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One-dimensional Fermi polaron in a combined harmonic and periodic potential

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We study an impurity in a one-dimensional potential consisting of a harmonic part and a periodic part using both the time-evolving block decay (TEBD) algorithm and a variational ansatz. Attractive and repulsive contact interactions with a sea of fermions are considered. We find excellent agreement between TEBD and variational results and use the variational ansatz to investigate higher lattice bands. We conclude that the lowest band approximation fails at sufficiently strong interactions and develop a method for computing the Tan contact parameter.

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I. INTRODUCTION

Impurities in lattices are of interest because of intriguing phenomena such as the Kondo effect [1], Anderson localization [2], and colossal magnetoresistance [3]. One-dimensional (1D) systems in particular are appealing because analytical results are available for the homogeneous fermionic impurity interacting through a δ function potential [4,5]. Various schemes such as the T-matrix approach, time-evolving block decimation (TEBD) [6], quantum Monte Carlo simulations, and a variational ansatz [7] have been successfully applied to the problem of an impurity interacting with fermions in higher dimensions [8–12] as well as one dimension [13–19] (for recent review articles, see Refs. [20,21]). Interest in 1D systems has further increased after the realization of such systems in ultracold gases using optical lattices, for instance, the Tonks-Girardeau gas [22,23]. Experimentally, the reduction in dimensionality is achieved by tightly confining the gas in two of the three spatial dimensions. Recent experiments studied impurities in 1D bosonic systems [24,25] and the 1D Fermi polaron in a few-body system [26]. Most theoretical studies of ultracold fermions in a lattice focus on the effects of the lattice and, for conceptual and numerical simplicity, neglect the effect of the harmonic trap. However, the inclusion of the harmonic trap changes the density of states [27], and in experimental practice a trapping potential is always present to confine the cloud of atoms.

Recently, it was proposed by Tan [28] that the high-momentum occupation probability \( n_q \) of fermions interacting through a short-range potential obeys the universal relation \( n_q \sim C/q^4 \), where \( q \) is momentum. The quantity \( C \) is called the contact because it is a measure of the probability of finding two particles in close proximity. Remarkably, the contact contains all the information about the many-body properties of the system and is furthermore appealing because of the relative ease with which it is measured, for example, using rf spectroscopy [29]. The Tan contact parameter was the subject of subsequent theoretical and experimental research (see Ref. [30] and references therein), although the majority of theoretical research was on homogeneous, spin-balanced systems (trapped systems have been discussed, e.g., in Refs. [31,32]). In this work, we look at the strongly spin-imbalanced, nonhomogeneous case.

We present a comprehensive study of an impurity in a 1D lattice with a harmonic trapping potential, interacting with a bath of majority component fermions. We note, however, that our variational model imposes no \textit{a priori} restrictions on the external potential or the dimensionality of the system. This paper is structured as follows. First, we investigate the problem in the lowest band approximation using both a variational ansatz and TEBD. Second, we consider higher lattice bands and evaluate the validity of the lowest band approximation. Finally, we discuss the high-energy excitations of the impurity and the associated contact parameter.

II. THE ONE-DIMENSIONAL FERMI POLARON

We consider an impurity (a “spin-down” atom) immersed in a sea of \( N \) (“spin-up”) fermions, with an external potential consisting of a harmonic part and a periodic part. This system is described in one dimension by the following Hamiltonian:

\[
\mathcal{H} = \sum_\sigma \int dx \psi_\sigma^\dagger(x) \left[ -\frac{\hbar^2}{2m_\sigma} \frac{d^2}{dx^2} + V(x) \right] \psi_\sigma(x) + g \int dx \psi_\uparrow^\dagger(x) \psi_\downarrow^\dagger(x) \psi_\downarrow(x) \psi_\uparrow(x) = \mathcal{H}_0 + \mathcal{H}_{\text{int}},
\]

where \( V(x) = v x^2 + \frac{h^2}{4} \left( 1 - \cos(2\pi k_L x) \right) \), \( x \) is position, \( m_\sigma \) is the mass of a particle, \( v \) is the strength of the harmonic potential, \( V_0 \) is the depth of the lattice, \( k_L \) determines the periodicity of the lattice, \( g \) determines the strength of the interparticle interaction (we assume contact interactions), and \( \psi_\sigma(1) \) destroys (creates) a particle in the spin state \( \sigma \in \{ \uparrow, \downarrow \} \). In practice, the “spin” states may, for instance, be different hyperfine states of the same atom.

