

Spectral functions of the half-filled one-dimensional Hubbard chain within the exchange-correlation potential formalism

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(Received 22 April 2022; accepted 7 July 2022; published 19 July 2022)

The spectral functions of the one-band half-filled one-dimensional Hubbard chain are calculated using the exchange-correlation potential formalism developed recently. The exchange-correlation potential is adopted from the exact potential derived from the Hubbard dimer. Within an approximation in which the full Green's function is replaced by a noninteracting one, the spectral functions can be calculated analytically. Despite the simplicity of the approximation, the resulting spectra are in favorable agreement with the more accurate results obtained from the dynamic density-matrix renormalization group method. In particular, the analytically calculated band gap as a function of U is in close agreement with the exact gap obtained from the Bethe ansatz. In addition, the formal general solution to the equation of motion of the Green's function is presented, and the difference between the traditional self-energy approach and the exchange-correlation potential formalism is also discussed and elaborated. A simplified Holstein Hamiltonian is considered to further illustrate the general form of the exchange-correlation potential.

DOI: [10.1103/PhysRevB.106.045123](https://doi.org/10.1103/PhysRevB.106.045123)

I. INTRODUCTION

Very recently, a completely different route for calculating the Green's function was proposed. The formalism replaces the traditional self-energy by a time-dependent exchange-correlation potential, $V_{xc}(r, r'; t)$, which acts as a multiplicative potential on the Green's function, in contrast to the self-energy, which acts as a convolution in space and time [1].

In Ref. [1], the formalism was illustrated by deriving the exact V_{xc} of the Hubbard dimer expressed in the site orbitals. In this paper, the formalism is applied to calculate the Green's function of the one-dimensional Hubbard chain at half filling by utilizing the V_{xc} derived from the Hubbard dimer, rewritten in the bonding and antibonding orbitals appropriate for extension to the one-dimensional (1D) chain. Under certain approximations, the Green's function can be calculated analytically, providing explicit insights into the dependence of the spectra on the parameters of the model. Despite the simple appearance of the Hamiltonian of the one-dimensional Hubbard chain, it is actually a rather stringent test for a many-electron theory. It is well known that the exact solution based on the Bethe ansatz yields two branches of collective excitations corresponding to the holon and the spinon [2,3]. While the Bethe-ansatz solution provides the dispersion of the holon and the spinon, it does not contain information about the spectral

distribution. The spectral functions, however, have been calculated within the dynamical density-matrix renormalization group method [4] and furnish comparison with the present work. Earlier calculations are limited to the large- U limit [5,6], and there are also related investigations on Luttinger liquids [7,8]. The 1D Hubbard model is physically relevant as shown, for example, in the case of SrCuO₂, which has been found to exhibit the spinon and holon excitations [9,10].

Apart from application to the 1D Hubbard chain, a formal solution of the equation of motion of the Green's function is derived, which provides an iterative scheme in practical calculations.

To contrast the traditional self-energy approach and the exchange-correlation formalism, comparison between the two is made and discussed from a historical perspective, and the differences are emphasized and elaborated.

In addition, the exchange-correlation potential of a simplified Holstein Hamiltonian, describing a coupling between a core electron and a set of bosons (e.g., plasmons or phonons), is derived analytically and serves as a further illustration of the exchange-correlation potential formalism. This sheds light on the form of V_{xc} , which offers a very simple physical interpretation.

II. THEORY

The exchange-correlation potential formalism developed in Ref. [1] is summarized, and the main results are presented.

A. Equation of motion of the Green's function

The zero-temperature time-ordered Green's function is defined as [11]

$$iG(rt, r't') = \langle T[\hat{\psi}(rt)\hat{\psi}^\dagger(r't')] \rangle, \quad (1)$$

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where $r = (\mathbf{r}, \sigma)$ labels both space and spin variables, $\hat{\psi}(rt)$ is the Heisenberg field operator, T is the time-ordering symbol, and $\langle \cdot \rangle$ denotes the expectation value in the ground state. Extension to finite temperature is quite straightforward. The many-electron Hamiltonian defining the Heisenberg operator is given by

$$\hat{H} = \int dr \hat{\psi}^\dagger(r) h_0(r) \hat{\psi}(r) + \frac{1}{2} \int dr dr' \hat{\psi}^\dagger(r) \hat{\psi}^\dagger(r') v(r-r') \hat{\psi}(r') \hat{\psi}(r), \quad (2)$$

where $h_0 = -\frac{1}{2}\nabla^2 + V_{\text{ext}}(r)$ and $v(r-r') = 1/|\mathbf{r}-\mathbf{r}'|$. In our notation, $\int dr = \sum_\sigma \int d^3r$, and atomic units are used throughout, in which the Bohr radius a_0 , the electron mass m_e , the electronic charge e , and \hbar are set to unity. For a system in equilibrium, the Hamiltonian is time independent, and t' may be set to zero. The equation of motion of the Green's function is given by

$$\left(i\frac{\partial}{\partial t} - h_0(r)\right)G(r, r'; t) + i \int dr'' v(r-r'') \langle T[\hat{\rho}(r''t) \hat{\psi}(rt) \hat{\psi}^\dagger(r')] \rangle = \delta(t)\delta(r-r'). \quad (3)$$

Since the Green's function was conceived in the 1950s, the traditional approach is to introduce the self-energy Σ and truncate the hierarchy of higher-order Green's functions such that [11]

$$-i \int dr'' v(r-r'') \langle T[\hat{\rho}(r''t) \hat{\psi}(rt) \hat{\psi}^\dagger(r')] \rangle = V_{\text{H}}(r)G(r, r'; t) + \int dr'' dt'' \Sigma(r, r''; t-t'')G(r'', r'; t''). \quad (4)$$

The equation of motion then becomes

$$\left(i\frac{\partial}{\partial t} - h(r)\right)G(r, r'; t) - \int dr'' dt'' \Sigma(r, r''; t-t'')G(r'', r'; t'') = \delta(r-r')\delta(t), \quad (5)$$

where $h = h_0 + V_{\text{H}}$ with V_{H} being the Hartree potential.

