Variational path-integral treatment of a translation invariant many-polaron system

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A translation invariant *N*-polaron system is investigated at arbitrary electron-phonon coupling strength, using a variational principle for path integrals for identical particles. An upper bound for the ground-state energy is found as a function of the number of spin up and spin down polarons, taking the electron-electron interaction and the Fermi statistics into account. The resulting addition energies and the criteria for multipolaron formation are discussed.

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I. INTRODUCTION

Thermodynamic and optical properties of interacting many-polaron systems are intensely investigated because they might play an important role in physical phenomena in high-T_c superconductors (see, e.g., Refs. 1 and 2, and references therein). In particular, numerous experiments on the infrared optical absorption of high-T_c materials (see, e.g., Refs. 3–8) reveal features that are associated with large polarons.[6,8,9]

For the case of weak electron-phonon coupling strength, a suitable variational approximation to the ground-state energy of an interacting many-polaron gas was already developed in Ref. 10 using a many-body canonical transformation for fermions in interaction with a phonon field. The static structure factor of the electron gas is the key ingredient of this theory. Based on the approach of Ref. 10, a many-body theory for the optical absorption at a gas of interacting polarons was developed.[11] The resulting optical conductivity turns out to be in fair agreement with the experimental "*d* band" by Lupi *et al.*[6] in the optical-absorption spectra of cuprates.

At arbitrary electron-phonon coupling strength, the many-body problem (including electron-electron interaction and Fermi statistics) in the *N*-polaron theory is not well developed. Within the random-phase approximation, the optical absorption of an interacting polaron gas was studied in Ref. 12, taking over the variational parameters of Feynman's polaron model,[13] which, however, are derived for a single polaron without many-body effects. For a dilute arbitrary-coupling polaron gas, the equilibrium properties[14,15] and the optical response[16] have been investigated using the path-integral approach taking into account the electron-electron interaction but neglecting the Fermi statistics. Recently, the formation of many-polaron clusters was investigated in Ref. 17 using the Vlasov kinetic equations.[18] However, this approach also does not take into account the Fermi statistics of electrons, and therefore it is valid only for sufficiently high temperatures.

The path integral treatment[19–21] of the quantum statistics of indistinguishable particles (bosons or fermions) provides a sound basis for including the many-body effects in a system of interacting polarons.[22] This approach was used[23–25] for calculating the ground-state energy and the optical conductivity spectra at arbitrary electron-phonon coupling strength for a finite number of interacting polarons in a parabolic confinement potential. However, the translation invariant polaron gas was not yet investigated within this approach.

In the present work, the ground-state properties of a translation invariant *N*-polaron system are theoretically studied in the framework of the variational path-integral method for identical particles, using a further development of the model introduced in Refs. 23–25. In Sec. II, the variational path-integral method and the chosen model system are described. In Sec. III, we discuss the numerical results for the ground-state energy of a translation invariant *N*-polaron system. Section IV is a summary of the obtained results with conclusions.

II. VARIATIONAL PATH-INTEGRAL METHOD FOR AN *N*-POLARON SYSTEM

A. The many-polaron system

In order to describe a many-polaron system, we start from the translation invariant *N*-polaron Hamiltonian

$$H=\sum_{j=1}^{N}\frac{\mathbf{p}_j^2}{2m}+\frac{1}{2}\sum_{j=1}^{N}\sum_{l=1,\neq j}^{N}\frac{e^2}{\epsilon_\infty|\mathbf{r}_j-\mathbf{r}_l|}+\sum_{\mathbf{k}}\hbar\omega_{\mathrm{LO}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\left(\sum_{j=1}^{N}\sum_{\mathbf{k}}V_k a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}_j}+\mathrm{H.c.}\right),\tag{1}$$

where m is the band mass, e is the electron charge, ω_{LO} is the longitudinal optical (LO) phonon frequency, and V_k are the amplitudes of the Fröhlich electron-LO-phonon interaction

$$V_k=i\frac{\hbar\omega_{\mathrm{LO}}}{k}\left(\frac{4\pi\alpha}{V}\right)^{1/2}\left(\frac{\hbar}{2m\omega_{\mathrm{LO}}}\right)^{1/4},$$

$$\alpha=\frac{e^2}{2\hbar\omega_{\mathrm{LO}}}\left(\frac{2m\omega_{\mathrm{LO}}}{\hbar}\right)^{1/2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right),\tag{2}$$

of course with the electron-phonon coupling constant $\alpha > 0$, the high-frequency dielectric constant $\epsilon_\infty > 0$, and the static dielectric constant $\epsilon_0 > 0$, and consequently

$$\frac{e^2}{\epsilon_\infty} > \hbar\left(\frac{2\hbar\omega_{\mathrm{LO}}}{m}\right)^{1/2}\alpha \Leftrightarrow \alpha\sqrt{2} < \left(\frac{H^*}{\hbar\omega_{\mathrm{LO}}}\right)^{1/2} \equiv U, \quad (3)$$

which is an important physical condition on the relative strength of the Coulomb interaction as compared to the electron-phonon coupling, as stressed in the earlier bipolaron work.[27] In the expression (3), H^* is the effective Hartree

$$H^* = \frac{e^2}{\epsilon_\infty a_B^*}, \quad a_B^* = \frac{\hbar^2}{me^2/\epsilon_\infty}, \quad (4)$$

where a_B^* is the effective Bohr radius. The partition function of the system can be expressed as a path integral over all electron and phonon coordinates. The path integral over the phonon variables can be calculated analytically.[26] Feynman's phonon elimination technique for this system is well known and leads to the partition function, which is a path integral over the electron coordinates only:

$$Z = \left(\prod_{\mathbf{k}} \frac{e^{1/2\beta\hbar\omega_{\mathrm{LO}}}}{2\sinh\frac{1}{2}\beta\hbar\omega_{\mathrm{LO}}}\right)\oint e^S \mathcal{D}\overline{\mathbf{r}}, \quad (5)$$

where $\overline{\mathbf{r}} = \{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$ denotes the set of electron coordinates, and $\oint \mathcal{D}\overline{\mathbf{r}}$ denotes the path integral over all the electron coordinates, integrated over equal initial and final points, i.e.,

$$\oint e^S \mathcal{D}\overline{\mathbf{r}} \equiv \int d\overline{\mathbf{r}} \int_{\overline{\mathbf{r}}(0)=\overline{\mathbf{r}}}^{\overline{\mathbf{r}}(\beta)=\overline{\mathbf{r}}} e^S \mathcal{D}\overline{\mathbf{r}}(\tau).$$

Throughout this paper, imaginary time variables are used. The effective action for the N-polaron system is retarded and given by

$$\begin{aligned} S = &-\int_0^\beta \left(\frac{m}{2}\sum_{j=1}^N \left(\frac{d\mathbf{r}_j(\tau)}{d\tau}\right)^2 + \frac{1}{2}\sum_{j=1}^N \sum_{l=1,\neq j}^N \frac{e^2}{\epsilon_\infty |\mathbf{r}_j(\tau) - \mathbf{r}_l(\tau)|}\right) d\tau \\ &+ \frac{1}{2}\int_0^\beta \int_0^\beta \sum_{j,l=1}^N \sum_{\mathbf{k}} |V_k|^2 e^{i\mathbf{k}[\mathbf{r}_j(\tau) - \mathbf{r}_l(\sigma)]} \\ &\times \frac{\cosh\hbar\omega_{\mathrm{LO}}\left(\frac{1}{2}\beta - |\tau - \sigma|\right)}{\sinh\frac{1}{2}\beta\hbar\omega_{\mathrm{LO}}} d\sigma d\tau. \end{aligned} \quad (6)$$

Note that the electrons are fermions. Therefore the path integral for the electrons with parallel spin has to be interpreted as the required antisymmetric projection of the propagators for distinguishable particles.

Below we use units in which $\hbar = 1$, $m = 1$, and $\omega_{\mathrm{LO}} = 1$. The units of distance and energy are thus the effective polaron radius $[\hbar/(m\omega_{\mathrm{LO}})]^{1/2}$ and the LO-phonon energy $\hbar\omega_{\mathrm{LO}}$.

