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The embedding potential for an interacting system

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Abstract. It is already known that for a quantum system of independent boson or fermion quasiparticles, calculations can be performed explicitly in only one part if the remainder is replaced by an energy-dependent *embedding potential*. Using path-integral methods, we extend this result to the case when arbitrary many-body interactions are permitted in the region where explicit calculation is to take place, provided that certain averaging (such as is involved in taking thermal expectation values), is carried out over the configurations of the other region. This result can be used to calculate the electronic structure and equilibrium atomic positions around defect structures where many-body effects are important locally. It is not necessary to solve the problem of the remaining part of the crystal in the absence of the local region; it is sufficient to know the solution in the perfect crystal. We compare the embedding potential to Feynman's 'influence functional' approach and use it to derive the well known scaling law for the Anderson model of a magnetic impurity.

1. Introduction

It is often desirable to perform a quantum-mechanical calculation on only one part of a solid. It might consist of a small region around a surface, grain boundary, line or point defect, or even of a single sublattice in the crystal structure. If the whole system may to an adequate approximation be regarded as consisting of non-interacting particles or quasi-particles moving in an external potential, it is known that the degrees of freedom in which one is not explicitly interested (here called 'region 2'), can be replaced by an energy- (or frequency-) dependent effective potential, known as the *embedding potential*, acting in that part of the Hilbert space ('region 1'), where we wish to calculate. This formalism contains exactly the same information as the Dyson equation for scattering of particles from a perturbation localised in region 1 and is equivalent in real space to imposing the requirement that the logarithmic derivative of the wavefunction be continuous across the boundary separating the two regions (Löwdin 1951, Baraff and Schlüter 1986, Inglesfield 1981, 1989, Fisher 1987, 1988).

In this paper we show that this result still holds in any calculation of ground-state or thermodynamic averages if the quasiparticles concerned, whether bosons or fermions, are allowed to interact with each other in region 1. (In the language of second quantization, this means that the Hamiltonian is no longer a quadratic form in the creation and annihilation operators for states in region 1.) We do this by using second quantized versions of the path-integral methods first employed by Feynman (1950, 1955), to

eliminate the photon and phonon fields to which electrons are coupled in quantum electrodynamics and in their motion through a polar crystal, respectively.

It is obvious that a result of this type holds in any equation which expresses one single-particle Green function in terms of other single-particle Green functions or of a proper self-energy. This is because such a self-energy must be confined to region 1 where interactions between the quasiparticles are permitted. Once the self-energy has been calculated we can simply include it in the single-particle 'optical potential' for region 1 and carry out exactly the same matrix manipulations as in the non-interacting case. The result of this paper is more general: in this language it tells us that we can also replace region 2 by the embedding potential when we calculate the self-energy itself.

We first show how the equation of motion for a field operator within region 1 contains, beside the 'embedding potential' term familiar from the independent-particle theory, an extra term that describes the behaviour of region 2 when it is decoupled from region 1. Such a term would be difficult to calculate for many of the systems described above; it would require, for example, finding the eigenvalues for a crystal in which the region around the defect of interest had been removed and replaced by empty space. However, this term has no effect on the equations of motion of Green functions for a system of independent particles; moreover we then show, by representing the matrix elements of the time evolution operator as a Feynman path integral, that this additional term in the equation of motion vanishes if we take a trace over all the fields in region 2. This corresponds to finding the total amplitude that one field configuration in region 1 evolves into another after a certain time while leaving the fields in region 2 in the same (unspecified) state. Next we extend the analysis to an imaginary-time path integral; when the trace is taken over all fields in regions 1 *and* 2 this yields the partition function and hence the complete thermodynamic behaviour of the system including all region 1 Green functions. Finally, we clarify the relationship of the embedding potential to the influence functional of Feynman, stressing the different sorts of averaging over the configurations of region 2 implied by the two methods, and use the embedding potential to give a rather simple picture of the scaling properties with band width of the Anderson model of a magnetic impurity.

2. The equation of motion

Suppose the system is defined by a set of single particle states $|i\rangle$, which we assume are discrete and orthonormal. The corresponding boson (or fermion) creation and annihilation operators obey the (anti-)commutation relations

$$[a_i, a_j^\dagger]_\zeta = a_i a_j^\dagger - \zeta a_j^\dagger a_i = \delta_{ij} \quad \zeta = +1 \text{ (bosons) or } -1 \text{ (fermions)}. \quad (1)$$

Divide the states $|i\rangle$ into two sets, 1 and 2. From this point on we use the subscripts $\{i, j, \dots, n\}$ to refer to states in set 1 and $\{p, q, \dots\}$ to refer to states in set 2. We suppose that the time-independent Hamiltonian H contains the operators of set 2 only in quadratic forms:

$$H = H_{11} + \sum_{ip} (t_{ip} a_i^\dagger a_p + t_{pi} a_p^\dagger a_i) + \sum_{qr} t_{qr} a_q^\dagger a_r \quad (2)$$

where H_{11} is an arbitrary polynomial in the annihilation and creation operators for states of set 1.