As shown in Ref. [1], it is possible to define an exchange-correlation potential V_{xc} so that the Green's function fulfills the following equation of motion:

$$\left(i\frac{\partial}{\partial t} - h(r) - V_{\text{xc}}(r, r'; t)\right)G(r, r'; t) = \delta(r-r')\delta(t), \quad (6)$$

where V_{xc} is the Coulomb potential of the time-dependent exchange-correlation hole, ρ_{xc} ,

$$V_{\text{xc}}(r, r'; t) = \int dr'' v(r-r'') \rho_{\text{xc}}(r, r', r''; t), \quad (7)$$

and ρ_{xc} is given by

$$\rho_{\text{xc}}(r, r', r''; t) = [g(r, r', r''; t) - 1]\rho(r''), \quad (8)$$

in which the correlator g is defined according to

$$\begin{aligned} & \langle T[\hat{\rho}(r''t) \hat{\psi}(rt) \hat{\psi}^\dagger(r')] \rangle \\ &= iG(r, r'; t)g(r, r', r''; t)\rho(r'') \\ &= iG(r, r'; t)[\rho(r'') + \rho_{\text{xc}}(r, r', r''; t)]. \end{aligned} \quad (9)$$

The exchange-correlation hole fulfills the sum rule

$$\int d^3r'' \rho_{\text{xc}}(r, r', r''; t) = -\delta_{\sigma\sigma'}\theta(-t), \quad (10)$$

and it has the property

$$\rho_{\text{xc}}(r, r', r; t) = -\rho(r) \quad (11)$$

for any r, r' , and t . The sum rule and the above property may be seen as the dynamic version of the corresponding properties of the static exchange-correlation hole [12] originating from the seminal work of Slater on the exchange hole [13,14]. For a given r' , $V_{\text{xc}}(r, r'; t)$ may be interpreted as a local time-dependent one-particle potential in which the added hole or electron moves.

In the language of the functional derivative technique, the exchange-correlation hole can be related to the functional derivative of the Green's function with respect to a probing field φ [15,16]. Since

$$\langle T[\hat{\rho}(3) \hat{\psi}(1) \hat{\psi}^\dagger(2)] \rangle = i\rho(3)G(1, 2) - \frac{\delta G(1, 2)}{\delta \varphi(3)}, \quad (12)$$

it follows that

$$i\rho_{\text{xc}}(1, 2, 3)G(1, 2) = -\frac{\delta G(1, 2)}{\delta \varphi(3)}, \quad (13)$$

where $1 = (r_1, t_1)$, etc. Using the identity

$$\delta G = -G(\delta G^{-1})G, \quad (14)$$

one obtains from the equation of motion of the Green's function

$$\begin{aligned} & \rho_{\text{xc}}(1, 2, 3)G(1, 2) \\ &= i \int d4G(1, 4) \left\{ \delta(4-3) + \frac{\delta V_{\text{H}}(4)}{\delta \varphi(3)} \right\} G(4, 2) \\ &= i \int d4G(1, 4)\epsilon^{-1}(4, 3)G(4, 2), \end{aligned} \quad (15)$$

where we have only kept the variation of the Hartree potential (random-phase approximation) and ϵ is the dielectric matrix. This provides an explicit formula for calculating the exchange-correlation hole in terms of the response function.

B. General iterative solution

From the equations of motion for G and G^{H} of the Hartree approximation, a Dyson-like equation can be constructed as follows:

$$\begin{aligned} G(r, r'; t) &= G^{\text{H}}(r, r'; t) \\ &+ \int dr'' dt' G^{\text{H}}(r, r''; t-t') \\ &\times V_{\text{xc}}(r'', r'; t')G(r'', r'; t'). \end{aligned} \quad (16)$$

By operating $i\partial/\partial t - h(r)$ on both sides of the equation, it can be verified that the above G fulfills the equation of motion.

This Dyson-like equation can be used as an iterative scheme for solving for G . The iteration is started by setting $G = G^H$ on the right-hand side and continued until self-consistency is achieved. One may choose a different starting point, such as the Kohn-Sham [17] Green's function G^{KS} , in which case V_{xc} must be replaced with $V_{xc} - V_{xc}^{KS}$.

In practice, it is convenient to express the equation of motion in a set of base orbitals $\{\varphi_i\}$:

$$i \frac{\partial}{\partial t} G_{ij}(t) - \sum_k h_{ik} G_{kj}(t) - \sum_{kl} V_{ik,lj}^{xc}(t) G_{kl}(t) = \delta_{ij} \delta(t), \quad (17)$$

where G_{ij} and h_{ik} are the matrix elements of G and h in the orbitals and

$$V_{ik,lj}^{xc}(t) = \int d^3 r d^3 r' \varphi_i^*(r) \varphi_k(r) V_{xc}(r, r'; t) \varphi_l^*(r') \varphi_j(r'). \quad (18)$$

The Dyson-like equation becomes

$$G_{ij}(t) = G_{ij}^H(t) + \sum_k \int dt' G_{ik}^H(t-t') F_{kj}(t'), \quad (19)$$

in which

$$F_{kj}(t') = \sum_{lm} V_{kl,mj}^{xc}(t') G_{lm}(t'). \quad (20)$$

Fourier transformation leads to

$$G_{ij}(\omega) = G_{ij}^H(\omega) + \sum_k G_{ik}^H(\omega) F_{kj}(\omega) \quad (21)$$

and

$$F_{kj}(\omega) = \sum_{lm} \int \frac{d\omega'}{2\pi} V_{kl,mj}^{xc}(\omega - \omega') G_{lm}(\omega'). \quad (22)$$

This yields an integral equation for $F(\omega)$:

$$F_{kj}(\omega) = \sum_{lm} \int \frac{d\omega'}{2\pi} V_{kl,mj}^{xc}(\omega - \omega') \times \left[G_{lm}^H(\omega') + \sum_n G_{ln}^H(\omega') F_{nm}(\omega') \right]. \quad (23)$$

Since G^H is a noninteracting Green's function, the integrals over ω' can be performed analytically.

Alternatively, by isolating the terms containing G_{ij} , the equation of motion can be rewritten as follows:

$$\left\{ i \frac{\partial}{\partial t} - h_{ii} - V_{ii,jj}^{xc}(t) - D_{ij}(t) \right\} G_{ij}(t) = \delta_{ij} \delta(t), \quad (24)$$

where

$$D_{ij}(t) = \frac{1}{G_{ij}(t)} \left\{ \sum_{k \neq i} h_{ik} G_{kj}(t) + \sum_{k \neq i, l \neq j} V_{ik,lj}^{xc}(t) G_{kl}(t) \right\}. \quad (25)$$

The formal iterative solution is given by

$$G_{ij}(t) = [G_{ij}(0^-) \theta(-t) + G_{ij}(0^+) \theta(t)] \times \exp \left\{ -i \int_0^t dt' [h_{ii} + V_{ii,jj}^{xc}(t') + D_{ij}(t')] \right\}, \quad (26)$$

where

$$iG_{ij}(0^+) - iG_{ij}(0^-) = \delta_{ij}, \quad (27)$$

which is obtained by integrating the equation of motion from 0^- to 0^+ . Since the Green's function to be solved appears on the right-hand side of the equation, the formal solution in Eq. (26) facilitates an iterative scheme for solving the Green's function.