B. Variational principle

For distinguishable particles, it is well known that the Jensen-Feynman inequality[13,26] provides a lower bound on the partition function Z (and consequently an upper bound on the free energy F)

$$\begin{aligned} Z &= \oint e^S \mathcal{D}\overline{\mathbf{r}} = \left(\oint e^{S_0}\mathcal{D}\overline{\mathbf{r}}\right)\langle e^{S-S_0}\rangle_0 \\ &\geqslant \left(\oint e^{S_0}\mathcal{D}\overline{\mathbf{r}}\right) e^{\langle S - S_0\rangle_0} \text{ with } \langle A\rangle_0 \equiv \frac{\oint A(\overline{\mathbf{r}}) e^{S_0}\mathcal{D}\overline{\mathbf{r}}}{\oint e^{S_0}\mathcal{D}\overline{\mathbf{r}}}, \end{aligned} \quad (7)$$

$$e^{-\beta F} \geqslant e^{-\beta F_0} e^{\langle S - S_0\rangle_0} \Rightarrow F \leqslant F_0 - \frac{\langle S - S_0\rangle_0}{\beta} \quad (8)$$

for a system with real action S and a real trial action S_0. The many-body extension (Ref. 19, p. 4476) of the Jensen-Feynman inequality, discussed in more detail in Ref. 22, requires (of course) that the potentials be symmetric with respect to all particle permutations, and that the exact propagator as well as the model propagator are defined on the same state space. This means that both the exact and the model propagator are antisymmetric for fermions (symmetric for bosons) at any time. The path integrals in Eq. (7) thus have to be interpreted in terms of an antisymmetric state space. Within this interpretation we consider the following generalization of Feynman's trial action:

$$\begin{aligned} S_0 = &-\int_0^\beta \left(\frac{1}{2}\sum_{j=1}^N \left(\frac{d\mathbf{r}_j(\tau)}{d\tau}\right)^2 + \frac{\omega^2 + w^2 - v^2}{4N} \right. \\ &\left. \times \sum_{j,l=1}^N [\mathbf{r}_j(\tau) - \mathbf{r}_l(\tau)]^2\right) d\tau - \frac{w}{8}\frac{v^2 - w^2}{N}\sum_{j,l=1}^N \int_0^\beta \int_0^\beta \\ &\times [\mathbf{r}_j(\tau) - \mathbf{r}_l(\sigma)]^2 \frac{\cosh w\left(\frac{1}{2}\beta - |\tau - \sigma|\right)}{\sinh\frac{1}{2}\beta w} d\sigma d\tau \end{aligned} \quad (9)$$

with the variational frequency parameters v, w, and ω. Because the coordinates of the fermions enter Eq. (9) only through the differences $r_j(\tau) - r_l(\sigma)$, this trial action is translation invariant.

Using the explicit forms of the exact (6) and the trial (9) actions, the variational inequality (8) takes the form

$$F(\beta|N_\uparrow,N_\downarrow) \leqslant F_0(\beta|N_\uparrow,N_\downarrow) + \frac{U}{2\beta}\int_0^\beta \left\langle \sum_{j,l=1,\neq j}^{N} \frac{1}{|\mathbf{r}_j(\tau)-\mathbf{r}_l(\tau)|}\right\rangle_0 d\tau - \frac{\omega^2+w^2-v^2}{4N\beta}\int_0^\beta \left\langle \sum_{j,l=1}^{N}[\mathbf{r}_j(\tau)-\mathbf{r}_l(\tau)]^2\right\rangle_0 d\tau$$
$$- \frac{w}{8}\frac{v^2-w^2}{N\beta}\int_0^\beta\int_0^\beta \left\langle \sum_{j,l=1}^{N}[\mathbf{r}_j(\tau)-\mathbf{r}_l(\sigma)]^2\right\rangle_0 \frac{\cosh w\left(\frac{1}{2}\beta-|\tau-\sigma|\right)}{\sinh\frac{1}{2}\beta w}d\sigma d\tau$$
$$- \frac{1}{2\beta}\int_0^\beta\int_0^\beta \sum_{\mathbf{k}}|V_k|^2\left\langle \sum_{j,l=1}^{N} e^{i\mathbf{k}[\mathbf{r}_j(\tau)-\mathbf{r}_l(\sigma)]}\right\rangle_0 \frac{\cosh\omega_{\mathrm{LO}}\left(\frac{1}{2}\beta-|\tau-\sigma|\right)}{\sinh\frac{1}{2}\beta\omega_{\mathrm{LO}}}d\sigma d\tau \tag{10}$$

and it is clear that the minimization automatically implies $v^2 \geqslant w^2$.

In the zero-temperature limit ($\beta\to\infty$), we arrive after some lengthy algebra at the following upper bound for the ground-state energy $E^0(N_\uparrow,N_\downarrow)$ of a translation invariant N-polaron system

$$E^0(N_\uparrow,N_\downarrow) \leqslant E_{var}(N_\uparrow,N_\downarrow|v,w,\omega),$$

with

$$E_{var}(N_\uparrow,N_\downarrow|v,w,\omega) = \frac{3}{4}\frac{(v-w)^2}{v} - \frac{3}{4}\omega + \frac{1}{2}\mathbb{E}_F(N_\downarrow) + \frac{1}{2}\mathbb{E}_F(N_\downarrow)$$
$$+ E_{C\parallel}(N_\uparrow) + E_{C\parallel}(N_\downarrow) + E_{C\uparrow\downarrow}(N_\uparrow,N_\downarrow)$$
$$+ E_{\alpha\parallel}(N_\uparrow) + E_{\alpha\parallel}(N_\downarrow) + E_{\alpha\uparrow\downarrow}(N_\uparrow,N_\downarrow), \tag{11}$$

where $\mathbb{E}_F(N)$ is the energy of N spin-polarized fermions confined to a parabolic potential with the confinement frequency ω, $E_{C\parallel}(N_{\uparrow(\downarrow)})$ is the Coulomb energy of the electrons with parallel spins, $E_{C\uparrow\downarrow}(N_\uparrow,N_\downarrow)$ is the Coulomb energy of the electrons with opposite spins, $E_{\alpha\parallel}(N_{\uparrow(\downarrow)})$ is the electron-phonon energy of the electrons with parallel spins, and $E_{\alpha\uparrow\downarrow}(N_\uparrow,N_\downarrow)$ is the electron-phonon energy of the electrons with opposite spins. The key steps in the derivation and the resulting analytical expressions for the terms of Eq. (11) can be found in the Appendix.

III. DISCUSSION OF RESULTS

In the present section we summarize and discuss the main results of the numerical minimization of $E_{var}(N_\uparrow,N_\downarrow|v,w,\omega)$ with respect to the three variational parameters v, w, and ω. The Fröhlich constant α and the Coulomb parameter

$$\alpha_0 \equiv \frac{U}{\sqrt{2}} \equiv \frac{\alpha}{1-\eta} \quad \text{with } \frac{1}{\eta} = \frac{\varepsilon_0}{\varepsilon_\infty} \tag{12}$$

characterize the strength of the electron-phonon and of the Coulomb interaction, obeying the physical condition $\alpha \geqslant \alpha_0$ [see Eq. (3)]. The optimal values of the variational parameters v, w, and ω are denoted v_{op}, w_{op}, and ω_{op}, respectively. The optimal value of the total spin was always determined by choosing the combination $(N_\uparrow,N_\downarrow)$ for fixed $N=N_\uparrow+N_\downarrow$, which corresponds to the lowest value $E^0(N)$ of the variational functional

$$E^0(N) \equiv \min_{N_\uparrow} E_{var}(N_\uparrow,N-N_\uparrow|v_{op},w_{op},\omega_{op}). \tag{13}$$

In Figs. 1–3 we present the ground-state energy per polaron (panel *a*), the addition energy (panel *b*), the optimal values of the variational parameters (panel *c*), and the total spin (panel *d*), as a function of the number of polarons. The addition energy is determined by the formula

$$\Delta(N) \equiv E^0(N+1) - 2E^0(N) + E^0(N-1). \tag{14}$$

In Fig. 1 we consider a highly polar system with $\alpha=\alpha_0=7$. The optimal value ω_{op} (see panel *c*) for the confinement frequency ω is strictly positive (at least for $N\leqslant 31$). Therefore the results of Fig. 1 are related to multipolaron states analogous to those investigated in Ref. 28. This interpretation is confirmed by the fact that (see panel *a* of Fig. 1) the ground-state energy per polaron for $N=2$ is lower than that for $N=1$. For $N>2$, the ground-state energy per polaron is an increasing function of N, which means that the effective electron-phonon coupling weakens due to screening when the number of polarons increases.

The addition energy (panel *b* of Fig. 1) oscillates, taking local maxima at even N and local minima at odd N. This oscillating behavior reflects the trend of a stable multipolaron state to have the minimal possible spin. This trend is an analog of the pairing of electrons in a superconducting state. For even N (see panel *d* of Fig. 1) the total spin S is equal to zero. For odd N, one electron remains nonpaired and $S=1/2$. Therefore one intuitively expects that the states with $S=0$ are energetically favorable as compared to states with $S=1/2$, and hence $\Delta(N)$ for odd N is lower than $\Delta(N)$ for even N. The plot of the addition energies in panel *b* of Fig. 1 confirms this expectation. Furthermore, pronounced maxima in $\Delta(N)$ correspond to closed-shell systems with $N=2,8,20,\ldots$.

