Partition function zeros of quantum many-body systems

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We present a method for calculating the Yang-Lee partition function zeros of a translationally invariant model of lattice fermions, exemplified by the Hubbard model. The method rests on a theorem involving the usual single-electron self-energy $\Sigma_\sigma(\vec{k}, i\omega_n|\mu)$ with chemical potential μ, in the imaginary time Matsubara formulation. The theorem maps the Yang-Lee zeros to a set of wave vector and spin labeled virtual energies $\xi_{\vec{k}\sigma}$. These, thermodynamically derived virtual energies, are solutions of the set of equations $\xi_{k\sigma} = \varepsilon_\sigma(\vec{k}) - \frac{1}{2}U + \Sigma_\sigma(\vec{k}, i\frac{\pi}{\beta}|\xi_{k\sigma} + \frac{1}{2}U - i\frac{\pi}{\beta}) = 0$. Examples of the method in simplified situations are provided.

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I. INTRODUCTION

Yang and Lee launched an important and fruitful direction in condensed matter physics by highlighting the significance of the zeros of the grand partition function of many-body systems [1]. Lee and Yang [2], soon thereafter, showed that for Ising ferromagnets, the zeros can be located exactly and lie on the unit circle in the complex fugacity plane. They showed that the density of the zeros closest to the real line provides fundamental insight into the critical singularities near a phase transition in two and higher dimensions. The work of Asano [3] gave an elegant reformulation of the Lee-Yang results using the method of contractions, and also enabled the surmounting of the added difficulties due to quantum mechanics in the ferromagnets [4]. The methodology used for these results was streamlined by Ruelle and Dyson [5], leading to several important further results over the intervening years [6,7], reviewed in Ref. [8]. The currently existing methods unfortunately do not appear to be generalizable for antiferromagnets and for broader classes of systems, including the ones considered here.

Our interest is in the study of quantum many-body systems, such as the Hubbard model [see Eq. (5)]. Locating the zeros and extracting meaningful information for these physically important systems has proceeded at a sedate pace. Here the major difficulty is the absence of systematic analytical methods. For numerical studies, a combination of the very high precision required for locating the zeros and the exponential growth of the Hilbert spaces with the system size, hamper direct enumeration techniques. Quantum Monte Carlo (QMC) methods for studying the repulsive Hubbard model with a complex chemical potential have been used earlier [9–12]. However the full spectrum of zeros seems difficult to obtain from QMC. Studies of related problems employing tensor networks show promise in overcoming some of these limitations [13,14]. There have also been recent studies of partition function zeros for related quantum many-body models in a variety of contexts, these include decoherence studies [15], quantum quenches [16], and in quantum computation [17]. These indicate a renewal of interest in this important subject.

The main objective of this paper is to introduce an analytical method for locating the zeros of the grand partition function of the Hubbard model [see Eq. (5)] in any dimension. This method requires a knowledge of the self-energy in the Matsubara imaginary-time framework [18]. While the self-energy is a highly nontrivial object to compute, a perturbative knowledge of the self-energy is available and may be used to give approximate location of the zeros. The method generalizes to nearby models in a straightforward way. The a few simple examples are provided below.

A. Heuristic perturbative approach to Yang-Lee zeros

Let us consider the Hubbard model Eq. (5) as an illustrative example. A perturbative approach is to expand the (grand) partition function as a series in the coupling constant [19] $Z = \mathrm{Tr}e^{-\beta(\mathcal{H}_0+V)} = Z_0(1 - \beta\langle T_\tau V\rangle_0) + \mathcal{O}(U^2)$, where $Z_0 = \prod_\alpha(1 + ze^{-\beta\varepsilon_\alpha})^2$ is the noninteracting result with the fugacity $z = e^{\beta\mu}$, T_τ the imaginary-time ordering operator, $\beta = \frac{1}{k_B T}$ and the correction term due to interactions is found by taking the noninteracting thermal average of the interaction term, so that

$$Z(z) = \prod_\alpha (1 + ze^{-\beta\varepsilon_\alpha})^2 \times \left[1 - \frac{\beta U}{N_s}\left(\sum_\alpha \frac{z}{z + e^{\beta\varepsilon_\alpha}}\right)^2 + \mathcal{O}(U^2)\right], \quad (1)$$

where the spin degeneracy leads to the square in the second term. For simplicity let us assume that all the energies ε_α are distinct. A simple minded estimate of the location of the zeros can be made as follows. Since the zeros of Z_0 are located at $z_\alpha \to -e^{\beta\varepsilon_\alpha}$, we might expect that the zeros of Z are continuously connected to these and hence try the expression $z_\alpha = -e^{\beta(\varepsilon_\alpha+\Delta_\alpha)}$ where the energy shift Δ_α vanishes as $U \to 0$. With a fixed α we substitute into Eq. (1) and the

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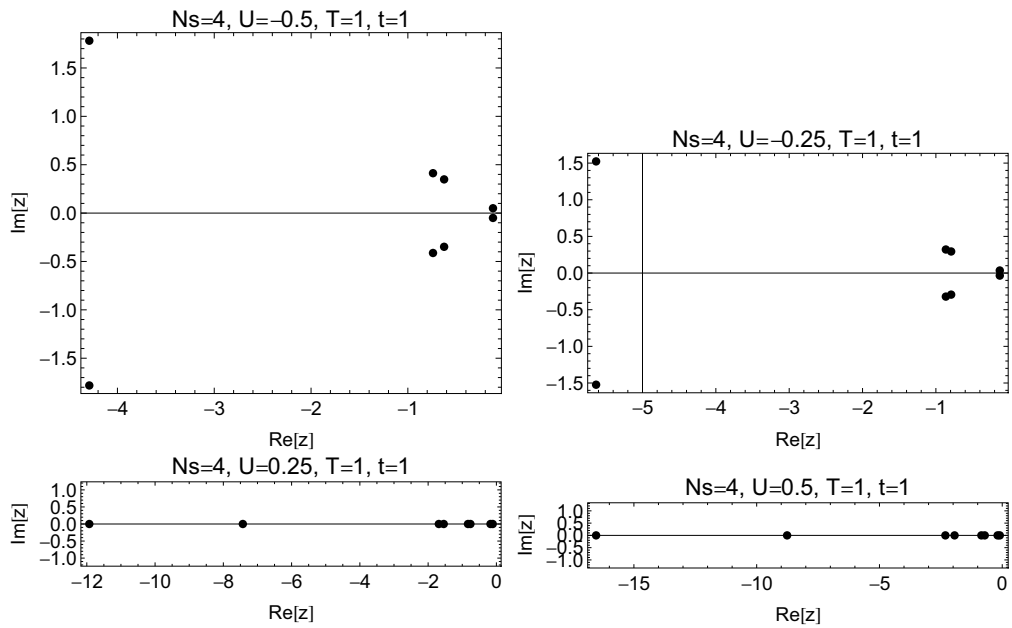

FIG. 1. Yang-Lee zeros of the partition function of the four-site Hubbard model at $T = 1$: top-left with $U = -0.5$; top-right with $U = -0.25$; bottom-left with $U = +0.25$; and bottom-right with $U = 0.5$. The partition function was calculated using the symbolic calculation programme DIRACQ [20]. From these figures we see that the attractive case leads to complex fugacities lying on a parabolaic curve- while the repulsive case leads to real fugacities. This is as expected from Eq. (3).

vanishing condition imposed on Z, thus requiring

$$\sum_{\gamma}\left(\frac{1}{1-e^{\beta(\varepsilon_\gamma-\varepsilon_\alpha-\Delta_\alpha)}}\right)=\pm\sqrt{\frac{N_s}{\beta U}}. \tag{2}$$

Solving to low orders we get

$$\Delta_\alpha=\pm\sqrt{\frac{Uk_BT}{N_s}}+\frac{U}{2N_s}\sum_{\gamma\neq\alpha}\coth\frac{\beta}{2}(\varepsilon_\gamma-\varepsilon_\alpha)+\dots \tag{3}$$

From this expression we infer that for $U > 0$ the energy shifts are real, and the fugacities z_α are on the negative real axis. On the other hand for any $U < 0$ the energy shifts are complex numbers occurring in complex conjugate pairs, and the fugacities z_α lie on a curve in the negative half-plane, which is symmetric about the real axis. In Fig. 1 we present the roots for the four-site Hubbard model, where the partition function was calculated using the software package DIRACQ [20] employing symbolic methods. We see that the exact roots behave in accordance with the above observation. The change in the nature of roots, from real for repulsive to nonreal for attractive interactions, is pronounced and easily visible. This provides a graphic demonstration of Dyson's comments [21] on the nature of perturbation theory in many-body systems, and is discussed further below.

