrm{Tr}\, e^{-\beta M\Omega^2 x^2/2} e^{-\beta(c^{+} e^{i\alpha p} T^{(0)}(\mu) e^{-i\alpha p} c + Un^2/2 + p^2/2M)} , \tag{37a}$$

$$= \mathrm{Tr}\, e^{-\beta M\Omega^2 (x - \alpha\hbar n)^2/2} e^{-\beta(c^{+} T^{(0)}(\mu) c + Un^2/2 + p^2/2M)} , \tag{37b}$$

$$= (\beta\hbar\Omega)^{-L} Z_{\mathrm{h}} \left(T, U, \mu - \frac{U}{2}\right) , \tag{37c}$$

where we have used the fact that $[p, B] = 0$ to perform the inverse transformation S^{-1} and we worked out the trace over the phonon coordinates analytically. From (37) it follows that the upperbound for Z contains the partition function

$$Z_{\mathrm{h}}(T, U, \mu) \equiv \mathrm{tr}\, e^{-\beta H_{\mathrm{h}}} = \mathrm{tr}\, e^{-\beta(c^{+} T^{(0)}(\mu + U/2) c + Un^2/2)} , \tag{38}$$

of the Hubbard model

$$H_{\mathrm{h}} = \sum_{i,j} \sum_{\sigma=\uparrow,\downarrow} c^{+}_{i,\sigma} T^{(0)}_{i,j}(0) c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} - \mu \sum_{i} (n_{i,\uparrow} + n_{i,\downarrow}) . \tag{39}$$

For the case at hand $U < 0$ so that Z_{h} is the partition function of the attractive Hubbard model.

A lower bound to Z in terms of the (attractive) Hubbard model follows from the application of (6) with $A = H_{\mathrm{h}} + H_{\mathrm{p}}$, $B = H - A$ and reads

$$Z \geq Z_{\mathrm{p}} Z_{\mathrm{h}} \left(T, U, \mu - \frac{U}{2}\right)$$
$$\times \exp\left[-\beta(e^{-\lambda^2 \coth(\beta\hbar\Omega/2)/2\hbar M\Omega^3} - 1) K_{\mathrm{h}} \left(T, U, \mu - \frac{U}{2}\right)\right] , \tag{40}$$

where $K_{\mathrm{h}}(T, U, \mu) \equiv \langle c^{+} T^{(0)}(\mu) c \rangle_{\mathrm{h}}$.

The corresponding bounds for the ground state energy read

$$E_0^{(h)}\left(T,U,\mu-\frac{U}{2}\right) \le E_0 \le E_0^{(h)}\left(Te^{-\lambda^2/2\hbar M\Omega^3},U,\mu-\frac{U}{2}\right)+\frac{L\hbar\Omega}{2}$$

$$\le E_0^{(h)}\left(T,U,\mu-\frac{U}{2}\right)$$

$$+\frac{L\hbar\Omega}{2}+(e^{-\lambda^2/2\hbar M\Omega^3}-1)K_0^{(h)}\left(T,U,\mu-\frac{U}{2}\right), \quad (41)$$

where the first upper bound was obtained from a straightforward application of the variational principle. In the anti-adiabatic limit $\hbar\Omega \to \infty$, $M\Omega^2 = K$ constant, the third term in the upper bound vanishes and the ground state energy of the Holstein model differs from the ground state energy of the Hubbard model by at most $\hbar\Omega/2$.