C. Self-energy versus exchange-correlation potential

A fundamental difference between the traditional self-energy and the exchange-correlation potential approaches is that the former acts on the Green's function as a convolution in space and time whereas the latter acts multiplicatively. The multiplicative property of V_{xc} has consequences. One of these is that the equation of motion in Eq. (6) separates into an equation for the hole Green's function ($t < 0$) and an equation for the electron Green's function ($t > 0$). In contrast, due to the convolution in time in the self-energy term, solving for the hole Green's function using the equation of motion in Eq. (5) requires explicit knowledge of the electron Green's function and vice versa. On the other hand, the self-energy formalism is advantageous when expressed in frequency space since the Dyson equation can be solved for each frequency whereas the exchange-correlation potential formalism involves a convolution in frequency. Thus the two approaches complement one another.

It was recently shown for the half-filled one-band Hubbard model in a square lattice that the use of the self-energy, calculated to a finite order of expansion in the interaction, to determine the Green's function via the Dyson equation can lead to incorrect physics [18]. While a direct expansion of the Green's function to the same order yields an insulating behavior, the Green's function obtained from the Dyson equation results in a metallic behavior. This discrepancy can be traced back to the reducible diagrams implicitly summed when solving the Dyson equation, which generally differ from those in the direct expansion of the Green's function at each order. This finding raises questions as to the appropriateness of using the Dyson equation. The exchange-correlation potential formalism, on the other hand, is not meant to rely upon many-body perturbation theory but rather on direct construction based on known exact or accurate results of model systems and on exact properties of the exchange-correlation hole.

The choice of the self-energy as a truncation scheme may be understandable from a historical perspective. In the 1950s and early 1960s it was presumably inconceivable to even consider many-body calculations on real materials. The commonly used model of solids at that time was the electron gas. For the electron gas, the definition of the self-energy acting on the Green's function as a convolution in space and time has a

great advantage in that it allows for a simple expression for the equation of motion or the Dyson equation when Fourier transformed:

$$G(k, \omega) = G_0(k, \omega) + G_0(k, \omega)\Sigma(k, \omega)G(k, \omega), \quad (28)$$

where G_0 is the Green's function of the free-electron gas. The self-energy has since then been synonymous with the Green's function and become the accepted route for calculating the Green's function to this day.

The important role that the self-energy has played in electronic structure theory is not to be undermined. In the self-energy formalism an iterative equation for the self-energy can be derived yielding [15,16]

$$\begin{aligned} \Sigma(1, 2) = & i \int d3d4v(1-3)G(1, 4) \\ & \times \left[\left\{ \delta(4-3) + \frac{\delta V_H(4)}{\delta \phi(3)} \right\} \delta(4-2) + \frac{\delta \Sigma(4, 2)}{\delta \phi(3)} \right]. \end{aligned} \quad (29)$$

Here, $1 = (r_1 t_1)$, etc., and ϕ is a probing field which is set to zero after the derivative is taken. Neglecting the term $\delta \Sigma / \delta \phi$ leads to the well-known *GW* approximation. This kind of iterative or perturbative equation is more difficult to establish for V_{xc} since the equation of motion in Eq. (6) cannot be easily inverted to obtain G^{-1} .

From the definition of the self-energy in Eq. (4), it can be seen that the Coulomb interaction has been lumped into the self-energy. While it is formally and mathematically correct, the definition makes no use of the fact that the Coulomb interaction is known explicitly. The definition of the correlator g in Eq. (9), on the other hand, is not explicitly dependent on the Coulomb interaction. The special property of the Coulomb interaction being dependent only on the distance between two electrons can be exploited leading to the conclusion that only the spherical average of the exchange-correlation hole is relevant [19,20]. This should greatly simplify the search for a good approximation for the exchange-correlation hole or potential.

III. MODEL SYSTEMS

To illustrate the form of the time-dependent exchange-correlation potential, the half-filled Hubbard dimer is considered. The exchange-correlation potential extracted from the Hubbard dimer is then used as an approximate V_{xc} for the 1D Hubbard chain.

Another example is a simplified Holstein model, describing a core electron coupled to a set of bosons such as plasmons or phonons. This Hamiltonian is appropriate to model solids in which the valence electrons are relatively delocalized, resembling electron gas. The alkalis and *s-p* semiconductors and insulators are examples of such systems.

The fourth example is the hydrogen atom. Although it is not a many-electron system, it illustrates explicitly the sum rule and condition fulfilled by the exchange-correlation hole.

A. Hubbard dimer

In Ref. [1], the exchange-correlation potential of the half-filled Hubbard dimer was worked out analytically. The Hamiltonian of the Hubbard dimer in standard notation is given by

$$\hat{H} = -\Delta \sum_{i \neq j} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad (30)$$

where $i, j = 1, 2$. The results are given by

$$V_{11,11}^{xc}(t > 0) = \frac{\alpha U}{2} \frac{1 + e^{-i2\Delta t}}{1 + \alpha^2 e^{-i2\Delta t}}, \quad (31)$$

$$V_{11,22}^{xc}(t > 0) = \frac{\alpha U}{2} \frac{1 - e^{-i2\Delta t}}{1 - \alpha^2 e^{-i2\Delta t}}, \quad (32)$$

where

$$\alpha = \frac{1-x}{1+x}, \quad (33)$$

$$x = \frac{1}{4\Delta} (\sqrt{U^2 + 16\Delta^2} - U) \quad (34)$$

is the relative weight of double-occupancy configurations in the ground state and

$$2\Delta = E_1^- - E_0^- = E_1^+ - E_0^+ > 0 \quad (35)$$

are the excitation energies of the $(N \pm 1)$ systems. From symmetry,

$$V_{22,22}^{xc} = V_{11,11}^{xc}, \quad V_{22,11}^{xc} = V_{11,22}^{xc}, \quad (36)$$

$$V_{xc}(-t) = -V_{xc}(t). \quad (37)$$

For convenience and for comparison, the results expressed in the site orbitals shown in Ref. [1] are shown in Figs. 1 and 2 but with different values of U .

It is perhaps more insightful to express V_{xc} in the bonding and antibonding orbitals, $V_{AA,AA}^{xc}$ and $V_{BB,BB}^{xc}$. In these orbitals, the Green's function is diagonal, and V_{xc} in the bonding state is identical to that in the antibonding one:

$$V^{xc}(t > 0) = \frac{1}{2} (V_{11,11}^{xc} + V_{11,22}^{xc}) = \frac{\alpha U}{2} \frac{1 - \alpha^2 e^{-i4\Delta t}}{1 - \alpha^4 e^{-i4\Delta t}}. \quad (38)$$

The other matrix element, $V_{AB,BA}^{xc} = V_{BA,AB}^{xc}$, is given by

$$\begin{aligned} \Delta V^{xc}(t > 0) &= \frac{1}{2} (V_{11,11}^{xc} - V_{11,22}^{xc}) \\ &= \frac{\alpha U}{2} \frac{(1 - \alpha^2) e^{-i2\Delta t}}{1 - \alpha^4 e^{-i4\Delta t}}. \end{aligned} \quad (39)$$

The results are shown in Fig. 3 for the real parts and in Fig. 4 for the imaginary parts. The dependence of the correlation strength on time is revealed clearly: the stronger the U , the more pronounced the variation of V_{xc} with time.