We therefore obtain some insight into the roots of the Hubbard model from the simple perturbation theory outlined above. However the theoretical argument is not completely satisfactory, since it mixes in factors of very different orders in N_s in the expression Eq. (1), or its higher-order generalizations. It is highly desirable to have a formulation where the fugacity, which is of the $\mathcal{O}(1)$ in N_s, is found from equations where all terms are of the same, i.e., $\mathcal{O}(1)$ order. We provide such a framework in this work.

B. Plan of the paper

In Sec. II we provide basic definitions of the Hamiltonian, the grand partition function and the fugacity. We define the virtual energies $\xi_{\vec{k}\sigma}$, and note some properties of these obtained from general considerations. In Sec. III we define the Matsubara finite temperature Green's functions, their unnormalized versions and the self-energy. In Sec. IV the main theorem of this work is proposed and established. The equation determining the virtual energy in terms of the self-energy is recorded in Eq. (29). In Sec. V we illustrate the application of the theorem to the problem of an exactly solvable single-site Hubbard model. Here the role of lifting of degeneracy of the single-site energy is also studied in detail. The exact self-energy is expanded to $\mathcal{O}(U^2)$, and to this order the perturbative results for ξ are shown to agree with the exact ones. This somewhat long section is mainly addressed to readers interested in details, and may be skipped by others. In Sec. VI we use the first-order (Hartree) approximation to the self-energy and extract the virtual energies $\xi_{\vec{k}\sigma}$ to $\mathcal{O}(U)$ for both signs of the interaction for the 1-d Hubbard ring of length 6. This is familiar as the idealized benzene molecule. These virtual zeros are compared with exact numerical values obtained by computing the grand partition function exactly using symbolic methods. In Sec. VII we note a few conclusions and prospects for further work.

In Appendix we recall the well-known results of Luttinger and Ward [22] for the grand partition function. Their result neatly expresses the result of an all-orders summation of perturbation theory. We observe that the key function $\Xi(\mu)$

in Eq. (28), whose zeros are all the virtual energies, is a multiplicative factor of the Luttinger-Ward partition function.

II. BASIC HAMILTONIAN AND THE PARTITION FUNCTION

Let us consider an interacting Fermi system described by the (grand-canonical) Hamiltonian

$$\mathcal{H} = H - \mu\mathcal{N} = \mathcal{H}_0 + V$$
$$\mathcal{H}_0 = \sum_{\vec{k}_\alpha\sigma} \varepsilon_{k_\alpha,\sigma}\, C^\dagger_{\vec{k}_\alpha\sigma} C_{\vec{k}_\alpha\sigma} - \mu\mathcal{N}, \tag{4}$$

where the (conserved) fermion number operator $\mathcal{N} = \sum_{k,\sigma} C^\dagger_{k\sigma} C_{k\sigma}$, μ the chemical potential, and the Hubbard Hamiltonian

$$H = \sum_{\vec{k}_\alpha\sigma} \varepsilon_{k_\alpha,\sigma}\, C^\dagger_{\vec{k}_\alpha\sigma} C_{\vec{k}_\alpha\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{5}$$

Here $\vec{k}_\alpha$ are the L^d box-quantized wave vectors. The kinetic energy term is the Fourier transform of the hopping Hamiltonian $T = -\sum_{\vec{r},\sigma,\vec{\eta}} (t_{\vec{\eta},\sigma} C^\dagger_{\vec{r}\sigma} C_{\vec{r}+\vec{\eta}\sigma} + \text{H.c.})$, and $\vec{\eta}$ is the nearest-neighbor vector on a d-dimensional hypercubic lattice. In the usual case the hopping matrix element $t_{\vec{\eta},\sigma}$ is independent of the spin σ. The generalized σ-dependent case is useful for studying the effect of lifting the spin degeneracy on the roots as discussed below. More general models can be obtained by replacing the interaction term with an appropriate V and the energy dispersion chosen suitably. We have assumed that the system has translation invariance and study a finite lattice (with lattice constant unity) with $N_s = L^d$ sites.

For the finite system under consideration the total number of (spin half) particles varies in the range $0 \leqslant N \leqslant 2N_s$. With the Boltzman constant $k_B = 1$ and $\beta = \frac{1}{T}$ we trace over all particle numbers and define the grand partition function:

$$Z(\mu) = \text{Tr}\, e^{-\beta(H-\mu\mathcal{N})} = \sum_{n,N} e^{-\beta E_n + \beta\mu N_n} = \sum_{N=0}^{2N_s} z^N Z_N(\beta), \tag{6}$$

where E_n and N_n are the eigenvalues of H and particle number for the state n [detailed definitions are given after Eq. (30)], Z_N is the canonical partition function for N particles and z is the fugacity $z(\mu) = e^{\beta\mu}$.$Z(\mu)$ is thus a polynomial in the fugacity z of degree $2N_s$, and by the fundamental theorem of algebra, it has exactly $2N_s$ zeros in the complex z plane, and hence expressible as $Z(\mu) = c_0 \prod_{\alpha=1}^{2N_s}(z - z_\alpha)$, where z_α are the Yang-Lee zeros of the given model. We will find it more convenient to work in the complex μ plane rather than with the fugacity z. We note the periodicity $z(\mu) = z(\mu + i\frac{2\pi}{\beta})$ and therefore the complex μ plane can be decomposed into infinite equivalent strips of width $i\frac{2\pi}{\beta}$. We restrict our attention to a conveniently chosen strip

$$\mathcal{S} = \left\{ -\frac{2\pi}{\beta} < \text{Im}\,\mu \leqslant 0, \quad \text{Re}\,\mu \in [-\infty, \infty] \right\}. \tag{7}$$

We remark further on the rationale underlying this convention below Eq. (10).

A. Definition of the virtual energies $\xi_{\vec{k}\sigma}$

We will write the partition function in the form

$$Z(\mu) = \prod_{\vec{k}\sigma} \left(1 + \frac{e^{\beta\mu}}{e^{\beta(\xi_{\vec{k}\sigma} + \frac{1}{2}U)}} \right). \tag{8}$$

With this convention, explained below, the roots of Z occur at

$$\mu \to -i\frac{\pi}{\beta} + \frac{1}{2}U + \xi_{\vec{k}\sigma}, \quad \text{or equivalently}$$
$$z_\alpha \to -e^{\beta(\xi_{\vec{k}\sigma} + \frac{1}{2}U)}, \tag{9}$$

where Eq. (9) anticipates a mapping $\alpha \leftrightarrow \vec{k}\sigma$, between the unlabeled Yang-Lee zeros z_α and the labeled virtual energies ξ. We remark that while Eq. (8) has the same form as that of an ideal Fermi gas with energies $\xi_{\vec{k}\sigma} + \frac{1}{2}U$, the latter are nontrivial complex functions of T, U. For an interacting system $\xi_{\vec{k}\sigma}$ are not viewed as eigenvalues of any Hermitean Hamiltonian, and are allowed to be nonreal. For this reason these may be regarded as thermodynamically derived virtual energies.

The imaginary part of $\xi_{\vec{k}\sigma}$ is constrained by

$$-\frac{\pi}{\beta} < \text{Im}\,\xi_{\vec{k}\sigma} \leqslant \frac{\pi}{\beta}. \tag{10}$$

The convention used in defining the strip $\mathcal{S}$ in Eq. (7), and the range of the imaginary part of ξ in Eq. (10), are such that complex conjugate roots in the fugacity variable $z = e^{\beta\mu}$ lead to complex conjugate energies ξ. The partition function being a polynomial in z with real coefficients, the roots in z are either real or come in complex conjugate pairs. It follows that the virtual energies are either real or they occur in complex conjugate pairs, i.e., if ξ is a virtual energy, then so is ξ^*.

The virtual energies ξ's are dependent on the temperature T, and also the interaction strength U. We also remark that if the virtual energies ξ are real and their density of states is nonsingular in a continuous interval of energies, then the system would behave like an almost ideal Fermi liquid for densities where μ lives in the same range. Such a situation seems to be realized in the repulsive Hubbard model at low T studied here. It is tempting to view Landau's Fermi liquids [19,23,24] as behaving in precisely such a fashion, with the energies $\xi_{\vec{k}\sigma}$ being closely related to Landau's quasiparticle energies [23].

We next record some general properties of the virtual energies for the Hubbard model.

(1) On bipartite lattices there is an invariance under a simultaneous particle-hole transformation for both directions of the spin, it is expressible in real space as $C_{i\sigma} \leftrightarrow e^{i\pi\phi_i} C^\dagger_{i\sigma}$ with a suitable phase factor ϕ_i. Collecting the extra coefficients generated by the transformation, we obtain an identity

$$Z(\mu) = e^{2\beta\mu N_s} e^{-\beta U N_s} Z(U - \mu). \tag{11}$$

This implies that the partition function zeros arise in particle-hole symmetric pairs $\{\mu, U - \mu\}$, or equivalently the virtual energies come in pairs, i.e.,

$$\xi_{k\sigma} = -\xi_{k'\sigma}, \tag{12}$$

for suitable momentum partners k and k'.