We study this Hamiltonian using two distinct approaches: the TEBD algorithm [6] and a different implementation of a variational ansatz proposed by Chevy [7]. The TEBD simulation employs the Hubbard Hamiltonian (with additional harmonic trapping):

\[
\mathcal{H}_{\text{Hubbard}} = -\sum_{i\sigma} J_\sigma c_i^\dagger c_{i+1\sigma} + \text{H.c.} + U \sum_i c_i^\dagger c_i^\dagger c_i c_i + V_0 \sum_{i\sigma} c_i^\dagger c_i c_i \sigma^2,
\]

where \( J_\sigma \) is the hopping parameter (which can depend on spin), \( U \) determines the strength of the interparticle interaction, \( c_i^\dagger(1) \) destroys (creates) a particle with spin \( \sigma \) at site \( i \) (we choose \( i = 0 \) as the center site), and \( V_0 \) measures the strength of the...
harmonic trap. The variational ansatz, on the other hand, is an approximative scheme where one restricts the Hilbert space to include at most a single particle-hole pair (while it is possible to generalize the ansatz to a higher number of particle-hole pairs [13], we will consider at most a single pair). We use a more general form of the variational ansatz of Ref. [7], where instead of a polaron at fixed momentum we consider a general superposition (similar extensions were derived in Refs. [33,34]):

$$|\Psi\rangle = \sum_i \phi_i a_i^\dagger |0\rangle + \sum_{mkn} \phi_{mnk} a_{i,m}^\dagger a_{i,n}^\dagger |0\rangle. \tag{3}$$

Here \(\phi_i\) and \(\phi_{mnk} (m \neq k)\) are variational parameters, which are to be determined, \(a_{i,m}^\dagger\) destroys (creates) a particle with spin \(\sigma\) in an occupied (empty) state \(m, m = 0\) denotes the ground state of the noninteracting system, and \(|0\rangle\) is a shorthand notation for the ground state of the noninteracting system of \(N\) fermions. The operators \(a_{i,m}^\dagger\) destroy (create) particles in the eigenstates of \(H_0\). On the other hand, the operators \(a_{i,n}^\dagger\) for the minority component atom correspond to the eigenstates of the “mean-field” Hamiltonian \(H_0 + \gamma n^\dagger(x) n^\dagger(x)\) [\(\gamma n_1(x)\) is the density of the majority component atoms, where the density distribution of the noninteracting gas is used], of which the ground state is expected to be closer to the ground state of the full Hamiltonian (1). The computation then requires calculating the expectation value of the Hamiltonian \(\langle \Psi | \hat{H} | \Psi \rangle\) and minimizing with respect to the variational parameters \(\phi_i\) and \(\phi_{mnk}\) using an iterative procedure (a detailed description is shown in the Appendix). In principle, one can do this in any basis for the minority and majority component atoms; our choice is simply a matter of computational convenience. We will consider eigenstates in real space only and henceforth refer to this method as the real-space variational ansatz (RSVA). Note that the ansatz (3) neglects contributions from a molecular state, in contrast to Refs. [15,35]. In one dimension, such a “molecular ansatz” is not required since there is no phase transition.

The Hubbard Hamiltonian (2) is known to describe physics limited to the first band of the lattice accurately. TEBD gives essentially exact numerical results for the Hubbard model (2) and does not restrict the number of particle-hole excitations. However, the Hubbard model does not reproduce all the features of the Hamiltonian (1); only the lattice sites are considered, and the effect of the lattice in the tight-binding approximation is accounted for through the simplified hopping parameter \(J\). While the RSVA gives only approximate results, it is easily extended beyond these limitations to enhance the spatial resolution and access higher bands. The method is also numerically efficient; our implementation of the RSVA is three orders of magnitude faster than our TEBD implementation.

To provide the mapping between the full Hamiltonian (1) and the Hubbard Hamiltonian (2), we express energies in terms of the recoil energy \(E_R = \frac{\hbar^2 L^2}{2m}\) and scale lengths by \(k_L\). We will first consider the case where the full Hamiltonian (1) is discretized in space with spacing \(1/k_L\), such that only the bottoms of the lattice wells are considered and the parameter \(V_0\) plays no role. This corresponds to the lowest band approximation (LBA) of the single-band Hubbard Hamiltonian. We use closed boundary conditions throughout this paper.

