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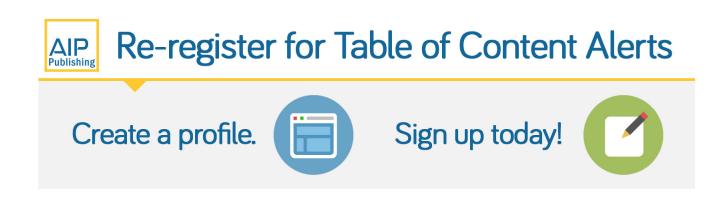
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Multiscale theory of collective and quasiparticle modes in quantum nanosystems

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A quantum nanosystem (such as a quantum dot, nanowire, superconducting nanoparticle, or superfluid nanodroplet) involves widely separated characteristic lengths. These lengths range from the average nearest-neighbor distance between the constituent fermions or bosons, or the lattice spacing for a conducting metal, to the overall size of the quantum nanosystem (QN). This suggests the wave function has related distinct dependencies on the positions of the constituent fermions and bosons. We show how the separation of scales can be used to generate a multiscale perturbation scheme for solving the wave equation. Results for electrons or other fermions show that, to lowest order, the wave function factorizes into an antisymmetric (fermion) part and a symmetric (bosonlike) part. The former manifests the short-range/exclusion-principle behavior, while the latter corresponds to collective behaviors, such as plasmons, which have a boson character. When the constituents are bosons, multiscale analysis shows that, to lowest order, the wave function can also factorize into short- and long-scale parts. However, to ensure that the product wave function has overall symmetric particle label exchange behavior, there could, in principle, be states of the boson nanosystem where both the short- and long-scale factors are either boson- or fermionlike; the latter "dual fermion" states are, due to their exclusion-principle-like character, of high energy (i.e., single particle states cannot be multiply occupied). The multiscale perturbation analysis is used to argue for the existence of a coarse-grained wave equation for bosonlike collective behaviors. Quasiparticles, with effective mass and interactions, emerge naturally as consequences of the long-scale dynamics of the constituent particles. The multiscale framework holds promise for facilitating QN computer simulations and novel approximation schemes. © *2008 American Institute of Physics.*
[DOI: 10.1063/1.2877226]

I. INTRODUCTION

In a quantum nanoparticle or nanodroplet (QN), there are at least two characteristic lengths: (1) the size of the QN and (2) the average distance between the nearest-neighbor constituent fermions or bosons. For a conductor or semiconductor, the latter is the spacing of the ion core lattice. For a superfluid or Fermi liquid droplet, the short scale is determined by the density of the constituent bosons or fermions. The approach presented here is based on the hypothesis the wave function for a QN reflects the multiple length scale character of the system, and this notion can be used to develop a scheme for constructing the wave function. In this and the next two sections we focus on fermions, while comments on bosons and conclusions are set forth in Sec. IV.

Multiscale techniques have been used to analyze a variety of natural and engineered systems. When there is a wide separation of scales, the ratio of the small to the large characteristic length, time, mass, or other quantity has been used to develop approximation schemes.[1–10] The multiscale perturbation approach of this type, which is closest to the one used here for the QN problem, was developed for the classical Liouville equation.[5,11–24]

Real-space decomposition techniques, the hybrid quantum-mechanics/molecular-mechanics (QM/MM) and hybrid quantum-mechanics/quantum-mechanics (QM/QM) approaches are used in electronic structure theory,[25–34] where a core region is designated to be treated with higher level of accuracy, along with the utilization of approximations of decreasing accuracy to solve the wave equation in regions of increasing distance from a local core site of interest. When there is no wide separation of scales, Laplace transformation techniques have been utilized to divide the interaction potential into a set of wave vector intervals to yield a discrete approximation.[25,27] In contrast, here we propose a scheme that utilizes a rigorous multiscale analysis with key advantages in applications to QNs.