(2) In the fully occupied subspace (i.e., particle number $N = 2N_s$ sector), there is only a single state. Here the kinetic

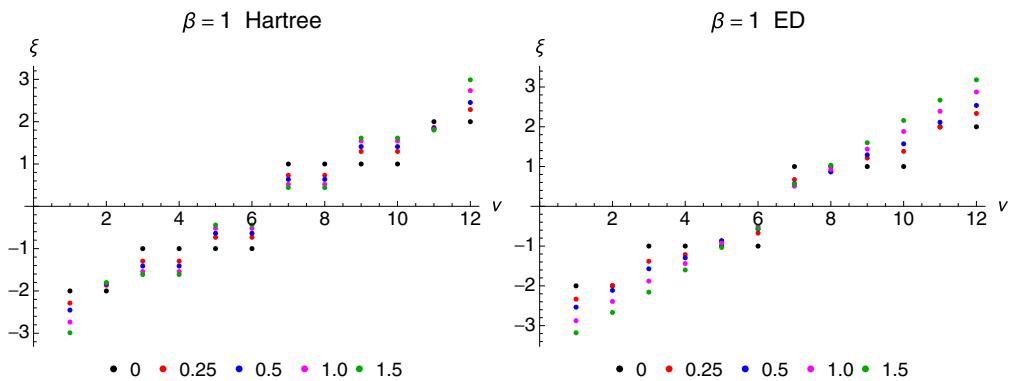

FIG. 2. The virtual energies ξ for the six-site Hubbard model from the Hartree equation Eq. (69) on **left**, and directly from the partition found from exact diagonalization (ED) on right, at various repulsive values of U marked below the plots. The virtual energies are all real in this case. On **left** the x-axis index ν combines six increasing values of $k = \frac{2\pi}{6}\{1, 2, \ldots 6\}$ with two values of the spin $\sigma = \{\uparrow, \downarrow\}$, into 12 indices $\{(k, \uparrow), (k, \downarrow)\}$ in ascending order, using the convention discussed below Eq. (69). As an example $\nu = 3$ corresponds to $k = \frac{2\pi}{3}$, $\sigma = \uparrow$, while $\nu = 4$ corresponds to $k = \frac{2\pi}{3}$, $\sigma = \downarrow$. On right the x-axis label ν is the sorting index of the increasing energies found from ED, which are blind to the wave vectors. We may thus overlap these indices, as in Fig. 3. The exact results show a smooth dispersion of the virtual energies, together with the expected $\xi \to -\xi$ symmetry. The approximate solutions have a similar scale and also satisfy the $\xi \to -\xi$ symmetry. We see that some of the parity related degeneracies of the noninteracting spectrum persist in the approximate results, and are likely to be lifted in a second-order calculation.

energy is inoperative due to the jammed nature of the state, and hence it is simple to compute the corresponding canonical partition function $Z_{2N_s} = e^{-\beta U N_s}$. Comparing with the coefficient of $e^{\beta N_s \mu}$ in Eq. (8), we find the first sum rule:

$$\sum_{\vec{k}\sigma} \xi_{\vec{k}\sigma} = 0. \tag{13}$$

The imaginary parts of ξ, if present, cancel out by the complex conjugate property of the roots. It is readily seen that Eq. (13) is satisfied when the ξ's satisfy the condition of particle hole symmetric pairs Eq. (12) by summing over all $\{\vec{k}\sigma\}$.

(3) A second sum rule can be readily found by comparing the results of the single-particle sector $N = 1$, i.e., the coefficient of $e^{\beta\mu}$ in Eq. (8). Its exact value is found using the observation that the two-particle interaction U is inoperative in this sector. We find the second sum rule:

$$e^{-\beta \frac{1}{2} U} \sum_{\vec{k}\sigma} e^{-\beta \xi_{\vec{k}\sigma}} = \sum_{\vec{k}\sigma} e^{-\beta \varepsilon_{\vec{k}\sigma}}. \tag{14}$$

We now define U_{eff} as a function of the parameters U, β and also the computed $\{\xi\}$. It is given by

$$U_{\text{eff}}(U, \beta, \{\xi\}) = \frac{2}{\beta} \ln \left(\frac{\sum_{k\sigma} e^{-\beta \xi_{k\sigma}}}{\sum_{k\sigma} e^{-\beta \varepsilon_{k\sigma}}} \right). \tag{15}$$

The sum-rule Eq. (14) may be cast in the form

$$U_{\text{eff}}(U, \beta, \{\xi\}) = U. \tag{16}$$

Clearly if the ξ's are exactly found, then the sum-rule is satisfied exactly. If ξ's are only found approximately, then the quality of the approximation is reflected in the difference between U_{eff} and U. This idea is illustrated below in Figs. 3 and 4.

(4) Further sum rules can be found by comparing other powers of $e^{\beta\mu}$, but they require exact knowledge of the canonical partition functions $Z_2, Z_3, \ldots$, and are therefore less tractable.

III. GREEN'S FUNCTION AND SELF-ENERGY IN MATSUBARA FREQUENCIES

It is useful to consider the unnormalized thermal Green's function, signified by an overbar

$$\bar{G}_\sigma(\vec{k}, \tau|\mu) = -(\text{Tr}\, e^{-\beta\mathcal{H}} (T_\tau C_{\vec{k}\sigma}(\tau) C^\dagger_{\vec{k}\sigma}(0))), \tag{17}$$

where $-\beta < \tau \leqslant \beta$, and T_τ denotes the (fermionic) imaginary-time ordering operator. For clarity we display the dependence on the chemical potential for $G, \Sigma, \ldots$, as in Eq. (17). For any operator $\mathcal{Q}$ the standard imaginary time Heisenberg picture time dependence is defined through $\mathcal{Q}(\tau) = e^{\tau\mathcal{H}} \mathcal{Q} e^{-\tau\mathcal{H}}$. This Green's function is related to the conventional normalized Green's function G [18,19] through

$$\bar{G}_\sigma(\vec{k}, \tau|\mu) = Z(\mu) G_\sigma(\vec{k}, \tau|\mu). \tag{18}$$

The usual antiperiodicity extends to the unnormalized $\bar{G}_\sigma(\tau + \beta) = -\bar{G}_\sigma(\tau)$, and used to obtain the Matsubara Fourier representation [18] $\bar{G}_\sigma(\vec{k}, i\omega_r|\mu) = \frac{1}{2\beta} \int_{-\beta}^{\beta} e^{i\omega_r \tau} \bar{G}_\sigma(\vec{k}, \tau|\mu) d\tau$, where the allowed Matsubara frequencies are $\omega_r = (2r + 1)\frac{\pi}{\beta}$ with integer r. We next record the equation of motion for $\bar{G}$ following from the Heisenberg dynamics $\partial_\tau C_{\vec{k},\sigma} = [\mathcal{H}, C_{k\sigma}(\tau)]$

$$(-\partial_\tau + \mu - \varepsilon_\sigma(k)) \bar{G}_\sigma(k, \tau|\mu) = \delta(\tau) Z(\mu) + \bar{\mathcal{A}}_\sigma(\vec{k}, \tau|\mu), \tag{19}$$

where

$$\bar{\mathcal{A}}(\vec{k}, \tau|\mu) = -\text{Tr}\, e^{-\beta\mathcal{H}} (T_\tau a_{\vec{k}\sigma}(\tau) C^\dagger_{\vec{k}\sigma}(0)) \tag{20}$$