### III. RESULTS

The polaron energy \(E_{pol}\) is defined as the energy of the impurity minus the energy of the impurity in the noninteracting system. In Fig. 1 we show \(E_{pol}\) as a function of \(U/J\) as computed by the RSVA and TEBD for various trapping frequencies. The agreement on the attractive (\(U/J < 0\)) side is excellent, while on the repulsive side we find good agreement for weak to moderate (\(0 < U/J \leq 4\)) interactions. For example, for a harmonic trap frequency of \(V_h/E_R = 0.0025\) we find a relative error of 1.7% at \(U/J = -5\) and an error of 0.2% at \(U/J = 1\). In the case of a finite trap, the iteration fails to converge at stronger (\(U/J \gtrsim 5\)) repulsive interactions. This is most likely due to the restrictions of the ansatz, which is not self-consistent in the majority component density. The inset of Fig. 1 also shows that while the energy matches very well with exact results, the prediction for the density profiles shows only qualitative agreement (see also the discussion concerning quasiparticle weight in Ref. [15]). Considering strongly repulsive interactions using the TEBD method we find, perhaps counterintuitively, the impurity in the center of the trap. Here it has a strong density overlap with the majority component. This is possible because of an arrangement where...
the doublon density \( \langle c_{\downarrow}^\dagger c_{\uparrow} c_{\downarrow} c_{\uparrow} \rangle \) is zero; the ground state is then a superposition of states with single occupancy (either \( \downarrow \) or \( \uparrow \)) of each lattice site.

The almost exact match on the attractive side is in agreement with results for the homogeneous case [13]. For strongly attractive interactions, the energy is given by \( E/E_R = U/J + \mathcal{E}_{\text{offset}}/E_R \), where \( \mathcal{E}_{\text{offset}} \) depends on the majority component number density \( \bar{n} \) near the center. This can be understood as follows. As the interaction becomes strongly attractive, the impurity will effectively pair with one of the majority component atoms, thus resulting in an interaction energy \( U/J \). However, this requires a rearrangement of the particles, resulting in a kinetic and trap energy penalty which depends only on \( V_h \) and \( N \). Indeed, we find that the energy of the trapped system with \( V_h/E_R = 0.0025 \) and number of lattice sites \( L = 80 \) is almost the same as the untrapped “lattice in a box” with \( L = 40 \). In both cases, \( \bar{n} \approx 0.5 \). This is consistent with the finding that a theory based on the local-density approximation works well [16]. In the tightly trapped limit \( V_h \rightarrow \infty \), particles are forced into the center of the trap, yielding unit filling \( \bar{n} = 1 \) for the \( N \) sites near the center, and we recover \( E_{\text{pol}} = U/J \).

Note that the special case of a harmonic trap with \( N = 1 \) was solved analytically [36].

With the RSVA on solid footing, we move to investigate the effect of higher lattice bands. While the Hubbard Hamiltonian is restricted to lattice sites, the variational approach allows spatially resolving the lattice, or, indeed, any spatially dependent potential, easily. This introduces a new free parameter \( V_0/E_R \), which describes the depth of the lattice. Figure 2 shows \( E_{\text{pol}} \) as a function of \( U/J \) for various values of \( V_0/E_R \) using six majority component particles and a harmonic trap \( V_h/E_R = 0.1 \). We resolve the lattice in real space with \( L = 16 \) sites using 128 points per lattice site and restrict the calculation to the first eight Bloch bands. Convergence with the number of points per lattice site is fast, and increasing the number further does not provide a significant change to the energy. Conversely, the convergence of the energy with the number of Bloch bands is slower [37]; including the ninth band gives a relative correction of 1.2% at \( U/J = -10 \) and \( V_0/E_R = 10 \). The proper rescaling of \( U/J \) as a function of \( V_0/E_R \) is obtained self-consistently by demanding that in the limit of small \( U/J \) the LBA is accurate. For high enough \( V_0/E_R \) the prediction from the LBA is quite accurate, even for strongly attractive interactions, as expected. However, as \( V_0/E_R \) is reduced, its accuracy quickly deteriorates. The effect of the harmonic trap (which varies significantly over lattice sites) increases the lattice depth required to be able to apply the LBA. In the lattice-only case, the LBA is known to be accurate as long as \( |U/J| \lesssim V_0/E_R \) (see [38] and references therein). We have verified by comparing to the case \( V_h = 0 \) that for \( U/J = −10 \) and \( V_0/E_R = 10 \), about two-thirds of the deviation from the LBA is due to harmonic confinement.