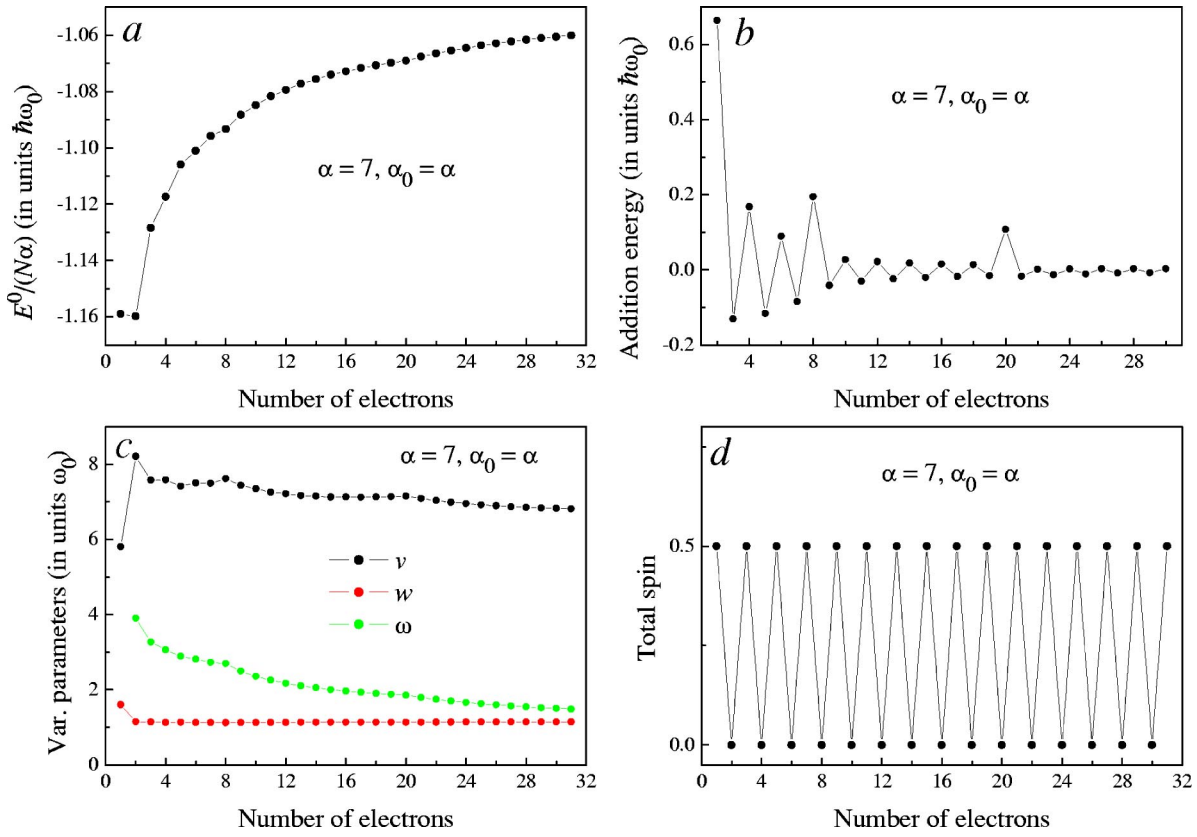

FIG. 1. (Color online) The ground-state energy per polaron (*a*), the addition energy (*b*), the optimal values of variational parameters (*c*), and the total spin (*d*) as a function of N for a translation invariant N-polaron system with $\alpha=7$, $\alpha_0=\alpha$.

The optimal values of the variational parameters (panel *c* of Fig. 1) reveal a general trend to decrease as a function of N, except the parameter v, which has a peak at $N=2$. This peak, as well as the minimum of $E^0(N)/N$ at $N=2$, shows that the two-polaron state in the extremely strong-coupling regime is especially stable with respect to the other multipolaron states with $N>2$. The dependence of the parameter ω on N starts from $N=2$ because the one-polaron variational functional does not depend on ω.

In Fig. 2, the ground-state energy, the additional energy, the variational parameters, and the total spin for N-polaron systems are plotted for $\alpha=3$, $\alpha_0=4.5$, and $\eta=1/3$. In this regime, the optimal value for the confinement frequency ω is $\omega_{op}=0$ (panel *c*). Therefore, in this regime, as well as at weaker electron-phonon coupling strengths, $N>1$ polarons do not form a multipolaron state. The addition energy, as seen from panel *b* of Fig. 2, has no oscillations or peaks in the case when N polarons do not form a multipolaron state. It should be noted that in the case when $\omega_{op}=0$, we deal with a finite number N of polarons in an infinite volume. So, at $\omega_{op}=0$ the many-body effects, related to the electron-electron interaction and to the Fermi statistics, are vanishingly small. The dependence of the ground-state energy of the total spin of a many-polaron system is just one of these many-body effects. As a consequence, the ground-state energy within the present model at $\omega_{op}=0$ does not depend on the total spin. For this reason, there is no panel *d* in Fig. 2.

Figures 1 and 2 represent two mutually opposite cases (with $\omega\neq 0$ and with $\omega_{op}=0$ for all N under consideration). Figure 3 describes the case when the regime with $\omega_{op}\neq 0$ (for $N\leqslant 16$) changes to the regime with $\omega_{op}=0$ (for $N\geqslant 17$). As seen from panel *a* of Fig. 3, the ground-state energy for $N\leqslant 16$ behaves similarly to that calculated for $\alpha=\alpha_0=7$ (panel *a* of Fig. 1), with the following distinction: for $\alpha_0/\alpha=1.01$ ($\alpha=7$) it appears that $E^0(N)/N|_{N=2} > E^0(N)/N|_{N=1}$, while for $\alpha_0/\alpha=1$ ($\alpha=7$), $E^0(N)/N|_{N=2} < E^0(N)/N|_{N=1}$. As seen from panel *c* of Fig. 3, when an extra polaron is added to $N=16$ polarons, the optimal value for ω switches to zero, and therefore the multipolaron state transforms to the ground state of N independent polarons. When N changes from $N=16$ to $N=17$, the ground-state energy per polaron slightly jumps down and is practically constant with further increasing N. The transition from a multipolaron state to a state of N independent polarons is clearly revealed in the dependence of the addition energy on the number of polarons (panel *b* of Fig. 3). At $N=16$, $\Delta(N)$ has a pronounced minimum, which is a manifestation of the transition from a multipolaron ground state to a ground state of N independent polarons.

The total spin, as seen from panel *d* of Fig. 3, takes its minimal possible value for $N\leqslant 13$, while for $N\geqslant 14$, the ground state is spin-polarized. So, the transition from the ground state with the minimal possible spin to the spin-polarized ground state with increasing N precedes the breakup of a multipolaron state. For $N\geqslant 17$, in the same way as in the case ($\alpha=3, \alpha_0=4.5$), the variational ground-state energy of an N-polaron system does not depend on the total spin.

In Fig. 4, the "phase diagrams" analogous to that of Ref. 27 are plotted for an N-polaron system in bulk with $N=2$, 3,

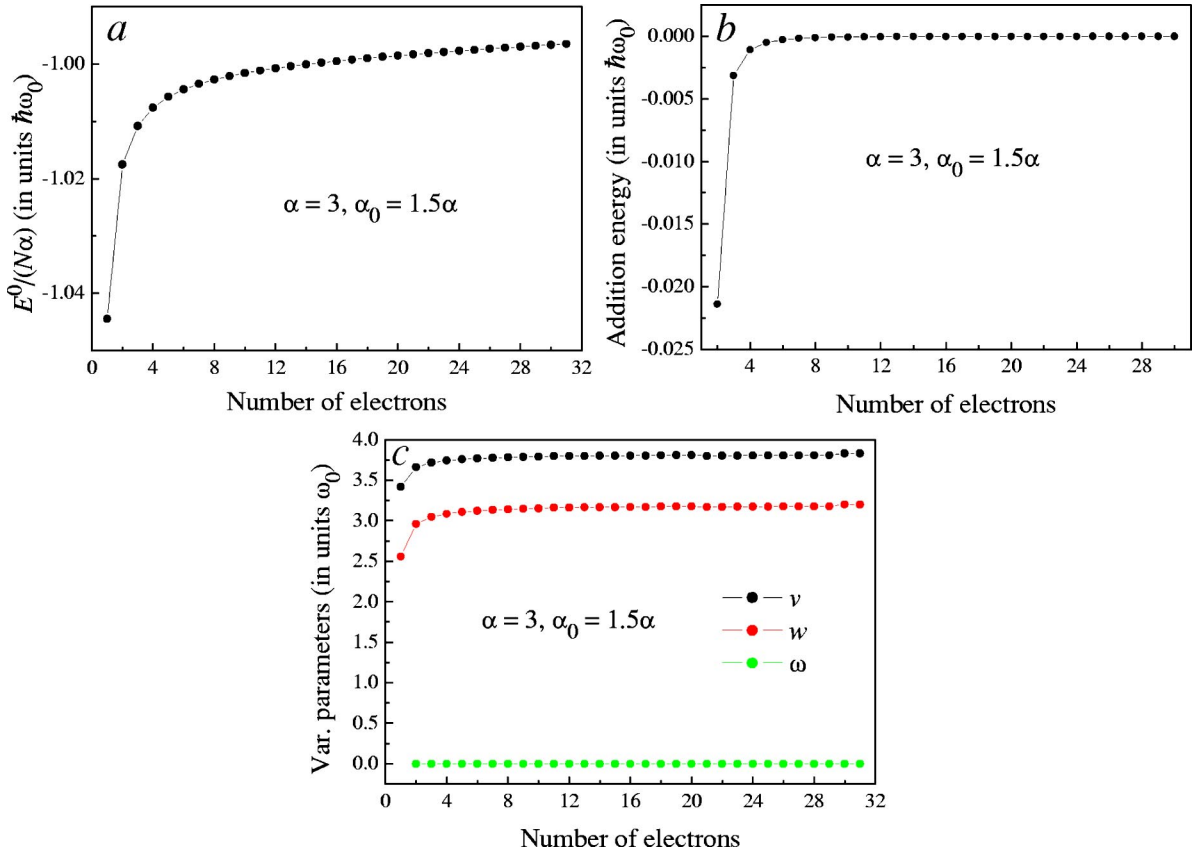

FIG. 2. (Color online) The ground-state energy per polaron (*a*), the addition energy (*b*), and the optimal values of variational parameters (*c*) as a function of N for a translation invariant N-polaron system with $\alpha=3$, $\alpha_0=1.5\alpha$.