Consider the Heisenberg equation of motion for an annihilation operator in set 1 (in units where $\hbar = 1$):

$$i(\partial/\partial t)a_j(t) = [a_j(t), H]_+ = [a_j, H_{11}(t)]_+ + \sum_p t_{jp} a_p(t). \quad (3)$$

Now the set 2 operators obey the coupled set of linear differential equations:

$$i(\partial/\partial t)a_p(t) = \sum_q t_{pq} a_q(t) + \sum_k t_{pk} a_k(t). \quad (4)$$

We rewrite this in terms of the changes in the region 2 operators relative to their values at $t = 0$:

$$\alpha_p(t) = a_p(t) - a_p(0) \quad (5)$$

These new operators satisfy the homogeneous boundary condition

$$\alpha_p(0) = 0 \quad (6)$$

and obey the following equations:

$$i(\partial/\partial t)\alpha_p(t) - \sum_q t_{pq} \alpha_q(t) = \sum_q t_{pq} a_q(0) + \sum_k t_{pk} a_k(t). \quad (7)$$

The solution can be written as an integral over a (*c*-number) retarded matrix Green function which also satisfies a homogeneous boundary condition:

$$G_{pq}(t - t') = 0 \quad \text{for } t < t' \quad (8)$$

in the form:

$$\alpha_p(t) = \sum_q \int_0^\infty dt' G_{pq}(t - t') \left(\sum_r t_{qr} a_r(0) + \sum_k t_{qk} a_k(t') \right). \quad (9)$$

Comparing the solution which would be obtained if the subspaces 1 and 2 were decoupled, (i.e., if $t_{qk} = 0$ for all k in 1, q in 2), we see that

$$a_p(t) = a_p^0(t) + \sum_q \int_0^\infty dt' G_{pq}(t - t') \sum_k t_{qk} a_k(t') \quad (10)$$

where $a_p^0(t)$ is the decoupled solution with the same initial conditions as the actual solution:

$$a_p(0) = a_p^0(0) \quad (11)$$

The equation of motion for our original region 1 operator therefore becomes:

$$i(\partial/\partial t)a_j(t) = [a_j(t), H_{11}(t)]_+ + \sum_{pqk} \int_0^\infty dt' t_{jp} G_{pq}(t - t') t_{qk} a_k(t') + \sum_p t_{jp} a_p^0(t). \quad (12)$$

The second term on the right-hand side is a retarded self-interaction which is second order in the coupling between regions 1 and 2 and which is the equivalent in the time domain of the energy-dependent embedding potential. It corresponds to a change in region 1 acting *through* region 2 and back onto region 1. The third term, however, is first order in the coupling and corresponds to the effect on region 1 of the *decoupled* behaviour of region 2. As explained above it may be difficult to calculate and it spoils what would otherwise be an expression that did not involve region 2 operators at all.

Its absence in the independent-particle derivations given previously is easily explained. Define, following Zubarev (1960), a single-particle Green function

$$\langle\langle a_j(t); a_k^+ \rangle\rangle_{\xi} = i\theta(t)\langle [a_j(t), a_k^+(0)]_{\xi} \rangle. \tag{13}$$

Observe that the third term in the equation of motion (12) for a_j makes no contribution to the equation of motion of the Green function, since the operator $a_p^0(t)$ is merely a linear combination of the $t = 0$ annihilation operators in region 2. It therefore (anti-)commutes with $a_k^+(0)$. However, this is not so in the equations of motion for n -particle Green functions ($n > 1$). Therefore in a many-body problem, when such higher Green functions do not trivially reduce to products of single-particle Green functions, we might expect this undesirable third term to contribute.

3. The path-integral representation of the evolution operator

The motivation for the next step is as follows. We observe that the decoupled behaviour of region 2 responsible for the undesirable term in equation (12) is governed entirely by the initial conditions we choose to impose upon it at $t = 0$. In any particular representation, this will depend on the relative phase of the initial wavefunction in regions 1 and 2. This is information in which we are not interested, because we normally consider a defect in thermal equilibrium and try to calculate ensemble averages; we therefore seek a way of taking an appropriate average over the initial conditions of region 2. The path integral formalism provides a convenient framework.