An interesting feature is the discontinuity of V^{xc} at $t = 0$, which is the difference between the particle ($t = 0^+$) and the hole ($t = 0^-$) values, reminiscent of the discontinuity in the exchange-correlation potential in density functional theory [21].

One also notices that the time dependence is dictated by the excitation energies of the $(N \pm 1)$ systems and, in general, these excitations include collective ones. For example,

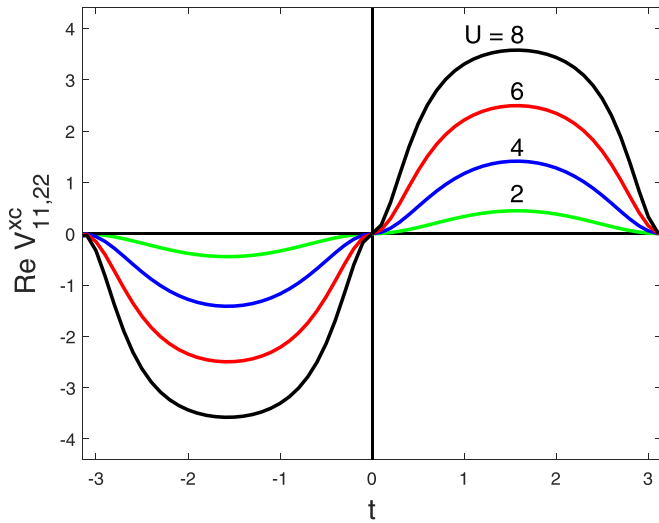
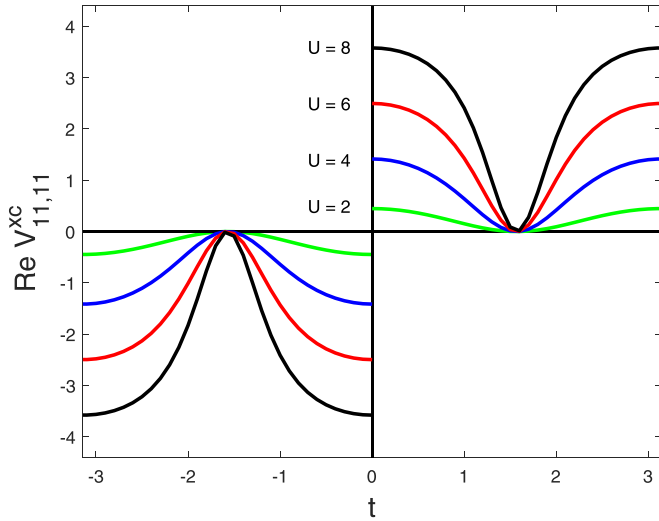


FIG. 1. The real parts of the exchange-correlation potentials $V_{11,11}^{xc}$ and $V_{11,22}^{xc}$ of the Hubbard dimer as a function of time for $U = 2, 4, 6,$ and 8 with $\Delta = 1$. Due to the particle-hole symmetry, $V_{xc}(-t) = -V_{xc}(t)$.

for solids one expects a time-dependent term of the form $\exp(-i\omega_p t)$, where ω_p is the plasmon energy. V_{xc} acts then as an effective external field, exchanging an energy ω_p with the system, as illustrated more explicitly later in the example on the Holstein Hamiltonian.

B. 1D Hubbard chain

To calculate the Green's function for the 1D Hubbard chain with the same Hamiltonian as in Eq. (30) but with $i, j = 1, \dots, \infty$, the V_{xc} of the Hubbard dimer will be used as a model. This approximation neglects components of V_{xc} beyond nearest neighbors. Due to translational lattice symmetry it is convenient to introduce Bloch base functions,

$$\varphi_k(r) = \frac{1}{\sqrt{N}} \sum_T e^{ikT} \varphi(r-T), \quad (40)$$

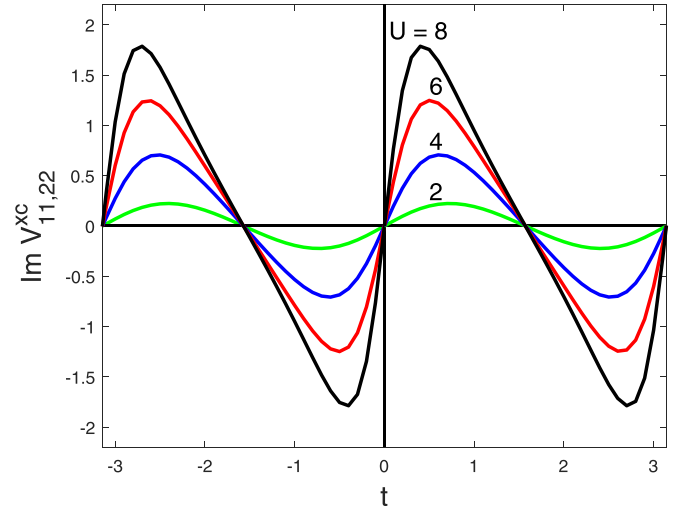
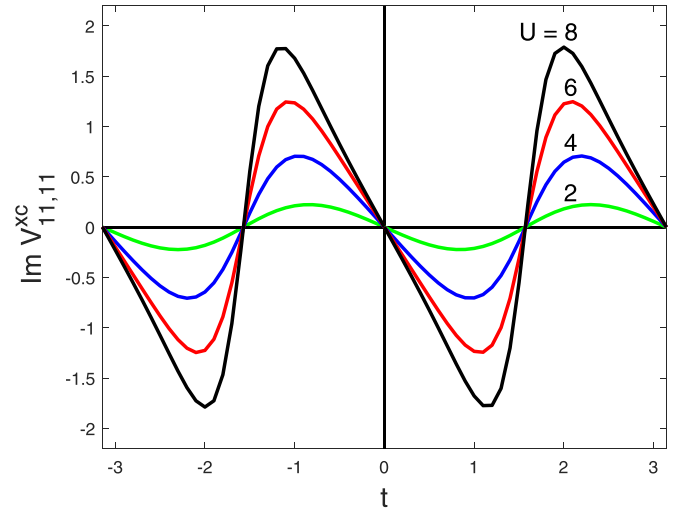


FIG. 2. The imaginary parts of the exchange-correlation potentials $V_{11,11}^{xc}$ and $V_{11,22}^{xc}$ of the Hubbard dimer as a function of time for $U = 2, 4, 6,$ and 8 with $\Delta = 1$. Due to the particle-hole symmetry, $V_{xc}(-t) = -V_{xc}(t)$.