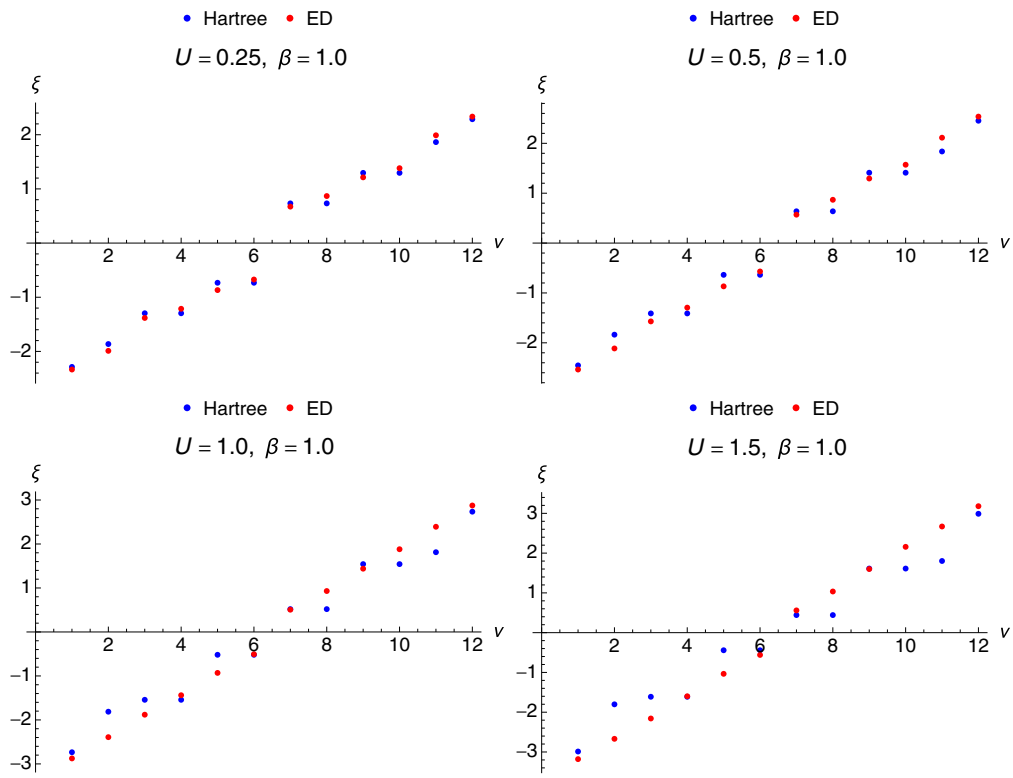

FIG. 3. Comparison between the exact virtual energies found from the partition function zeros (red dots) and the solutions of the first-order equations Eq. (69) (blue dots) at four different repulsive values of U marked in the plots. The x axis label index ν is as defined in Fig. 2 for the Hartree solution and also the sorting index for the energies found from ED. For the displayed U and β, the solutions of Eq. (69) can be used to compute $U_{\rm eff}$, see Eqs. (15) and (16). The pairs $(U, U_{\rm eff})$ are (0.25, 0.149), (0.5, 0.289), (1.0, 0.55), (1.5, 0.804), indicating that the first-order approximation worsens with increasing U.

with

$$a_{\vec{k}\sigma} \equiv [C_{\vec{k}\sigma}, V]. \tag{21}$$

Note that we can also write the unnormalized $\bar{\mathcal{A}} = Z(\mu)\mathcal{A}$, in analogy with the corresponding G's. Taking the Matsubara-Fourier series of both sides we get

$$\{i\omega_r + \mu - \varepsilon_\sigma(k)\}\bar{G}_\sigma(\vec{k}, i\omega_r|\mu) = Z(\mu) + \bar{\mathcal{A}}_\sigma(\vec{k}, i\omega_r|\mu). \tag{22}$$

Defining the Dyson self-energy Σ as

$$\Sigma_\sigma(\vec{k}, i\omega_r|\mu) = \frac{\bar{\mathcal{A}}_\sigma(\vec{k}, i\omega_r|\mu)}{\bar{G}_\sigma(\vec{k}, i\omega_r|\mu)} \tag{23}$$

this leads to the unnormalized version of Dyson's equation

$$\{i\omega_r + \mu - \varepsilon_\sigma(k) - \Sigma_\sigma(\vec{k}, i\omega_r|\mu)\}\,\bar{G}_\sigma(\vec{k}, i\omega_r|\mu) = Z(\mu). \tag{24}$$

It should be noted that in $\Sigma_\sigma(\vec{k}, i\omega_r|\mu)$, every occurrence of $i\omega_r$ is in the combination $i\omega_r + \mu$. In terms with $r \neq 0$ we note that $\omega_r - \omega_0 = r\frac{2\pi}{\beta}$, this shift can be absorbed into μ and using the periodicity $Z(\mu) = Z(\mu + ir\frac{2\pi}{\beta})$. We also note that Eqs. (31), (22), and (23) implies the periodicity in the complex μ plane for integer s

$$\bar{G}_\sigma\left(\vec{k}, i\omega_r|\mu + is\frac{2\pi}{\beta}\right) = \bar{G}_\sigma(\vec{k}, i\omega_{r+s}|\mu), \tag{25}$$

and similar relations for $\Sigma_\sigma(\vec{k}, i\omega_r)$. Therefore studying $\bar{G}_\sigma(\vec{k}, i\omega_r|\mu)$ with $r \neq 0$ does not lead to anything new and in the following we confine ourselves to $r = 0$. Displaying the μ dependence of G and Σ explicitly and defining Ψ through

$$\Psi_{\vec{k}\sigma}(\mu) \equiv G_\sigma^{-1}\left(\vec{k}, i\frac{\pi}{\beta}|\mu\right) = \mu + i\frac{\pi}{\beta} - \varepsilon_\sigma(\vec{k}) - \Sigma_\sigma\left(\vec{k}, i\frac{\pi}{\beta}|\mu\right), \tag{26}$$

we write Eq. (24) as

$$\Psi_{\vec{k}\sigma}(\mu) \times \bar{G}_\sigma\left(\vec{k}, i\frac{\pi}{\beta}|\mu\right) = Z(\mu). \tag{27}$$

The total number of such equations is $2N_s$, including the two spin projections and the N_s values of $\vec{k}$.

IV. THEOREM FOR LOCATING THE YANG-LEE ZEROS OF $Z(\mu)$.

We now discuss the connection between Yang-Lee zeros of $Z(\mu)$ and the vanishing of $\Psi_{\vec{k}\sigma}(\mu)$ [see Eq. (26)]. Recalling Eq. (7) we will establish below.