We choose to work in the basis of coherent states which diagonalizes the annihilation operators. For boson annihilation operators the eigenvalues are complex numbers but for fermions they are anti-commuting Grassmann variables. (For further details of Grassmann variables and of the coherent state path integrals used in this section and the next see Negele and Orland 1988, whose notation we follow here.) The amplitude A_{fi} for the evolution of a field configuration $|\varphi_i\rangle$ (where these eigenvalues are φ_{ai}) at time t_i into $|\varphi_f\rangle$ (where these eigenvalues are φ_{af}) at time t_f is given by the Feynman path integral:

$$\begin{aligned} A_{fi} &= \langle \varphi_f | \exp[-i(t_f - t_i)H] | \varphi_i \rangle \\ &= \lim_{M \rightarrow \infty} \int \prod_a \prod_{k=1}^{M-1} (1/N) d\varphi_a^*(t_k) d\varphi_a(t_k) \exp \left[- \sum_{k=1}^{M-1} \sum_a \varphi_a^*(t_k) \varphi_a(t_k) \right. \\ &\quad \left. + \sum_{k=1}^M \left(\sum_a \varphi_a^*(t_k) \varphi_a(t_{k-1}) \right) - i\varepsilon H(\varphi_a^*(t_k), \varphi_a(t_{k-1})) \right] \\ &= \int D(\varphi_a^*, \varphi_a) \exp \left[- \sum_a \varphi_a^*(t_f) \varphi_a(t_f) \right. \\ &\quad \left. + i \int_{t_i}^{t_f} dt \left(\sum_a \varphi_a^*(t) i(\partial/\partial t) \varphi_a(t) \right) - H(\varphi_a^*(t), \varphi_a(t)) \right] \end{aligned} \tag{14}$$

where the functional integral is over all field configurations subject to the initial and final conditions $\varphi_a(t_i) = \varphi_{ai}$, $\varphi_a^*(t_f) = \varphi_{af}^*$, $\varepsilon = (t_f - t_i)/M$, and $N = 2\pi i$ (bosons) or $N = 1$ (fermions). Here and subsequently, a sum or product over the subscript a implies inclusion of all fields in both regions 1 and 2.

We wish to carry out the functional integrations over the fields φ_a corresponding to boson (fermion) operators in region 2 to obtain an effective functional of the fields in region 1 that can be integrated to obtain the matrix elements of the evolution operator between two states specified by their configurations in region 1. It is clear that with the present form of (14), such an effective functional will depend on the initial and final configurations $\varphi_p(t_i)$ and $\varphi_p(t_f)$ of the fields in region 2. The form of this dependence can be seen from studying the integral (14) in the stationary phase approximation; the dominant contributions then come from the paths $\varphi_p^s(t)$ for which the exponent is stationary with respect to variations in the fields and which therefore obey the equations of motion:

$$\delta S / \delta \varphi_p^s(t) = 0 \quad \delta S / \delta \varphi_p^{s*}(t) = 0 \tag{15}$$

where S is the exponent in (14). However these equations are algebraically identical to the Heisenberg equations of motion for the creation and annihilation operators, respectively. For the region 2 operators that enter the exponent only quadratically, *all* the dependence on the end-points is contained in the contribution from the stationary paths (Feynman and Hibbs 1965), and is therefore just as given by the undesirable term in the Heisenberg equation of motion (9).

We now take the trace of expression (14) over the fields in set 2. That is to say we ask for the total amplitude for evolution of some given field configuration within region 1 into another between times t_i and t_f while leaving the fields in region 2 in their unspecified initial state (bosons) or with their phase altered by π (fermions). It is clear that in this way the dependence on the initial conditions in region 2 will be eliminated. It is convenient to define a Green function for region 2 which satisfies the equation:

$$\sum_q (\delta_{pq} i\partial/\partial t - t_{pq}) G_{qr}(t - t') = \delta_{pr} \delta(t - t') \tag{16}$$

subject to the (anti-)periodic boundary conditions

$$G_{qr}(t + t_f - t_i) = \zeta G_{qr}(t). \tag{17}$$

Then we can write the contribution to the exponent in (14) which involves the region 2 fields as:

$$\begin{aligned} & i \int_{t_i}^{t_f} dt \left(\sum_p \varphi_p^*(t) i(\partial/\partial t) \varphi_p(t) - \sum_{ip} (t_{ip} \varphi_i^*(t) \varphi_p(t) + t_{pi} \varphi_p^*(t) \varphi_i(t)) \right. \\ & \quad \left. - \sum_{pq} t_{pq} \varphi_p^*(t) \varphi_q(t) \right) \\ & = i \int_{t_i}^{t_f} dt \sum_{pq} \left[\left(\varphi_p^*(t) - \sum_{ir} \int_{t_i}^{t_f} dt' G_{pr}^*(t - t') t_{ri}^* \varphi_i^*(t') \right) \right. \\ & \quad \left. \times (\delta_{pq} i\partial/\partial t - t_{pq}) \left(\varphi_q(t) - \sum_{js} \int_{t_i}^{t_f} dt'' G_{qs}(t - t'') t_{sj} \varphi_j(t'') \right) \right] \\ & \quad - \sum_{ij} \sum_{pq} \int_{t_i}^{t_f} dt' \varphi_i^*(t') t_{ip} G_{pq}(t - t') t_{qj} \varphi_j(t'). \end{aligned} \tag{18}$$

The last term is the familiar embedding potential. In deriving (18) we have used (16) and the hermiticity of H to show that

$$\sum_q (\delta_{pq} i\partial/\partial t - t_{pq}) \sum_{js} \int_{t_i}^{t_f} dt'' G_{qs}(t-t'') t_{sj} \varphi_j(t'') = \sum_j t_{pj} \varphi_j(t) \quad (19)$$

and integration by parts combined with the (anti-) periodic boundary conditions on the region 2 operators and the Green function to show that

$$\begin{aligned} & \int_{t_i}^{t_f} dt \sum_{pq} \sum_{ir} \int_{t_i}^{t_f} dt' G_{pr}^* t_{ri}^* \varphi_i^*(t') (\delta_{pq} i\partial/\partial t - t_{pq}) \varphi_q(t) \\ &= \int_{t_i}^{t_f} dt \sum_{qi} t_{iq} \varphi_i^*(t) \varphi_q(t). \end{aligned} \quad (20)$$

If we now make the change of variables in region 2

$$\varphi_q(t) \rightarrow \varphi_q(t) - \sum_{js} \int_{t_i}^{t_f} dt'' G_{qs}(t-t'') t_{sj} \varphi_j(t'') \quad (21)$$

then we can carry out the integration over the region 2 fields. It is a Gaussian integral whose value depends on whether the fields are bosonic or fermionic. The answer is irrelevant since it combines with the Jacobian of the transformation (21) to give an overall multiplicative factor in the evolution operator which is independent of the region 1 Hamiltonian H_{11} . It therefore cancels when comparing the amplitudes for different processes within region 1.

Therefore in order to find, within a multiplicative constant, a matrix element of the time development operator between two region 1 field configurations, it suffices to carry out a functional integration over the region 1 fields only with an effective Hamiltonian

$$H_{\text{eff}} = H_{11}(\varphi_i(t), \varphi_i(t)) + \sum_{ij} \sum_{pq} \int_{t_i}^{t_f} dt' \varphi_i^*(t) t_{ip} G_{pq}(t-t') t_{qj} \varphi_j(t'). \quad (22)$$

This corresponds to adding to the region 1 Hamiltonian a single-particle time-dependent embedding potential whose matrix elements are

$$M_{ij}(t-t') = \sum_{pq} t_{ip} G_{pq}(t-t') t_{qj}. \quad (23)$$

Note that because we imposed boundary conditions at two different times the effective potential or self-interaction we have derived for region 1 is neither wholly retarded nor wholly advanced.

4. The partition function

The partition function can be written as a path integral in imaginary time. It is then straightforward to apply the same techniques as above to show that the free energy of the system is given to within an additive constant by taking the path integral over just the region 1 degrees of freedom with an extra term similar to that in (22) added to the Hamiltonian.

Specifically, the partition function in the grand canonical ensemble is given by

$$\begin{aligned}
 Z &= \text{tr} \exp[-\beta(H - \mu N)] \\
 &= \int (1/N) \prod_a d\varphi_a^* d\varphi_a \exp\left(-\sum_a \varphi_a^* \varphi_a\right) \langle \xi\varphi | \exp[-\beta(H - \mu N)] | \varphi \rangle \\
 &= \int D(\varphi_a^*(\tau), \varphi_a(\tau)) \exp\left[-\int_0^\beta d\tau \left(\sum_a \varphi_a^*(\tau)(\partial/\partial\tau - \mu)\varphi_a(\tau) \right. \right. \\
 &\quad \left. \left. + H(\varphi_a^*(\tau), \varphi_a(\tau))\right)\right]. \tag{24}
 \end{aligned}$$