where T denotes a lattice site. The Green's function expressed in these Bloch functions takes the form

$$G(r, r'; t) = \sum_k \varphi_k(r) G(k, t) \varphi_k^*(r'), \quad (41)$$

where

$$G(k, t) = \int dr dr' \varphi_k^*(r) G(r, r'; t) \varphi_k(r'). \quad (42)$$

The equation of motion in the Bloch base functions is given by

$$(i\partial_t - \varepsilon_q) G(q, t) - F(q, t) = \delta(t), \quad (43)$$

where

$$\begin{aligned} \varepsilon_q &= \int dr \varphi_q^*(r) h(r) \varphi_q(r) \\ &= \frac{1}{N} \sum_{TT'} e^{-iq(T-T')} \varphi^*(r-T) h(r) \varphi(r-T') \\ &= -2\Delta \cos q \end{aligned} \quad (44)$$

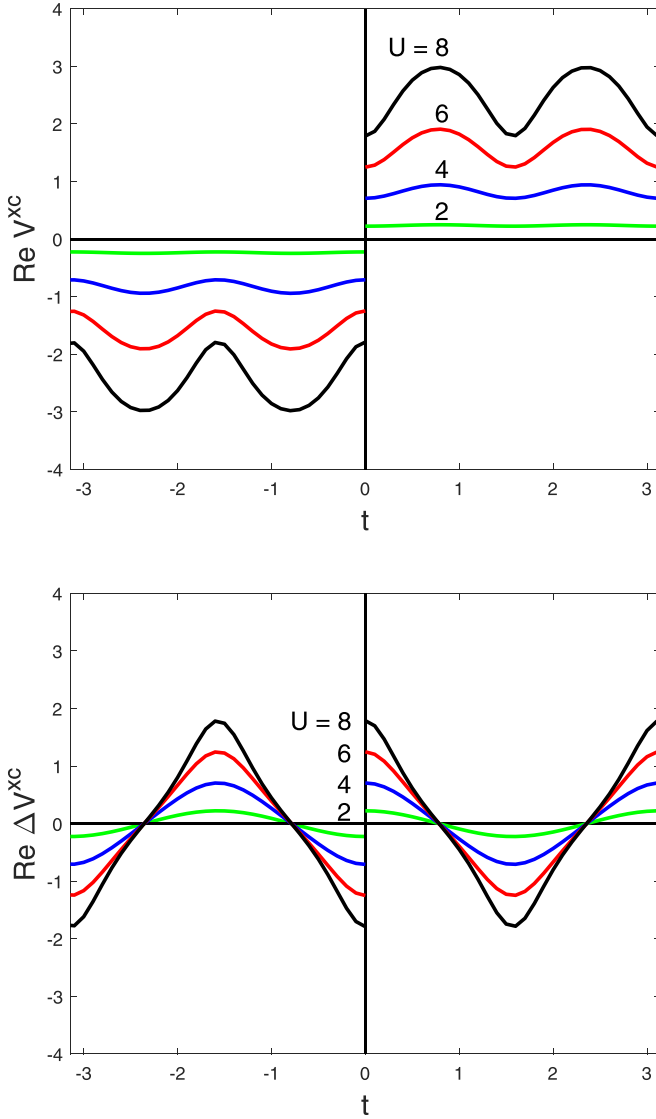


FIG. 3. The real parts of the exchange-correlation potential in the bonding state $\phi_B = \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2)$ and antibonding state $\phi_A = \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2)$ as a function of time for $U = 2, 4, 6,$ and 8 with $\Delta = 1$.

and

$$F(q, t) = \sum_k \int dr dr' \times \varphi_q^*(r) \varphi_k(r) V_{xc}(r, r'; t) \varphi_k^*(r') \varphi_q(r') \times G(k, t). \quad (45)$$

Since the Hartree potential is a constant, it can be absorbed into the chemical potential.

To solve the equation of motion, one makes use of the V^{xc} deduced for the Hubbard dimer. The equations of motion of the Green's function in the bonding and antibonding orbitals are given by

$$[i\partial_t - \varepsilon_A - V^{xc}(t)]G_A(t) - \Delta V^{xc}(t)G_B(t) = \delta(t), \quad (46)$$

$$[i\partial_t - \varepsilon_B - V^{xc}(t)]G_B(t) - \Delta V^{xc}(t)G_A(t) = \delta(t), \quad (47)$$

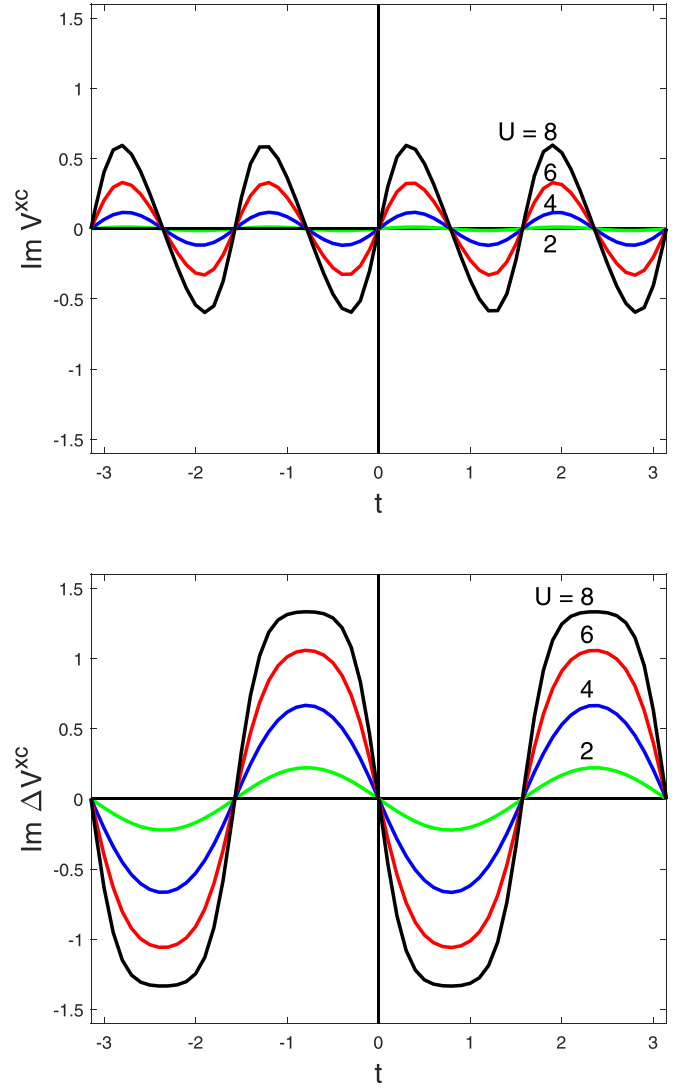


FIG. 4. The imaginary parts of the exchange-correlation potential in the bonding and antibonding states as a function of time for $U = 2, 4, 6,$ and 8 with $\Delta = 1$.

where

$$\varepsilon_A = \Delta, \quad \varepsilon_B = -\Delta \quad (48)$$

are the one-particle antibonding and bonding energies. V^{xc} and ΔV^{xc} are given in Eqs. (38) and (39), respectively.