Additional upper bounds to the partition function of the Holstein and Hubbard model follow from the decomposition

$$H = H_5 + H_6, \qquad H_5 = \frac{p^2}{2M}+\frac{M\Omega^2x^2}{2}+\lambda xn, \qquad H_6 = c^+T^{(0)}(\mu)c, \quad (42)$$

and the identity

$$e^{-\beta(p^2/2M+M\Omega^2x^2/2+\lambda xn)}$$

$$= e^{\beta\lambda^2n^2(1-t)/2M\Omega^2}e^{-\beta\lambda txn/2}e^{-\beta(p^2/2M+M\Omega^2x^2/2)}e^{-\beta\lambda txn/2}, \quad (43a)$$

where

$$43(b)t = \frac{\tanh(\beta\hbar\Omega/2)}{\beta\hbar\Omega/2}. \quad (43b)$$

Application of the GTS inequality and the identity

$$e^{\beta\lambda^2n^2(1-t)/2M\Omega^2} = \int du\ \rho_3\left(u,\frac{1}{1-t}\right)e^{-\beta\lambda(1-t)un}, \quad (44a)$$

where

$$\rho_3(u,a) \equiv \left(\frac{\beta M\Omega^2}{2a\pi}\right)^{L/2} e^{-\beta M\Omega^2u^2/2a}, \quad (44b)$$

yields, after some algebra,

$$Z \le Z_3 \equiv \operatorname{Tr} e^{-\beta H_5}e^{-\beta H_6}, \quad (45a)$$

$$Z_3 = Z_3(\mu) = Z_{\mathrm{p}}\int dx\ \rho_3(x,1)\operatorname{tr} e^{-\beta\lambda xn/2}e^{-\beta c^+T^{(0)}(\mu)c}e^{-\beta\lambda xn/2}, \quad (45b)$$

$$= Z_{\mathrm{p}}\int dx\ \rho_3(x,1)\det(1+e^{-\beta\lambda D(x)/2}e^{-\beta T^{(0)}(\mu)}e^{-\beta\lambda D(x)/2})^2, \quad (45c)$$

where $D = D(x) = \delta_{i,j}x_i$ is a diagonal matrix. Note that the determinant in (45) is strictly positive. Obviously inequality (45) becomes an equality if $\lambda = 0$.

The electronic part in the upper bound (45) is identical to an upper bound to the partition function of the attractive Hubbard model. Indeed, invoking the GTS inequality and identity (44) once more we find

$$
\begin{aligned}
Z_{\mathrm{p}} Z_{\mathrm{h}}(T,U,\mu) &\leq Z_{\mathrm{p}} Z_4 \\
&\equiv Z_{\mathrm{p}} \mathrm{tr}\, e^{-\beta c^{+} T^{(0)}(\mu+U/2)c} e^{-\beta U n^2/2}\,, && \text{(46a)} \\
&= Z_{\mathrm{p}} \int dx\; \rho_3(x,1)\, \mathrm{tr}\, e^{-\beta c^{+} T^{(0)}(\mu+U/2)c} e^{-\beta\lambda x n}\,, && \text{(46b)} \\
&= Z_{\mathrm{p}} \int dx\; \rho_3(x,1)\, \mathrm{tr}\, e^{-\beta\lambda x n/2} e^{-\beta c^{+} T^{(0)}(\mu+U/2)c} e^{-\beta\lambda x n/2}\,, && \text{(46c)} \\
&= Z_3\left(\mu + \frac{U}{2}\right). && \text{(46d)}
\end{aligned}
$$

The numerical calculation of upper bounds (45) and (46) is more complicated than the computation of Z_1 or $Z_2(g)$.

From (29) and (45) it follows that

$$
\begin{aligned}
&\min_x \left[\frac{M\Omega^2 x^2}{2} - 2\lim_{\beta\to\infty} \beta^{-1} \mathrm{Sp}\, \ln(1 + e^{-\beta\lambda D(x)/2} e^{-\beta T^{(0)}(\mu)} e^{-\beta\lambda D(x)/2})\right] \\
&\quad \leq E_0 - \frac{L\hbar\Omega}{2} \\
&\quad \leq \min_x \left[\frac{M\Omega^2 x^2}{2} - 2\lim_{\beta\to\infty} \beta^{-1} \mathrm{Sp}\, \ln(1 + e^{-\beta(T^{(0)}(\mu)+\lambda D(x))})\right], \qquad \text{(47)}
\end{aligned}
$$

