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Fermi-polaron problem: Diagrammatic Monte Carlo method for divergent sign-alternating series

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We use the diagrammatic Monte Carlo approach to solve the problem of a single spin-down fermion resonantly interacting with a Fermi gas of spin-up particles. Our solution is important for understanding the phase diagram and properties of the crossover from the BCS regime to the Bose-Einstein condensate in the strongly imbalanced regime. On the technical side, we develop a generic sign-problem-tolerant method for exact numerical solution of polaron-type models. This is a characteristic example of how Monte Carlo methods can be used to simulate divergent sign-alternating diagrammatic series.

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The polaron problem is canonical across all fields in physics and for more than 70 years[1] the same generic questions are asked whenever one has to study properties of particles coupled to the environment.[2] The diversity and novelty lie in the nature of the particle, the environment, and the coupling between them: there are electron-phonon polarons (optical and/or acoustic), spin polarons, exciton polarons, polarons coupled to Bose-Einstein condensates (BECs), etc. The polaron parameters, such as its energy, effective mass, and coupling to other excitations in the system, to a large extent determine the basic properties of all condensed matter systems at low temperature. Strictly speaking, studies of the effect of coupling to fluctuations of the respective physical vacuum on properties of elementary particles fall in the same category of problems.

Recently, investigations of the BCS-BEC crossover in the strongly imbalanced regime focused on properties of minority (spin-down) fermions resonantly coupled to the majority (spin-up) fermions.[3,4] To be more specific, one is interested in knowing the effective quasiparticle parameters for the Hamiltonian

$$H = H_F - \Delta_R/2m + \int d\boldsymbol{r}\, V(\boldsymbol{r}-\boldsymbol{R})n(\boldsymbol{r}), \qquad (1)$$

where H_F is the Hamiltonian of the ideal spin-up Fermi gas with the density n and Fermi momentum k_F, $\boldsymbol{R}$ is the particle coordinate, and $V(\boldsymbol{r}-\boldsymbol{R})$ is the interaction potential of finite range r_0 between the particle and the Fermi gas. Here, the particle and the Fermi gas have the same bare mass m. In what follows we refer to (1) as the Fermi-polaron problem, and use units such that $m=1/2$ and $k_F=1$.

For the BCS-BEC crossover physics in the limit of vanishing density $k_F \to 0$ and divergent s-scattering length a, so that $k_F a$ remains fixed but $k_F r_0 \to 0$, the nature of the interaction potential is irrelevant, e.g., the same results will be obtained for neutron matter and cesium atoms. The polaron parameters hold the key to the phase diagram of the strongly polarized gas. If the state with a dilute gas of spin-down fermions is stable at all values of $k_F a$, then the solution of the single-particle problem defines the phase diagram in the vicinity of the multicritical point discussed by Sachdev and Yang.[5] At this point the spin-down fermion forms a bound state with a spin-up fermion, thus becoming a spin-zero composite boson, i.e., the quasiparticles radically change their statistics. The multicritical point, however, may be thermodynamically unstable if the effective scattering length between the composite bosons and spin-up electrons is large enough, and the analysis of Ref. 6 based on fixed-node Monte Carlo (MC) simulations finds evidence in favor of this scenario. It is worth noting that the model (1) (in general, the particle mass is different from that of the Fermi gas) is also known as the Anderson orthogonality problem with recoil.[7,8]

Despite broad interest in the polaron problem, there is no reliable numerical technique to address it in full complexity, i.e., in all dimensions, for an arbitrary environment, bare particle dispersion relation, and interaction potential. Here we develop a technique based on the MC simulation of Feynman diagrams for the proper polaron self-energy which overcomes all previously existing limitations and allows an unbiased solution of the generic formulation of the problem. The diagrammatic Monte Carlo (diag-MC) technique was proved to be an efficient method for solving electron-phonon polaron problems[9,10] which are characterized by convergent, sign-positive series. (The essence of the diag-MC method is in interpreting the sum of all Feynman diagrams as an ensemble averaging procedure over the corresponding configuration space.) Although the series for the Fermi polaron are more involved, there is no fundamental difficulty in simulating the corresponding distribution. The crucial difference is that in the Fermi system we have to deal with a sign-alternating, divergent (at least for strong coupling) series. Under these conditions a direct summation of all relevant Feynman diagrams for the Green's functions is not possible, and one has to develop additional tools for (i) reducing the number of diagrams by calculating self-energies rather than Green's functions, and (ii) extrapolating diag-MC results to the infinite diagram order for divergent series. We find that the series for the Fermi polarons are Riesz summable and a numerically exact solution within the diag-MC approach does exist. We believe that our findings are important in a much broader context since the diag-MC approach to the many-body problem has essentially the same structure.