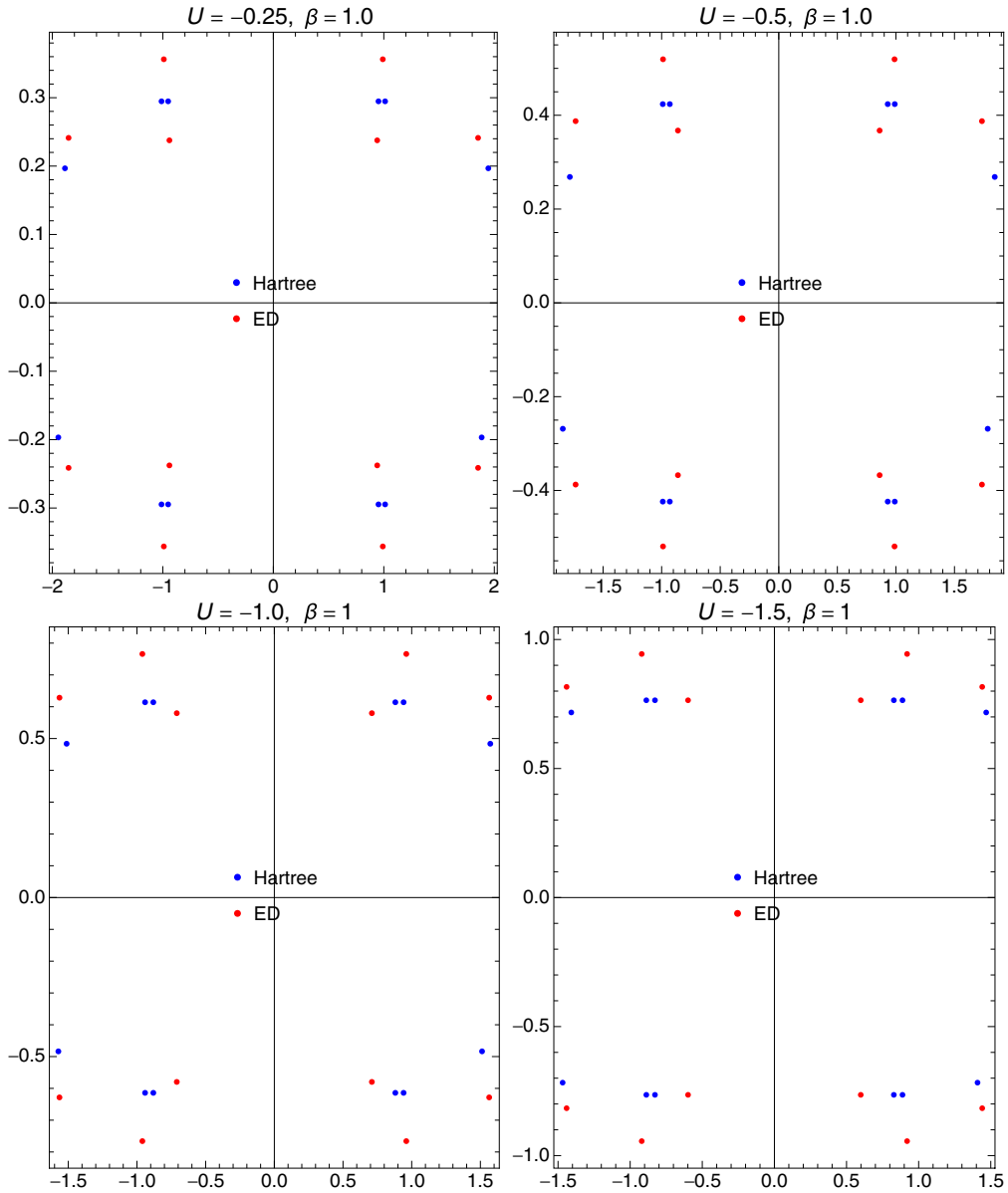

FIG. 4. Attractive interactions. All the attractive cases lead to complex virtual energies, as expected from arguments given in the text. Complex plots of the virtual energies with the real (imaginary) part on the x (y) axis. We compare the exact virtual energies found from the partition function zeros (red dots) and the solutions of Eq. (69) (blue dots) at four different attractive values of U marked in the plots. We picture the degenerate roots by introducing a slight displacement in the real part. For the displayed U and β, the solutions of Eq. (69) can be used to compute U_{eff} [see (15) and (16)]. The pairs (U, U_{eff}) are $(-0.25, -0.162)$, $(-0.5, -0.344)$, $(-1.0, -0.709 + 0.237i)$, $(-1.5, -0.916 + 0.334i)$, indicating as in the repulsive case Fig. 3, that the first order approximation worsens with increasing U. The plots at larger $|U|$ show a tendency for the real parts of energies to contract. This is understandable since an attractive U encourages spin-paired electrons to hop together- while discouraging spin-unpaired electron hops- so as to avoid losing their pairing energy [25]. The correlated hopping bandwidth tends to shrink with increasing $|U|$.

Theorem. For a fixed $(\vec{k}\,\sigma)$, if a complex number $\mu^* \in \mathcal{S}$ is a zero of $\Psi_{\vec{k}\sigma}(\mu)$ [i.e., $\Psi_{\vec{k}\sigma}(\mu^*) = 0$], then μ^* is also a zero of the partition function [i.e., $Z(\mu^*) = 0$].

Remarks. We record a few relevant comments below.

(1) In principle the self-energy $\Sigma_\sigma(\vec{k}, i\omega_r|\mu)$ can be calculated to arbitrary orders in the interaction, using the standard rules of the Feynman-Dyson-Matsubara perturbation theory in the imaginary time [18,19,22]. Given an approximation for Σ to a certain order in the coupling, the theorem can be used to find the corresponding momentum-labeled virtual energy $\xi_{\vec{k}\sigma}$, and from their total set, the (unlabeled) Yang-Lee zeros of the partition function.

(2) If the noninteracting virtual energies (i.e., the band energies $\varepsilon_{\vec{k}\sigma}$) are completely nondegenerate, then using continuity in the coupling, all zeros of Z can be located perturbatively from the theorem by varying $\vec{k}, \sigma$.

(3) Equation (27) also admits the possibility that μ^*, a root of Z, satisfies $\bar{G}_\sigma(\vec{k}, i\frac{\pi}{\beta}|\mu^*) = 0$ for a fixed $\vec{k}\sigma$, while

$\Psi_{\vec{k}\sigma}(\mu^*) \neq 0$. This type of root is much less amenable to a systematic perturbative treatment since $\bar{G}$, unlike $\Psi_{\vec{k}\sigma}$, is generally a function of almost the entire set of $\vec{k}\sigma$. However, we may bypass this class of roots, by studying the union over the $\vec{k}$, σ of the class of roots for each individual $\vec{k}$, σ's.

(4) With the nondegeneracy assumption noted above, our result is that all zeros of Z coincide with the zeros of a function $\Xi(\mu)$ defined by

$$\Xi(\mu) = \prod_{\vec{k}\sigma} \Psi_{\vec{k}\sigma}(\mu). \tag{28}$$

(5) When the single electron levels $\varepsilon_{\vec{k}\sigma}$ have degeneracies due to spin invariance or parity, this case can be viewed as a limiting case of the nondegenerate one. In the discussion following Eq. (69) we remark on how the degenerate case, treated to lowest order in U, allows for two perturbed solutions arising from a single (unperturbed) degenerate one, so that one can assign them one virtual energy to each spin projection.

(6) Using Eqs. (9) and (26) we summarize the final equation determining the virtual energy $\xi_{\vec{k}\sigma}$ as

$$\xi_{\vec{k}\sigma} = \varepsilon_{\vec{k}\sigma} - \frac{1}{2}U + \Sigma_\sigma\left(\vec{k}, i\frac{\pi}{\beta}|\xi_{k\sigma} + \frac{1}{2}U - i\frac{\pi}{\beta}\right). \tag{29}$$

Proof. To prove the theorem, a glance at Eq. (27) shows that it is sufficient to show that $\bar{G}$ is a holomorphic function of μ in the strip $\mathcal{S}$ [Eq. (7)] (i.e., without any poles or other singular points). We can establish this property using the standard eigenbasis representation

$$\bar{G}_\sigma(\vec{k}, i\omega_r|\mu) = \sum_{n,m} \frac{e^{-\beta\epsilon_n} + e^{-\beta\epsilon_m}}{\epsilon_n - \epsilon_m + i\frac{\pi}{\beta}(2r+1)} |\langle n|C_\sigma(\vec{k})|m\rangle|^2, \tag{30}$$

where $\{|n\rangle\}$ denotes a complete set of (Fock) states $\mathcal{H}|n\rangle = \epsilon_n|n\rangle, H|n\rangle = E_n|n\rangle, \mathcal{N}|n\rangle = N_n|n\rangle$, so that $\epsilon_n = E_n - \mu N_n$. This spectral representation follows from Eq. (17) by inserting complete sets of eigenstates followed by a Fourier transform from τ to the Matsubara frequencies ω_r. Recall that the destruction operator C_σ acting to the right either destroys the state or decreases the number of particles by 1, i.e., $N_n - N_m = -1$. Making the μ dependence explicit we write

$$\frac{e^{-\beta\epsilon_n} + e^{-\beta\epsilon_m}}{\epsilon_n - \epsilon_m + i\frac{\pi}{\beta}(2r+1)} = e^{\beta(\mu N_n - E_n)} \frac{1 + e^{\beta(E_n - E_m + \mu)}}{E_n - E_m + \mu + i\frac{\pi}{\beta}(2r+1)}, \tag{31}$$

and hence

$$\bar{G}_\sigma\left(\vec{k}, i\frac{\pi}{\beta}|\mu\right) = \sum_{n,m} e^{\beta(\mu N_n - E_n)} \frac{1 + e^{\beta(E_n - E_m + \mu)}}{E_n - E_m + \mu + i\frac{\pi}{\beta}} \times |\langle n|C_\sigma(\vec{k})|m\rangle|^2. \tag{32}$$

The reality of the eigenvalues E_n shows that $\bar{G}$ has no poles in the strip Eq. (7) due to the cancellation of a possible pole at $E_n - E_m + \mu + i\frac{\pi}{\beta} = 0$ by the vanishing of the numerator $1 + e^{\beta(E_n - E_m + \mu)}$ at the same location. Noting also that $0 \leqslant |\langle n|C|m\rangle|^2 \leqslant 1$, $\bar{G}$ is therefore a holomorphic function of μ in the strip $\mathcal{S}$. From Eq. (27) we obtain the theorem.