This time the functional integration is over all field configurations in regions 1 and 2 which satisfy the boundary conditions $\varphi_a(\beta) = \zeta\varphi_a(0)$. N is the number operator, μ the chemical potential, $\beta = 1/(kT)$ and other symbols continue to carry the same meaning. We proceed as before, defining a region 2 Green function which is (anti-)periodic on the interval $[0, \beta]$:

$$\sum_q [\delta_{pq}(\partial/\partial\tau - \mu) - t_{pq}]G_{qr}(\tau - \tau') = \delta_{qr}\delta(\tau - \tau') \tag{25}$$

$$G_{qr}(\tau + \beta) = \zeta G_{qr}(\tau) \tag{26}$$

and completing the square in the region 2 fields. On integrating out these fields the partition function becomes, to within a multiplicative constant which is independent of the Hamiltonian and the fields in region 1:

$$\begin{aligned}
 Z &= \int D(\varphi_i^*(\tau), \varphi_i(\tau)) \exp\left[-\int_0^\beta d\tau \left(\sum_i \varphi_i^*(\tau)(\partial/\partial\tau - \mu)\varphi_i(\tau) \right. \right. \\
 &\quad \left. \left. + H_{11}(\varphi_i^*(\tau), \varphi_i(\tau)) + \sum_{ij} \sum_{pq} \int_0^\beta d\tau' \varphi_i^*(\tau)t_{ip}G_{pq}(\tau - \tau')t_{qj}\varphi_j(\tau')\right)\right]. \tag{27}
 \end{aligned}$$

The multiplicative constant in the partition function will correspond to an additive constant in the total free energy. We can simplify the structure of the last term and increase its resemblance to the energy-dependent form of the embedding potential derived previously (Fisher 1988 and references therein), by transforming from the integration over (anti-)periodic paths in imaginary time to integration over the Fourier transforms of the paths, defined so that:

$$\varphi_a(\tau) = \sum_n \varphi_a(i\omega_n) \exp(-i\omega_n\tau) \tag{28}$$

$$G_{pq}(\tau - \tau') = \sum_n G_{pq}(i\omega_n) \exp[-i\omega_n(\tau - \tau')] \tag{29}$$

with $\omega_n = 2n\pi/\beta$ (bosons) or $\omega_n = (2n + 1)\pi/\beta$ (fermions). Then (27) becomes:

$$\begin{aligned}
 Z &= \int D(\varphi_i^*(i\omega)\varphi_i(i\omega)) \exp\left[-\beta \sum_n \left(\sum_i \varphi_i^*(i\omega_n)(-i\omega_n - \mu)\varphi_i(i\omega_n) \right. \right. \\
 &\quad \left. \left. + \sum_{ij} \sum_{pq} \varphi_i^*(i\omega_n)t_{ip}G_{pq}(i\omega_n)t_{qj}\varphi_j(i\omega_n)\right) - I(\varphi_i^*(i\omega), \varphi_i(i\omega))\right] \tag{30}
 \end{aligned}$$

where the functional I of the Fourier-transformed fields is defined to be equal to the

imaginary time integral of H_{11} along the path. Since H_{11} is supposed to contain terms higher than quadratic in the fields, the structure of I will be more complicated than a single summation over frequencies ω_n .

The convolution in (24) and (27) has now been replaced by an energy-dependent potential just as in the independent-particle case. Note that we can add arbitrary source terms for fields within region 1 to H_{11} without affecting the result:

$$H_{11} \rightarrow H_{11} + \sum_i \int_0^\beta d\tau (J_i^*(\tau)\varphi_i(\tau) + J_i(\tau)\varphi_i^*(\tau)) \quad (31)$$

where J is a complex (Grassmann) source for bosons (fermions). This gives us a generating functional that can be differentiated with respect to the sources J to yield the expectation values of τ -ordered products of the region 1 fields. Therefore Green functions of all orders within region 1 are correctly generated by this embedding procedure. Double-time Green functions may be obtained by analytic continuation to real time in the usual way. Similarly the expectation value of any operator which acts entirely within region 1 may be calculated.

Finally, note that since the embedding corrections in (22), (27) and (30) are independent of H_{11} they can be found by solving the complete problem for *any* region 1 that is convenient. This will generally mean adopting in region 1 the same independent quasiparticle approximation that is to be used in region 2 and diagonalizing the Hamiltonian of highest symmetry that can be formed by varying H_{11} , i.e., performing a band-structure calculation for the perfect solid. Therefore the problem of region 2 in the absence of region 1 (the 'crystal with a hole in it'), need never be solved to obtain the embedding corrections. This is most important for the practical implementation of the embedding scheme; for further details of this point and of the methods that can be used in the independent quasiparticle approximation see Fisher (1988).