Recent multiscale formulations of the Liouville equation for classical *N* particle systems introduce order parameters corresponding to collective, slow behaviors.[23,24,35] It was shown how such order parameters can be introduced without the need for tedious book keeping to conserve the number of degrees of freedom. In particular, it was shown that this can be accomplished when there is a clearer separation of scales. In the present application to QNs, convenient order parameters are found to be vectors that track the long-scale migration of the constituent particles as they traverse the QN. This

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approach also treats all constituent particles, both within and outside the nanoparticle, in a symmetric manner, and enables the N-body potential to be simultaneously expressed in terms of particlelike variables and the order parameters. This approach captures the coarse-grained configuration of the constituent particles and the associated disturbances of density-like variables. More precisely, we derive a coarse-grained wave equation for the collective and "dressed" particlelike excitations.

A key to the present approach is the existence of a small parameter ε, the length scale ratio, and the ansatz that the wave function depends on both the positions of the constituent particles and the scaled positions, and that these two dependencies can be determined when ε is small. By construction, the scaled constituent particle positions change by one unit as it traverses the QN, while the short-scale position variable changes by many units, i.e., by ε^{-1}, as the constituent particle traverses the QN. With this, we solve the wave equation via perturbation expansion in ε. To the lowest order in ε, we find solutions to the wave equation that factorizes into two parts. The first captures short-scale motion and associated close encounters between constituent particles. For fermions, close encounters are strongly constrained by the exclusion principle; thus, the short-scale factor in the lowest order wave function is antisymmetric with respect to a permutation of particle labels. The second factor captures the overall profile (or envelope) of the wave function. Such long-scale behavior does not have a dominant exclusion principle flavor and, consequently, it is symmetric, as required to keep the overall fermion wave function antisymmetric. For electrons, the long-scale factor is expected to capture plasmons, while for other Fermi systems it is related to density or spin waves. Selected comments are made on boson nanodroplets and future applications.

II. MULTISCALE PERTURBATION APPROACH

The proposed multiscale analysis of quantum nanosystems proceeds in several steps. (1) The N-particle potential energy is rewritten to make the multiscale character of the QN explicit. (2) A set of descriptive variables (order parameters) is introduced that evolve much more slowly than the short-scale, particle-particle collisional dynamics. The lattice spacing for the ion cores in a conducting solid and the average nearest-neighbor distance for a liquid are much smaller than the size of the QN (essentially by definition of a QN). This suggests that the wave function has multiscale structure. (3) Identify a perturbation parameter ε, notably the ratio of the short to long characteristic lengths, and construct solutions to the wave equation as an expansion in ε.

The N-particle potential V and wave function Ψ are written in the multiscale form; for example,

$$V = V(\vec{r}_1, \ldots, \vec{r}_N; \varepsilon\vec{r}_1, \ldots, \varepsilon\vec{r}_N) \equiv V(r,R), \tag{2.1}$$

where $\vec{r}_i$ is the position of the ith of N particles and $\vec{R}_i = \varepsilon\vec{r}_i$. The dependence on $r(\equiv\{\vec{r}_1, \ldots, \vec{r}_N\})$ reflects the average interparticle spacing within the QN. The dependence on $R(\equiv\{\varepsilon\vec{r}_1, \ldots, \varepsilon\vec{r}_N\})$ reflects variations in the potential energy due to the long-range interactions experienced across the

QN, i.e., and not limited to nearest numbers. For a metal, the R dependence also represents the effect of the ion cores that confine the electrons to the QN. Since ε is the ratio of the average interparticle distance to overall QN size, the potential as in Eq. (2.1) is expressed in terms of its ε^0 and ε^{-1} length scale dependencies on particle positions. This suggests that the wave function should also express this dual dependence

$$\Psi(r,R,\varepsilon). \tag{2.2}$$

In this multiscale formulation, the $\vec{R}_i$ dependence reflects the long-range character of Ψ due to particle motion across the QN. However, R should not be regarded as a distinct dynamical variable. Rather the presence of R reflects a distinct way in which Ψ depends on r, i.e., both directly and via R. We show below that one can construct both the r and the R dependencies of Ψ in a self-consistent manner if ε is small, e.g., the average interparticle spacing is much less than QN size. In fact, for a QN constituted of N particles, ε is $O(N^{-1/3})$ so we expect the multiscale approach should be of interest for QNs consisting of 1000 particles or more. Due to the dependence of Ψ on R, the multiscale theory discussed here is reminiscent of the Born–Oppenheimer separation. It is, however, important to note that R, here, is not a distinct dynamical variable. In this sense, the approach also differs from standard coordinate transformations[36] well known in scattering theory.