5, and 10. The area where $\alpha_0 \leqslant \alpha$ is the nonphysical region. For $\alpha > \alpha_0$, each sector between a curve corresponding to a well-defined N and the line indicating $\alpha_0=\alpha$ shows the stability region where $\omega_{op} \neq 0$, while the white area corresponds to the regime with $\omega_{op}=0$. When comparing the stability region for $N=2$ from Fig. 4 with the bipolaron "phase diagram" of Ref. 27, the stability region in the present work starts from the value $\alpha_c \approx 4.1$ (instead of $\alpha_c \approx 6.9$ in Ref. 27). The width of the stability region within the present model is also larger than the width of the stability region within the model of Ref. 27. Also, the absolute values of the ground-state energy of a two-polaron system given by the present model are smaller than those given by the approach of Ref. 27.

The difference between the numerical results of the present work and of Ref. 27 is due to the following distinction between the used model systems. The model system of Ref. 27 consists of two electrons interacting with two fictitious particles and with each other through quadratic interactions. But the trial Hamiltonian given by Eq. (6) of Ref. 27 is not symmetric with respect to the permutation of the electrons. It is only symmetric under the permutation of the pairs "electron+fictitious particle." As a consequence, this trial system is only applicable if the electrons are distinguishable, i.e., have opposite spin. In contrast to the model of Ref. 27, the model used in the present paper is described by the trial action (9), which is fully symmetric with respect to the permutations of the electrons, as is required to describe identical particles. Up to now we have been unable to construct such a model with two retardation sources. As a consequence, the trial model of Ref. 27 is superior to our model for describing two polarons because it has more variational parameters, but its applicability is limited to two polarons. The generalization of the model of Ref. 27 to $N>2$ is currently under investigation.

The "phase diagrams" for $N>2$ demonstrate the existence of stable multipolaron states (see Ref. 28). As distinct from Ref. 28, here the ground state of an N-polaron system is investigated supposing that the electrons are fermions. As seen from these figures, for $N>2$, the stability region for a multipolaron state is narrower than the stability region for $N=2$, and its width decreases with increasing N. The critical value α_c for the electron-phonon coupling constant increases with increasing N. From this behavior we can deduce a general trend, which explains the behavior of the ground-state energy and related quantities as a function of N shown in Fig. 3. For fixed values of α and η, the width of the stability region for a multipolaron state is a decreasing function of the number of electrons. Therefore for any (α, η) there exists a critical number of electrons $N_0(\alpha, \eta)$ such that a multipolaron state exists for $N \leqslant N_0(\alpha, \eta)$ and does not exist for $N > N_0(\alpha, \eta)$. For example, for the N-polaron system described in Fig. 1, N_0 is at least larger than 20. For the system shown in Fig. 2, $N_0=1$, and for the system in Fig. 3, $N_0=16$. If we add electrons to an N-polaron system one by one, the multipolaron state breaks up when the number of electrons exceeds a critical value $N_0(\alpha, \eta)$.

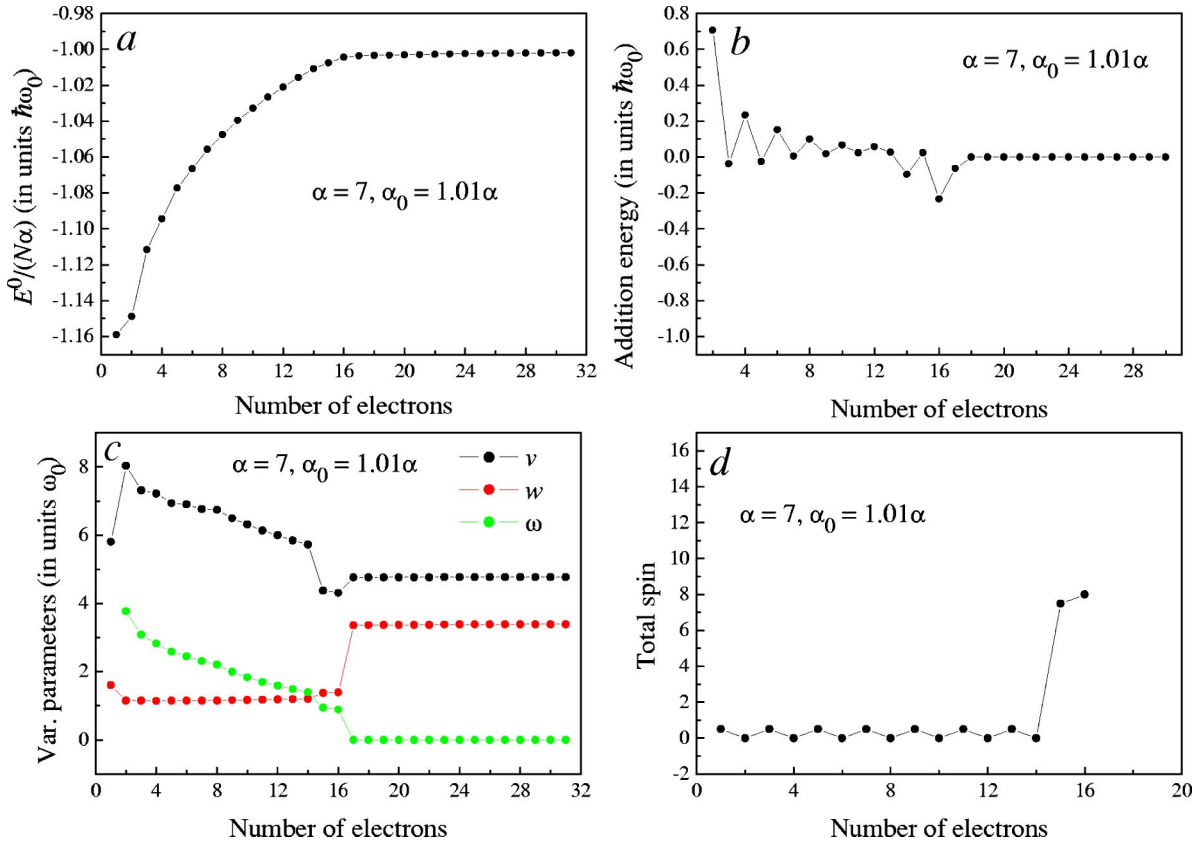

FIG. 3. (Color online) The ground-state energy per polaron (a), the addition energy (b), the optimal values of variational parameters (c), and the total spin (d) as a function of N for a translation invariant N-polaron system with $\alpha=7$, $\alpha_0=1.01\alpha$.

In order to analyze the consequences of the Fermi statistics for the ground-state properties of an N-polaron system, we compare the ground-state energies calculated with and without the Fermi statistics. In Table I the results are presented for the ground-state energy per particle in units of the one-polaron strong-coupling energy E_1,

$$\mathcal{E}_N = \frac{E^0(N)}{NE_1}\left(E_1 \equiv \frac{1}{3\pi}\alpha^2\right), \tag{15}$$

with $\alpha=10$, $\eta=0$ for three cases: the many-body path-integral approach of the present work with fermion statistics ($\mathcal{E}_N^{(F)}$), the same approach for distinguishable particles ($\mathcal{E}_N^{(d)}$), and the strong-coupling approach of Ref. 28, which also does not take into account the Fermi statistics ($\mathcal{E}_N^{(d,sc)}$).

