Comment on "Bethe Ansatz Results for the 4f-Electron Spectra of a Degenerate Anderson Model"

In a recent Letter [1], Zvyagin calculates the spectral density for $4f$ electrons coupled to a conduction band using the Bethe ansatz (BA) solution for the degenerate Anderson impurity model (AIM). It is claimed that the results *qualitatively disagree* with the results obtained using a variational approach [2]. The *high energy* feature in the f-spectral function near the $4f$-level energy ϵ_f, i.e., the "normal" ionization peak (NIP), is argued to be *qualitatively* different in the two approaches. Here we point out that this is *not* the case.

We concentrate on the $U \to \infty$, N-fold degenerate Anderson model. Zvyagin assumed constant hopping matrix elements $V_{m,k} \equiv V$ and conduction electron density of states $\rho(E) \equiv \rho$. He presented BA results in the large band width limit $B \gg |\epsilon_f|$ which showed that the NIP is shifted towards the chemical potential from ϵ_f in the Kondo limit $n_f \approx 1$, where n_f is the f occupancy. He then stated that the peak shifts in the opposite direction in our variational calculation [2]. This is *not* the case, as is obvious from our results in the Kondo limit presented in Appendix C of Ref. [2]. This is also shown very clearly in Fig. 5 of Ref. [3] and in Fig. 1 [the spectra are broadened by a Lorentzian (FWHM $= 0.10\Delta$) and normalized to their maximum values].

The NIP position is called $\tilde{\epsilon}_f$ in Appendix C of Ref. [2]. For large N and the Kondo limit this *real* quantity is determined by

$$\tilde{\epsilon}_f = \epsilon_f + \mathrm{Re}\tilde{\Gamma}(\tilde{\epsilon}_f), \tag{1}$$

where

$$\tilde{\Gamma}(z) = N \int_{-B}^{0} d\epsilon |V(\epsilon)|^2/(z - \epsilon). \tag{2}$$

$\mathrm{Re}\tilde{\Gamma}(\tilde{\epsilon}_f - i0^+)$ is *positive* for negative $\tilde{\epsilon}_f$ with $|\tilde{\epsilon}_f| \ll B$ [for a constant $V(\epsilon)$ it is given by $NV(0)^2 \ln(B/|\tilde{\epsilon}_f|)$]. It immediately follows that in our variational calculation the NIP shifts *towards* the chemical potential, as in the BA solution. Zvyagin claims that the solution to this equation was found by us "in the *complex* form" [1]. Apparently he was confused by an unfortunate misprint in the second equality of our equation which determines $\tilde{\epsilon}_f$. It should read $|\tilde{\epsilon}_f|$ instead of $\tilde{\epsilon}_f$ in the argument of the logarithm. From the first part of the equation, presented above, it should be obvious that this was in fact a misprint.

Zvyagin compared his results with Eqs. (1) and (2), which give the NIP position correctly only to zeroth order in $(1/N)$. We have, however, also presented methods which are correct to higher orders in $(1/N)$ [2], which were used in most calculations. In Fig. 1 we included all terms of order $(1/N)^0$ and some terms of order $(1/N)^1$.

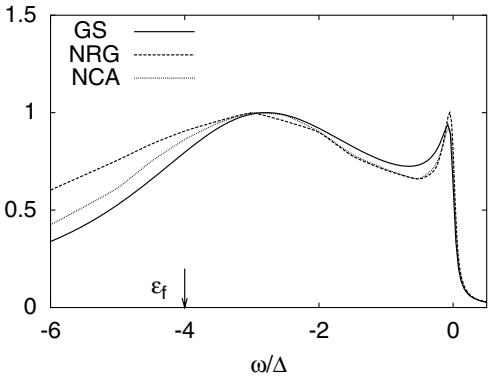

FIG. 1. Photoemission spectrum of the AIM according to our variational method (GS), a numerical renormalization group calculation (NRG) [4], and the NCA [4]. The parameters are $\Delta = \pi V^2/(2B) = 0.01B$, $\epsilon_f/\Delta = -4$, and $N = 2$. The NIP is shifted *towards* the chemical potential also in our variational approach, contrary to claims in Ref. [1].

Real compounds typically have strongly varying hopping matrix elements $V(\varepsilon)$, which was taken into account in most of our previous calculations. In such cases the NIP can indeed be shifted away from the chemical potential. This is, however, not in contradiction to the work of Zvyagin, since he assumed a constant $V(\varepsilon)$.

As noted by Zvyagin [1] other low energy characteristics obtained within our scheme qualitatively coincide with the BA ones. Our method has been used successfully in the description of cerium compounds [3,5].

In conclusion, in contrast to the claims in Ref. [1], our variational results for the high energy feature in the f-spectral function for the degenerate Anderson model qualitatively *agree* with the BA results for models where the assumptions of the Ref. [1] are valid.

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