The wave equation for N identical particles reads, neglecting spin effects,

$$(K + V)\Psi = E\Psi \tag{2.3}$$

for kinetic and potential energies K and V, and energy eigenvalue E. It is convenient to introduce the gradient ∇_0 and associated Laplacian ∇_0^2 in $3N$ dimensional r space and, similarly, ∇_1 and ∇_1^2 for R space. The chain rule and the multiscale form for Ψ in Eq. (2.2) imply

$$\left[H_0 - \varepsilon\nabla_0 \cdot \nabla_1 - \frac{\varepsilon^2}{2}\nabla_1^2 + \varepsilon^2 V_2 \right]\Psi = E\Psi, \tag{2.4}$$

$$H_0 = -\tfrac{1}{2}\nabla_0^2 + V_0. \tag{2.5}$$

A key first step in the multiscale analysis is to separate the long- and short-scale dependencies in the N-particle potential. We have expressed the potential as $V = V_0(r) + \varepsilon^2 V_2(r,R)$. We neglect any first order contributions to V in ε. In the limit of small ε, an adiabatic separation between the short and long range is valid in which case infinitesimal changes in the scaling parameter ε do not change the full potential V. Hence, we assume that V is stationary with respect to small changes in ε and a first order term need not be included. We have separated V into contributions to various orders in ε: the lowest order problem is taken to reflect the short-range interactions while the perturbative term has mixed character. We adopt this separation scheme because it yields a transparent picture as the multiscale analysis unfolds. Specific formulation of the separation of the N-particle potential into short- and long-range parts can be accomplished in a number of ways, including a scheme, as sug-

gested elsewhere, involving the separation of the Laplace transformation of the two body potential into short- and long-scale contributions. The Laplace transformation scheme[25,27] could be used in this way. ∇_0 is a gradient with respect to r at constant R when operating on Ψ in the multiscale form [Eq. (2.2)], and conversely for ∇_1.

Writing Ψ as an expansion in ε and examining the wave equation to each order in ε, we construct the solution. The lowest order problem reads

$$H_0\Psi_0 = E_0\Psi_0. \tag{2.6}$$

There are solutions to the lowest order equation of the form

$$\Psi_0 = \hat{\Psi}(r)\Phi(R). \tag{2.7}$$

Note that E_0 has no R dependence since V_0 is independent of R. Thus, $\hat{\Psi}$ only describes the short-range character of the wave function; Φ expresses its long-scale character. However, Φ does not reflect the short-scale detail that could enable it to support the many quasi-single-particle states needed to fill all levels up to the Fermi energy. This suggests that for fermions $\hat{\Psi}$ is antisymmetric and, hence, Φ must be symmetric, i.e., Φ is bosonlike. It is concluded that fermion systems support bosonlike, collective modes as described by Φ.

The above analysis and scaling of V are consistent with the notion that the ∇_1 terms ensure that Ψ has no short-scale behavior in R. Since these gradient terms enter at higher order in ε, then, so should the R dependence of the potential. Thus, we assumed that V_0 is independent of R to arrive at a self-consistent picture.

To $O(\varepsilon)$, the wave equation implies

$$H_1\Psi_0 + H_0\Psi_1 = E_1\Psi_0 + E_0\Psi_1, \quad H_1 = -\nabla_0 \cdot \nabla_1. \tag{2.8}$$