The bonding and antibonding states of the Hubbard dimer are the analog of the Bloch states of the 1D chain corresponding to the centers of the occupied and unoccupied bands, respectively. Based on the form of the equations of motion of the bonding and antibonding Green's functions of the Hubbard dimer, a physically motivated approximation is to replace $G_A(G_B)$ by $G(q, t)$ and $G_B(G_A)$, which represents the rest of the Green's functions, by the average $\frac{1}{N} \sum_k G(k, t)$:

$$[i\partial_t - \varepsilon_q - V^{xc}(t)]G(q, t) - \frac{1}{N} \sum_k \Delta V^{xc}(t)G(k, t) = \delta(t). \quad (49)$$

Formally, this approximation can also be seen to follow from Eqs. (43) and (45), in which the off-diagonal components of

V^{xc} in the Bloch functions φ_k , which express the coupling between different k points, are approximated by ΔV^{xc} of the Hubbard dimer, independent of k .

One may rewrite the above equation as follows:

$$[i\partial_t - \varepsilon_q - V^{\text{xc}}(t) - \Delta V^{\text{xc}}(q, t)]G(q, t) = \delta(t), \quad (50)$$

where

$$\Delta V^{\text{xc}}(q, t) = \frac{1}{N} \sum_k \Delta V^{\text{xc}}(t) \frac{G(k, t)}{G(q, t)}. \quad (51)$$

The solution for the electron case is assumed to be given by

$$G^e(q, t) = -i\theta(t)e^{-i\varepsilon_q t - i \int_0^t dt' [V^{\text{xc}}(t') + \Delta V^{\text{xc}}(q, t')]} \quad (52)$$

A similar result can be readily derived for the hole Green's function, keeping in mind that $V^{\text{xc}}(-t) = -V^{\text{xc}}(t)$.

To proceed further analytically, the Green's function appearing in Eq. (51) is approximated by a noninteracting one,

$$G(k, t) \approx G_0(k, t) = ie^{-i\varepsilon_k t} [\theta(-t) - \theta(t)], \quad (53)$$

leading to

$$\Delta V^{\text{xc}}(q, t) \approx \frac{1}{N} \sum_k \Delta V^{\text{xc}}(t) e^{-i(\varepsilon_k - \varepsilon_q)t}. \quad (54)$$

This approximation keeps the main excitation component of G but neglects the incoherent part, which would contribute to some structure in the spectral functions at high energy but is not expected to alter the main spectral features at low energy. The presence of the gap in the renormalized Green's function has no effect since it is the ratio that matters.

Furthermore, to facilitate analytical calculations, V^{xc} and ΔV^{xc} in Eqs. (38) and (39) are expanded as follows:

$$V^{\text{xc}}(t) \approx \frac{\alpha U}{2}, \quad (55)$$

$$\Delta V^{\text{xc}}(t) \approx \frac{\alpha U}{2} (1 - \alpha^2) e^{-i2\Delta t}. \quad (56)$$

In the above approximation the constant term that shifts the one-particle energy and the main excitation term $\exp(-i2\Delta t)$ that generates the main satellites are kept, whereas the higher-excitation term $\exp(-i4\Delta t)$ is neglected. One obtains to first order in ΔV^{xc}

$$\begin{aligned} G^e(q, t) &= -i\theta(t) e^{-i(\varepsilon_q + \frac{\alpha U}{2})t} \\ &\times \left\{ 1 - i \frac{\alpha U}{2} (1 - \alpha^2) \frac{1}{N} \sum_k \int_0^t dt' e^{-i(\varepsilon_k - \varepsilon_q + 2\Delta)t'} \right\}. \end{aligned} \quad (57)$$

Performing the time integral, one finds

$$\begin{aligned} G^e(q, t) &= -i\theta(t) e^{-i(\varepsilon_q + \frac{\alpha U}{2})t} \\ &\times \left\{ 1 + \frac{\alpha U}{2} (1 - \alpha^2) \frac{1}{N} \sum_k \frac{e^{-i(\varepsilon_k - \varepsilon_q + 2\Delta)t} - 1}{\varepsilon_k - \varepsilon_q + 2\Delta} \right\}. \end{aligned} \quad (58)$$

Fourier transformation to the frequency domain yields

$$\begin{aligned} G^e(q, \omega) &= \frac{A_0^e}{\omega - (\varepsilon_q + \frac{\alpha U}{2}) + i\eta} \\ &+ \frac{1}{N} \sum_k \frac{A^e(k)}{\omega - (\varepsilon_k + \frac{\alpha U}{2} + 2\Delta) + i\eta}, \end{aligned} \quad (59)$$

where

$$A_0^e = 1 - \frac{\alpha U}{2} (1 - \alpha^2) \frac{1}{N} \sum_k \frac{1}{\varepsilon_k - \varepsilon_q + 2\Delta}, \quad (60)$$

$$A^e(k) = \frac{\alpha U}{2} (1 - \alpha^2) \frac{1}{\varepsilon_k - \varepsilon_q + 2\Delta}. \quad (61)$$

A similar derivation can be carried out for the hole Green's function, and the result is given by

$$\begin{aligned} G^h(q, t) &= i\theta(-t) e^{-i(\varepsilon_q - \frac{\alpha U}{2})t} \\ &\times \left\{ 1 - \frac{\alpha U}{2} (1 - \alpha^2) \frac{1}{N} \sum_k \frac{e^{-i(\varepsilon_k - \varepsilon_q - 2\Delta)t} - 1}{\varepsilon_k - \varepsilon_q - 2\Delta} \right\}, \end{aligned} \quad (62)$$

$$\begin{aligned} G^h(q, \omega) &= \frac{A_0^h}{\omega - (\varepsilon_q - \frac{\alpha U}{2}) - i\eta} \\ &- \frac{1}{N} \sum_k \frac{A^h(k)}{\omega - (\varepsilon_k - \frac{\alpha U}{2} - 2\Delta) - i\eta}, \end{aligned} \quad (63)$$

where

$$A_0^h = 1 + \frac{\alpha U}{2} (1 - \alpha^2) \frac{1}{N} \sum_k \frac{1}{\varepsilon_k - \varepsilon_q - 2\Delta}, \quad (64)$$

$$A^h(k) = \frac{\alpha U}{2} (1 - \alpha^2) \frac{1}{\varepsilon_k - \varepsilon_q - 2\Delta}. \quad (65)$$

For the electron or hole case it is understood that both ε_k and ε_q correspond to unoccupied or occupied states.