For any finite interaction strength, a fraction of the particles occupy all higher lattice bands. This allows access to the occupation probability of highly excited states, from which one can obtain the Tan contact parameter \( C \). Indeed, we find (see the inset of Fig. 2) that the high-\( n \) asymptote of the occupation probability \( \sum |\phi_{mkn}\rangle^2 \sim 1/n^4 \). These high-\( n \) states are just plane waves near the center of the trap where the polaron is localized because at very high energies the details of the potential are irrelevant. We thus obtain the characteristic decay \( \bar{n}_q \sim C/E_n^q \sim C/q^4 \), where \( q \) is momentum. For small values of \( |U/J| \) we recover the weakly interacting limit \( C \propto U^2 \).

Our approach highlights a general problem with single-band models in the sense that effects related to the contact may be neglected in an uncontrolled way; the \( 1/q^4 \) regime is entered when \( r_0 \ll 1/q \ll \mathcal{L} \), where \( r_0 \) is the range of the interparticle potential and \( \mathcal{L} \) is any relevant length scale of the problem [30]. In the results of Fig. 2, the contact regime is reached only for length scales shorter than the lattice spacing \( k^{-1}_l \) for a wide range of interaction strengths \( U/J \). Therefore, caution should be applied when using single-band models even in the weakly interacting regime, as essential physics may be missed.

It would also be of interest to investigate the influence of \( \bar{n} \) on the crossover to the contact regime. In the limit where the gas is very dilute, i.e., \( \bar{n} \ll 1 \), the interparticle spacing will become very large relative to the lattice spacing. Then it is plausible that the universal behavior will show up for \( k < k_l \). Unfortunately, it is not numerically feasible with our method to study the case of large \( L \) with a sufficient number of majority component particles, so that \( \bar{n} \ll 1 \).

IV. CONCLUSIONS

In conclusion, we have performed a detailed analysis of a (spin-down) impurity immersed in a sea of \( N \) (spin-up) fermions in a lattice with an additional harmonic trapping potential. We find that the RSVA is accurate over a large range of the interaction strength \( U \), from strongly attractive to moderately repulsive interactions. Furthermore, we compute the contribution from higher bands in this system and find
that the lowest band approximation breaks down even at relatively high values of the lattice depth $V_0/E_k$ if a sufficiently strong harmonic trapping potential is also present. Finally, we derive a method to compute the Tan contact parameter using the RSVA in trapped highly polarized systems. Our variational approach is general, simple, and numerically efficient and can be readily generalized to an arbitrary external potential $V(x)$, higher dimensions, and mass-imbalanced systems.

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APPENDIX: DETAILED DERIVATION OF THE VARIATIONAL METHOD

To describe the impurity, we consider the following Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}},$$

(A1)

where $\mathcal{H}_0$ is the single-particle Hamiltonian without interparticle interactions (in the canonical ensemble). This noninteracting Hamiltonian is given by

$$\mathcal{H}_0 = \int dx \sum_{\sigma} \psi^\dagger_\sigma(x) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi^{\dagger}_\sigma(x),$$

(A2)

where $\psi^{(\dagger)}_\sigma(x)$ destroys (creates) a particle with spin $\sigma \in \{\uparrow, \downarrow\}$, $m$ is the mass of a particle (we assume no mass imbalance), $V(x)$ measures the strength of the harmonic trapping potential, $V_0$ measures the depth of the periodic part of the potential, and $\psi^{(\dagger)}_\sigma$ determines the periodicity of the lattice. The interaction part of the Hamiltonian is (assuming contact interactions)

$$\mathcal{H}_{\text{int}} = g \int dx \sum_{\sigma} \psi^\dagger_\sigma(x) \psi^{\dagger}_\sigma(x) \psi^{\dagger}_\sigma(x) \psi^{\dagger}_\sigma(x).$$

(A3)