In what follows, we will be using the term "polaron" in a narrower sense, i.e., only for the unbound fermionic spin-down excitation. For the composite boson we will be using the term "molecule." If the polaron is a well-defined elemen-

tary excitation, its energy $E(\boldsymbol{p})$ can be extracted from the pole in the particle Green's function in the frequency-momentum representation, by solving the equation

$$[G_{\downarrow}^{(0)}(\omega = E(\boldsymbol{p}),\boldsymbol{p})]^{-1} = \Sigma_{\downarrow}(\omega = E(\boldsymbol{p}),\boldsymbol{p}), \tag{2}$$

where $G_{\downarrow}^{(0)}$ is the vacuum Green's function for the particle and $\Sigma_{\downarrow}$ is its self-energy. In the diag-MC technique we use the imaginary-time–momentum representation to circumvent the problem of dealing with the singular structure of free propagators and alleviate the sign problem. Remarkably, in order to find the polaron energy, we do not have to perform a numeric analytic continuation from imaginary to real frequencies, because in the imaginary-time–momentum representation Eq. (2) translates into

$$[G_{\downarrow}^{(0)}(\omega = E(\boldsymbol{p}),\boldsymbol{p})]^{-1} = \int_0^{\infty} \Sigma_{\downarrow}(\tau,\boldsymbol{p}) e^{E(\boldsymbol{p})\tau} d\tau. \tag{3}$$

The equivalence of Eqs. (2) and (3) readily follows from the fact that for the particle there is a freedom of choosing the chemical potential $\mu_{\downarrow}$ (for a single particle this is just a uniform external potential which does not affect its physical properties). This freedom can be utilized for fine-tuning $\mu_{\downarrow} = E(\boldsymbol{p})$, in which case the solution of Eq. (2) corresponds to zero frequency, no matter whether it is real or imaginary. Then, by utilizing the trivial dependence of self-energy on $\mu_{\downarrow}$, namely, $\Sigma_{\downarrow}(\tau,\boldsymbol{p},\mu_{\downarrow}) = \Sigma_{\downarrow}(\tau,\boldsymbol{p}) e^{\mu_{\downarrow}\tau}$, one proves Eq. (3).

We obtain $\Sigma_{\downarrow}(\tau,\boldsymbol{p})$ by the diag-MC method, which simulates the standard diagrammatic expansion by interpreting it as a statistical ensemble. In our case, the diagrams are constructed from the following lines: (i) the vacuum particle propagators $G_{\downarrow}^{(0)}(\tau,p) = e^{(\mu_{\downarrow} - p^2/2m)\tau}$, represented by thin horizontal straight lines, (ii) the spin-up propagators $G_{\uparrow}(\tau,p > k_F) = e^{(\epsilon_F - p^2/2m)\tau}$ and $G_{\uparrow}(\tau,p < k_F) = e^{-(\epsilon_F - p^2/2m)\tau}$ (ϵ_F is the Fermi energy of spin-up particles), depicted with thin-line arcs, and (iii) the T-matrix propagator $\Gamma(\tau,p)$. A requirement of the resonant problem is that the T matrix has to be considered as a separate diagrammatic element which sums ladder diagrams for the short-range potential $V(r)$. This summation takes the ultraviolet physics into account exactly and allows $\Gamma(\tau,p)$ to be expressed in terms of the s-scattering length a. The ladder structure of diagrams absorbed in the T-matrix explains why we treat it as a "pair propagator" and depict it with a (dashed heavy) line. The exact expression for Γ in the frequency-momentum representation reads (see, e.g., Ref. 11)

$$\Gamma^{-1}(\eta,p) = \frac{m}{4\pi a} - \frac{m}{8\pi}\sqrt{p^2 - 4m\eta} - \Pi(p,\eta), \tag{4}$$

$$\Pi(p,\eta) = \int_{q \le k_F} \frac{d\boldsymbol{q}/(2\pi)^3}{q^2/2m + (\boldsymbol{p}-\boldsymbol{q})^2/2m - \eta}, \tag{5}$$

where $\eta = \omega + \epsilon_F$. As an illustration, in Fig. 1 we present the first-order diagram for $\Sigma_{\downarrow}$.