The calculated total spectral functions for $U = 2, 4, 6$, and 8 are shown in Fig. 5, and the k -resolved spectra are illustrated in Fig. 6 for a few k points corresponding to $U = 7.74$. This value has been chosen in order to make a comparison with the results obtained using the dynamical density-matrix renormalization group method [4]. Due to the approximation made in replacing G with G^0 in Eq. (51), there is no spectral weight below the chemical potential arising from the electron Green's function, and similarly, there is no spectral weight above the chemical potential arising from the hole Green's function. For this reason, there is no spectral weight below the chemical potential for $k = \frac{75\pi}{91}$ and $k = \frac{90\pi}{91}$ when compared with the results shown in Fig. 11 of Benthien and Jeckelmann [4]. Furthermore, the peaks are sharp δ functions but with some weight transferred to higher or lower energy. It is known that for a one-dimensional interacting system, a removal or addition of an electron results in two branches consisting of a spinless holon or antiholon dispersion with a hole or electron charge and a charge-neutral spinon dispersion of spin $\frac{1}{2}$.

Although the approximations used are very simple, the k -resolved spectra shown in Fig. 6 are in favorable agreement with those calculated using the dynamical density-matrix

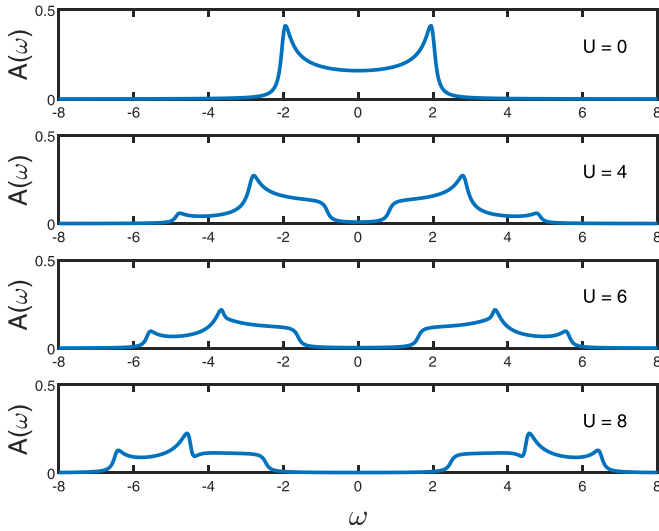


FIG. 5. The calculated total spectral functions of the 1D Hubbard chain for $U = 0, 4, 6,$ and 8 using approximations described in the text. A broadening of 0.1 has been used.

renormalization group method [4]. A notable discrepancy is the dispersion widths for both the spinon and the holon branches. Thus the peak positions at small k are lower in energy compared with those in the work of Benthien and Jeckelmann [4]. This is understandable since within the approximations used, the dispersion is pinned down by the noninteracting G^0 and the use of the Hubbard dimer V^{xc} neglects long-range correlations, which tend to narrow the band dispersion.

The structure of the calculated k -resolved hole spectra in Fig. 6 can be understood from the explicit expression for the

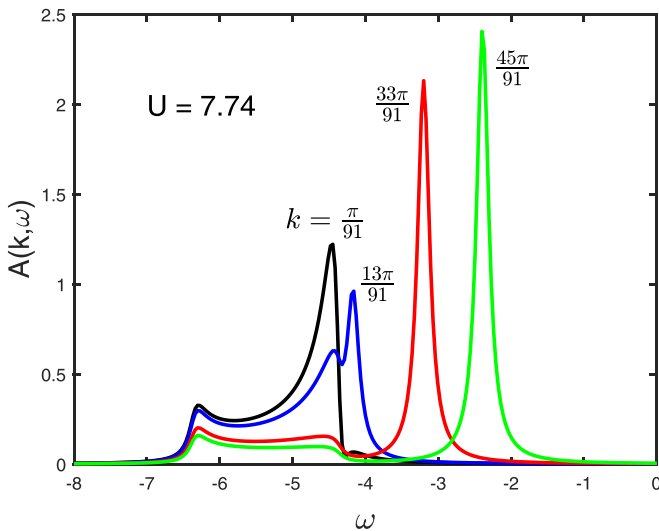


FIG. 6. The k -resolved spectral functions of the 1D Hubbard chain for $U = 7.74$. The U and k values have been chosen to facilitate comparison with Fig. 11 of Benthien and Jeckelmann [4]. Within the approximations used, there is no spectral weight for $k = \frac{75\pi}{91}$ and $\frac{90\pi}{91}$ below the chemical potential, as explained in the text. A broadening of 0.1 has been used.

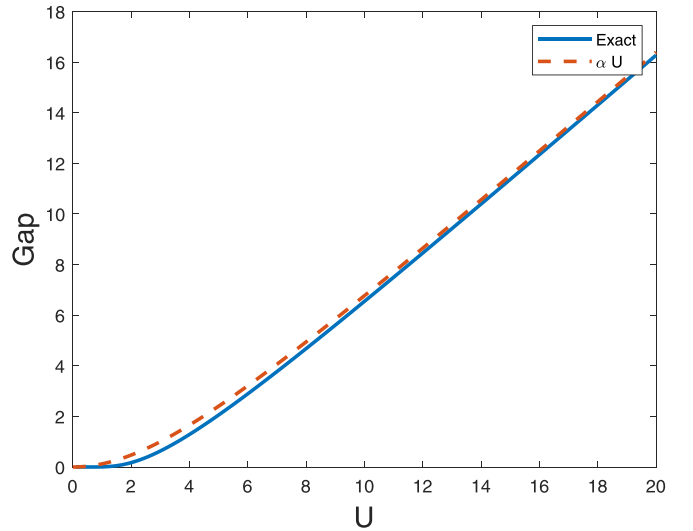


FIG. 7. The calculated band gap, αU , compared with the exact gap obtained from the Bethe ansatz as a function of U . The calculated gap approaches the exact result as U increases.

hole Green's function in Eq. (63). The imaginary part of the first term is the main peak centered at $\omega = \varepsilon_q - \frac{\alpha U}{2}$, which is interpreted as the spinon excitation. The imaginary part of the second term with the weight $A^h(k)$ set to unity is the noninteracting occupied density of states shifted by $-(\frac{\alpha U}{2} + 2\Delta)$. For $q = \frac{45\pi}{91}$ (green curve), the one-particle energy, ε_q , is approximately zero, and the main peak is located at the top of the band edge at $\omega = -\frac{\alpha U}{2}$. The remaining spectrum stretching approximately from -6.5 to -4.5 is the shifted occupied density of states weighted by $A^h(k)$. The peak feature at the lower edge at -6.5 reflects the same feature present in the shifted noninteracting occupied density of states ($U = 0$ in Fig. 5) and may be interpreted as the holon excitation. The structure at the upper edge at around -4.5 , on the other hand, arises from the enhanced weight of $A^h(k)$, which is largest for q around the bottom of the noninteracting band, giving rise to a steplike structure [4]. For $q = \frac{\pi}{91}$ (black curve), the main peak is centered at $\omega = -\frac{\alpha U}{2} - 2\Delta$, and it merges with the shifted density of states. For $q = \frac{13\pi}{91}$ the main peak still lies outside the shifted density of states, and a three-peak structure is then observed, as also found in the calculated spectra using the dynamical density-matrix renormalization group method [4]. It is not immediately evident from the expressions for the Green's function in Eqs. (59) and (62) how to interpret the two branches as spinon and holon excitations. Such an interpretation would probably require analysis in terms of state vectors.