We can calculate the eigenfunctions and eigenvalues of $\mathcal{H}_0$ numerically. Let us define the creation operators for the particles in the eigenstates of the Hamiltonian $\mathcal{H}_0$ as $a^\dagger_{\alpha n}$, where $\alpha \in \{\text{spin orientations}\}$ and $n = 0$ is the ground state. A possible technique for finding the approximate ground state for this Hamiltonian is a variational ansatz [7]. In the ansatz, one restricts the possible particle-hole excitations of the system to one and neglects the probability of multiple particle-hole excitations. In our basis of choice, it reads (note that in order to avoid double counting, it is necessary to demand that $m \neq k$)

$$|\Psi\rangle = \sum_l \phi_l a^{\dagger}_{l\uparrow}|0\rangle + \sum_{mkn} \phi_{mkn} a^{\dagger}_{kn\uparrow} a_{k\uparrow} a^{\dagger}_{n\downarrow} |0\rangle,$$

(A4)

where $|0\rangle$ represents the vacuum, that is, the majority component atoms filled up until the Fermi surface in the noninteracting ($g = 0$) state. Since we are considering a fixed number $N$ of majority component particles, determining the state $|0\rangle$ is trivial: it just consists of the lowest $N$ eigenstates. The coefficients $\phi_l$ and $\phi_{mkn}$ are variational parameters, which are to be determined. Note that in the case of zero interparticle interactions ($g = 0$), the solution is obtained by setting $\phi_0 = 1$, $\phi_l = 0$ for $l > 0$ and $\phi_{mkn} = 0$.

We are interested in the ground-state energy of the impurity. For this purpose, let us now calculate the expectation value of the Hamiltonian $\langle \mathcal{H} \rangle = \langle \mathcal{H}_0 \rangle + \langle \mathcal{H}_{\text{int}} \rangle$. First, consider the noninteracting part of the Hamiltonian:

$$\langle \mathcal{H}_0 \rangle = \sum_l \phi^2_l a^\dagger_{l\uparrow} a_{l\uparrow}$$

$$\times \left( \sum_{mkn} \phi_{mkn} a^\dagger_{m\uparrow} a_{m\uparrow} a^\dagger_{n\downarrow} |0\rangle \right)$$

$$= \sum_{l\downarrow} E_l |\phi_l|^2 + \sum_{mkn} \Delta E_{mkn} |\phi_{mkn}|^2.$$

(A5)

Here the energies $E_l$ are the eigenvalues of the Hamiltonian $\mathcal{H}_0$ ($l = 0$ is the ground state of the noninteracting system) and $\Delta E_{mkn} = (E_m - E_k + E_n)$. It is straightforward to see that since $E_m > E_k$ (the operator $a^\dagger_{m\uparrow}$ cannot create particles in states that are already occupied), the ground state of the noninteracting system is the polaron in the lowest eigenstate of $\mathcal{H}_0$ with unit probability, as expected.

Now consider the interaction part of the Hamiltonian. First, we write it in the eigenfunction basis:

$$\mathcal{H}_{\text{int}} = g \sum_{ijpq} U_{ijpq}^\dagger a^\dagger_{i\uparrow} a_{j\downarrow} a^\dagger_{p\downarrow} a_{q\uparrow},$$

(A6)

where $U_{ijpq} = \int dx \phi^{\dagger}_{i\uparrow}(x) \phi^{\dagger}_{j\downarrow}(x) \phi_{p\downarrow}(x) \phi_{q\uparrow}(x)$. Here the $\alpha$ and $\beta$ functions correspond to the eigenfunctions for the majority component and the impurity, respectively, so that, for instance, $\phi^{\dagger}_{i\uparrow}(x) = \sum_i \phi^{\dagger}_{i\uparrow}(x) a^\dagger_{i\uparrow}$. These eigenfunctions can be chosen to be the same, although it will turn out to be useful to choose a different basis for the impurity. We remark that in our implementation the Hamiltonian is real and symmetric and both the eigenfunctions and the variational coefficients can be taken to be real. However, for the sake of completeness, we will continue to treat these quantities as complex.

It now follows that $\langle \mathcal{H}_{\text{int}} \rangle = \langle \mathcal{H}_{\text{int}} \rangle^{1} + \langle \mathcal{H}_{\text{int}} \rangle^{2} + \langle \mathcal{H}_{\text{int}} \rangle^{3}$, where the first term is a mean-field term and some careful bookkeeping is required when we consider the other terms.