At zero-temperture (47) yields

$$
\begin{aligned}
&\min_x \left[\frac{M\Omega^2 x^2}{2} - 2\lim_{\beta\to\infty} \beta^{-1} \mathrm{Sp}\, \ln(1 + e^{-\beta\lambda D(x)/2} e^{-\beta T^{(0)}(\mu)} e^{-\beta\lambda D(x)/2})\right] \\
&\quad \leq E_0^{(h)}\left(T, U, \mu + \frac{U}{2}\right). \qquad \text{(48)}
\end{aligned}
$$

It is also of interest to adopt instead of the Hubbard model Hamiltonian, the standard BCS trial Hamiltonian

$$
H^{(\mathrm{BCS})} = \sum_k \sum_{\sigma=\uparrow,\downarrow} \widehat{\epsilon}_k c^{+}_{k,\sigma} c_{k,\sigma} + \widehat{\Delta} \sum_k \left(c^{+}_{k,\uparrow} c^{+}_{-k,\downarrow} + c_{-k,\downarrow} c_{k,\uparrow}\right), \qquad \text{(49)}
$$

to derive an upper bound to the free energy of the Holstein model. Specializing to the ground state for simplicity, simultaneous minimization of the resulting upper bound with respect to $\widehat{\epsilon}_k$ and $\widehat{\Delta}$ gives

$$
E_0 - \frac{L\hbar\Omega}{2} \leq \frac{U\langle n\rangle^2}{4} - \frac{\Delta^2}{U} - \sum_k \frac{\tilde{\epsilon}_k(\tilde{\epsilon}_k - \tilde{\mu})}{\sqrt{(\tilde{\epsilon}_k - \tilde{\mu})^2 + \Delta^2}}\,, \qquad \text{(50a)}
$$

where

$$\tilde{\epsilon}_k = \epsilon_k e^{U/2\hbar\Omega}, \tag{50b}$$

and the gap Δ and the chemical potential $\tilde{\mu}$ are the solutions of the set of equations

$$1 = -\frac{U}{2}\sum_k \frac{1}{\sqrt{(\tilde{\epsilon}_k - \tilde{\mu})^2 + \Delta^2}}, \tag{50c}$$

$$\langle n \rangle = 1 - \sum_k \frac{(\tilde{\epsilon}_k - \tilde{\mu})}{\sqrt{(\tilde{\epsilon}_k - \tilde{\mu})^2 + \Delta^2}}, \tag{50d}$$

where $\langle n \rangle$ denotes the density of electrons. In deriving (50) we have assumed that a Fourier transformation of $T^{(0)}(\mu)$ with respect to the site indices yields a diagonal matrix with elements ϵ_k.

5.1. *Application*

In Fig. 1 we show numerical results for the lower and upper bounds (30), as obtained by simulated annealing of the phonon coordinates of a system of $L = 120$ sites together with the results obtained by solving the BCS equations (50) for the same system. The results for the latter do not change if the number of sites is increased