The energy of the molecule, has to be extracted from the pole in the two-particle (spin-up + spin-down) or "pair" channel. The rest of the theory is in exact analogy with the

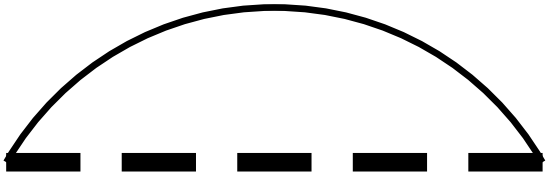

FIG. 1. First-order diagram for $\Sigma_{\downarrow}$, consisting of the T-matrix propagator Γ (heavy dashed line) and the spin-up propagator (solid arc).

Dyson-equation theory of the polaron pole. Diagrammatically, it arises from the summation of geometric series of products $\Gamma K \Gamma K \Gamma K \ldots$ where K is the Γ-irreducible diagram in the two-particle channel—a direct analog of the single-particle self-energy (see Fig. 2 for an illustration). Correspondingly, the molecular energy is found by solving the equation

$$\Gamma^{-1}(\omega = E_m(\boldsymbol{p}),\boldsymbol{p}) = \int_0^{\infty} K(\tau,\boldsymbol{p}) e^{E_m(\boldsymbol{p})\tau} d\tau. \tag{6}$$

We found neither an analytical expression for $\Gamma(\tau,p)$, nor a fast way of tabulating it with high accuracy using the inverse Laplace transform of the frequency-momentum representation Eq. (4). Instead, we applied the recently developed bold diag-MC technique[12] to obtain $\Gamma(\tau,p)$ numerically, by relating it to the vacuum T matrix, the analytic expression for which in the (τ,p) representation is readily available. This was the first practical application of the bold MC technique; see Ref. 12 for details.

The updates used to sample diagrams do not differ dramatically from the ones described in the literature; we leave the corresponding discussion to a full-sized paper. Instead, we concentrate on the convergence issues. In contrast to previous examples of diag-MC applications, the series for the resonant Fermi polaron turns out to be divergent. However, the Cesàro-Riesz summation method solves the problem. For the quantity of interest—polaron or molecule self-energy—we construct partial sums $\Sigma(N_*) = \Sigma_{N=1}^{N_*} D_N F_N^{(N_*)}$, defined as the sums of all diagrams up to order N_* (the diagram order N is defined by the number of spin-up propagators), with the Nth-order terms being multiplied by the factor

$$F_N^{(N_*)} = [(N_* - N + 1)/N_*]^{\delta} \quad \text{(Cesàro-Riesz)}. \tag{7}$$

Here $\delta > 0$ is a fixed parameter ($\delta = 1$ corresponds to the Cesàro method). If the series is Riesz summable for some

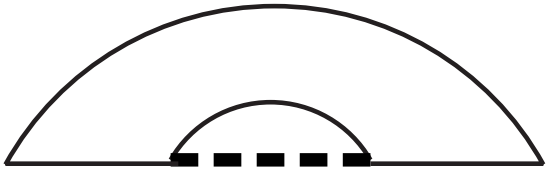

FIG. 2. First diagram for the molecular self-energy K, consisting of one T-matrix propagator (heavy dashed line), two spin-up propagators (solid arcs), and two spin-down propagators (solid straight lines).

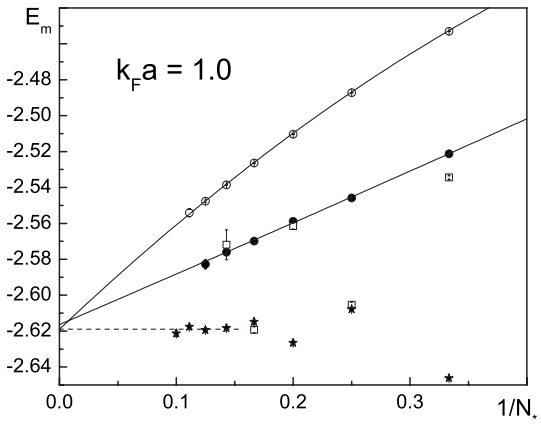

FIG. 3. Molecule energy (at $k_F a=1$) as a function of truncation parameter $N*$ for different summation techniques: Cesàro (open squares), Riesz $\delta=2$ (filled circles, fitted with the parabola $y=-2.6164+0.280\,13x+0.016\,38x^2$), Riesz $\delta=4$ (open circles, fitted with the parabola $y=-2.6190+0.616\,35x-0.3515x^2$), Eq. (8) (stars fitted with the horizontal dashed line).