5. The embedding potential and the influence functional

Feynman and co-workers (Feynman and Vernon 1963, Feynman and Hibbs 1965), have developed a general formalism within the path-integral framework for problems where one is interested in the behaviour of a quantum system (analogous to our region 1), coupled to a second quantum system (analogous to our region 2). Suppose the system of interest (system 1), is described by coordinate or coordinates Q and the remaining part (system 2), by coordinate or coordinates X . We decompose the action as a functional of the path in the form

$$S(Q, X) = S_1(Q) + S_2(X) + S_{12}(Q, X). \quad (32)$$

Then the *probability* that system 1 is in state ψ_f and system 2 in state χ_f at final time t_f given that they were in states ψ_i and χ_i , respectively, at initial time t_i is given by the path-integral expression:

$$P_{fi} = \int \psi_f^*(Q_f)\psi_i(Q_i)\chi_f^*(X_f)\chi_i(X_i) \exp[i(S(Q, X) - S(Q', X'))] \\ \times \psi_i^*(Q_i)\psi_i(Q_i)\chi_i^*(X_i)\chi_i(X_i) dX_i dX_i' dQ_i dQ_i' dX_f dX_f' \\ \times dQ_f dQ_f' DX(t) DX'(t) DQ'(t) DQ(t)$$

$$\begin{aligned}
 &= \int \psi_i^*(Q_i) \psi_f(Q_f) \exp[i(S_1(Q) - S_1(Q'))] F_{fi}(Q, Q') \psi_i^*(Q_i') \psi_i(Q_i) \\
 &\quad \times dQ_i dQ_i' dQ_f dQ_f' DQ'(t) DQ(t)
 \end{aligned} \tag{33}$$

where the path-integral runs over all paths starting at $\{Q_i, Q_i', X_i, X_i'\}$ and finishing at $\{Q_f, Q_f', X_f, X_f'\}$, and

$$\begin{aligned}
 F_{fi}(Q, Q') &= \int \chi_f^*(X_f) \chi_f(X_f) \exp[i(S_2(X) + S_{12}(Q, X) - S_2(X') - S_{12}(Q', X'))] \\
 &\quad \times \chi_i^*(X_i) \chi_i(X_i) DX(t) DX'(t) dX_i dX_i' dX_f dX_f' \\
 &= \exp(i\Phi_{fi}(Q, Q'))
 \end{aligned} \tag{34}$$

F_{fi} is the *influence functional*, containing all the information about the influence of system 2 on system 1. It depends on S_2 and S_{12} , i.e., both on the properties of the isolated system 2 and on the coupling between the two systems, but not on the properties of system 1. The above expression also defines Φ_{fi} , the *influence phase*. If the final state of system 2 is of no interest, the total probability of a transition from ψ_i to ψ_f may be obtained by summing over final states χ_f and taking some appropriate average over initial states χ_i . For example, Feynman and Vernon (1963) consider some problems at zero temperature and take as the initial state χ_i the ground state of the isolated system 2. If the Lagrangians for system 2 and for the coupling between the systems are quadratic in the coordinates and their time derivatives then the integrals in (34) are Gaussian integrals and can be performed to yield an influence phase Φ which is itself quadratic in the coordinates Q, Q' .

We make contact with the embedding potential description as follows. Suppose that instead of the probability P_{fi} for the above transition we calculate the quantum-mechanical *amplitude*:

$$\begin{aligned}
 A_{fi} &= \int \psi_i^*(Q_i) \chi_f^*(X_f) \exp(iS(Q, X)) \psi_i(Q_i) \chi_i(X_i) DQ(t) DX(t) dQ_i dX_i dQ_f dX_f \\
 &= \int \psi_i^*(Q_i) \exp[i(S_1(Q) + R_{fi}(Q))] \psi_i(Q_i) DQ(t) dQ_i dQ_f
 \end{aligned} \tag{35}$$

where

$$\exp(iR_{fi}(Q)) = \int \chi_f^*(X_f) \exp[i(S_2(X) + S_{12}(Q, X))] \chi_i(X_i) DX(t) dX_i dX_f.$$

The influence phase defined in (33) is related to this quantity R by

$$\Phi_{fi}(Q, Q') = R_{fi}(Q) - R_{fi}^*(Q'). \tag{36}$$

Now we shall relate R to the embedding potential: we impose the condition that the initial and final states of system 2 be the same, sum over initial states and use a closure relation to obtain

$$\exp[iR(Q)] = \int \exp[(i(S_2(X) + S_{12}(Q, X)))] DX(t) \tag{37}$$

where the integral now runs over the set of all paths which return at time t_f to their starting points.