To simplify the equations introduce a bracket notation so that Ψ_0 is written $\Phi|0\rangle$. Labeling the states of the unperturbed system $n=0,1,\ldots$, taking them to be orthonormal ($\langle m|n\rangle = \delta_{mn}$), and $|0\rangle$ to be nondegenerate, one obtains

$$E_1 = -\langle 0|\nabla_0|0\rangle \cdot \nabla_1\Phi/\Phi. \tag{2.9}$$

Note that the quantity $\langle 0|\nabla_0|0\rangle$ implies an integration in r, as is standard in the bracket notation. Considering the system to be finite (so that $|0\rangle$ vanishes at infinity), the matrix element of ∇_0 in Eq. (2.9), i.e., $\langle 0|\nabla_0|0\rangle$, is zero; hence E_1 vanishes. For example, we have $\int d^{3N}r\Psi_{(0)}^* \partial\Psi_0/\partial x_1$ for the component of ∇_0 for particle one along the x axis. If Ψ_0 is real, this reduces to $\frac{1}{2}\int d^{3N}r\partial(\Psi_0^2)/\partial x_1$, which is zero since $\Psi_0 \to 0$ for the finite nanostructure. Collecting terms in Eq. (2.8), one obtains

$$\Psi_1 = \sum_{n>0} |n\rangle \frac{\langle n|\nabla_0|0\rangle}{[E_{(0)} - E_{(n)}]}\nabla_1\Phi. \tag{2.10}$$

Note that $E_{(n)}$ is the energy of the nth level of H_0, i.e., $H_0|n\rangle = E_{(n)}|n\rangle$.

To $O(\varepsilon^2)$, one obtains

$$H_0\Psi_2 - \nabla_0 \cdot \nabla_1\Psi_1 - \tfrac{1}{2}\nabla_1^2\Psi_0 + V_2\Psi_0 = E_0\Psi_2 + E_2\Psi_0. \tag{2.11}$$

Since V_0 is independent of R, all $E_{(n)}$ and $|n\rangle$ are also independent of R. Taking the inner product of Eq. (2.11) with $\langle 0|$ yields

$$\left[-\tfrac{1}{2}\nabla_1 \cdot \underline{\underline{\Lambda}}\nabla_1 + U\right]\Phi = E_2\Phi, \tag{2.12}$$

$$U(R) = \langle 0|V_2|0\rangle, \tag{2.13}$$

$$\Lambda_{i\alpha i'\alpha'} = \delta_{ii'}\delta_{\alpha\alpha'} + 2\sum_{n>0} \frac{\langle 0|\nabla_{0i\alpha}|n\rangle\langle n|\nabla_{0i'\alpha'}|0\rangle}{[E_{(n)} - E_{(0)}]},$$
$$\alpha,\alpha' = 1,2,3; \; i,i' = 1,\ldots,N. \tag{2.14}$$

The matrix elements in Eq. (2.14) are independent of i and i' due to the exchange symmetry of the states $|n\rangle$, $n=0,1,\ldots$, and that they involve integration over all particle coordinates. Thus, $\Lambda_{i\alpha i'\alpha'}$ takes the form

$$\Lambda_{i\alpha i'\alpha'} = \delta_{ii'}\delta_{\alpha\alpha'} + \Gamma_{\alpha\alpha'}, \tag{2.15}$$

where the second term has no dependence on particle label and the Γ tensor is defined upon comparing Eqs. (2.13) and (2.14).

The matrix $\Gamma_{\alpha\alpha'}$ expresses the anisotropy of the short-scale states $|n\rangle$, $n=0,1,\ldots$, and Eq. (2.14) shows in detail the structure of $\underline{\underline{\Lambda}}$ as it appears in Eq. (2.12).

A few comments are in order regarding Eq. (2.12). Equation (2.12) is a *coarse-grained Schrödinger equation*, where the eigenvalues of the inverse of $\underline{\underline{\Lambda}}$ act like effective masses for the long-range motion of the constituent particles as described by Φ. Furthermore, $\underline{\underline{\Lambda}}$ is defined by the short-range character of the wave function. While $\underline{\underline{\Lambda}}$ is symmetric in particle label ii', it is not diagonal so that the effective masses, defined as the eigenvalues of the inverse of $\underline{\underline{\Lambda}}$, are truly many-body quantities. Thus, the effective masses can depart dramatically from those of the particles themselves (the latter being one in the present units where $\hbar$ is one as well). Thus, $\Gamma_{\alpha\alpha'}$ expresses the departure of the quasiparticles, described by the coarse-grained wave equation, from that of the behavior of the original constituent particles. The perturbation analysis yields a course-grained equation for Φ with E_2 as an eigenvalue. The quantity $\underline{\underline{\Lambda}}$ in Eq. (2.12) may also be interpreted as a gauge transformation, or a metric tensor, where the long-range variables are now coupled as a result of the off-diagonal elements of $\underline{\underline{\Lambda}}$. The choice of gauge depends on the momentum (or flux), i.e., ∇_0 at the short range. Thus, one may interpret the coupling of long-range and short-range behaviors (through $\underline{\underline{\Lambda}}$) as predominantly flux dependent. Note the initially orthogonal set of long-range variables are now coupled as a result of the gauge transformation.