Another proof of Eqs. (24) and (27)

We note a spectral representation for $\bar{A}$ [of the same form as Eq. (30)]

$$\bar{A}_\sigma(\vec{k}, i\omega_r) = \sum_{n,m} \frac{e^{-\beta\epsilon_n} + e^{-\beta\epsilon_m}}{\epsilon_n - \epsilon_m + i\frac{\pi}{\beta}(2r+1)} \times \langle n|a_\sigma(\vec{k})|m\rangle\langle m|C_\sigma^\dagger(\vec{k})|n\rangle. \tag{33}$$

Using this relation and Eq. (30) we rearrange Eq. (22) with $r = 0$ as

$$Z(\mu) = \left\{i\frac{\pi}{\beta} + \mu - \varepsilon_\sigma(\vec{k})\right\} \sum_{nm} \frac{e^{-\beta\epsilon_n} + e^{-\beta\epsilon_m}}{\epsilon_n - \epsilon_m + i\frac{\pi}{\beta}} |\langle n|C_\sigma(\vec{k})|m\rangle|^2 - \sum_{n,m} \frac{e^{-\beta\epsilon_n} + e^{-\beta\epsilon_m}}{\epsilon_n - \epsilon_m + i\frac{\pi}{\beta}} \langle n|a_\sigma(\vec{k})|m\rangle\langle m|C_\sigma^\dagger(\vec{k})|n\rangle, \tag{34}$$

which can be simplified using

$$\begin{aligned}\langle n|a_\sigma(\vec{k})|m\rangle &= \langle n[C_\sigma(\vec{k}), \mathcal{H}]|m\rangle - (\varepsilon_\sigma(\vec{k}) - \mu)\langle n|C_\sigma(\vec{k})|m\rangle, \\ &= (\epsilon_m - \epsilon_n + \mu - \varepsilon_\sigma(\vec{k}))\langle n|C_\sigma(\vec{k})|m\rangle\end{aligned} \tag{35}$$

so that combining the two terms Eqs. (34) and (35), and simplifying gives

$$\begin{aligned}Z(\mu) &= \sum_{nm}\sum_{nm}(e^{-\beta\epsilon_n} + e^{-\beta\epsilon_m})|\langle n|C_\sigma(\vec{k})|m\rangle|^2 \\ &= \mathrm{Tr}e^{-\beta\mathcal{H}}\{C_\sigma(\vec{k}), C_\sigma^\dagger(\vec{k})\} \\ &= \mathrm{Tr}e^{-\beta\mathcal{H}},\end{aligned} \tag{36}$$

i.e., we recover the exact definition of Z Eq. (6). Summarizing, we see that Eqs. (24) and (27) consistently represents the vanishing of the partition function $Z(\mu)$ Eq. (6).

V. SOME ILLUSTRATIVE EXAMPLES

A. Noninteracting Fermi system

We note that the noninteracting Fermi model with a partition function

$$Z_{\mathrm{non}}(\mu) = \prod_{\vec{k}\sigma}\left(1 + \frac{e^{\beta\mu}}{e^{\beta\varepsilon_\sigma(\vec{k})}}\right), \tag{37}$$

provides a simple illustration of our ideas, since a vanishing condition of the noninteracting Fermion Green's function

$$G_{(0)\sigma}^{-1}\left(\vec{k}, i\frac{\pi}{\beta}|\mu\right) = i\frac{\pi}{\beta} + \mu - \varepsilon_\sigma(\vec{k}), \tag{38}$$

gives a zero of $Z_{\mathrm{non}}(\mu)$. The added imaginary part $i\frac{\pi}{\beta}$ to μ converts the Fermi factor into a Bose factor. It is therefore amusing to note that root finding is performed on the Bosonized partition function.

B. Exact Green's function in the atomic limit

We study a less trivial example of a single-site Hubbard model in the so called atomic limit, where electrons are localized on an atom. Here the partition function, its roots and the exact Green's function are all calculable explicitly, and show that the theorem applies well to the exact solution for G and also enables us to check the perturbative solution, which is carried out to $\mathcal{O}(U^2)$.

We consider the atomic limit of the Hubbard model with spin dependent energies $\varepsilon_{i\sigma}$

$$H = \sum_{i\sigma} \varepsilon_{i\sigma} C^\dagger_{i\sigma} C_{i\sigma} + U \sum_i C^\dagger_{i\uparrow} C_{i\uparrow} C^\dagger_{i\downarrow} C_{i\downarrow}, \tag{39}$$

which is uncoupled in the sites i and therefore easily solvable. Let us first consider the partition function which is easily evaluated in terms of the fugacity z and other parameters as

$$Z(\mu) = \prod_{i=1,N_s} \mathcal{Z}_i(\mu),$$
$$\mathcal{Z}_i(\mu) = 1 + z(e^{-\beta\varepsilon_{i\uparrow}} + e^{-\beta\varepsilon_{i\downarrow}}) + z^2 e^{-\beta(U+\varepsilon_{i\uparrow}+\varepsilon_{i\downarrow})}. \tag{40}$$

We simplify the notation using $\varepsilon_{i\sigma} = \varepsilon_{i0} + \sigma\delta_\varepsilon$, so that

$$\mathcal{Z}_i(\mu) = 1 + 2ze^{-\beta\varepsilon_{i0}} \cosh\beta\delta_\varepsilon + z^2 e^{-\beta(U+2\varepsilon_{i0})}, \tag{41}$$

so that the two roots of $\mathcal{Z}_i(\mu)$ in the fugacity variable $z = e^{\beta\mu}$, which are denoted as $z_{i\sigma}$, can be calculated as

$$z_{i\sigma} = -1 \times e^{\beta(U+\varepsilon_{i0})}(\cosh\beta\delta_\varepsilon + \sigma\{\sinh^2(\beta\delta_\varepsilon) + 1 - e^{-\beta U}\}^{\frac{1}{2}}). \tag{42}$$

At $U = 0$ the roots are $z_{i\sigma} = -e^{\beta\varepsilon_{i\sigma}}$ the free particle roots, while for nonzero U the roots are either on the negative real z line (U positive) or off the z real line (U negative). We can also express this result in terms of virtual energies $\xi_{i\sigma}$ defined in Eq. (9) as

$$\xi_{i\sigma} = \frac{1}{2}U + \varepsilon_{i0} + \frac{1}{\beta}\ln(\cosh\beta\delta_\varepsilon + \sigma\{\sinh^2(\beta\delta_\varepsilon) + 1 - e^{-\beta U}\}^{\frac{1}{2}}). \tag{43}$$

We now drop the site index i, and compute the average number of particles using $n_\sigma = -\frac{1}{\beta}\frac{\partial}{\partial\varepsilon_\sigma}\ln\mathcal{Z}$

$$n_\sigma(\mu) = \frac{1}{\mathcal{Z}(\mu)}(e^{\beta(\mu-\varepsilon_\sigma)} + e^{\beta(2\mu-U-2\varepsilon_0)}). \tag{44}$$

Now we write down the exact atomic limit Green's function- known from Hubbard's work [26]

$$G_\sigma(i\omega_n|\mu) = \frac{1 - n_{\bar\sigma}(\mu)}{i\omega_n + \mu - \varepsilon_\sigma} + \frac{n_{\bar\sigma}(\mu)}{i\omega_n + \mu - U - \varepsilon_\sigma}, \tag{45}$$

which can be rewritten in the form of a single term with a self-energy

$$G_\sigma(i\omega_n|\mu) = \frac{1}{i\omega_n + \mu - \varepsilon_\sigma - \Sigma_\sigma(i\omega_n|\mu)},$$
$$\Sigma_\sigma(i\omega_n|\mu) = Un_{\bar\sigma} + \frac{U^2 n_{\bar\sigma}(1 - n_{\bar\sigma})}{i\omega_n + \mu - \varepsilon_\sigma - U(1 - n_{\bar\sigma})}. \tag{46}$$

We alternately calculate n_σ from Eq. (45) using the familiar formula $n_\sigma = \frac{1}{\beta}\sum_n e^{i\omega_n 0^+} G_\sigma(i\omega_n)$. After some algebra one can verify that the result is the same as in Eq. (44).

Note also that the un-normalized Greens function Eq. (18) is given by

$$\bar G_\sigma(i\omega_n|\mu) = \frac{1 + e^{\beta(\mu-\varepsilon_\sigma)}}{i\omega_n + \mu - \varepsilon_\sigma} + \frac{e^{\beta(\mu-\varepsilon_{\bar\sigma})}(1 + e^{\beta(\mu-\varepsilon_\sigma-U)})}{i\omega_n + \mu - \varepsilon_\sigma - U}. \tag{47}$$

It is easily seen that $\bar G_\sigma(i\omega_0)$ is a holomorphic function of μ in the strip $\mathcal{S}$ Eq. (7), due to the vanishing of the numerator at every location of the vanishing denominators.

1. Roots for small U: Nondegenerate case $\delta_\varepsilon > 0$

We find by expanding Eq. (43)

$$\xi_\uparrow = \epsilon_0 + \delta_\varepsilon + \frac{1}{2}U\coth\beta\delta_\varepsilon - \beta U^2\frac{1}{8}\frac{\cosh\beta\delta_\varepsilon}{\sinh^3\beta\delta_\varepsilon} + \mathcal{O}(U^3). \tag{48}$$

We can find $\xi_\downarrow$ from the above by setting $\delta_\varepsilon \to -\delta_\varepsilon$.