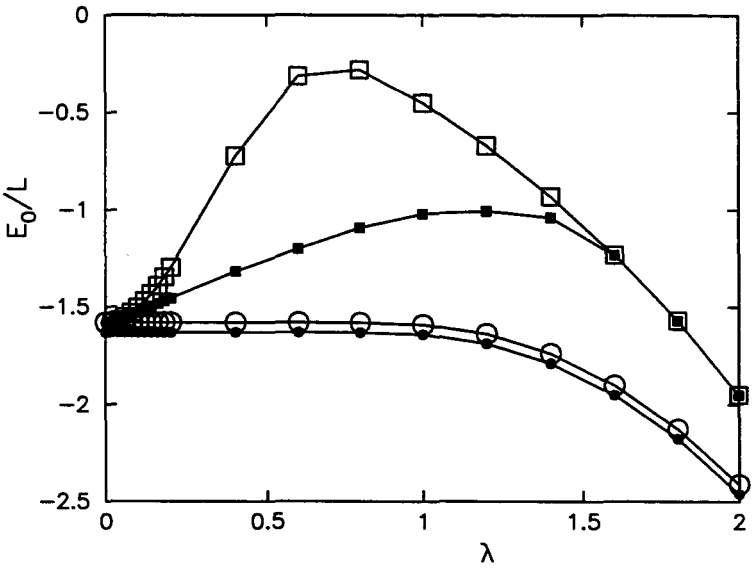

Fig. 1. Numerical results for upper and lower bounds to the ground state energy per site E_0/L of the two-dimensional Holstein model as a function of the EP coupling λ. Open squares: Variational results using the BCS trial Hamiltonian with a fixed oscillator frequency. Solid squares: Variational results using the BCS trial Hamiltonian and an adjustable oscillator frequency. Circles: Upperbounds as obtained from a simulated-anneal minimization of the r.h.s. of (30) for a lattice of 12×10 sites. Bullets: Lowerbounds as obtained from a simulated-anneal minimization of the l.h.s. of (23) for a lattice of 12×10 sites. In all cases the density of electrons $\langle n \rangle = 1$.

by several orders of magnitude so that we believe they are extremely close to their infinite-system values. The first set (open squares) of BCS-variational data has been obtained for fixed Ω. For the second set (solid squares) of data we also allowed for a different phonon frequency and used this frequency as an additional minimization

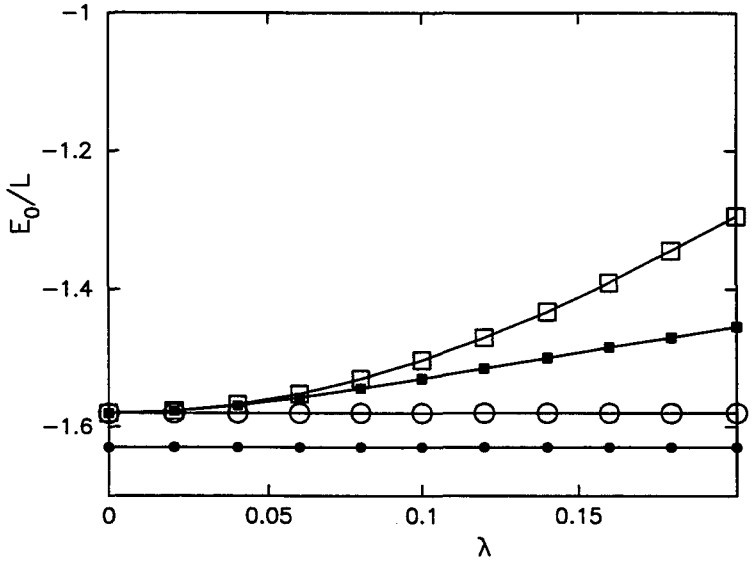

Fig. 2. Blow-up of Fig. 1 for small λ. BCS results for the ground-state energy are consistently larger than those obtained from the r.h.s. of (30).