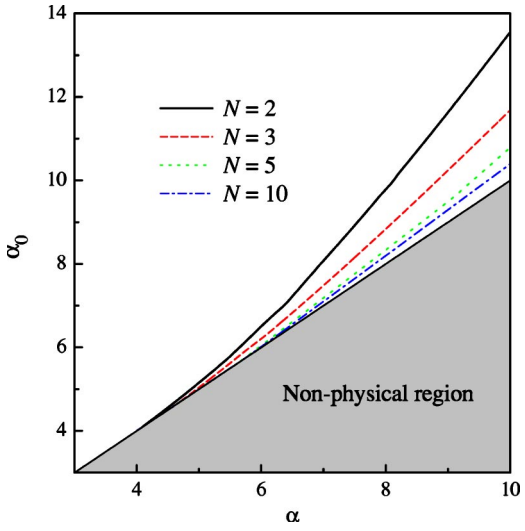

FIG. 4. (Color online) The "phase diagrams" of a translation invariant N-polaron system. The gray area is the nonphysical region, for which $\alpha > \alpha_0$. The stability region for each number of electrons is determined by the equation $\alpha_c < \alpha < \alpha_0$.

As seen from Table I, the ground-state energy per particle for N identical polarons $\mathcal{E}_N^{(F)}$ is higher than that for N distinguishable polarons $\mathcal{E}_N^{(d)}$. Furthermore, $\mathcal{E}_N^{(F)}$ increases whereas $\mathcal{E}_N^{(d)}$ decreases with an increasing number of polarons. Note, however, that $E_N^{(d)} < E_N^{(d,sc)}$ for the considered values of α and η, which means that the path-integral variational method provides better results for the N-polaron ground-state energy

TABLE I. The polaron characteristic energy $\mathcal{E}_N$ calculated using different methods.

N	$\mathcal{E}_N^{(F)}$	$\mathcal{E}_N^{(d)}$	$\mathcal{E}_N^{(d,sc)}$
2	−1.349	−1.349	−1.148
3	−1.308	−1.415	−1.241
4	−1.296	−1.468	−1.308
5	−1.279	−1.508	−1.361
6	−1.272	−1.536	−1.404

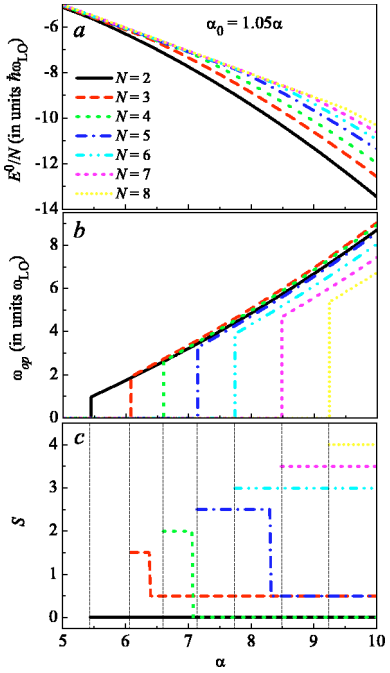

FIG. 5. (Color online) The ground-state energy per particle (a), the optimal value ω_{op} of the confinement frequency (b), and the total spin (c) of a translation invariant N-polaron system as a function of the coupling strength α for $\alpha_0/\alpha=1.05$. The vertical dashed lines in the panel c indicate the critical values α_c separating the regimes of $\alpha>\alpha_c$, where the multipolaron ground state with $\omega_{op}\neq 0$ exists, and $\alpha<\alpha_c$, where $\omega_{op}=0$.

than the strong-coupling approach[28] (at least for $\alpha\leqslant 10$).

Another consequence of the Fermi statistics is the dependence of the polaron characteristics and of the total spin of an N-polaron system on the parameters (α,α_0,N). In Fig. 5 we present the ground-state energy per particle, the confinement frequency ω_{op}, and the total spin S as a function of the coupling constant α for $\alpha_0/\alpha=1.05$ and for a different number of polarons. The ground-state energy turns out to be a continuous function of α, while ω_{op} and S reveal jumps. For all considered numbers of polarons $N>2$, there is a region of α in which S takes its maximal value, while $\omega_{op}\neq 0$. When lowering α, this spin-polarized state with parallel spins precedes the transition from the regime with $\omega_{op}\neq 0$ to the regime with $\omega_{op}=0$ (the breakup of a multipolaron state). For $N=2$ (the case of a bipolaron), we see from Fig. 5 that the ground state has a total spin $S=0$ for all values of α, i.e., the ground state of a bipolaron is a singlet. This result is in agreement with earlier investigations of the large-bipolaron problem (see, e.g., Ref. 31).

IV. CONCLUSIONS

Using the extension of the Jensen-Feynman variational principle to the systems of identical particles, we have derived a rigorous upper bound for the free energy of a translation invariant system of N interacting polarons. In the zero-temperature limit, the variational free energy provides the variational functional for the ground-state energy of the N-polaron system. The developed approach is valid for an arbitrary coupling strength. The resulting ground-state energy is obtained taking into account the Fermi statistics of electrons.

For sufficiently high values of the electron-phonon coupling constant and of the ratio $1/\eta=\varepsilon_0/\varepsilon_\infty$, the system of N interacting polarons can form a stable multipolaron ground state. When this state is formed, the total spin of the system takes its minimal possible value. The larger the number of electrons, the narrower the stability region of a multipolaron state becomes. So, when adding electrons one by one to a stable multipolaron state, it breaks up for a definite number of electrons N_0, which depends on the coupling constant and on the ratio of the dielectric constants. This breakup is preceded by the change from a spin-mixed ground state with a minimal possible spin to a spin-polarized ground state with parallel spins.

For a stable multipolaron state, the addition energy reveals peaks corresponding to closed shells. At $N=N_0$, the addition energy has a pronounced minimum. These features of the addition energy, as well as the total spin as a function of the number of electrons, might be resolved experimentally using, e.g., capacity and magnetization measurements.

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APPENDIX: MATHEMATICAL DETAILS

1. Generalization of the Hellman-Feynman theorem

For the averages of the quadratic terms in Eq. (10), we can derive a generalization of the Hellman-Feynman theorem for the case where we have a (trial) action but no Hamiltonian. Indeed, since $F_0=-1/\beta\ln Z_0$ it follows that

$$\frac{d}{d\gamma}F_0=-\frac{1}{\beta}\frac{d}{d\gamma}\ln Z_0=-\frac{1}{\beta}\frac{1}{Z_0}\frac{d}{d\gamma}Z_0=-\frac{1}{\beta}\left\langle\frac{dS_0}{d\gamma}\right\rangle_0 \tag{A1}$$

for any parameter γ in the trial action. Taking the derivative of S_0 [Eq. (9)] with respect to ω and v then gives

$$\int_0^\beta\left\langle\sum_{j,l=1}^{N}[\mathbf{r}_j(\tau)-\mathbf{r}_l(\tau)]^2\right\rangle_0 d\tau=-\frac{2N}{\omega}\left\langle\frac{dS_0}{d\omega}\right\rangle_0=\frac{2N\beta}{\omega}\frac{dF_0}{d\omega},$$

$$\sum_{j,l=1}^{N}\int_0^\beta\int_0^\beta\left\langle\sum_{j,l=1}^{N}[\mathbf{r}_j(\tau)-\mathbf{r}_l(\sigma)]^2\right\rangle_0\frac{\cosh w\left(\frac{1}{2}\beta-|\tau-\sigma|\right)}{\sinh\frac{1}{2}\beta w}d\sigma d\tau=\frac{4N\beta}{wv}\left(\frac{dF_0}{dv}+\frac{v}{\omega}\frac{dF_0}{d\omega}\right),$$

and therefore the variational inequality becomes

$$F(\beta|N_\uparrow,N_\downarrow)\leqslant F_0(\beta|N_\uparrow,N_\downarrow)-\frac{1}{2}\omega\frac{dF_0(\beta|N_\uparrow,N_\downarrow)}{d\omega}-\frac{1}{2}\frac{v^2-w^2}{v}\frac{dF_0(\beta|N_\uparrow,N_\downarrow)}{dv}+\frac{U}{2\beta}\int_0^\beta\left\langle\sum_{j,l=1,\neq j}^{N}\frac{1}{|\mathbf{r}_j(\tau)-\mathbf{r}_l(\tau)|}\right\rangle_0 d\tau$$
$$-\frac{1}{2\beta}\int_0^\beta\int_0^\beta\sum_{\mathbf{k}}|V_k|^2\left\langle\sum_{j,l=1}^{N}e^{i\mathbf{k}[\mathbf{r}_j(\tau)-\mathbf{r}_l(\sigma)]}\right\rangle_0\frac{\cosh\omega_{\mathrm{LO}}\left(\frac{1}{2}\beta-|\tau-\sigma|\right)}{\sinh\frac{1}{2}\beta\omega_{\mathrm{LO}}}d\sigma d\tau. \tag{A2}$$