values of δ, then the answer in the $N*\to\infty$ limit does not depend on δ (moreover, the answer should be the same and independent of the appropriate summation technique). The freedom of choosing the value of the Riesz exponent δ is used to optimize the convergence.

For the $N*$-truncated and F-reweighted series, we first determine the polaron and molecule energies and then study their dependence on $N*$ as $N*\to\infty$. Figure 3 illustrates the procedure. The odd-even oscillations are very pronounced for $\delta=1$, hinting at the absence of convergence of the original series, but are strongly suppressed for larger values of δ. With $\delta=4$ we were not able to resolve odd-even oscillations, but the smoothness of the curve here comes at the expense of increased curvature, which renders the extrapolation to the $1/N*\to 0$ limit more vulnerable to systematic errors. Empirically, we constructed a factor $F_N^{(N*)}$, which leads to a faster convergence [see Figs. 3 and 4 (error bars are mentioned in all plots but are typically smaller than symbol sizes)]

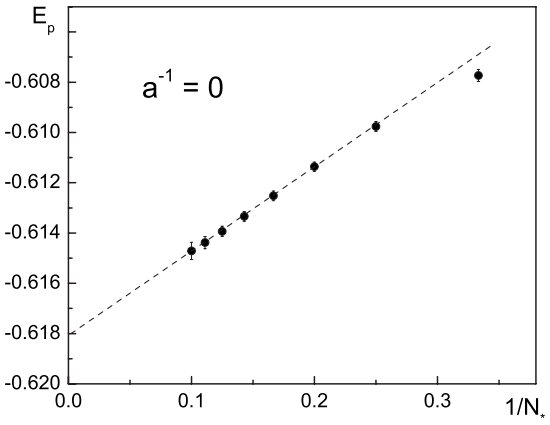

FIG. 4. Polaron energy (at the unitarity point $a^{-1}=0$) as a function of truncation parameter $N*$ using Eq. (8). The asymptotic behavior at $1/N*\to 0$ is perfectly fitted by a straight line.

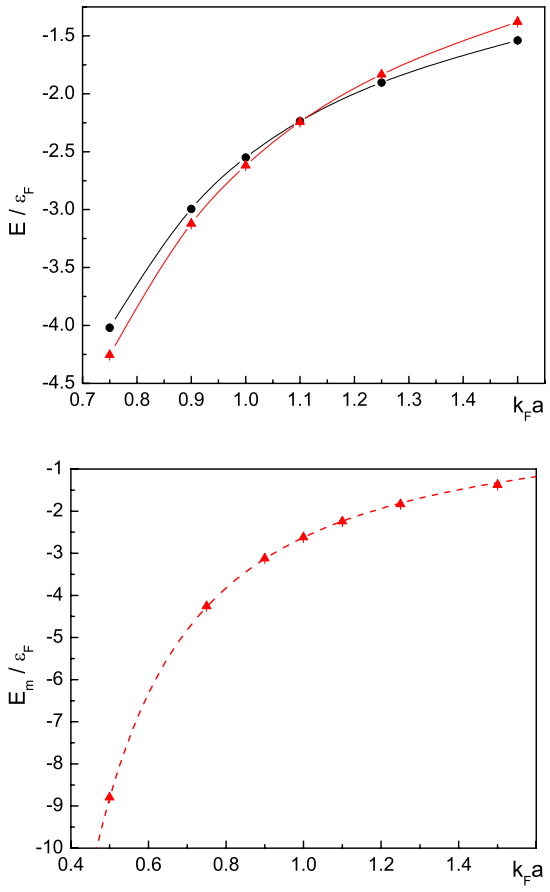

FIG. 5. (Color online) Polaron (black circles) and molecule [red (gray) triangles] energies (in units of ϵ_F) as functions of $k_F a$. The dashed line on the lower panel corresponds to Eq. (9).

$$F_N^{(N*)} = C_{N*} \sum_{m=N}^{N*} \exp\left(-\frac{(N*+1)^2}{m(N*-m+1)}\right), \tag{8}$$

where C_{N*} is the normalization factor.