This is the first-quantised equivalent of (18); when substituted into (35), it tells us the total *amplitude* for the transition between ψ_i and ψ_f while leaving system 2 in the

same unspecified state. Furthermore, if system 2 is harmonic so that (37) is a Gaussian integral, $R(Q)$ becomes a bilinear functional form in the coordinates Q :

$$R(Q) = \int_{t_i}^{t_f} dt dt' \Sigma(t-t') Q(t) Q(t'). \quad (38)$$

This is in the same form as the last term in (18) and the quantity Σ is just the first-quantised version of the time-dependent embedding potential.

Of course a second-quantised influence functional could be defined equally well for the many-body problems treated in previous sections by replacing the word *coordinate* by *field configuration* and by using Grassmann variables for fermion fields. As usual, the simplifications of a harmonic system then correspond to those for non-interacting bosons or fermions.

Relating the influence functional to the embedding potential in this way establishes the connection between influence functional theory and scattering theory. Apart from this, the influence functional and the embedding potential approaches each have their own advantages. In favour of the embedding potential method is the fact that once we have used the path-integral approach to prove, in some sense, the *equivalence* of a system 1 plus a harmonic system 2 to the same system 1 plus a time-dependent embedding potential, we can apply this equivalence in any way we choose and our calculation need not involve path integrals at all. This is illustrated by the use of elementary matrix methods for independent electron problems (Fisher 1988). The original influence functional, however, is by contrast of use *only* within a path-integral framework. On the other hand, whereas the embedding potential method, motivated by the appearance of a trace in the expression for the partition function, simply takes a trace over system 2, there is much more flexibility available in the averaging process if an influence functional is used. In particular, the system considered need not be in thermal equilibrium and quantities at finite temperature can be obtained directly in real time without the need for analytic continuation. These differences can all be traced to the fact that the embedding potential approach concentrates on the amplitude for a quantum-mechanical process and the influence functional approach on the probability.

6. The scaling behaviour of the asymmetric Anderson model

The simplest model Hamiltonian describing a fermion problem which contains many-body terms is the Anderson model of an impurity atom, with an on-site Coulomb repulsion U , hybridising with a band of non-interacting electrons:

$$H = \sum_{\sigma} [\varepsilon_d d_{\sigma}^{\dagger} d_{\sigma} + (U/2) d_{\sigma}^{\dagger} d_{\sigma} d_{-\sigma}^{\dagger} d_{-\sigma}] + \sum_{k\sigma} V_k (d_{\sigma}^{\dagger} c_{k\sigma} + c_{k\sigma}^{\dagger} d_{\sigma}) + \sum_{k\sigma} c_{k\sigma}^{\dagger} c_{k\sigma}. \quad (39)$$

This model has been intensively studied. An exact solution of great complexity is now known, based on the Bethe ansatz (Bethe 1931, Weigmann and Tsel'ick 1983), but understanding of the model's behaviour is based on its scaling properties under changes in the band width (Haldane 1978, Krishna-murthy *et al* 1975, 1980a,b). Here we attempt the modest target of deriving these scaling properties in the 'asymmetric' case $U \gg \varepsilon_d$ as an example of the use of the embedding potential in a true many-body problem. The resulting physical picture of the scaling in terms of the suppression of fluctuations in the

occupancy of one impurity spin state due to the occupation of the other is closely related to the more usual description as given by Haldane (1978); in fact it bears almost the same relation to it as did the original scaling theory of the related Kondo problem (Anderson *et al* 1970) to the later ‘poor man’s’ version (Anderson 1970).

We take region 1 to be the impurity atom and region 2 to be the host band. The embedding potential is given by equation (19) of Fisher (1988):

$$\Sigma(E, W) = \int_{-W}^W \frac{\rho(\epsilon_k) |V_k|^2 d\epsilon_k}{E - \epsilon_k} \tag{40}$$

and its derivative with respect to the half-band width W , assuming a symmetric band, by

$$\frac{\partial \Sigma(E, W)}{\partial W} = \rho(W) |V_W|^2 \left(\frac{1}{E - W} + \frac{1}{E + W} \right). \tag{41}$$

Here ρ is the density of states and we allow the energy E to be complex. It is usual to take $\rho(\epsilon_k) |V_k|^2$ as approximately constant over the band:

$$\rho(\epsilon_k) |V_k|^2 \approx \Delta/\pi \quad \text{for } -W < \epsilon_k < W \tag{42}$$

where Δ is the Lorentzian broadening of a single-particle state hybridizing with the band. On the imaginary energy axis, regardless of the detailed form of the band structure, $\partial \Sigma/\partial W$ is peaked near $E = \pm iW$ and is of order $\Delta/(\pi W)$ at these points.