2. Roots for small U: Degenerate case $\delta_\varepsilon = 0$

Expanding the $\delta_\varepsilon = 0$ limit of Eq. (43) we get

$$\xi_+ = \varepsilon_0 - \sqrt{\frac{U}{\beta}} + \frac{\sqrt{\beta}}{12}U^{\frac{3}{2}} + \mathcal{O}(U^{\frac{5}{2}})$$
$$\xi_- = \varepsilon_0 - \sqrt{\frac{U}{\beta}} - \frac{\sqrt{\beta}}{12}U^{\frac{3}{2}} + \mathcal{O}(U^{\frac{5}{2}}). \tag{49}$$

3. Perturbative roots from G: Nondegenerate case

We next show how the small U roots given in Eqs. (48) and (49) can be obtained using the perturbative expansion of the Dyson self-energy, as remarked below the theorem, i.e., the condition $\Psi_{\bar k\sigma}(\mu) = 0$. Recall that

$$G_\sigma^{-1}\left(i\frac{\pi}{\beta}| - i\frac{\pi}{\beta} + x\right) = x - \varepsilon_\sigma - \Sigma_\sigma(x) \tag{50}$$

with

$$\Sigma_\sigma(x) = Un_{\bar\sigma} + \frac{U^2 n_{\bar\sigma}(1 - n_{\bar\sigma})}{x - \varepsilon_\sigma - U(1 - n_{\bar\sigma})}. \tag{51}$$

For the purpose of this calculation we use the convenient variable x, which is related to the virtual energy through $\xi = x - \frac{1}{2}U$. We next expand the exact occupation n_σ appearing above, using Eq. (44), in a series in U. In terms of the Fermi function

$$f_{z,\sigma} = \frac{z}{z + e^{\beta\varepsilon_\sigma}} \tag{52}$$

we find

$$n_\sigma = f_\sigma - \beta U f_\sigma f_{\bar\sigma}(1 - f_{\bar\sigma}) + \mathcal{O}(U^2), \tag{53}$$

where $\bar\sigma = -\sigma$. We setup the root equation to $\mathcal{O}(U^2)$ for $G_\sigma^{-1} = 0$. Recall we are temporarily using $x = i\frac{\pi}{\beta} + \mu$, so that $z \to -e^{\beta x}$, and in terms of x

$$f_{z,\sigma}|_{z\to -e^{\beta x}} \equiv f_\sigma(x) = \frac{e^{\beta x}}{e^{\beta x} - e^{\beta\varepsilon_\sigma}}$$
$$f'(x) = \beta f_\sigma(x)[1 - f_\sigma(x)]. \tag{54}$$

Expanding n_σ using Eq. (53), and truncating to $\mathcal{O}(U^2)$ or from diagrammatics directly, we get

$$\Sigma_\sigma(x) = U f_{\bar\sigma} - \beta U^2 f_{\bar\sigma}(x)[1 - f_{\bar\sigma}(x)] f_\sigma(x) + \frac{U^2 f_{\bar\sigma}(1 - f_{\bar\sigma})}{x - \varepsilon_\sigma} + \mathcal{O}(U^3). \tag{55}$$

In Eq. (50) we substitute the above, and so the condition for a root is

$$x - \varepsilon_\sigma - U f_{\bar\sigma}(x) + \beta U^2 f_\sigma(x) f_{\bar\sigma}(x)[1 - f_{\bar\sigma}(x)] - U^2 \frac{f_{\bar\sigma}(x)[1 - f_{\bar\sigma}(x)]}{(x - \varepsilon_\sigma)} = 0 \tag{56}$$

and for therefore for $\sigma = \uparrow$

$$\begin{aligned} x &= \varepsilon_\uparrow + U f_\downarrow(x) - \beta U^2 f_\uparrow(x) f_\downarrow(x)[1 - f_\downarrow(x)] + U^2 \frac{f_\downarrow(x)[1 - f_\downarrow(x)]}{x - \varepsilon_\uparrow} = 0 \\ &= \varepsilon_\uparrow + U f_\downarrow(x) - U^2 \beta f_\downarrow(x)[1 - f_\downarrow(x)]\left[f_\uparrow(x) - \frac{k_B T}{x - \varepsilon_\uparrow}\right]. \end{aligned} \tag{57}$$

We can solve iteratively

$$x = x_0 + U x_1 + U^2 x_2 + \dots \tag{58}$$

so that

$$x_0 = \varepsilon_\uparrow + \eta = \varepsilon_0 + \delta_\varepsilon + \eta \tag{59}$$

$$x_1 = f_\downarrow(x_0) = \frac{e^{\delta_\varepsilon}}{2 \sinh \beta \delta_\varepsilon}, \tag{60}$$

where we set $\eta = 0$ at the end. To get the full second-order result, we need to expand

$$\begin{aligned} f_\downarrow(x_0 + U x_1) &= f_\downarrow(x_0) + U x_1 f'_\downarrow(x_0) + .. \\ &= f_\downarrow(x_0) + \beta U f_\downarrow^2(x_0)[1 - f_\downarrow(x_0)] + \dots \end{aligned} \tag{61}$$

Hence

$$x_2 = \beta f_\downarrow^2(x_0)(1 - f_\downarrow(x_0)) - U^2 \beta f_\downarrow(x_0)(1 - f_\downarrow(x_0)) \times \left[f_\uparrow(x_0 + \eta) - \frac{k_B T}{x_0 - \varepsilon_\uparrow + \eta}\right]. \tag{62}$$

The term in square brackets on the right equals $\frac{1}{2}$ by taking the limit $\eta \to 0$. On simplification this leads to

$$x_2 = -\frac{\beta}{8} \frac{\cosh \beta \delta_\varepsilon}{\sinh^3(\beta \delta_\varepsilon)}. \tag{63}$$

We therefore verify that Eqs. (59), (60), and (63) combine to give the first three terms obtained directly Eq. (48).

4. Degenerate case

For the degenerate case $\varepsilon_\sigma = \varepsilon_0$ (i.e., $\delta_\varepsilon = 0$), we show how the leading behavior in Eq. (49) is obtained from the condition $\Psi_{\vec k\sigma}(\mu) = 0$ from the theorem. We write the leading, i.e., $\mathcal{O}(U)$ terms of Eq. (56)

$$x - \varepsilon_0 = U \frac{1}{1 - e^{\beta(\varepsilon_0 - x)}} + \dots, \tag{64}$$

and expand the Bose factor for $x \sim \varepsilon_0$ and rearrange to obtain the leading solution

$$x - \varepsilon_0 = \pm \sqrt{\frac{U}{\beta}} + \dots \tag{65}$$

To get the next correction we note that the right-hand side of Eq. (64) is expressible as

$$\frac{U}{\beta(x - \varepsilon_0)(1 - \frac{1}{2}\beta(x - \varepsilon_0) + \dots)},$$

so in the spirit of a perturbative expansion we substitute the leading result Eq. (65) in the denominator and expanding we get the next correction as

$$x_\pm = \varepsilon_0 \pm \sqrt{\frac{U}{\beta}} + \frac{1}{2} U + \mathcal{O}(U^{3/2}), \tag{66}$$

giving the first few terms in Eq. (49).

This expression shows that the doubly degenerate root of the $U = 0$ system evolves into a pair of roots at nonzero U. The pair of roots are real for $U > 0$ and complex conjugates for $U < 0$. The reader will notice a similarity between this result, and the results from the heuristic argument presented in Eqs. (2) and (3) in Sec. I.

5. Satisfying the two sumrules Eqs. (13) and (14)

We note that the perturbative solutions Eqs. (48), (49), and (66) satisfy the first sum-rule Eq. (13), one checks that terms of orders other than $\mathcal{O}(U)$ cancel out. The solutions Eqs. (48), (49), and (66) also satisfy the second sumrule Eq. (14), here terms of $\mathcal{O}(U^n)$ with $n \neq 0$ cancel out. These sumrules are therefore of interest in numerical schemes, providing nontrivial constraints.

VI. VIRTUAL ENERGIES FROM SELF-ENERGY TO $\mathcal{O}(U)$.

The self-energy of the Hubbard model on N_s sites to $\mathcal{O}(U)$ is readily obtained from standard perturbation theory [19] as

$$\Sigma_\sigma(\vec k, i\omega_n) = \frac{U}{N_s} \sum_{\vec p} \frac{1}{e^{\beta(\varepsilon_{p\bar\sigma} - \mu)} + 1}, \tag{67}$$

where $\bar\sigma = -\sigma$. Substituting into Eq. (29) we get the equation determining the virtual energy as

$$\xi_{\vec k\sigma} = \varepsilon_{\vec k\sigma} - \frac{1}{2} U + \frac{U}{N_s} \sum_p \frac{1}{1 - e^{\beta(\varepsilon_{p\bar\sigma} - \xi_{k\sigma} - \frac{1}{2}U)}} + \mathcal{O}(U^2). \tag{68}$$

Below we will present the numerical solutions of a simplified version

$$\xi_{\vec k\sigma} = \varepsilon_{\vec k\sigma} + \frac{U}{2N_s} \sum_p \coth \frac{\beta}{2}(\xi_{k\sigma} - \varepsilon_{p\bar\sigma}), \tag{69}$$

where we dropped a term of the $\mathcal{O}(U^2)$ arising from expanding the coth. The dropped term is added back to other second-order terms in the self-energy, and the results of such a calculation to $\mathcal{O}(U^2)$ will be reported later [27]. From the structure of Eq. (69) and since $\sum_p \varepsilon_{p\bar\sigma} = 0$, we see that the sum-rule Eq. (13) is automatically satisfied.