The calculated band gap, which is given by αU , is displayed in Fig. 7 and compared with the exact result [22],

$$E_{\text{gap}} = \frac{16\Delta^2}{U} \int_1^\infty dy \frac{\sqrt{y^2 - 1}}{\sinh\left(\frac{2\pi\Delta y}{U}\right)}, \quad (66)$$

obtained from the Bethe ansatz. The agreement between the analytically calculated gap and the exact gap is very close, despite the simplicity of the approximation. The

calculated gap approaches the exact gap in the limit of large U , and a gap opens as soon as U is finite, as in the exact case. The discrepancy is largest at small values of U , which may be understood from the lack of long-range screening effects in V^{xc} of the Hubbard dimer. It should be noted that in the widely used dynamical mean-field theory (DMFT) [23] within the single-site approximation, the gap is not opened up until $U > 6$. Only within the cluster DMFT with an even number of sites does the gap form for any finite U , whereas with an odd number of sites a metallic region remains until U exceeds a certain value before entering the Mott insulating phase through a coexistence region [24].

C. Holstein Hamiltonian

A simplified Holstein Hamiltonian describing a coupling between a core electron and a set of bosons, such as plasmons or phonons, is given by [25]

$$\hat{H} = \varepsilon \hat{c}^\dagger \hat{c} + \sum_q \hat{c} \hat{c}^\dagger g_q (\hat{b}_q + \hat{b}_q^\dagger) + \sum_q \omega_q \hat{b}_q^\dagger \hat{b}_q, \quad (67)$$

where ε is the core electron energy, ω_q is the boson energy of wave vector q , and \hat{c} and \hat{b}_q are the core electron and the boson operators, respectively. This Hamiltonian can be solved analytically, and the algebra is simplified if it is assumed that the boson is dispersionless with an average energy ω_p . Under this assumption, the exact solution for the core-electron removal spectra yields [25]

$$A(\omega) = \sum_{n=0}^{\infty} f_n \delta(\omega - \varepsilon - \Delta\varepsilon + n\omega_p), \quad (68)$$

where

$$f_n = \frac{e^{-a} a^n}{n!}, \quad a = \sum_q \left(\frac{g_q}{\omega_p} \right)^2, \quad \Delta\varepsilon = a\omega_p. \quad (69)$$

This exact solution can also be obtained using the cumulant expansion [26–28]. The hole Green's function corresponding to the above spectra is given by

$$G(t < 0) = i \sum_{n=0}^{\infty} f_n e^{-i(\varepsilon + \Delta\varepsilon - n\omega_p)t} \theta(-t). \quad (70)$$

It can be verified that the time-dependent exchange-correlation potential corresponding to the Holstein Hamiltonian reads

$$V_{\text{xc}}(t < 0) = \Delta\varepsilon (1 - e^{i\omega_p t}). \quad (71)$$

This expression provides a very simple interpretation: The first term corrects the noninteracting core-electron energy, whereas the second term describes the bosonic mode interacting with the core electron, which can exchange not only one but also multiple quanta of ω_p with the field. This is precisely what is accomplished by the cumulant expansion [26–28] within the self-energy formulation but in an *ad hoc* and complicated manner.

D. Hydrogen atom

It may seem trivial to consider the hydrogen atom since it is not a many-electron system. Nevertheless, it illustrates a number of exact results such as the sum rule in Eq. (10) and the condition in Eq. (11). For the hydrogen atom, the hole Green's function is given by

$$G(r, r'; t < 0) = i\varphi_s(r)\varphi_s(r') \exp(-i\varepsilon_s t) \theta(-t), \quad (72)$$

where φ_s and ε_s are the $1s$ orbital and its energy. The exchange-correlation potential for $t < 0$ can be readily deduced yielding

$$V_{\text{xc}}(r, r'; t < 0) = -V_{\text{H}}(r) = - \int dr'' v(r - r'') |\varphi_s(r'')|^2, \quad (73)$$

independent of r' and t , canceling the spurious Hartree potential. The corresponding exchange-correlation hole is then given by

$$\rho_{\text{xc}}(r, r', r''; t < 0) = -|\varphi_s(r'')|^2. \quad (74)$$

It can also be seen that the condition in Eq. (11),

$$\rho_{\text{xc}}(r, r', r; t < 0) = -\rho(r), \quad (75)$$

as well as the sum rule in Eq. (10),

$$\int dr'' \rho_{\text{xc}}(r, r', r''; t < 0) = - \int dr'' |\varphi_s(r'')|^2 = -1, \quad (76)$$

are both fulfilled, as they should be.

IV. CONCLUSION

The exchange-correlation formalism has been applied to determine the Green's function of the 1D Hubbard chain by utilizing the exchange-correlation potential derived from the Hubbard dimer. Under the approximation corresponding to replacing the full Green's function by a noninteracting Green's function in the first iteration, the spectral functions can be calculated analytically. Despite the very simple approximation, the results compare favorably with the more accurate results calculated using the dynamical density-matrix renormalization group method. Peak structures corresponding to the holon and spinon collective excitations are correctly reproduced, although the positions are too low for small k , due to the use of a noninteracting Green's function and the neglect of long-range correlations in the exchange-correlation potential of the Hubbard dimer. The calculated gap agrees very well with the exact result obtained from the Bethe ansatz. These very encouraging results may indicate the robustness of the exchange-correlation potential, insensitive to the system size, allowing for extrapolation from a small to a large system. By using the exact V^{xc} of the Hubbard dimer, it is ensured that the sum rule is fulfilled.

An example from the Holstein Hamiltonian further illustrates the potential of the exchange-correlation formalism. The exact V^{xc} has a very simple form, offering a clear physical interpretation. The main collective charge excitation (plasmon) determines the characteristic energy of the time-dependent part of V^{xc} , while the constant term provides a correction to the one-particle energy. One may speculate

that a generic structure of the exchange-correlation potential consists of a constant term and a series of time-dependent terms of exponential form with energies characteristic of the excitations of $(N \pm 1)$ systems.

The example of the hydrogen atom illustrates the exact properties of the exchange-correlation hole.

ACKNOWLEDGMENT

Financial support from the Knut and Alice Wallenberg Foundation (KAW 2017.0061) and the Swedish Research Council (Vetenskapsrådet, VR 2021-04498_3) is gratefully acknowledged.

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