2. Correlation and density functions

In order to calculate the Coulomb and the electron-phonon energies [the terms in the second and third lines of Eq. (A2), respectively], we only need the pair correlation function g_F and the two-point correlation function C_F for fermions that we define as

$$g_F(r,\beta|N_\uparrow,N_\downarrow)=\frac{1}{N(N-1)}\sum_{j,l=1;j\neq l}^{N}\langle\delta(\mathbf{r}-\mathbf{r}_j+\mathbf{r}_l)\rangle_0, \tag{A3}$$

$$C_F(\mathbf{q},\tau,\beta|N_\uparrow,N_\downarrow)=\frac{1}{N^2}\sum_{j,l=1}^{N}\langle e^{-i\mathbf{q}\cdot\mathbf{r}_l(\tau)}e^{i\mathbf{q}\cdot\mathbf{r}_j(0)}\rangle_0, \tag{A4}$$

where $\langle\cdots\rangle_0$ denotes a path-integral average with the action functional S_0. After a separation of the center-of-mass motion (see Ref. 25), these correlation functions take the form

$$g_F(r,\beta|N_\uparrow,N_\downarrow)=\frac{1}{N}\frac{1}{N-1}\sum_{j,l=1;j\neq l}^{N}\langle\delta(\mathbf{r}-\mathbf{r}_j+\mathbf{r}_l)\rangle_F, \tag{A5}$$

$$C_F(q,\tau,\beta|N_\uparrow,N_\downarrow)$$
$$=\mathbb{C}_F(q,\tau,\beta|N_\uparrow,N_\downarrow)\exp\left[-\frac{q^2}{N}\left(\frac{w^2\tau(\beta-\tau)}{2v^2\beta}+\frac{v^2-w^2}{v^3}\frac{\sinh\left(\frac{1}{2}v\tau\right)\sinh\left(\frac{1}{2}v(\beta-\tau)\right)}{\sinh\left(\frac{1}{2}v\beta\right)}-\frac{\sinh\left(\frac{1}{2}\omega\tau\right)\sinh\left(\frac{1}{2}\omega(\beta-\tau)\right)}{\omega\sinh\left(\frac{1}{2}\omega\beta\right)}\right)\right] \tag{A6}$$

with

$$\mathbb{C}_F(\mathbf{q},\tau,\beta|N_\uparrow,N_\downarrow)=\frac{1}{N^2}\sum_{j,l=1}^{N}\langle e^{-i\mathbf{q}\cdot\mathbf{r}_l(\tau)}e^{i\mathbf{q}\cdot\mathbf{r}_j(0)}\rangle_F, \tag{A7}$$

where $\langle\cdots\rangle_F$ denotes a path-integral average with the action functional

$$S_F=-\frac{1}{2}\int_0^\beta\sum_{j=1}^{N}\left[\left(\frac{d\mathbf{r}_j(\tau)}{d\tau}\right)^2+\omega^2\mathbf{r}_j^2(\tau)\right]d\tau \tag{A8}$$

for $N=N_\uparrow+N_\downarrow$ independent fermions in a 3D parabolic potential with the confinement frequency ω. We shall also use the density function

$$\tilde{n}_F(\mathbf{q},\beta|N_\uparrow,N_\downarrow)=\frac{1}{N}\sum_{j=1}^{N}\langle e^{-i\mathbf{q}\cdot\mathbf{r}_j}\rangle_F. \tag{A9}$$

The functions (A5), (A7), and (A9) were already derived before (see Refs. 25, 29, and 30).

Both the Coulomb energy and the electron-phonon energy in Eq. (A2) are effectively Coulomb terms but with two important differences. First, the standard Coulomb repulsion between the electrons is static, whereas the effective Coulomb attraction due to the polaron effect is retarded. A direct consequence of this difference is that the center of mass plays no role in the Coulomb repulsion, whereas it is essen-

tial in the retarded contribution. Second, the self-interaction has to be excluded from the Coulomb repulsion, whereas it contributes in the electron-phonon contribution. This is the main reason why we treat the Coulomb repulsion via the pair correlation function (in real space), and the retarded interaction with the two-point correlation function $C_F(\mathbf{k},\tau,\beta|N)$ (i.e., in wave-number space). In principle we have the choice to handle both terms either in real space or in wave-number space.

Having the definitions of the pair correlation function and the two point correlation function in mind, we thus obtain for the free energy (performing the angular integrations at once)

$$\begin{aligned} F(\beta|N_\uparrow,N_\downarrow) \leqslant F_0(\beta|N_\uparrow,N_\downarrow) &- \frac{1}{2}\omega\frac{dF_0(\beta|N_\uparrow,N_\downarrow)}{d\omega} \\ &- \frac{1}{2}\frac{v^2-w^2}{v}\frac{dF_0(\beta|N_\uparrow,N_\downarrow)}{dv} \\ &+ 2\pi U\int_0^\infty rN(N-1)g_F(r,\beta|N_\uparrow,N_\downarrow)dr \\ &- \frac{\sqrt{2}\alpha}{\pi}\int_0^{\beta/2}\int_0^\infty N^2 C_F(q,\tau,\beta|N_\uparrow,N_\downarrow)dq \\ &\times\frac{\cosh\left(\frac{1}{2}\beta-\tau\right)}{\sinh\left(\frac{1}{2}\beta\right)}d\tau. \end{aligned} \tag{A10}$$

For the ground-state energy ($\beta\to\infty$) we thus find

$$E^0(N_\uparrow,N_\downarrow) \leqslant E_{var}(N_\uparrow,N_\downarrow|v,w,\omega),$$

where the variational functional is

$$\begin{aligned} E_{var}(N_\uparrow,N_\downarrow|v,w,\omega) &= E_0(N_\uparrow,N_\downarrow) - \frac{1}{2}\omega\frac{dE_0(N_\uparrow,N_\downarrow)}{d\omega} - \frac{1}{2}\frac{v^2-w^2}{v}\frac{dE_0(N_\uparrow,N_\downarrow)}{dv} \\ &+ 2\pi U\int_0^\infty rN(N-1)g_F(r,\beta\to\infty|N_\uparrow,N_\downarrow)dr \\ &- \frac{\sqrt{2}\alpha}{\pi}\int_0^\infty\int_0^\infty N^2 C_F(q,\tau,\beta\to\infty|N_\uparrow,N_\downarrow)dqe^{-\tau}d\tau. \end{aligned} \tag{A11}$$

Here, E_0 is the ground-state energy corresponding to the trial action, given by

$$E_0(N_\uparrow,N_\downarrow) = \frac{3}{2}(v-w-\omega) + \mathbb{E}_F(N_\uparrow) + \mathbb{E}_F(N_\downarrow), \tag{A12}$$

where $\mathbb{E}_F(N)$ is the ground-state energy of N fermions with parallel spins and with energy levels $\epsilon_n=\left(n+\frac{3}{2}\right)\omega$:

$$\mathbb{E}_F(N) = \frac{1}{8}L(L+2)(L+1)^2\omega + (N-N_L)\left(L+\frac{3}{2}\right)\omega, \tag{A13}$$

L denotes the lowest partially filled or empty level, and

$$N_L = \frac{1}{6}L(L+1)(L+2)$$

is the number of fermions in the fully occupied levels. Filling out E_0 in E_{var} we thus obtain

$$\begin{aligned} E_{var}(N_\uparrow,N_\downarrow|v,w,\omega) &= \frac{3}{4}\frac{(v-w)^2}{v} - \frac{3}{4}\omega + \frac{1}{2}\mathbb{E}_F(N_\uparrow) + \frac{1}{2}\mathbb{E}_F(N_\downarrow) \\ &+ 2\pi U\int_0^\infty rN(N-1)g_F(r,\beta\to\infty|N_\uparrow,N_\downarrow)dr \\ &- \frac{\sqrt{2}\alpha}{\pi}\int_0^\infty\int_0^\infty N^2 C_F(q,\tau,\beta\to\infty|N_\uparrow,N_\downarrow)dqe^{-\tau}d\tau, \end{aligned} \tag{A14}$$

where the factor $1/2$ in front of $\mathbb{E}_F$ is a consequence of the subtraction $\mathbb{E}_F-\frac{1}{2}\omega(d\mathbb{E}_F/d\omega)$, not surprising because of the virial theorem for harmonic oscillators. The term $\frac{3}{4}(v-w)^2/v$ is precisely the same as in Feynman's treatment of the polaron, but of course the values of v and w will be different if many-particle effects will be taken into account.