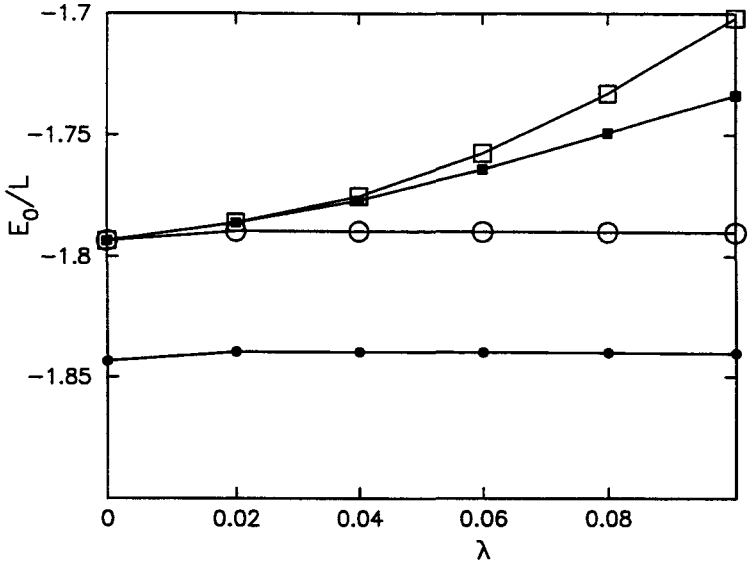

Fig. 3. Same as Fig. 1 except that $\langle n \rangle = 1.383$.

parameter. In our numerical work we used a hypercubic lattice subject to periodic boundary conditions.

In Fig. 2 we show the data of Fig. 1 for small λ on an expanded scale demonstrationg that also in this regime the ground-state energy of the Holstein model, as obtained from the BCS variational treatment, is larger than the ground-state energy obtained from the variational ansatz based on the adiabatic limit. In the case of the latter, for sufficiently small λ the energy is extremely close to the free-electron value. Within the BCS approach the decrease of the energy resulting from the attractive interaction is more than compensated for by the increase in kinetic energy resulting from the reduction of the bandwidth. Changing the density of electrons does not alter this picture, as is illustrated in Fig. 3. The qualitative features of the results depicted in Figs. 1–3 seem to be generic for simple hypercubic lattices. For the whole range of EP couplings covered, the BCS variational ansatz never yields an energy that is lower than the one obtained from the upperbound (30).

6. Off-Diagonal Long-Range Order

Bose–Einstein condensation in boson systems is characterized by the existence of ODLRO in the reduced one-particle density matrix.[20,21] Yang has shown that the concept of ODLRO can also be used to characterize the superconducting state of fermion systems.[4] Recently it has been shown that, under certain simplifying assumptions, ODLRO implies the existence of the Meissner effect and magnetic flux quantization.[22,23]

We now address the question of the existence of ODLRO in EP lattice models described by Hamiltonian (1). Following Yang there is ODLRO in a fermion system if the largest eigenvalue λ_0 of the $2L^2 \times 2L^2$ matrix

$$\rho_{r,s} \equiv \rho(i,j,\sigma;k,l,\sigma') = \langle c^+_{i,\sigma} c^+_{j,-\sigma} c_{l,-\sigma'} c_{k,\sigma'} \rangle \,, \tag{51}$$

grows with the size of the system (assuming the density of fermions is kept constant). Here $r = (i,j,\sigma)$ and $s = (k,l,\sigma')$ and we have confined ourselves to the case of singlet pairing.

As also pointed out by Yang, it is possible for a system to exhibit ODLRO in e.g. the three-body, four-body, ... density matrices but not in the two-body density matrix.[4] Here we will confine ourselves to the study of the largest eigenvalue of the two-body density matrix, and we will use the term ODLRO, always meaning ODLRO in the two-body density matrix.

Let us introduce the $L \times L$ matrix Λ and define the most general singlet-pair operator by

$$\Delta^\dagger = \sum_{i,j} \Lambda_{i,j} c^+_{i,\uparrow} c^+_{j,\downarrow} \,. \tag{52}$$

Without loss of generality we may assume that Λ is normalized, i.e.