Associated with the coarse-grained Schrödinger equation (2.12) is the functional $E_2[\Phi]$:

$$E_2[\Phi] = \frac{\int d^{3N}R\left(\frac{1}{2}\nabla_1\Phi^*\underline{\underline{\Lambda}}\nabla_1\Phi + U|\Phi|^2\right)}{\int d^{3N}|\Phi|^2}. \tag{2.16}$$

Minimization of E_2 with respect to Φ yields Eq. (2.12) and therefore provides a starting point for a variational technique.

These results can be used to generate a QN theory based on a numerical or approximate analytical solution of the lowest order problem. These results can also serve as the starting point of a phenomenological theory, or to motivate a variational approach as in the next section.

III. MEAN-FIELD, PHENOMENOLOGICAL FERMION MODEL

The analysis of the previous section suggests that for low energy states of a fermion system, the coarse-grained wave function $\Phi(R)$ is symmetric with respect to particle label exchange. As the lowest order wave function is a product of a rapidly fluctuating factor $\hat{\Psi}$ and a smoothly varying factor Φ, Φ acts like an "envelope" for the "wave packet" $\hat{\Psi}$. This implies the eigenstates of the coarse-grained wave equation correspond to collective modes of a QN. In the following, we explore this picture via a phenomenological approach.

Assume that $U(R)$ contains effective one and two body interactions:

$$U = \sum_i \upsilon(\vec{R}_i) + \sum_{i<j} u(\vec{R}_i, \vec{R}_j). \tag{3.1}$$

Here, υ is an effective "external" field representing confinement effects (as from the ion core lattice in a conductor or an average interaction in liquid helium III); correlations between the long-scale motions of the particles are accounted for via the effective two body interaction υ. Since Φ is symmetric, we consider mean field solutions Φ that are a product of single-particle functions, i.e.,

$$\Phi = \varphi(\vec{R}_1)\cdots\varphi(\vec{R}_N) \tag{3.2}$$

involving one single-particle function φ. Recalling [Eqs. (2.13) and (2.14)] the elements of $\underline{\underline{\Lambda}}$, a variational calculation based on Eqs. (3.2) and (2.16) implies

$$-\frac{1}{2}\sum_{\alpha,\alpha'}\left[\delta_{\alpha\alpha'} + \Gamma_{\alpha\alpha'}\right]\frac{\partial^2\varphi}{\partial X_\alpha\partial X_{\alpha'}} + (N-1)\sum_{\alpha,\alpha'}\Gamma_{\alpha\alpha'}$$
$$\times \int d^3R' \frac{\partial\varphi(\vec{R}')}{\partial X'_{\alpha'}}\frac{\partial\varphi(\vec{R})}{\partial X_\alpha} + \upsilon(\vec{R})\varphi(\vec{R}) + (N-1)$$
$$\times \int d^3R' u(\vec{R},\vec{R}')|\varphi(\vec{R}')|^2\varphi(\vec{R}) = E^*\varphi(\vec{R}) \tag{3.3}$$

for α component X_α of $\vec{R}$ and single-particle energy E^s. Note terms from $\int d^3R\partial\varphi/\partial X_\alpha$ vanish as φ approaches zero at infinity. Small eigenvalues of $\Gamma_{\alpha\alpha'}$ correspond to a large effective mass associated with collective behavior. Thus, it is expected that small eigenvalues of $\delta_{\alpha\alpha'} + \Gamma_{\alpha\alpha'}$ indicate an excitation that simultaneously involves many particles moving in a coordinated fashion. The energetics and precise character [i.e., profile $\varphi(\vec{R})$] depends on the interplay of effective

mass and the coarse-grained potential $U(\vec{R}_1,\ldots,\vec{R}_N)$.