We now split g_F and C_F for a mixture of fermions with different spin projections into the parts corresponding to parallel and opposite spins. The case of $N_\uparrow$ electrons with spin up and $N_\downarrow$ electrons with spin down can be found after some reflection in terms of the spin-polarized quantities:

$$N\tilde{n}_F(\mathbf{q},\beta|N=N_\uparrow+N_\downarrow) = N_\uparrow\tilde{n}_F(\mathbf{q},\beta|N_\uparrow) + N_\downarrow\tilde{n}_F(\mathbf{q},\beta|N_\downarrow), \tag{A15}$$

$$\begin{aligned} N(N-1)g_F(r,\beta|N_\uparrow,N_\downarrow) &= N_\uparrow(N_\uparrow-1)g_F(r,\beta|N_\uparrow) + N_\downarrow(N_\downarrow-1)g_F(r,\beta|N_\downarrow) \\ &+ \frac{2N_\uparrow N_\downarrow}{(2\pi)^3}\int e^{i\mathbf{q}\cdot\mathbf{r}}\tilde{n}_F(\mathbf{q},\beta|N_\uparrow)\tilde{n}_F(\mathbf{q},\beta|N_\downarrow)d\mathbf{q}, \end{aligned} \tag{A16}$$

$$\begin{aligned} N^2\mathbb{C}_F(\mathbf{q},\tau,\beta|N_\uparrow,N_\downarrow) = N_\uparrow^2\mathbb{C}_F(\mathbf{q},\tau,\beta|N_\uparrow) + N_\downarrow^2\mathbb{C}_F(\mathbf{q},\tau,\beta|N_\downarrow) \\ + 2N_\uparrow N_\downarrow\tilde{n}_F(\mathbf{q},\beta|N_\uparrow)\tilde{n}_F(\mathbf{q},\beta|N_\downarrow). \end{aligned} \tag{A17}$$

3. Coulomb and electron-phonon energies

Using Eqs. (A15)–(A17) in the variational functional (A11), we arrive at the expression with three Coulomb terms and three electron-phonon terms as follows:

$$E_{var}(N_\uparrow,N_\downarrow|v,w,\omega)=\frac{3}{4}\frac{(v-w)^2}{v}-\frac{3}{4}\omega+\frac{1}{2}\mathbb{E}_F(N_\downarrow)+\frac{1}{2}\mathbb{E}_F(N_\downarrow)+E_{C\|}(N_\uparrow)+E_{C\|}(N_\downarrow)+E_{C\uparrow\downarrow}(N_\uparrow,N_\downarrow)+E_{\alpha\|}(N_\uparrow)+E_{\alpha\|}(N_\downarrow)+E_{\alpha\uparrow\downarrow}(N_\uparrow,N_\downarrow) \tag{A18}$$

with the contributions

$$E_{C\|}(N)=2\pi N(N-1)U\int_0^\infty rg_F(r,\beta\to\infty|N)dr, \tag{A19}$$

$$E_{C\uparrow\downarrow}(N_\uparrow,N_\downarrow)=4\pi N_\uparrow N_\downarrow U\int_0^\infty r\frac{1}{(2\pi)^3}\int e^{i\mathbf{q}\cdot\mathbf{r}}\tilde{n}_F\times(\mathbf{q},\beta\to\infty|N_\uparrow)\tilde{n}_F(\mathbf{q},\beta\to\infty|N_\downarrow)d\mathbf{q}dr, \tag{A20}$$

$$E_{\alpha\|}(N)=-\frac{\sqrt{2}\alpha}{\pi}N^2\int_0^\infty\int_0^\infty e^{-q^2/2(N_\uparrow+N_\downarrow)[(w^2/v^2)\tau+(v^2-w^2)/v^3(1-e^{-v\tau})-(1-e^{-\omega\tau})/\omega]-\tau}\mathbb{C}_F(\mathbf{q},\tau,\beta\to\infty|N)dqd\tau, \tag{A21}$$

$$E_{\alpha\uparrow\downarrow}(N_\uparrow,N_\downarrow)=-\frac{2\sqrt{2}\alpha}{\pi}N_\uparrow N_\downarrow\int_0^\infty dq\int_0^\infty d\tau e^{-q^2/2(N_\uparrow+N_\downarrow)[(w^2/v^2)\tau+(v^2-w^2)/v^3(1-e^{-v\tau})-(1-e^{-\omega\tau})/\omega]-\tau}\tilde{n}_F(\mathbf{q},\beta\to\infty|N_\uparrow)\tilde{n}_F(\mathbf{q},\beta\to\infty|N_\downarrow). \tag{A22}$$

The integrations over $\mathbf{q}$ and over r in Eqs. (A19)–(A22) are performed using the explicit form of the density and correlation functions [see Eq. (A25)]

$$\tilde{n}_F(\mathbf{q},\beta\to\infty|N)=\frac{1}{N}\sum_{k=0}^{L}n_k(q)f_1(k|\beta\to\infty,N), \tag{A23}$$

$$\mathbb{C}_F(\mathbf{q},\tau,\beta\to\infty|N)=\frac{1}{N^2}\sum_{k=0}^{L}\sum_{k'=L}^{\infty}M_{kk'}(q)\times e^{(k-k')\omega\tau}[f_1(k|\beta\to\infty,N)-f_2(k,k'|\beta\to\infty,N)], \tag{A24}$$

$$g_F(r,\beta\to\infty|N)=\frac{1}{N(N-1)}\frac{1}{(2\pi)^3}\int d\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}\sum_{k=0}^{L}\sum_{k'=L}^{\infty}M_{kk'}(q)\times[f_1(k|\beta\to\infty,N)-f_2(k,k'|\beta\to\infty,N)] \tag{A25}$$

with the matrix elements

$$n_k(q)=\exp\left(-\frac{q^2}{4\omega}\right)L_k^{(2)}\left(\frac{q^2}{2\omega}\right), \tag{A26}$$

$$M_{kk'}(q)=e^{-q^2/2\omega}\left(\frac{q^2}{2\omega}\right)^{k_>-k_<}\sum_{j=0}^{k_<}(j+1)\frac{(k_<-j)!}{(k_>-j)!}\times\left[L_{k_<-j}^{(k_>-k_<)}\left(\frac{q^2}{2\omega}\right)\right]^2\begin{pmatrix}k_<\equiv\min(k,k')\\ k_>\equiv\max(k,k')\end{pmatrix}, \tag{A27}$$

where $L_k^{(\alpha)}(x)$ are the Laguerre polynomials, and with one-particle and two-particle distribution functions

$$f_1(k|\beta\to\infty,N)=\begin{cases}1, & k<L\\ 0, & k>L\\ \dfrac{N-N_L}{N_{L+1}-N_L}, & k=L,\end{cases} \tag{A28}$$

$$f_2(k,k'|\beta\to\infty,N)=\begin{cases}f_1(k|\beta\to\infty,N)f_1(k'|\beta\to\infty,N), & k\neq k'\\ 1, & k=k'<L\\ 0, & k=k'>L\\ \dfrac{N-N_L}{N_{L+1}-N_L}\dfrac{N-N_L-1}{N_{L+1}-N_L-1}, & k=k'=L.\end{cases} \tag{A29}$$

Using Eqs. (A23)–(A29), after performing integrations we arrive at the following formulas for the Coulomb and electron-phonon energies (A19)–(A22).

(i) The Coulomb energy for opposite spins is given by the expression

$$E_{C\uparrow\downarrow}(N_\uparrow,N_\downarrow)=U\sqrt{\frac{2\omega}{\pi}}\sum_{k=0}^{L_\uparrow}\sum_{l=0}^{L_\downarrow}(-1)^{k+l}\begin{pmatrix}k-\frac{1}{2}\\ k\end{pmatrix}\begin{pmatrix}k+l-\frac{1}{2}\\ l\end{pmatrix}\times\left[\begin{pmatrix}L_\uparrow+2\\ k+3\end{pmatrix}+\frac{N_\uparrow-N_{L_\uparrow}}{N_{L_\uparrow+1}-N_{L_\uparrow}}\begin{pmatrix}L_\uparrow+2\\ k+2\end{pmatrix}\right]\times\left[\begin{pmatrix}L_\downarrow+2\\ l+3\end{pmatrix}+\frac{N_\downarrow-N_{L_\downarrow}}{N_{L_\downarrow+1}-N_{L_\downarrow}}\begin{pmatrix}L_\downarrow+2\\ l+2\end{pmatrix}\right]. \tag{A30}$$

(ii) The Coulomb energy for parallel spins is

$$E_{C\|}(N) = U\sqrt{\frac{\omega}{2\pi}}\sum_{k=0}^{L}\sum_{l=0}^{L}(-1)^{k+l}\binom{k-\frac{1}{2}}{k}\binom{k+l-\frac{1}{2}}{l}$$
$$\times\left[\binom{L+2}{k+3}\binom{L+2}{l+3}+\frac{N-N_L}{N_{L+1}-N_L}\binom{L+2}{k+2}\binom{L+2}{l+3}\right.$$
$$+\frac{N-N_L}{N_{L+1}-N_L}\binom{L+2}{l+2}\binom{L+2}{k+3}$$
$$\left.+\frac{N-N_L}{N_{L+1}-N_L}\frac{N-N_L-1}{N_{L+1}-N_L-1}\binom{L+2}{k+2}\binom{L+2}{l+2}\right]$$
$$-U\sqrt{\frac{\omega}{2\pi}}\sum_{k=0}^{L}\sum_{k'=0}^{L}f_2(k,k'|\beta\to\infty,N)$$
$$\times\sum_{l=0}^{k_<}\sum_{j=0}^{l}(-1)^{l+j}\binom{j-\frac{1}{2}}{j}\binom{k_>-k_<+l+j-\frac{1}{2}}{l+k_>-k_<}$$
$$\times\binom{k_>+2}{k_<-l}\binom{2(l+k_>-k_<)}{l-j}.$$