$$\mathrm{Sp}\, \Lambda^\dagger \Lambda = 1 \,. \tag{53}$$

From the derivation of the upper and lowerbounds to the partition function we may expect that

$$e^{-\beta H} \approx e^{-\beta H_3/2} e^{-\beta H_4} e^{-\beta H_3/2}\,, \tag{54}$$

will be an excellent approximation for small $\beta\hbar \max_k(\omega_k)$ and/or weak EP interaction. For the Holstein model we could, as an alternative, use decomposition (42) instead of (54). As $[H_3, \Delta] = [H_3, \Delta^\dagger] = 0$ we have

$$\langle c^+_{i,\sigma} c^+_{j,-\sigma} c_{l,-\sigma'} c_{k,\sigma'} \rangle_4 \equiv \frac{\mathrm{Tr}\, e^{-\beta H_3} e^{-\beta H_4} c^+_{i,\sigma} c^+_{j,-\sigma} c_{l,-\sigma'} c_{k,\sigma'}}{\mathrm{Tr}\, e^{-\beta H_3} e^{-\beta H_4}}\,, \tag{55a}$$

$$= \langle\langle (1 + e^{\beta T(x,\mu)})^{-1}_{i,k} (1 + e^{\beta T(x,\mu)})^{-1}_{j,l} \rangle\rangle_4\,, \tag{55b}$$

where

$$\langle\langle F(x) \rangle\rangle_n \equiv \int dx\ \rho_n(x) F(x)\,, \tag{55c}$$

and

$$\rho_4(x) \equiv \rho_4(x,g) = \frac{\rho_2(x,g)\ \det(1 + e^{-\beta T(x,\mu)})^2}{\int dx \rho_2(x,g)\ \det(1 + e^{-\beta T(x,\mu)})^2} > 0\,, \tag{55d}$$

is a proper, normalized probability distribution. For the most general singlet pairing operator

$$\langle \Delta^\dagger \Delta \rangle_4 = \int dx \rho_4(x)\, \mathrm{Sp}\, N^{\mathrm{T}}(x,\mu) \Lambda N(x,\mu) \Lambda^\dagger\,, \tag{56}$$

where $N(x,\mu) = (1 + e^{\beta T(x,\mu)})^{-1}$. As all the eigenvalues of $N(x,\mu)$ are nonzero and smaller than one we have,

$$0 \leq \mathrm{Sp}\, N^{\mathrm{T}}(x,\mu) \Lambda N(x,\mu) \Lambda^\dagger \leq \mathrm{Sp}\, \Lambda \Lambda^\dagger = 1\,, \tag{57}$$

implying

$$0 \leq \langle \Delta^\dagger \Delta \rangle_4 \leq 1\,. \tag{58}$$

We now set Λ equal to the eigenvector that corresponds to the largest eigenvalue of the reduced two-particle density matrix. For this choice

$$\lambda_0 = \langle \Delta^\dagger \Delta \rangle_4 \leq 1\,, \tag{59}$$

demonstrating the absence of ODLRO in EP models of the type (1), for all approximations to the density matrix that are strictly positive.

As we have seen above, for the Holstein model already the most simple approximation of this type yields an upper bound to the ground state energy that is better than the one obtained from the BCS variational treatment. Whereas the latter has ODLRO build in, the former has not and as (59) shows, it will never display ODLRO.

From the exact expression

$$\langle \Delta^\dagger \Delta \rangle = \lim_{m\to\infty} \int dx_1 \dots dx_m \rho(x_1, \dots, x_m) \times \mathrm{Sp}\, N^{\mathrm{T}}(x_1, \dots, x_m, \mu) \Lambda N(x_1, \dots, x_m, \mu) \Lambda^\dagger , \tag{60}$$

where $\rho(x_1, \dots, x_m)$ is a Gaussian distribution of the variables $(x_1, \dots, x_m)$ and

$$N(x_1, \dots, x_m, \mu) = (1 + e^{\beta T(x_1,\mu)/m} \dots e^{\beta T(x_1,\mu)/m})^{-1} , \tag{61}$$

it follows immediately that a necessary condition for EP models of the type (1) to exhibit ODLRO is that $e^{\beta T(x_1,\mu)} \dots e^{\beta T(x_m,\mu)}$ has at least one eigenvalue that is less than zero.

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