The total energy E_2, as a deviation from $E_{(0)}$, associated with the coarse-grained Φ dynamics is given by

$$E_2 = NE^* \tag{3.4}$$

for the N-particle QN. The forms of u and υ determine the allowed E^* values, i.e., the spectrum of the bosonlike excitations of the fermion nanosystem. Since all particles move in a coordinated fashion in these φ-produce states, it is suggested that this corresponds to the spectrum of collective, QN-wide modes.

If the effective potential υ^{ff},

$$\upsilon^{\text{ff}}(\vec{R}) = \upsilon(\vec{R}) + (N-1)\int d^3R' u(\vec{R}_1\vec{R}')|\varphi(\vec{R}')|^2 \tag{3.5}$$

has a minimum for a range of φ profiles, then the QN supports self-sustained local zones of accumulating constituent particle density. For conducting QNs, one suspects that this corresponds to surface plasmons or localizations along a superconducting nanowire.

If u has a strongly attracting tail and a hard repulsive core, quasiparticle density is nearly constant on the $\vec{R}$ scale within a nanodroplet.[37] In that case, excitations take the form of dynamic changes in the shape of a droplet. These morphological excitations could couple to QN rotation. Using boundary layer techniques as in Refs. 5 and 37, one can derive equations for the quantized morphological dynamics of a nanodroplet.

IV. CONCLUSIONS FOR FERMION AND BOSON SYSTEMS

A main difficulty in QN theory is that the wave function simultaneously involves variations on two or more distinct scales. In this study, it was shown that when these length scales are well separated one may construct the wave function to account for these distinct dependencies. To do so, place-holder variables, i.e., "order parameters," are introduced to keep track of the long-scale behavior.[23,24,35,38] If ε is the ratio of the short to the long characteristic length, then the $\vec{R}_i = \varepsilon\vec{r}_i$ serve this role by capturing the long-scale behaviors. Thereby, the wave function takes the form $\Psi(r,R;\varepsilon)$ and r and R are the sets of the positions $\vec{r}_1,\ldots,\vec{r}_N$ and scaled positions $\vec{R}_1,\ldots,\vec{R}_N$ respectively. When ε is small, i.e., the scales are well separated, one may construct the dual dependence of Ψ on r and R. Recognizing that R is not a set of distinct dynamical variables, but rather is a way to keep track of the multiple (both r and R) dependencies in Ψ on the configuration of the particles is an important conceptual advance.

The multiscale approach reveals QN collective and single-particle excitations. This framework elucidates the cross-talk between short-scale, highly fluctuating single-particle-like phenomena and long-scale collective modes as follows. The multiscale perturbation analysis provides evidence for the notion of a coarse-grained wave equation for collective degrees of freedom that correspond to excitations spanning the whole QN. Key elements in the coarse-grained

wave equation, notably the inverse mass matrix $\underline{\underline{\Lambda}}$ and the coarse-grained N-body interaction U, involve averages over the short-scale dynamics. As suggested in Sec. III, the coarse-grained behavior is accounted for via the factor $\Phi(\varepsilon \vec{r}_1, \ldots, \varepsilon \vec{r}_N)$ that acts like an overall "envelope function" modulating the short-scale behavior of the factor $\hat{\Psi}(\vec{r}_1, \ldots, \vec{r}_N)$ that expresses the antisymmetric exchange behavior of fermions. As suggested in Sec. III, Φ can be written to good approximation as an N-fold product of single particle functions $\varphi(\varepsilon \vec{r})$ that correspond to an overall densitylike variable, i.e., $|\varphi(\varepsilon \vec{r})|^2$ is a coarse-grained density.