Consider the partition function as a path integral of the type (27) or (30) over histories of the occupancies of the impurity spin states in imaginary time. Each history consists of a succession of fluctuations in the occupancy of the two spin states of the impurity and while both states are occupied the large on-site Coulomb energy penalty U is incurred. If U is very large and one spin state is occupied, the other state cannot be occupied for ‘times’ longer than about $1/U$ without incurring a prohibitive energy penalty. Hence fluctuations in the occupancy of the other state with (imaginary) frequencies less than U are damped out, and if $U \gg W$ then an increment $(\partial \Sigma/\partial W) dW$ in the embedding potential due to a change dW in the band width can have no effect, since it is peaked at (imaginary) frequency W . If, however, the first spin state is unoccupied then there is no such damping of low (imaginary) frequency occupancy fluctuations and the embedding potential increment makes a contribution of order $\Delta dW/(\pi W)$ to the effective energy of the state.

Since the presence or absence of this term in the energy depends only on whether the first spin state is occupied or not, the effect of the extra term in the embedding potential is the same as a change in the effective one-electron energy of the impurity state:

$$d\epsilon_d^{\text{eff}} = \frac{-\Delta dW}{\pi W} \tag{43}$$

in agreement with the result of Haldane (1978). (The minus sign appears because the embedding potential contributes to the energy when the other spin state is *unoccupied*.) Clearly this scaling behaviour breaks down when either $W \geq U$ (in which case fluctuations at imaginary frequencies near the peaks of the embedding potential increment are no longer suppressed), or when $\beta \leq 1/W$ (in which case the path integral is taken over such a small ‘time’ interval that fluctuations of characteristic frequency as low as W cannot occur, regardless of the occupancy of the other state). Scaling also breaks down when ϵ_d^{eff} is driven outside the band interval $[-W, W]$ or when W becomes of the same

order as Δ (whichever occurs first as W is decreased), since then *all* occupancy fluctuations are damped out, in the first case by the energy cost to remove a particle or hole from the band and in the second by the large size of the embedding potential.

We see that the simple physical picture of suppression of double occupancy fluctuations below a certain frequency, coupled with elementary considerations concerning the form of the embedding potential, have enabled us to derive the scaling behaviour of the many-body problem.

7. Conclusion

We have shown that the problem of one part of a quantum-mechanical system where boson or fermion quasiparticles are allowed to interact (region 1) which is embedded in a second part where they do not interact (region 2) is equivalent to the problem of the isolated region 1 with an extra term added to the Hamiltonian. In the case considered here, where the coupling between regions 1 and 2 simply takes the form of particle hopping between them, the extra term is a contribution to the one-body part of the Hamiltonian. For a system such as a fermion sea (region 1) coupled to bosons (region 2), where the fermions can emit or absorb bosons and therefore the coupling between the two regions contains both region 1 annihilation and creation operators, we would obtain instead the familiar boson-mediated interaction between the fermions.

The result holds only if a trace is taken over the possible configurations of the fields in region 2 that might accompany a given evolution of the fields in region 1. In particular, it holds if a trace is taken over *all* the fields to find the partition function and hence the free energy of the system. The additional term in the Hamiltonian is both advanced and retarded in real or imaginary time, or alternatively is frequency (energy) dependent.

We stress that the method involves no prescription as to how the many-body problem within region 1 is to be tackled. Indeed, since the transformation between the complete system and region 1 alone plus the embedding potential is exact, its strength lies in the fact that it can be combined with *any* treatment of the many-body terms.

As we suggested in the Introduction, this result has wide applications in the theory of solids. For example a calculation can be performed on a cluster of atoms around some defect where many-electron interactions are important locally and the bulk solid can be represented (assuming the independent-electron approximation is sufficient in the bulk), by the embedding potential. Since the free energy is given correctly to within an additive constant, this method will yield the correct interatomic forces and the correct atomic equilibrium positions provided that atomic displacements generate a negligible change in the Hamiltonian outside region 1. An example of a defect system in which such an approach might be especially useful is provided by the diamond vacancy.

Applications are not confined to cases where region 1 is spatially localized. For example, consider the periodic Anderson model (PAM), where an array of rare earth ions like the impurity studied in § 6 and with very large on-site electron–electron repulsion U hybridises with a wide conduction band treated in the independent-electron approximation. By taking the rare earth ions as region 1 and the conduction band as region 2 we can reduce the problem within the rare earth lattice to a Hubbard model with complex and energy- (frequency-) dependent hopping parameters. It has recently been discovered (Harrington *et al* 1988), that the solution of the PAM reduces to that of the Hubbard model if the direct f–f hopping is sufficiently large. This may be interpreted from the present point of view to mean that in this limit the energy dependence of the conduction

band mediated hopping is swamped by the direct hopping and simple Hubbard model behaviour is recovered.

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