The first term is given by

$$\mathcal{H}_{\text{int}}^{1} = g \sum_{ijpq} U_{ijpq}^\dagger a^\dagger_{i\uparrow} a_{j\downarrow} a^\dagger_{p\downarrow} a_{q\uparrow}.$$  

(A7)

For the inner product to be nonzero (the states are obviously orthogonal) we must have $q = l'$, $i = j$, and $p = l$, so that

$$\langle \mathcal{H}_{\text{int}} \rangle^{1} = g \sum_{llll'} U_{l'll'}^\dagger \phi^\dagger_l \phi_l = g \sum_{llll'} U_{l'll'}^\dagger \phi^\dagger_l ^{}.$$  

(A8)

where $U_{ll'} = \int dx \phi^{\dagger}_{l\uparrow}(x) \phi_{l\uparrow}(x)$. This is a Hartree energy-like term, where $n^\uparrow(x)$ is the majority component density. The
We can now determine the variational coefficients. Analogous to the previous case, we have

\[ \langle H_{m} \rangle_{2} = \sum_{m' k' n'} \left( \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}} \right) \left( g \sum_{ijpq} U_{ijpq} a_{i}^{\dagger} a_{j} a_{k} a_{q} \right) \times \sum_{m' k'n'} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}}. \]  

(A9)

Now there are three ways to make sure the inner product is nonzero:

\[ k = k', \quad m = m', \quad i = j, \]  

(A11)

\[ k = i, \quad m = m', \quad k' = j, \]  

(A12)

\[ k = k', \quad m = j, \quad i = m', \]  

(A13)

so that (note the minus sign because of the change in the ordering of operators, i.e., Wick’s theorem)

\[ \langle H_{m} \rangle_{2} = g \sum_{m' k' n'} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}} \left( \sum_{ijpq} U_{ijpq} a_{i}^{\dagger} a_{j} a_{k} a_{q} \right) \times \sum_{m' k'n'} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}}. \]  

(A10)

The occupation number probabilities \( n_{i} \) for a certain state \( i \) at zero temperature are now implicit in the summation. Writing them explicitly,

\[ \langle H_{m} \rangle_{2} = g \sum_{m' k' n'} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}} \left( \sum_{ijpq} U_{ijpq} a_{i}^{\dagger} a_{j} a_{k} a_{q} \right) \times \sum_{m' k'n'} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}}. \]  

(A14)

The occupation number probabilities \( n_{i} \) for a certain state \( i \) at zero temperature are now implicit in the summation. Writing them explicitly,

\[ \langle H_{m} \rangle_{2} = g \sum_{m' k' n'} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}} \left( \sum_{ijpq} U_{ijpq} a_{i}^{\dagger} a_{j} a_{k} a_{q} \right) \times \sum_{m' k'n'} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}}. \]  

(A15)

The third term is less complicated and is given by

\[ \langle H_{m} \rangle_{3} = \sum_{m' k' n'} \langle \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}} \rangle \times \left( g \sum_{ijpq} U_{ijpq} a_{i}^{\dagger} a_{j} a_{k} a_{q} \right) + \text{H.c.} \]  

(A16)

We can now determine the variational coefficients \( \phi_{i} \) and \( \phi_{mkn} \). Consider the sum of terms \( \langle H \rangle = \langle H_{0} \rangle + \langle H_{m} \rangle_{1} + \langle H_{m} \rangle_{2} + \langle H_{m} \rangle_{3} \). It follows that \( \frac{\partial}{\partial \phi_{i}} \langle H \rangle = \frac{\partial}{\partial \phi_{i}} E(\psi|\psi) = E\phi_{i} \). The constant \( E \) is a Lagrange multiplier, which can be identified with the energy of the impurity. A similar procedure gives another set of equations for the coefficients \( \phi_{mkn} \). Following this recipe, we obtain

\[ \frac{\partial E(\Psi|\Psi)}{\partial \phi_{mkn}} = E\phi_{l} + g\phi_{l} \sum_{j} U_{lj} + g \sum_{mkn} \phi_{mkn} U_{kln} n_{k}(1 - n_{m}) \]  

\[ = E\phi_{l}. \]  

(A17)

The differentiation with respect to \( \phi_{mkn} \) gives

\[ \frac{\partial E(\Psi|\Psi)}{\partial \phi_{mkl}} = (E_{n} - E_{k} + E_{m} \phi_{mkn} + g\phi_{l} U_{kln} n_{k}(1 - n_{m}) + g \sum_{n' m' k' n} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}} \times \sum_{m' k'n'} \phi_{m' k' n' a_{i} a_{j} a_{k} a_{m}}. \]  

\[ \text{A18} \]

Now we can write

\[ E\phi_{i} = E_{i}\phi_{i} + g \sum_{l} \phi_{i} U_{i} + g \sum_{mkn} \phi_{mkn} U_{mkn} \]  

\[ \text{A20} \]

\[ E\phi_{mkn} = \Delta E_{mkn} \phi_{mkn} + g \Gamma_{mkn} + g \sum_{l} \phi_{i} U_{mkn} \]  

\[ \text{A21} \]

This system of equations can be solved iteratively starting, e.g., from an initial state where \( \phi_{0} = 1 \) and all other coefficients are zero, i.e., the ground state of the noninteracting system.