(iii) The electron-phonon energy for opposite spins is

$$E_{\alpha\uparrow\downarrow}(N_\uparrow,N_\downarrow) = -2\alpha\sqrt{\frac{\omega}{\pi}}\int_0^\infty d\tau e^{-\tau}\sum_{k=0}^{L_\uparrow}\sum_{l=0}^{L_\downarrow}\frac{(-1)^{k+l}\binom{k-\frac{1}{2}}{k}\binom{k+l-\frac{1}{2}}{l}}{[2\omega P(\tau)+1]^{k+l+1/2}}$$
$$\times\left[\binom{L_\uparrow+2}{k+3}+\frac{N_\uparrow-N_{L_\uparrow}}{N_{L_\uparrow+1}-N_{L_\uparrow}}\binom{L_\uparrow+2}{k+2}\right]\left[\binom{L_\downarrow+2}{l+3}+\frac{N_\downarrow-N_{L_\downarrow}}{N_{L_\downarrow+1}-N_{L_\downarrow}}\binom{L_\downarrow+2}{l+2}\right] \tag{A31}$$

with the function

$$P(\tau)\equiv\frac{1}{2(N_\uparrow+N_\downarrow)}\left(\frac{w^2}{v^2}\tau+\frac{v^2-w^2}{v^3}(1-e^{-v\tau})-\frac{1-e^{-\omega\tau}}{\omega}\right). \tag{A32}$$

(iv) Finally, the electron-phonon energy for parallel spins takes the form

$$E_{\alpha\|}(N) = -\frac{\sqrt{2}\alpha}{\pi}\int_0^\infty d\tau e^{-\tau}E_{\alpha\|}(N,\tau), \tag{A33}$$

where the time-dependent function $E_{\alpha\|}(N,\tau)$ is a sum of three terms:

$$E_{\alpha\|}(N,\tau) = E^{(0)}_{\alpha\|}(N,\tau)+\frac{N-N_L}{N_{L+1}-N_L}E^{(1)}_{\alpha\|}(N,\tau)+\frac{N-N_L}{N_{L+1}-N_L}\frac{N-N_L-1}{N_{L+1}-N_L-1}E^{(2)}_{\alpha\|}(N,\tau). \tag{A34}$$

The terms $E^{(j)}_{\alpha\|}(N,\tau)$ can be written down in two equivalent alternative forms. The first form is relevant for the numerical calculation in the region of small and intermediate values of $(\omega\tau)$,

$$E^{(0)}_{\alpha\|}(N,\tau) = \sqrt{\frac{\pi\omega}{2}}\left(\sum_{j=0}^{L-1}\frac{[2(\cosh\omega\tau-1)]^j\binom{L+2}{j+3}\binom{j-\frac{1}{2}}{j}}{[2\omega P(\tau)+1-e^{-\omega\tau}]^{j+1/2}}\right.$$
$$-\sum_{j=1}^{L-1}(e^{j\omega\tau}+e^{-j\omega\tau})\sum_{n=0}^{L-j-1}\sum_{m=0}^{n}\frac{(-1)^{n+m}\binom{L+2}{j+n+3}\binom{2(j+n)}{n-m}\binom{m-\frac{1}{2}}{m}\binom{j+n+m-\frac{1}{2}}{j+n}}{[2\omega P(\tau)+1]^{j+n+m+1/2}}$$
$$\left.-\sum_{j=0}^{L-1}\sum_{n=0}^{j}(-1)^{j+n}\frac{\binom{2j}{j-n}\binom{L+2}{j+3}\binom{j-\frac{1}{2}}{j}\binom{j+n-\frac{1}{2}}{n}}{[2\omega P(\tau)+1]^{j+n+1/2}}\right)$$

$$+\sum_{j=0}^{L-1}\sum_{n=0}^{L-1}\frac{(-1)^{j+n}\binom{L+2}{j+3}\binom{L+2}{n+3}\binom{j-\frac{1}{2}}{j}\binom{j+n-\frac{1}{2}}{n}}{[2\omega P(\tau)+1]^{j+n+1/2}}\Bigg), \tag{A35}$$

$$E_{\alpha\|}^{(1)}(N,\tau)=\sqrt{\frac{\pi\omega}{2}}\Bigg(\sum_{j=0}^{L}\frac{[2(\cosh\omega\tau-1)]^{j}\binom{L+2}{j+2}\binom{j-\frac{1}{2}}{j}}{[2\omega P(\tau)+1-e^{-\omega\tau}]^{j+1/2}}$$
$$-\sum_{j=1}^{L}(e^{j\omega\tau}+e^{-j\omega\tau})\sum_{n=0}^{L-j}\sum_{m=0}^{n}\frac{(-1)^{n+m}\binom{L+2}{j+n+2}\binom{2(j+n)}{n-m}\binom{m-\frac{1}{2}}{m}\binom{j+n+m-\frac{1}{2}}{j+n}}{[2\omega P(\tau)+1]^{j+n+m+1/2}}$$
$$+2\sum_{j=0}^{L-1}\sum_{n=0}^{L}\frac{(-1)^{j+n}\binom{L+2}{j+3}\binom{L+2}{n+2}\binom{j-\frac{1}{2}}{j}\binom{j+n-\frac{1}{2}}{n}}{[2\omega P(\tau)+1]^{j+n+1/2}}\Bigg), \tag{A36}$$

$$E_{\alpha\|}^{(2)}(N,\tau)=\sqrt{\frac{\pi\omega}{2}}\Bigg(-\sum_{j=0}^{L}\sum_{n=0}^{j}(-1)^{j+n}\frac{\binom{2j}{j-n}\binom{L+2}{j+2}\binom{j-\frac{1}{2}}{j}\binom{j+n-\frac{1}{2}}{n}}{[2\omega P(\tau)+1]^{j+n+1/2}}$$
$$+\sum_{j=0}^{L}\sum_{n=0}^{L}\frac{(-1)^{j+n}\binom{L+2}{j+2}\binom{L+2}{n+2}\binom{j-\frac{1}{2}}{j}\binom{j+n-\frac{1}{2}}{n}}{[2\omega P(\tau)+1]^{j+n+1/2}}\Bigg). \tag{A37}$$

The second form is relevant for intermediate and large values of $(\omega\tau)$,

$$E_{\alpha\|}^{(0)}(N,\tau)=\sqrt{\frac{\pi\omega}{2}}\Bigg(\sum_{j=1}^{\infty}e^{-j\omega\tau}\sum_{n=0}^{L-1}\sum_{m=0}^{n}\frac{(-1)^{n+m}\binom{L+j+2}{n+j+3}\binom{2(n+j)}{n-m}\binom{m-\frac{1}{2}}{m}\binom{j+n+m-\frac{1}{2}}{j+n}}{[2\omega P(\tau)+1]^{j+n+m+1/2}}$$
$$-\sum_{j=1}^{L-1}e^{-j\omega\tau}\sum_{n=0}^{L-j-1}\sum_{m=0}^{n}\frac{(-1)^{n+m}\binom{L+2}{n+j+3}\binom{2(n+j)}{n-m}\binom{m-\frac{1}{2}}{m}\binom{j+n+m-\frac{1}{2}}{j+n}}{[2\omega P(\tau)+1]^{j+n+m+1/2}}$$
$$+\sum_{n=0}^{L-1}\sum_{m=0}^{L-1}\frac{(-1)^{n+m}\binom{L+2}{n+3}\binom{L+2}{m+3}\binom{n-\frac{1}{2}}{n}\binom{n+m-\frac{1}{2}}{m}}{[2\omega P(\tau)+1]^{n+m+1/2}}\Bigg), \tag{A38}$$

$$E_{\alpha\|}^{(1)}(N,\tau)=\sqrt{\frac{\pi\omega}{2}}\left(\sum_{j=0}^{\infty}e^{-j\omega\tau}\sum_{n=0}^{L}\sum_{m=0}^{n}\frac{(-1)^{n+m}\binom{L+j+2}{n+j+2}\binom{2(n+j)}{n-m}\binom{m-\frac{1}{2}}{m}\binom{j+n+m-\frac{1}{2}}{j+n}}{[2\omega P(\tau)+1]^{j+n+m+1/2}}\right.$$
$$-\sum_{j=1}^{L}e^{-j\omega\tau}\sum_{n=0}^{L-j}\sum_{m=0}^{n}\frac{(-1)^{n+m}\binom{L+2}{n+j+2}\binom{2(n+j)}{n-m}\binom{m-\frac{1}{2}}{m}\binom{j+n+m-\frac{1}{2}}{j+n}}{[2\omega P(\tau)+1]^{j+n+m+1/2}}$$
$$\left.+2\sum_{n=0}^{L}\sum_{m=0}^{L-1}\frac{(-1)^{n+m}\binom{L+2}{n+2}\binom{L+2}{m+3}\binom{n-\frac{1}{2}}{n}\binom{n+m-\frac{1}{2}}{m}}{[2\omega P(\tau)+1]^{n+m+1/2}}\right). \tag{A39}$$

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