In the limit of $k_F a\to 0$ the molecule energy is given by the asymptotic expression

$$E_m = -\frac{1}{ma^2} - \epsilon_F + \frac{2\pi\tilde{a}}{(2/3)m} n_\uparrow \quad (k_F a \to 0), \tag{9}$$

where the last term comes from the interaction between the composite molecule with the Fermi gas. Correspondingly, $\tilde{a}\approx 1.18a$ is the molecule-fermion s-scattering length[13] obtained from the nonperturbative solution of the three-body problem. This result provides a robust test to the entire numerical procedure of sampling and extrapolating divergent sign-alternating diagrammatic series. Our data are in perfect agreement with the $\tilde{a}\approx 1.18a$ result within the statistical uncertainty of the order of 5% (see the lower panel in Fig. 5).

In Fig. 5, we show polaron and molecule energies in the region of $k_F a\sim 1$ where the nature of the quasiparticle state changes. The crossing point is found to be at $(k_F a)_c = 1.11(2)$. The values of both polaron and molecule energies are in excellent agreement with the fixed-node Monte Carlo

simulations.[4,6] Interestingly, the polaron self-energy is nearly exhausted by the first-order diagram considered in Ref. 11; see also Fig. 4.

The crossing of the polaron and molecule solutions is exact since the hybridization between the two is zero at $(k_F a)_c$. This is guaranteed by the phase-space argument. The conservation of energy, momentum, and spin projection dictates that the leading decay channel involves four quasiparticles in the final state (the polaron decays into a molecule, two holes, and one spin-up particle); correspondingly, the final-state phase volume gets negligibly small as compared to the energy difference $|E_p - E_m|$ at and in the vicinity of the crossing point.

The data for the effective mass are presented in Fig. 6. As expected, at the crossing point the effective mass curve is discontinuous. Note that good agreement with Eq. (9) for E_m at all couplings is somewhat misleading since Eq. (9) assumes that molecules are compact and their mass is $2m$. The actual effective mass is significantly enhanced in the vicinity of $(k_F a)_c$.

Summarizing, the problem of the resonant Fermi polaron is solved here by the diag-MC technique, and the point where the ground state switches from the single-particle (fermionic) sector to the two-particle (bosonic) sector is found to be at $k_F a = 1.11(2)$. We discovered that, while the diagrammatic series is divergent, the fermionic sign of the diagrams renders the series summable by Cesàro-Riesz-type methods and suitable for numerical analysis. We do not see any limitations for the technique to be successfully used for arbitrary polaron models, and, possibly, arbitrary interacting many-body systems. The technique offers an acceptable solution to the sign problem, i.e., in the space of Feynman diagrams it is possible to extrapolate simulation results to infinite diagram order before error bars go out of control due to an exponentially or factorially expanding configuration space. Whether this *sign blessing* is a specific feature of the problem solved here, or a generic feature of fermionic and, possibly, other diagrammatic expansions, is a major question that we will address in future.

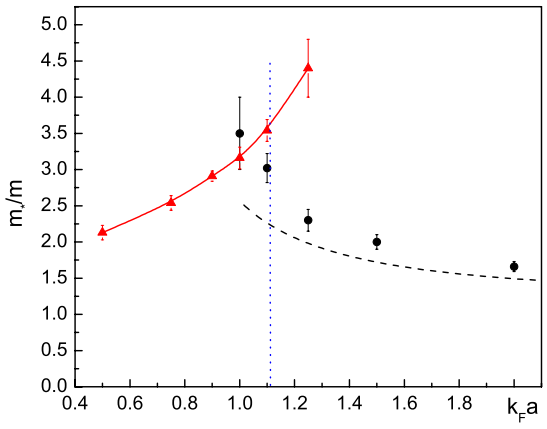

FIG. 6. (Color online) Polaron (black circles) and molecule [red (gray) triangles] effective mass as functions of $k_F a$. The vertical dotted line stands for $(k_F a)_c = 1.11$. The dashed line is the contribution from the first diagram (Ref. 11).

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