Let us now consider only the degenerate case where the energies $\varepsilon_{\vec{k}\sigma}$ shed any dependence of σ. This is a somewhat subtle case relative to the nondegenerate case, where continuity in U can be used. For the degenerate case our treatment shows how a degenerate level can lead to a pair of distinct virtual energies at this order. We note that the second term in Eq. (69), regarded as a function of ξ, has a pole at each ε_p on the real line. Very close to ε_a the equation can be approximated by retaining only the dominant term, giving two solutions $\xi^* = \varepsilon_a \pm \sqrt{\frac{U}{N_s}}$ straddling ε_a. This pair of solutions can then by refined by adding in the neglected terms. For any nonzero U we then expect $\sim 2L$ solutions. For a fixed $\vec{k}$, we want the energies to coincide with the noninteracting value $\varepsilon_{\vec{k}}$ as $U \to 0$. Therefore we pick two solutions closest to this value. We can use a convention where the solution with lower (higher) real part of ξ is regarded as arising from spin up (down), assuming continuity when a magnetic field in the $+z$ direction is tuned to zero. This and keeping in mind the condition of complex conjugation, i.e., ξ and ξ^* occuring in pairs [discussed below Eq. (10)], this gives us a total of $2L$ virtual energies, each evolving from a specific $\varepsilon_{\vec{k}}$. Solving these equations for finite systems is fairly straightforward. We display the results of solving Eq. (69), and compare with the exact energies found by numerical means for a small Hubbard. The partition function for a six-site Hubbard model with periodic boundary conditions, i.e., the benzene ring, was found using the dirac-q symbolic computation program [20]. A comparison is presented for both repulsive and attractive signs of U at $\beta = 1$ (all energies are relative to the hopping t). In Fig. 2 we compare the virtual energies for a few typical values of positive U found by solving Eq. (69) in the left panel, and by numerically finding the roots of the partition function in the right panel.

In Fig. 3 we compare the exact virtual energies and the approximate ones from Eq. (69) at four typical values of U. For smaller $U \leqslant 0.25$ the results are quite close. They suggest that it is reasonable to label the numerical solutions with the k values read off from the approximate solutions. For the larger values of U the agreement is poorer, although the extremities show a closer convergence.

In Fig. 4 we display results for the attractive case, at a few negative values of U. All virtual energies are nonreal in these calculations, requiring only a negative sign of U. The solutions of Eq. (69) capture the shrinking range of the real part of the virtual energies at the extremities in all cases. The quantitative agreement with the imaginary parts is not as good.

The formation of bound (Cooper) pairs in this case is similar to that of electron-electron binding posited in Dyson's well known argument [21] about the instability of quantum electrodyamics with a flipped sign of e^2. The resulting nonconvergence of perturbation theory in field theory, is based on the instability of the ground state due to pair formation, under the standard assumption of an infinite system. For the conventionally measured variables (energy, susceptibilities etc) related effects can only be seen in the limit of a large number of particles, i.e., in the thermodynamic limit. In the present case, we see that the distinct behavior of the virtual states between the repulsive and attractive cases, namely the energies going from real values for repulsion to complex pairs for attraction. This striking change is visible even for small systems.

VII. CONCLUDING REMARKS

We have argued that the roots of the grand partition function of many-body models, such as the Hubbard model, can be found perturbatively in the interaction. Our method gives virtual energies $\xi_{\vec{k}\sigma}$, which are assigned (crystal) momentum and spin labels. The condition Eq. (29), can be used to systematically estimate the virtual energies $\xi_{\vec{k}\sigma}$, starting from the non-interacting values $\xi_{\vec{k}\sigma}|_{U\to 0} \to \varepsilon_\sigma(\vec{k})$. We have illustrated this idea with two examples (i) the single-site Hubbard model, by solving for the thermodynamically derived virtual energies by perturbation theory to second order in U and compared with expansion in U of the exact values that are readily found (ii) the benzene molecule, i.e., a six-site Hubbard ring by solving for the virtual energies in a six-site Hubbard model by first-order perturbation theory in U of either sign and compared with the exact numerical results.

For repulsive U, the virtual energies are real in the lowest-order calculations. Assuming that a substantial fraction of the virtual roots are real at low T in certain energy ranges, their level density should control the compressibility, heat capacity and susceptibility for the corresponding densities. In this sense the methods developed here may be expected to connect with the Landau Fermi liquid and its many variants [28]. Towards this end it seems important to study the virtual energy distribution for larger systems, and to study its variation with the strength of the interaction U. For the case of attractive interaction, the results presented here give nonreal virtual energies, already to first order in U and for very small lattice sizes. Further applications of these ideas are subjects for future research [27].

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX: ZEROS FROM THE LUTTINGER-WAR D FORMULA

In this section we discuss another expression for the partition function of a many-body system found in the well-known work of Luttinger and Ward (LW) [22]. LW found a formally exact expression for the thermodynamic potential Ω (and therefore the partition function) in terms of the Green's function $G_\sigma(\vec{k}, i\omega_r)$, from perturbation theory to all orders in the coupling. The LW result follows from a clever rearrangement of the thermal perturbation theory, whose convergence is implicitly assumed to be sufficiently benign. Their result for

the grand potential Ω

$$\Omega = -\frac{1}{\beta}\ln Z(\mu) \tag{A1}$$

can be written in terms of the partition function in the following way:

$$Z(\mu) = Z_A(\mu)\times Z_B(\mu)\times Z_C(\mu), \tag{A2}$$

where

$$\ln Z_A(\mu) = \sum_{\vec{k}\,r\sigma} e^{i\omega_r 0^+}\ \ln\big[-G_\sigma^{-1}(\vec{k}, i\omega_r)\big] \tag{A3}$$

$$\ln Z_B(\mu) = \sum_{\vec{k}\,r\sigma} e^{i\omega_r 0^+}\big\{G_0^{-1}(\vec{k}, i\omega_r)G_\sigma(\vec{k}, i\omega_r) - 1\big\} \tag{A4}$$

and

$$\ln Z_C(\mu) = -\sum_{\nu\geqslant 1}\sum_{\vec{k}\,r\sigma} e^{i\omega_r 0^+}\frac{1}{2\nu}\widetilde{\Sigma}_\sigma^{(\nu)}(\vec{k}, i\omega_r)\ G_\sigma(\vec{k}, i\omega_r), \tag{A5}$$

where G_0 is the noninteracting Greens function, $\widetilde{\Sigma}_\sigma^{(\nu)}(\vec{k}, i\omega_r)$ is the total νth-order skeleton self-energy part, where the order of the diagram ν counts all explicit powers of the interaction, in this case U. In these expressions the term $e^{i\omega_r 0^+}$ is required for convergence of the sum. Note that Z_B and Z_C vanish in the limit of free Fermions. Readers might recognize that $\ln Z_C$ Eq. (A5) is the Luttinger-Ward functional of G, with the property that its functional derivative gives the exact self-energy, and thereby Ω is a stationary functional of $G_{\vec{k}\sigma}$.

From Eq. (A3) we obtain the product form

$$\begin{aligned} Z_A(\mu) &= \prod_{\vec{k}\sigma\, r} e^{i\omega_r 0^+}\big\{-G_\sigma^{-1}(\vec{k}, i\omega_r)\big\}, \\ &= \prod_{\vec{k}\sigma}(-1)\Psi_{\vec{k}\sigma}(\mu)\times\left(\prod_{\vec{k}\sigma\, r\neq 0} e^{i\omega_r 0^+}\ \big\{-G_\sigma^{-1}(\vec{k}, i\omega_r|\mu)\big\}\right) \end{aligned} \tag{A6}$$

using Eq. (26). Indeed the complete partition function Z_0 of the free Fermi theory is of this form with G_0 replacing G. It is seen from this expression that Z_A [and hence $Z(\mu)$] contains the factor $\Xi(\mu)$ given in Eq. (28), and their quotient is expressible as a functional of G. The quotient is required to be a holomorphic function of μ in the strip $\mathcal{S}$, with no other zeros. This result not easy to prove directly, but must be true if all the zeros are given by the function $\Xi(\mu)$ given in Eq. (28).

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