The problem with the above scheme is that the fixed-point iteration is not guaranteed to converge, especially if the initial state is far from the ground state. We may find a metastable state, or worse, the iteration might not converge at all. A convenient alternative choice (although not necessarily the best) is writing the polaron eigenstates in terms of a “mean-field” basis. We consider a slightly different Hamiltonian to describe the polaron:

\[ \mathcal{H}_{0, \text{MF}} = \int dx \psi_{\dagger}(x) \left\{ -\frac{\hbar^{2}}{2m} \frac{\partial^{2}}{\partial x^{2}} + \frac{1}{2} m \omega^{2} x^{2} + \frac{V_{0}}{2} \left[ -\cos(2\pi k_{L} x) + 1 \right] + g n_{\dagger}(x) \right\} \psi_{\dagger}(x) \]  

(A22)

where \( n_{\dagger}(x) \) is the majority component density in the noninteracting system. The eigenfunctions of this Hamiltonian can still be obtained through an eigenvalue solver; one just needs to
calculate the eigenfunctions of the noninteracting Hamiltonian first, compute \( n_i(x) \) from the resulting eigenbasis, and use the result to compute the eigenfunctions in the new basis for the polaron. Since the total Hamiltonian describing the system is unchanged, we subtract the term that was added from the polaron. Since the total Hamiltonian describing the system result to compute the eigenfunctions in the new basis for the polaron. Since the total Hamiltonian is unchanged, we subtract the term that was added from the polaron. Since the total Hamiltonian describing the system is unchanged, we subtract the term that was added from the polaron. Since the total Hamiltonian describing the system is unchanged, we subtract the term that was added from the polaron. Since the total Hamiltonian describing the system is unchanged, we subtract the term that was added from the polaron.

\[
\mathcal{H} = \mathcal{H}_{0,\text{MF}} + \mathcal{H}_{\text{int}} + \mathcal{H}_{\text{MF}},
\]

(A23)

and we calculate the expectation value:

\[
\langle \mathcal{H}_{\text{MF}} \rangle = -g \left( \sum_i \phi_i^* a_i^\dagger + \sum_{mkn} \phi_{mkn}^* a_i^\dagger a_k^\dagger a_m^\dagger \right)
\]

\[
\times \sum_{ij} U_{ij} a_i^\dagger a_j^\dagger \left( \sum_l \phi_l^* \right)
\]

\[
+ \sum_{m'kn'} \phi_{m'kn'}^* a_{m'k}^\dagger a_{n'n}^\dagger \right) \right). \quad \text{(A24)}
\]

We have four terms. The first one is simple:

\[
\left( \sum_{l'l'} \sum_{ij} \phi_i^* a_{ij}^\dagger a_{ij}^\dagger \phi_{l'l'} \right) = -g \left( \sum_{l'l'} \phi_i^* a_{ij}^\dagger a_{ij}^\dagger \phi_{l'l'} \right), \quad \text{(A25)}
\]

which precisely cancels the \( U_{l'l'} \) term in Eq. (A20). The second and third terms (the cross-terms) drop out because of the requirement that \( m \neq k \). The final term is given by

\[
-g \left( \sum_{mkn} \phi_{mkn}^* a_i^\dagger a_j^\dagger a_{k+m}^\dagger a_{l+m}^\dagger \right) \times \sum_{m'kn'} \phi_{m'kn'}^* a_{m'k}^\dagger a_{l'n}^\dagger a_{n'n}^\dagger
\]

\[
= -g \sum_{mkn} \phi_{mkn}^* \phi_{mkn} (1 - n_m) U_{n'n'}, \quad \text{(A26)}
\]

which cancels the term containing the density in \( \Gamma_{mkn} \), the first term in Eq. (A19). The change of basis thus conveniently simplifies the variational calculation by removing two of the terms.

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