For a metal or semiconducting QN, the multiscale approach illustrates how collective behaviors in the N-electron QN emerge as bosonlike excitations in the form of long-scale electron density oscillations, i.e., through $|\varphi|^2$. To lowest order in the perturbation hierarchy, there are states wherein the wave function separates into a short-scale, antisymmetric fermion factor $\hat{\Psi}(r)$ and a long-scale symmetric, bosonlike factor $\Phi(R)$. The latter satisfies a coarse-grained wave equation involving an effective potential created by averaging the N-electron potential over short-scale variations. To construct this effective potential, one solves a short-scale problem for $\hat{\Psi}$. The perturbation method illustrates the emergence of an effective mass for the long-scale, QN-wide dynamics of the electrons, revisiting the notion of a dressed particle with effective mass. The long-scale dependence of the wave function captures excitations with effective mass that can greatly exceed the mass of a single constituent particle strongly suggests that the low-lying eigenstates of the coarse-grained wave equation correspond to collective modes, and that when the assumption is made that $\Phi(R) \approx \varphi(\vec{R}_1) \cdots \varphi(\vec{R}_N)$, $|\varphi(\vec{R})|^2$ emerges as the density profile for these collective, high effective-mass modes. However, if the long-scale correlations are accounted for in $\Phi(R)$ then it is tempting to approximate $\hat{\Psi}$ as a Slater determinant of single-electron functions, one for each of the N lowest single-particle energy states, comprising the fermion ground state. This picture of $\hat{\Psi}(r)\Phi(R)$ composite states suggests that excitations from the ground state are of several distinct types classified via effective mass and the associated density $|\varphi(\vec{R})|^2$, as well as the number of single-particle states above the Fermi level.

For fermion liquids (e.g., helium III) the long-range excitations, emerging as states of the coarse-grained wave function Φ, correspond to surface waves, i.e., fluctuations in droplet shape. As for the electron phenomena noted above, the spectrum of these excitations is reflected in the range of effective masses supported by the $\underline{\underline{\Lambda}}$ matrix of Secs. II and III. Since Φ is symmetric with respect to particle label exchange, these excitations are bosonlike in character.

The collective excitations described by the long-scale equation for conductors or semiconductors are likely related to surface plasmas and quantum dot fluorescence. In a more general approach, the phonons of the ion core lattice of the nanoparticle are expected to support superconductivity effects.

For boson systems, the requirement of overall symmetry of the wave function could be met by the lowest order solution in the perturbation analysis being a product of two factors, $\hat{\Psi}$ and Φ, both of which are either antisymmetric or symmetric. However, there can be more complex states which, in analogy to Slater determinants, can be a linear combination of $\hat{\Psi}\Phi$ terms that is symmetric overall, even though any one $\hat{\Psi}\Phi$ term is not symmetric. Thus, there could be low energy solutions to the wave equation of complex structure as follows.

To illustrate the potential for more complex excited states in a boson QN, let $A_{ij}(r)$ be antisymmetric with respect to the exchange of the particle label indices i and j, but symmetric with respect to all other index permutations, and similarly for $B_{ij}(R)$. Then, the following function is overall symmetric:

$$\sum_{i<j} A_{ij}(r) B_{ij}(R).$$

This state has some antisymmetric character but is not necessarily of high energy, i.e., there is no analog to the Fermi level. In boson systems, the multiscale approach appears promising for discovering the excitations of quantum nanodroplets, i.e., their quantized surface waves and coupled morphological-rotational dynamics.

For the relatively simple boson system states, wherein both $\hat{\Psi}$ and Φ are symmetric, the results of Sec. II suggest the existence of a coarse-grained wave equation for Φ that can be used to analyze the surface waves and other morphological dynamics of superfluid nanodroplets. Considering the peculiar behavior of low temperature Bose condensates, the application of a multiscale approach to analyze boson nanodroplets is likely to reveal unexpected behaviors.

For boson nanodroplets, the collective factor corresponds to droplet shape, rotation, and density waves propagating internally or on the surface. However, there may be more complex lowest order solutions whereby neither factor is antisymmetric or symmetric, but the product or sum of product solutions has the correct particle label exchange symmetry. One expects that the dual antisymmetric solutions $\hat{\Psi}\Phi$ are of high energy. This is suggested by the argument that both factors should have the character of a Slater determinant of single-particle-like functions with only single occupancy per single-particle state allowed. This is in sharp contrast to the case where both $\hat{\Psi}$ and Φ are symmetric, so that most particles would occupy the single-particle ground state.

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